Accurate Approximations for One-, Two- and Three-Dimensional Groundwater Mass Transport From an Exponentially Decaying Contaminant Source

A Thesis Presented to

the Faculty of the Interdisciplinary Graduate

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In Partial Fulfillment

of the Requirements for the Degree

Master of Science in Environmental Engineering

by

Danxu Yuan

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ABSTRACT

Three models were established through the extension of Domenico-Robbins' model to simulate one-dimensional, two-dimensional and three-dimensional contaminant transport from an exponentially decaying source of finite size. The models incorporate one-dimensional groundwater velocity, longitudinal and transverse dispersion. The models are tested against three exact solutions obtained by numerical convolution of exponentially decaying impulse sources and the agreement is excellent. Use of the models shows that the output contaminant concentrations in column tests simulated by the models are very close to those produced by experiments. Other possible applications include simulations of contaminant transport from sources which have exactly the form of the source term in the models, and the estimation of concentration at some receptor downstream of a source for an exposure assessment calculation. Appendices show how to perform the required calculation for use in computer spreadsheets and programs are included.

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SYMBOL	DEFINITION	TYPICAL UNITS	DIMENSION
C	concentration	mg/L	M/L^3
n	porosity	unitless	L^3/L^3
v	linear velocity	ft/day	L/T
V	volume	ft^3	L^3
A	area	ft^2	L^2
M	mass	mg	M
S	solubility	mg/L	M/L
$\mathbf{m_i}$	mass fraction	unitless	M/M
$\mathbf{D_x}$	dispersion coefficient along flow	ft^2/day	L^2/T
$\mathbf{D_{y,z}}$	dispersion coefficient perpendicular to flow	ft^2/day	L^2/T
t	time	day	T
τ	time	day	T
x	coordinate parallel to flow	ft	L
y, z	coordinates perpendicular to flow	ft	L
λ	decay rate	1/day	1/T
Pe	ratio of advective flux to dispersive flux	unitless	$(L^2/T)/(L^2/T)$

Chapter 1 Introduction

This chapter starts with summarizing mathematical models of contaminant transport in subsurface porous media, briefly describing Domenico-Robbins' model, and finally ends at bringing up the problem dealt in this project.

1.1 Mathematical Models of Contaminant Fate and Transport

Recent concerns over the environmental impact of land disposal of hazardous wastes have led to the rapidly increasing use of transport models to predict leachate plume migration in groundwater systems. A number of mathematical models of contaminant fate and transport in the subsurface are now available to help address contaminant transport problems and they are used in the exposure component of risk assessment, evaluating alternative risk-based source management strategies, designing remediation systems, and interpreting soil flushing and leaching experiments. These mathematical models can be divided into two categories: numerical and analytical models.

The numerical models offer great flexibility and capability to handle complex field conditions. However, their application is often constrained by computational difficulties (convergence and stability problems) inherent in the numerical approximations, and excessive computational requirements, particularly for three-dimensional problems. Analytical solutions are limited in scope compared to numerical simulators, but they are useful for providing rapid initial estimates of alternative corrective actions, especially when implemented over large spatial and temporal scales. The analytical models are also more economical and convenient in applications, and they also provide simple and effective means for gaining insight into the relative importance of the various transport parameters. When the limited precision of data describing most field situations is considered, analytical estimates of expected concentrations may be as meaningful as detailed numerical simulations. Furthermore, the analytical solutions, often being more efficient to compute than the numerical solutions, are more conductive to uncertainty analyses via stochastic techniques.

1.2 Domenico-Robbins' Model

Many analytical solutions for various source functions and geometrices are available. The more complex analytical models generally require some type of numerical integration. In the more simple closed-form category for instantaneous pulses are the models of Baetsle (1969) and Hunt (1978). For continuous source problems, the relatively simple two-dimensional model of Wilson and Miller (1978) and the three-dimensional solution of Hunt (1978) are typical examples. However, these models require that the source be treated as a point and, consequently, are only applicable to the far field.

Domenico and Robbins (1985) developed an analytical expression for contaminant transport from a source of finite size in a continuous flow regime. The model requires some numerical integration and its degree of accuracy for near-field problems depends on discretization procedures applied to the source boundary. Meanwhile, they developed a second model for a continuous source by extending a well-known pulse model. This second model is particularly useful in that it permits the determination of several potential unknowns directly from a concentration distribution. These include the source concentration, source dimensions, the position of the center of the mass that is the product of the seepage velocity and the time since the contaminant first entered the groundwater, and up to three dispersivities for three-dimensional problem. As a demonstration of its utility, this second model was applied with reasonable success to a well-defined field condition. Domenico and Robbins (1985) also made a comparison of the two models, indicating that, except for minor differences in the very near field, the results from each were virtually identical.

The model described above is referred to as an "extended pulse" type model in that it was derived by an infinite spatial extension of an instantaneous finite source pulse model. Based on this extended pulse model, Domenico (1987) developed another mathematical model for a finite source that incorporated one-dimensional groundwater velocity, longitudinal and transverse dispersion, and some form of decay for either radionuclides or biodegradable organics.

1.3 The Extension of Domenico-Robbins' Model

While Domenico-Robbins' (1985) model is useful, a similar model that can approximate the case of a source whose concentration exponentially decays with time (as distinct from a decaying contaminant) would extend the utility of their approach. Such an intermediate source term where the source concentration decreases over time might be more realistic and could significantly affect decisions relating to risk-based closure and remediation.

This project presents three analytical fate and transport models that use concepts from the Domenico-Robbins model, but incorporating a more realistic term for making the observed receptor concentration (ORC) calculations in groundwater. These solutions are limited in scope compared to numerical models, but they are useful in providing rapid initial estimates of alternative risk-based source management strategies, and are intended to serve as a screening tool to help a generator decide whether a more complicated and detailed numerical modeling study is worthwhile. The flushing of an immobile residual contaminant that can enter the aqueous phase by dissolution is an example of a source zone that could be modeled by an exponentially decaying source.

1.4 The Organization of This Thesis

This thesis begins by considering the overall mathematical models of contaminant transport in subsurface porous media, with particular emphasis on describing Domenico-Robbins' model, and bringing up the problem dealt with in this project. The second chapter reviews the literature of analytical models and concludes that models for decaying contaminant sources are in need. Chapter 3 briefly states the problems faced by model users.

Chapter 4 presents the model development procedure. The proposed models, called approximation no.1, additional models, called approximation no.2, and the exact solutions are provided. Model testing is illustrated in Chapter 5. Fifteen test cases, each having different values of dispersion coefficient, groundwater velocity and source decaying rate, are selected to test the proposed models and additional solutions against the exact solutions. Computer Spreadsheets are used as tools to carry out the model testing.

Chapter 6 includes four examples of model application, with emphasis on application no.4 to simulate leaching tests from hydrocarbon residuals. Chapter 7 presents the conclusions and limitations. Finally, the FORTRAN programs used to evaluate all the solutions are attached as appendices. A typical computer Spreadsheet of model evaluation is provided in the appendices as well.

Chapter 2 Literature Review

The process through which a dissolved mass moves in a porous medium is referred to as advection-dispersion transport. Interest in mass advection-dispersion transport in porous media has resulted from groundwater quality considerations of artificial recharge and waste disposal, especially hazardous waste disposal such as oil tank leakage, into and through the groundwater system. Mathematical modeling of the transport of contaminant mass in groundwater involves the application of analytical or numerical solutions of the advection-dispersion equation. Numerical models are more versatile and can provide more accurate solutions of complex situations. Analytical models are simplified approximations of reality due to the many required assumptions, but can provide reliable and accurate results for simulations that do not involve complex aquifer heterogeneity or boundary conditions.

By the early 1970s, many analytical solutions had been obtained and applied. Examples are Carslaw and Jaeger (1959), Ogata and Banks (1961), Harleman and Rumer (1963), Hoopes and Harleman (1965), Bruch and Street (1966), Shamir and Harleman (1966), Ogata (1970), and Codell and Schreiber (1972). Common to these studies is the assumption of a step function for input concentration, i.e., the input concentration is changed instantaneously from zero to some value and is maintained at this value thereafter. Marino (1974) derived mathematical solutions to two simplified dispersion problems involving variable input concentrations of contaminants. For the first problem the concentration of the displacing fluid at the starting point was expressed as an exponential function (decaying or increasing over time). The second problem specified the concentration at the starting point as an initial concentration minus an exponential function. The solutions predict the distribution of contaminants in saturated porous media resulting from the variable source concentrations. Marino's solutions were developed for one-dimensional problems only, while longitudinal and transverse dispersion problems are more useful in practical application.

Yeh and Tsai (1976) developed a transient, three-dimensional turbulent diffusion equation describing the concentration distribution of a substance or heat in a time-dependent flow field analytically. Their approach was based on Green's functions. The solutions were developed for cases in which the velocity field could be described as any integratable function of time. There are no limitations on the type of source conditions, however numerical convolution is required and their work is more appropriate for heat transfer problems.

Hunt's (1978) solutions are the fundamental basis on which many analytical models in contaminant hydrology have been developed. Hunt (1978) reported solutions for instantaneous, continuous, and steady-state point sources of the pollution in a uniform groundwater flow field. These solutions have been used to determine how long a continuous source must be in place before steady-state conditions are approached, determine the effect of a finite aquifer depth upon solutions for an aquifer of infinite depth, calculate maximum concentrations for instantaneous sources under two different sets of conditions, and determine the time required for solutions for a point source and a source of finite size to approach each other. Hunt's solutions have limited applications since they are obviously constrained with point sources.

Wison *et al.* (1978) presented analytical solution for a common groundwater contamination problem, i.e., two-dimensional plume problem. The definition of the two-dimensional plume is the following. Suppose a source of contaminant enters the saturated zone at the water table, if the contaminant continually flows into the aquifer, a process referred to as injection, a plume will develop downstream of the source, spreading out to the side and below. When the aquifer is relatively thin, the vertical extent of the plume is limited by the bottom impermeable boundary. The contaminant quickly mixes over the vertical, and its concentration becomes essentially uniform with depth. When that occurs the plume can be regarded as essentially two dimensional. Obviously, the application of this two-dimensional approach is limited by conditions of contaminant sources and aquifer systems.

Prakash (1982) developed simple analytical models to predict the spatial distribution of steady-state concentrations caused by continuous release of contaminants from a point, line, rectangular, or parallelepiped source in a groundwater environment with one- or two-dimensional uniform flow. The applicability of this model to certain types of field situations was demonstrated by examples. Once again, an assumption is made that the source concentration is constant and thus this model can not be used to deal with problems of variable concentration sources.

In modeling practice, continuous sources of finite size are quite often used to simulate the transport of contaminants. Based on Hunt's (1978) work, Domenico and

Robbins (1985) derived two analytical expressions for contaminant transport from a finite source in a continuous flow regime. The first model required numerical integration and the second model was developed by extending a pulse model. This second model is particularly useful since it permits the determination of several potential unknowns directly from a concentration distribution. A comparison of these two models indicates that, except for minor differences in the very near field, the results from each are virtually identical. Domenico-Robbins model is very useful in applications of early estimation of concentration distribution but might not be appropriate for late estimation as it still does not include any variable source terms.

The majority of previous three-dimensional analytical models are based on a rather restrictive assumption of infinite aquifer thickness (Shen, 1976; Hunt, 1978; Domenico and Palciauska, 1982; Sagar, 1982; and Domenico and Robbins, 1985); therefore, Huyakorn *et al.* (1987) proposed a new three-dimensional analytical solution. This solution predicts transient and steady state concentration distributions resulting from a partially penetrating strip source in a finite thickness aquifer. The plane of the source is assumed to be perpendicular to the longitudinal direction of groundwater velocity, and the prescribed source is assumed to be Gaussian in the transverse direction and uniform over the penetration thickness. This model has been compared with three other analytical models and the results of the comparison indicate certain advantages of the model over its previous counterparts. This solution does not include a variable source term either.

While Ogata (1970) and Codell and Schreiber (1972) present solutions for transport and dispersion in groundwater from a vertical plane source, Galya (1987) used a horizontal plane source to more appropriately model dispersive transport from landfills or land treatment facilities. This model extends the model of Codell and Schreiber (1977) and Yeh (1981) in adopting Green's function and incorporates retardation and decay (this decay occurs while the contaminant mass transports through a porous medium). This model provides more accurate results than point-source solutions, particularly near the source; but it cannot handle the transport of an temporally decaying source which is more realistic.

The fate and transport of contaminants in the groundwater are a rather complex process and there are many other factors rather than dispersion (such as decaying) involved. Among the solutions dealing with the transport of a decaying contaminant species, Domenico's (1987) is one of the most convenient models for a finite source that incorporates one-dimensional groundwater velocity, longitudinal and transverse dispersion, and some form of decay for either radionuclides or biodegradable organics. This model can be used in a calibration procedure that permits the determination of up to seven parameters, including the velocity of the contaminant, source size and concentration, and up to three dispersivities for a three dimensional problem, from a known spatial distribution of concentrations. This model is intended to solve multidimensional transport problems of a decaying contaminant species that is different from an exponentially decaying source, which is the subject of this thesis.

Based on the literature reviewed, there is a need to develop approximations that account for a time-variable source term. Approximations are preferred because exact solutions appear to be obtainable only by convolution of elementary impulse solutions, and closed-form solutions may not be available.

The subject of this thesis is to extend the Domenico-Robbins approach for an exponentially decaying source term (for which closed-form solutions exist) and compare this approach to an exact solution obtained by numerical convolution and a simplified approximation approach.

Chapter 3 Problem Statement

Risk Reduction Standards of Texas contain guidelines for calculating an allowable medium specific (soil, air, water, ground water) concentration (MSC) at a receptor (well, receiving water, property lines) (Texas Administrative Code, 1994). If the generator can convincingly show that its source of the contamination can be controlled so that it does not exceed this value at the nearest likely receptor, then an avenue for negotiating a clean-up standard is opened with the regulatory agency. In Texas this is called a Risk Reduction Standard Number-3 Closure. The intent is to reduce the number of contamination sources that are cleaned-up to background or health-based standards where such an effort is unnecessary. Generally, the rules incorporate certain deed recordings to prevent a Number-3 site from being sold in a manner such that any receptors' exposure is increased, and various other safeguards.

While these rules are specific to Texas, the concept has evolved from Federal Guidelines, and similar programs will likely be implemented in other states and nations. The rules contain very specific calculation procedures to determine the MSC, but the generator is free to compute the potential observed receptor concentration (PORC) using any reasonably defensible method. Typically some modeling study is conducted using an acceptable numerical model. The goal of the modeling exercise is to determine what changes in the source mass and distribution are necessary to ensure that the PORC is less than the MSC at the nearest receptor. For example, if the modeling exercise shows that a ten percent uniform reduction in mass at the source is sufficient to achieve the risk-reduction standard, then the remediation strategy will be much different (and probably less expensive) than a ninety percent clean-up strategy.

Many analytical models for contaminant fate and transport exist, but most that have been used involve either a constant source term or an impulse source term. The subject of this project is to develop a model for an exponentially decaying source. A constant source is inappropriate as the mass of contaminants will eventually be depleted. An impulse source is inappropriate because it is unlikely that all the mass will dissolve immediately.

Chapter 4 Model Development

4.1 Introduction

Marino (1974) developed a mathematical model for the transport of a variable concentration source of contaminants. In 1978, an attempt was made by Hunt (1978) to establish models of the transport for an instantaneous and a continuous point contaminant source and then for an instantaneous source of finite size. Several years later, Domenico and Robbins (1985) developed a model for contaminant transport from a finite source in a continuous flow regime based on the previous work. In 1987, Domenico (1987) extended his 1985 model for a finite source that incorporated some form of decay for radionuclides or biodegradable organics.

The models developed in this thesis stemmed from Marino's (1974) solutions to dispersion problems involving variable input concentrations of contaminants in a one-dimensional groundwater flow field. The concepts used in Domenico-Robbins' (1985) model was employed to extend this one-dimensional model into two and three dimensions. Hunt's (1978) solutions to the transport of point contaminant sources were also the starting points to obtain exact solutions (more rigorous compared to the proposed models) against which the models were tested. Additional approximate solutions that are less rigorous than the exact ones, or the Domenico-Robbins' model were also derived for model testing and potential application. The procedure of model development will be illustrated in the following sections in this chapter.

4.2 Solutions for Instantaneous and Continuous Point Sources

If the uniform flow field has a constant velocity, *v*, in the positive x direction, then the groundwater advection-dispersion equation is

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

where C is the concentration in mass per unit volume of water; D_x, D_y, D_z are the principal values of the dispersion tensor; x, y, z, represent the Cartesian coordinates that are presumed to be collinear with the principal directions of dispersion; and v is the average linear velocity of the groundwater (specific discharge divided by the porosity).

An instantaneous point source is contaminant mass injected at the origin (x = 0) instantaneously at time t = 0. A continuous point source is contaminant mass injected at the origin continuously for all time t > 0. The solutions, C_i, for instantaneous sources can be obtained by using the following initial conditions to define the masses, M_i, of contaminant that are injected at the origin instantaneously at t = 0:

$$M_1 = \int_{-\infty}^{\infty} C_i(x,0)n\,dx, \tag{2}$$

$$M_2 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} C_i(x,y,0)n\,dx\,dy, \tag{3}$$

$$M_3 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} C_i(x,y,z,0)n\,dx\,dy. \tag{4}$$

In each of Eqs. (2)-(4), the initial distributions of C_i are approximated with the Dirac delta function, and the porosity, *n*, will be assumed constant. The solutions, C_c, for continuous sources can be obtained by using the following definition for the constant mass flow rate, M_i, which is injected continuously into the aquifer for $0 < t < \infty$:

$$\overline{M}_i = \frac{dM_i}{dt}; \qquad i = 1, 2, 3. \tag{5}$$

Equations (1)-(4) then become a special form of the analogous equations in heat conduction. Hunt (1978) reported the one-dimensional and three-dimensional solutions to be

$$C_i(x,t) = \frac{M_1}{2n\sqrt{\pi D_x t}} \exp[-\frac{(x-vt)^2}{4D_x t}], \tag{6}$$

$$C_c(x,t) = \frac{\overline{M}_1 \exp(\frac{xv}{2D_x})}{2nv}[\exp(-\frac{xv}{2D_x})\text{erfc}(\frac{x-vt}{2\sqrt{D_x t}}) - \exp(\frac{xv}{2D_x})\text{erfc}(\frac{x+vt}{2\sqrt{D_x t}})], \tag{7}$$

$$C_i(x,y,z,t) = \frac{M_3 \exp[-\frac{(x-vt)^2}{4D_x t} - \frac{y^2}{4D_y t} - \frac{z^2}{4D_z t}]}{8n\sqrt{\pi^3 t^3 D_x D_y D_z}}, \tag{8}$$

$$C_c(x,y,z,t) = \frac{\overline{M}_3 \exp(\frac{xv}{2D_x})}{8\pi n R\sqrt{D_y D_z}}[\exp(-\frac{Rv}{2D_x})\text{erfc}(\frac{R-vt}{2\sqrt{D_x t}}) + \exp(\frac{Rv}{2D_x})\text{erfc}(\frac{R+vt}{2\sqrt{D_x t}})], \tag{9}$$

where erfc is the complementary error function, and R is defined as

$$R = \sqrt{x^2 + y^2 \frac{D_x}{D_y} + z^2 \frac{D_x}{D_z}}. \tag{10}$$

The two-dimensional solution for an instantaneous source was also reported by Hunt (1978) as

$$C_i(x,y,t) = \frac{M_2 \exp[-\frac{(x-vt)^2}{4D_x t} - \frac{y^2}{4D_y t}]}{4\pi n t\sqrt{D_x D_y}} \qquad (11)$$

The continuous source solution to two-dimensional flow was derived by Hunt (1978) from Eq. (11) by replacing M_2 with $\overline{M_2}\, d\tau$, t with t - τ, and integrating from τ = 0 to τ = t as

$$C_c(x,y,t) = \frac{\overline{M}_2 \exp(\frac{xv}{2D_x})}{4\pi n\sqrt{D_x D_y}} \int_0^t \exp[-\frac{\frac{x^2}{D_x} + \frac{y^2}{D_y}}{4(t-\tau)} - \frac{v^2(t-\tau)}{4D_x}]\frac{d\tau}{t-\tau}. \qquad (12)$$

Equations (6), (8), and (11) will be used later in Section 4.5 to derive the exact solutions to the transport problem of a continuous source of finite size when M_i/n is replaced by $C_0 v d\tau$ (C_0 is the initial concentration of the contaminant) which is the elementary solution to the transport of contaminants in groundwater. The integral in Eq. (13) has a solution that is defined recursively using exponential integrals.

4.3 Solutions for an Instantaneous Source of Finite Size

The solution for an instantaneous source of finite size, which will be referred as a "pulse" is shown schematically in Figure 1, will be taken to satisfy Eq. (1) and the initial condition,

$$C_i(x,y,z,0) = \frac{M_3}{n}L^3, \qquad \text{when } 0 \le x,y,z, < \frac{L}{2}$$

$$= 0, \qquad \text{when } \frac{L}{2} < x,y,z < \infty, \qquad (13)$$

where L is side length of the cubical region occupied by the contaminant at t = 0.

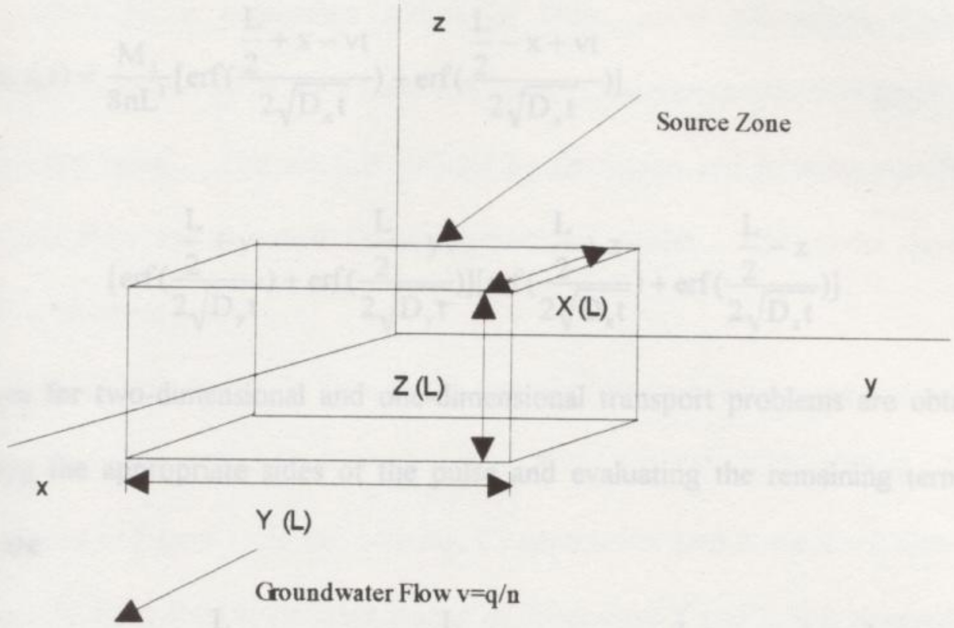

Figure 1. Schematic of Finite Size "Pulse" Source Zone
(Centroid of region shown is located at (0, 0, 0,))

According to Hunt (1978), a solution to Eq. (1) is

$$C_i(x,y,z,t) = \frac{1}{8\pi^3} \int \int_{-\infty}^{\infty} \int F(\alpha,\beta,\gamma) \exp(i\alpha x + i\beta y + i\gamma z + \delta t) d\alpha d\beta d\gamma, \tag{14}$$

where $\delta(\alpha,\beta,\gamma) = -i\alpha v - \alpha^2 D_x - \beta^2 D_y - \gamma^2 D_z$.

Setting t = 0 in Eq. (15), using the initial condition, Eq. (14), and inverting the three-dimensional Fourier integral gives

$$F(\alpha,\beta,\gamma) = \frac{M_3}{8nL^3} \frac{\sin\frac{\alpha L}{2}}{\alpha} \frac{\sin\frac{\beta L}{2}}{\beta} \frac{\sin\frac{\gamma L}{2}}{\gamma}. \tag{15}$$

Finally, substitution of Eq. (16) into Eq. (15) and evaluating the integrals give the solution for a source of finite size,

$$C_i(x,y,z,t)=\frac{M_3}{8nL^3}[\mathrm{erf}(\frac{\frac{L}{2}+x-vt}{2\sqrt{D_x t}})+\mathrm{erf}(\frac{\frac{L}{2}-x+vt}{2\sqrt{D_x t}})]$$

$$[\mathrm{erf}(\frac{\frac{L}{2}+y}{2\sqrt{D_y t}})+\mathrm{erf}(\frac{\frac{L}{2}-y}{2\sqrt{D_y t}})][\mathrm{erf}(\frac{\frac{L}{2}+z}{2\sqrt{D_z t}})+\mathrm{erf}(\frac{\frac{L}{2}-z}{2\sqrt{D_z t}})]. \qquad (16)$$

Solutions for two-dimensional and one-dimensional transport problems are obtained by extending the appropriate sides of the pulse and evaluating the remaining terms. The results are

$$C_i(x,y,t)=\frac{M_2}{4nL^3}[\mathrm{erf}(\frac{\frac{L}{2}+x-vt}{2\sqrt{D_x t}})+\mathrm{erf}(\frac{\frac{L}{2}-x+vt}{2\sqrt{D_x t}})]\,[\mathrm{erf}(\frac{\frac{L}{2}+y}{2\sqrt{D_y t}})+\mathrm{erf}(\frac{\frac{L}{2}-y}{2\sqrt{D_y t}})], \qquad (17)$$

$$C_i(x,t)=\frac{M_1}{2nL^3}[\mathrm{erf}(\frac{\frac{L}{2}+x-vt}{2\sqrt{D_x t}})+\mathrm{erf}(\frac{\frac{L}{2}-x+vt}{2\sqrt{D_x t}})]. \qquad (18)$$

The procedure to develop Eqs.(17) and (18) will be shown later in Section 4.4 when Domenico-Robbins' model is presented.

4.4 Solutions for a Continuous Source of Finite Size -- Domenico and Robbins' Model

To extend that model for an instantaneous source of finite size presented in Section 4.3 to a continuous source model, one would be required to either numerically solve the convolution integral associated with this instantaneous source, or perform the required spatial integration of the continuous point source model presented in Section 4.2. Rather than perform these integrations, Domenico and Robbins (1985) created a useful approximation for a continuous source of finite spatial dimensions from Hunt's instantaneous solution by taking a finite size "pulse" and superposing it in space to create an "extended pulse". The solution derived by Domenico and Robbins was for three-dimensional flow and is called Domenico-Robbins' model. This model development process is described below.

The solution shown in Section 4.3 describes the convection and dispersion of a substance deposited at time $t = 0$ in the region $-X/2 < x < X/2$, $-Y/2 < y < Y/2$, $-Z/2 < z < Z/2$, as shown in Figure 1. In this solution, C_0 approaches zero in the $x = 0$ plane as time gets large. For the continuous plane source of dimensions Y and Z, it is required that the concentration be maintained at C_0 for all time in the $x = 0$ plane and be equal to zero at $x > 0$ for time equal to zero. This effect can be accomplished with the box of Figure 2 by extending the box to infinity in the minus x direction as shown in Figure 2.

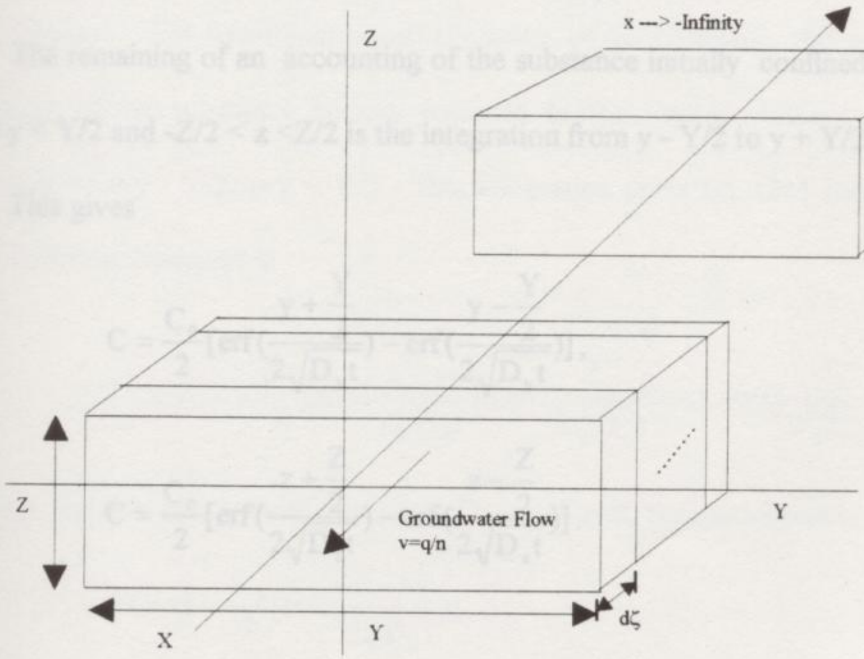

Figure 2. Schematic of "Extended Pulse" Model

The process is described by an infinite number of area sources each slightly displaced in the - x direction from each other resulting in an infinite number of elementary solutions which must be superposed, i.e., integrated from some *x* to infinity (Crank, 1979). The result is

$$C(x,t) = \frac{C_0}{2\sqrt{\pi D_x t}} \int_x^{\infty} \exp(-\frac{\varsigma^2}{4D_x t}) d\varsigma$$

$$= \frac{C_0}{\sqrt{\pi}} \int_{x/2\sqrt{D_x t}}^{\infty} \exp(-\eta^2) d\eta, \qquad (19)$$

where $\eta = \frac{\zeta}{2\sqrt{D_x t}}$, and $\zeta = x - vt$.

Equation (19) has the closed form complementary error function solution of

$$C(x,t) = \frac{C_0}{2} \operatorname{erfc}(\frac{x - vt}{2\sqrt{D_x t}}), \qquad (20)$$

which describes continuous mass flow from the *x* = 0 plane.

The remaining of an accounting of the substance initially confined in this region -Y/2 < y < Y/2 and -Z/2 < z <Z/2 is the integration from y - Y/2 to y + Y/2 and z -Z/2 to z + Z/2. This gives

$$C = \frac{C_0}{2}[\operatorname{erf}(\frac{y + \frac{Y}{2}}{2\sqrt{D_y t}}) - \operatorname{erf}(\frac{y - \frac{Y}{2}}{2\sqrt{D_y t}})], \qquad (21)$$

$$C = \frac{C_0}{2}[\operatorname{erf}(\frac{z + \frac{Z}{2}}{2\sqrt{D_z t}}) - \operatorname{erf}(\frac{z - \frac{Z}{2}}{2\sqrt{D_z t}})]. \qquad (22)$$

The product of these three integral solutions (Eqs. (20), (21) and (22)) describes a semi-infinite contaminated parcel which moves in the positive x direction with a one-dimensional velocity but which continually expands in size in directions transverse to x throughout the whole domain of x, i.e., in the positive and negative regions.

Domenico and Robbins tested this approach against a superposition model that represented a "truncated" spatial integration of the point source model of Hunt (Section 4.2). The agreement was excellent and their resulting model for three-dimensional transport is

$$C(x,y,z,t) = \frac{C_0}{8}[\text{erfc}(\frac{x - vt}{2\sqrt{D_x t}})][\text{erf}(\frac{y + \frac{Y}{2}}{2\sqrt{D_y x / v}}) - \text{erf}(\frac{y - \frac{Y}{2}}{2\sqrt{D_y x / v}})]$$

$$[\text{erf}(\frac{z + \frac{Z}{2}}{2\sqrt{D_z x / v}}) - \text{erf}(\frac{z - \frac{Z}{2}}{2\sqrt{D_z x / v}})]. \qquad (23)$$

Similarly, for two-dimensional transport of contaminant, the remaining of an accounting of the substance initially confined in the region -Y/2 < y < Y/2 is the integration from y - Y/2 to y + Y/2. This integration gives Eq. (21) and the model for two-dimensional transport is

$$C(x,y,t) = \frac{C_0}{4}[\text{erfc}(\frac{x - vt}{2\sqrt{D_x t}})][\text{erf}(\frac{y + \frac{Y}{2}}{2\sqrt{D_y x / v}}) - \text{erf}(\frac{y - \frac{Y}{2}}{2\sqrt{D_y x / v}})] \qquad (24)$$

Moreover, for one-dimensional transport of contaminant, the model simply is

$$C(x,t) = \frac{C_0}{2}[\text{erfc}(\frac{x - vt}{2\sqrt{D_x t}})]. \qquad (25)$$

In all cases, the fundamental form of the solutions to the governing partial deferential equation (PDE) are products of exponential functions, e.g.,

$$C(x,y,z,t) = f_1(x)f_2(y)f_3(z)f_4(t) \tag{26}$$

that satisfy the partial deferential equation.

4.5 Exact Solutions for a Continuous Source of Finite Size

Domenico and Robbins' model is only an approximate approach to a continuous source of finite size. In order to properly extend those models for an instantaneous source of finite size to continuous source models to obtain more rigorous solutions (referred as to exact solutions), it would be required to either numerically solve the convolution integral associated with this instantaneous source, or perform the required spatial integration of the continuous point source models presented in Section 4.2. In this section, the convolution integration associated with instantaneous sources was selected.

First of all, the continuous source solution to one-dimensional case can be derived from Eq. (6) by replacing M_1/n with $C_0 v d\tau$, t with $t - \tau$, and integrating with respect to τ from $\tau = 0$ to $\tau = t$ to give

$$C(x,t) = \int_0^t \frac{C_0 v}{2\sqrt{\pi D_x (t-\tau)}} \exp[-\frac{(x - v(t-\tau))^2}{4D_x (t-\tau)}] d\tau . \tag{27}$$

Secondly, the continuous source solution to the two-dimensional case can be derived from Eq. (11) by replacing M_2/n with $C_0 v d\tau$, t with $t - \tau$, and integrating with respect to τ from $\tau = 0$ to $\tau = t$ and with respect to y' from $y' = -Y/2$ to $y' = Y/2$ to give

$$C\ (x,y,t) = \int_{-\frac{Y}{2}}^{\frac{Y}{2}} \int_0^t \frac{C_0 v \exp[-\frac{(x-v(t-\tau))^2}{4D_x(t-\tau)} - \frac{(y-y')^2}{4D_y(t-\tau)}]}{4\pi(t-\tau)\sqrt{D_x D_y}} d\tau dy', \quad (28)$$

where Y is the source dimension in the y direction.

Thirdly, the continuous source solution to the three-dimensional case can be derived from Eq. (8) by replacing M_3/n with $C_0 v d\tau$, t with $t - \tau$, and integrating with respect to τ from $\tau = 0$ to $\tau = t$ and with respect to y' from $y' = -Y/2$ to $y' = Y/2$ and with respect to z' from $z' = -Z/2$ to $z' = Z/2$ to give

$$C(x,y,z,t) = \int_{-\frac{Z}{2}}^{\frac{Z}{2}} \int_{-\frac{Y}{2}}^{\frac{Y}{2}} \int_0^t \frac{C_0 v}{8\sqrt{\pi^3 (t-\tau)^3 D_x D_y D_z}}$$

$$\exp[-\frac{(x-v(t-\tau))^2}{4D_x(t-\tau)} - \frac{(y-y')^2}{4D_y(t-\tau)} - \frac{(z-z')^2}{4D_z(t-\tau)} d\tau dy' dz'. \quad (29)$$

Equations (27), (28) and (29) are in integral form and closed-form results for either the time or spatial integrations are available, but not for both. Numerical integration is required to evaluate the exact models and the evaluation procedure is rather complicated and time consuming.

4.6 Solutions for a Decaying Contaminant Species

Domenico (1987) developed a model for a finite source that incorporated one-dimensional groundwater velocity, longitudinal and transverse dispersion, and some form of decay (decay rate λ) for either radionuclides or biodegradable organics. In this work

Domenico outlined an approach where three-dimensional approximations could be constructed from the product of three orthogonal one-dimensional solutions. They are

$$C(x,t) = \frac{C_0}{2}\exp[\frac{x(v-\sqrt{v^2+4\lambda D_x})}{2D_x}]\,\mathrm{erfc}(\frac{x-t\sqrt{v^2+4\lambda D_x}}{2\sqrt{D_x t}}), \tag{30}$$

$$C(x,y,t) = \frac{C_0}{4}\exp[\frac{x(v-\sqrt{v^2+4\lambda D_x})}{2D_x}]\mathrm{erfc}(\frac{x-t\sqrt{v^2+4\lambda D_x}}{2\sqrt{D_x t}})$$

$$[\mathrm{erf}(\frac{y+\frac{Y}{2}}{2\sqrt{D_y\frac{x}{v}}})-\mathrm{erf}(\frac{y-\frac{Y}{2}}{2\sqrt{D_y\frac{x}{v}}})], \tag{31}$$

$$C(x,y,z,t) = \frac{C_0}{8}\exp[\frac{x(v-\sqrt{v^2+4\lambda D_x})}{2D_x}]\mathrm{erfc}(\frac{x-t\sqrt{v^2+4\lambda D_x}}{2\sqrt{D_x t}})$$

$$[\mathrm{erf}(\frac{y+\frac{Y}{2}}{2\sqrt{D_y\frac{x}{v}}})-\mathrm{erf}(\frac{y-\frac{Y}{2}}{2\sqrt{D_y\frac{x}{v}}})]\,[\mathrm{erf}(\frac{z+\frac{Z}{2}}{2\sqrt{D_z\frac{x}{v}}})-\mathrm{erf}(\frac{z-\frac{Z}{2}}{2\sqrt{D_z\frac{x}{v}}})]. \tag{32}$$

4.7 The Proposed Models -- Solutions to Approximation No.1 to Exponentially Decaying Sources

The extension finite-source model to account for an exponentially decaying source term is accomplished using Domenico's (1987) approach with different source models. For one-dimensional flow, the initial and boundary conditions are

$C(x,0) = 0$,

$C(0,t) = C_0 \exp(-\lambda t)$,

$$\frac{\partial C}{\partial x}(\pm\infty, t) = 0. \qquad (33)$$

The one-dimensional source model (Marino, 1974) is

$$C(x,t) = \frac{C_0}{2}\exp(-\lambda t)[\exp(\frac{vx - x\sqrt{v^2 - 4\lambda D_x}}{2D_x})$$

$$\mathrm{erfc}(\frac{x - t\sqrt{v^2 - 4\lambda D_x}}{2\sqrt{D_x t}}) + \exp(\frac{vx + x\sqrt{v^2 - 4\lambda D_x}}{2D_x})\ \mathrm{erfc}(\frac{x + t\sqrt{v^2 - 4\lambda D_x}}{2\sqrt{D_x t}})]. \qquad (34)$$

Application of Domenico's approach leads to the following models (two-dimensional and three-dimensional) for sources centered at x = 0, y = 0, and z = 0 with concentration in the source of $C(0, t) = C_0 \exp(-\lambda t)$:

$$C(x,y,t) = \frac{C_0}{4}\exp(-\lambda t)[\exp(\frac{vx - x\sqrt{v^2 - 4\lambda D_x}}{2D_x})$$

$$\mathrm{erfc}(\frac{x - t\sqrt{v^2 - 4\lambda D_x}}{2\sqrt{D_x t}}) + \exp(\frac{vx + x\sqrt{v^2 - 4\lambda D_x}}{2D_x})$$

$$\mathrm{erfc}(\frac{x + t\sqrt{v^2 - 4\lambda D_x}}{2\sqrt{D_x t}})][\mathrm{erf}(\frac{y + \frac{Y}{2}}{2\sqrt{D_y \frac{x}{v}}}) - \mathrm{erf}(\frac{y - \frac{Y}{2}}{2\sqrt{D_y \frac{x}{v}}})], \qquad (35)$$

$$C(x,y,z,t) = \frac{C_0}{8}\exp(-\lambda t)[\exp(\frac{vx - x\sqrt{v^2 - 4\lambda D_x}}{2D_x})$$

$$\text{erfc}(\frac{x - t\sqrt{v^2 - 4\lambda D_x}}{2\sqrt{D_x t}}) + \exp(\frac{vx + x\sqrt{v^2 - 4\lambda D_x}}{2D_x})$$

$$\text{erfc}(\frac{x + t\sqrt{v^2 - 4\lambda D_x}}{2\sqrt{D_x t}})][\text{erf}(\frac{y + \frac{Y}{2}}{2\sqrt{D_y \frac{x}{v}}}) - \text{erf}(\frac{y - \frac{Y}{2}}{2\sqrt{D_y \frac{x}{v}}})]$$

$$[\text{erf}(\frac{z + \frac{Z}{2}}{2\sqrt{D_z \frac{x}{v}}}) - \text{erf}(\frac{z - \frac{Z}{2}}{2\sqrt{D_z \frac{x}{v}}})]. \quad (36)$$

4.8 Solutions to Approximate No.2 to Exponentially Decaying Sources

In addition to the application of Domenico's approach to obtain models for exponentially decaying sources, another attempt was made to approximate solutions to the problems. The process of developing the models is to superpose an infinite number of impulse solutions, all starting at the same time but each being displaced from $x = 0$ by $-v\tau$ units. Figure 3 is the schematic depicting this procedure.

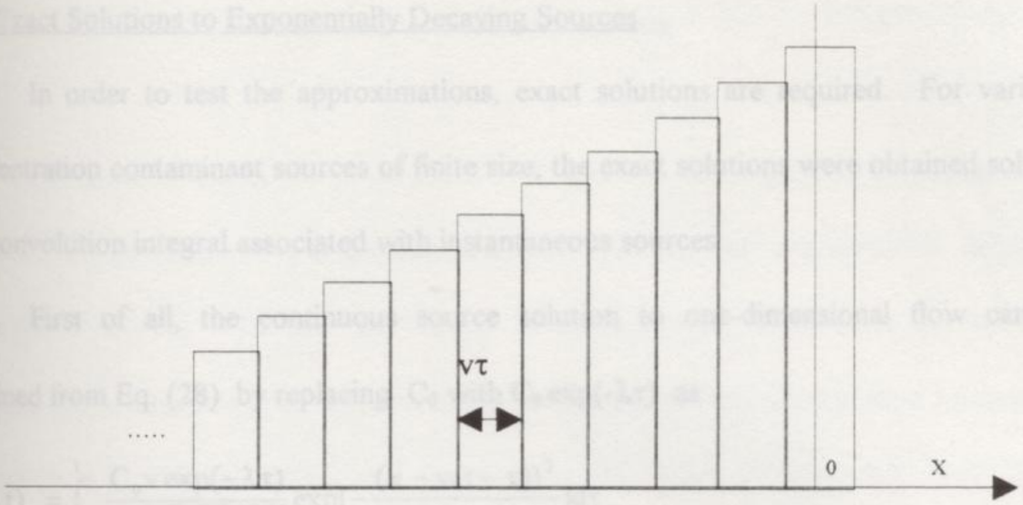

Figure 3. Schematic for the Developing of Approximation No.2

The solutions are

$$C(x,t) = \int_{-\infty}^{0} \frac{C_0 \exp(-\lambda \frac{\xi}{v})}{2\sqrt{\pi D_x t}} \exp[-\frac{(x-\xi-vt)^2}{4D_x t}]d\xi \,, \tag{37}$$

$$C(x,y,t) = \int_{-\frac{Y}{2}}^{\frac{Y}{2}} \int_{-\infty}^{0} \frac{C_0 \exp(-\lambda \frac{\xi}{v}) \exp[-\frac{(x-\xi-vt)^2}{4D_x t} - \frac{(y-y')^2}{4D_y t}]}{4\pi t\sqrt{D_x D_y}} d\xi dy', \tag{38}$$

$$C(x,y,z,t) = \int_{-\frac{Z}{2}}^{\frac{Z}{2}} \int_{-\frac{Y}{2}}^{\frac{Y}{2}} \int_{-\infty}^{0} \frac{C_0 v \exp(-\lambda \frac{\xi}{v})}{8\sqrt{\pi^3 t^3 D_x D_y D_z}} \exp[-\frac{(x-\xi-vt)^2}{4D_x t} - \frac{(y-y')^2}{4D_y t}$$

$$- \frac{(z-z')^2}{4D_z t} d\xi dy' dz'. \tag{39}$$

These equations are in integral form yet and can be evaluated analytically. The analytical expressions were found using the Mathematica.

4.9 Exact Solutions to Exponentially Decaying Sources

In order to test the approximations, exact solutions are required. For variable concentration contaminant sources of finite size, the exact solutions were obtained solving the convolution integral associated with instantaneous sources.

First of all, the continuous source solution to one-dimensional flow can be obtained from Eq. (28) by replacing C_0 with $C_0 \exp(-\lambda\tau)$ as

$$C(x,t) = \int_0^t \frac{C_0 v \exp(-\lambda\tau)}{2\sqrt{\pi D_x (t-\tau)}} \exp[-\frac{(x - v(t-\tau))^2}{4D_x(t-\tau)}] d\tau . \tag{40}$$

Secondly, the continuous source solution to two-dimensional flow can be obtained from Eq. (29) by replacing C_0 with $C_0 \exp(-\lambda\tau)$ as

$$C(x,y,t) = \int_{-\frac{Y}{2}}^{\frac{Y}{2}} \int_0^t \frac{C_0 v \exp(-\lambda\tau) \exp[-\frac{(x - v(t-\tau))^2}{4D_x(t-\tau)} - \frac{(y-y')^2}{4D_y(t-\tau)}]}{4\pi(t-\tau)\sqrt{D_x D_y}} d\tau dy' \tag{41}$$

Thirdly, the continuous source solution to three-dimensional flow can be obtained from Eq. (30) by replacing C_0 with $C_0 \exp(-\lambda\tau)$ as

$$C(x,y,z,t) = \int_{-\frac{Z}{2}}^{\frac{Z}{2}} \int_{-\frac{Y}{2}}^{\frac{Y}{2}} \int_0^t \frac{C_0 v \exp(-\lambda\tau)}{8\sqrt{\pi^3 (t-\tau)^3 D_x D_y D_z}} \exp[-\frac{(x - v(t-\tau))^2}{4D_x(t-\tau)} - \frac{(y-y')^2}{4D_y(t-\tau)}$$

$$-\frac{(z-z')^2}{4D_z(t-\tau)}] d\tau dy' dz' . \tag{42}$$

As Eqs. (27), (28), and (29), Eqs. (40), (41), and (42) are in integral forms and again either the spatial or temporal integrations have closed-form solutions, but not both. Numerical convolution is required to evaluate these expressions.

Chapter 5 Model Testing

The models presented in Sections 4.7 and 4.8 are regarded as approximate solutions to the adevective-dispersion transport problem of exponentially decaying contaminant sources. To test the validity of the approximations, these approximate solutions are compared to the exact solutions (requiring numerical integration) presented in Section 4.9. Model testing will be made in the order of one-, two- and three-dimensional groundwater flow fields with each having three test cases.

5.1 Model Testing for One-Dimensional Flow

In Section 4.9, the exact solution was presented as an integral form and this integration can not be solved analytically. Gaussian Quadrature (Press *et al.*, 1995) using Legendre polynomial weighting functions were used to perform the convolutions. One1_dll.for is a computer FORTRAN program (Appendix 1) used to perform the integration numerically. Testing of the program showed that this numerical integration method was accurate enough by dividing the range of the argument, which is the computation time of interest, into 3072 elements for the positions near the contaminant source and 1024 elements for rest of the distance.

On the other hand, the proposed model presented in Section 4.7 is simply composed of exponential functions and complimentary error functions and can be evaluated directly. One2_dll.for is a computer FORTRAN program (Appendix 2) employed to evaluate the model. It is worthy noting here that the complimentary error functions are evaluated numerically.

Finally, approximation no.2 depicted in Section 4.8 is also presented in an integral form and can be solved analytically. The Mathematica (Wolfram, 1994) software package is used to perform the required integration and the result is

$$C(x,t)=\frac{C_0}{2}\exp\left[\frac{\lambda(D_x\lambda t+tv^2-vx)}{v^2}\right]\operatorname{erfc}\left(\frac{-\frac{\lambda}{v}-\frac{v}{2D_x}+\frac{x}{2D_x t}}{\sqrt{\frac{1}{D_x t}}}\right) \tag{43}$$

Then a computer FORTRAN program was coded to evaluate the above expression. See Appendix 3 for a listing of One3_dll.for.

The model was tested in three cases and the numerical values of the parameters used in the model for testing are shown in Table 1.

Table 1. Parameters Used for One-Dimensional Model Testing

Parameters	Test Case 1	Test Case 2	Test Case 3
C_0, mg/L	1000	1000	1000
V, ft/day	10	10	100
D_x	0.1	1.0	10.0
λ, 1/day	0.0	0.1	1.0

The first test case was to compare the results of the approximations with the exact results when the source decay rate was zero. This case was the closest that corresponded to Domenico's original model and is equivalent to a constant source at $x = 0$. The second test case was identical to the first case except a source decay rate of 0.1 was imposed. The third case was also identical to the first case except a source decay rate of 1.0 was imposed. No particular length or time scale was considered, so these numerical values must be viewed as generic values all in appropriate units.

Figure 4 shows a plot of the concentration profiles for the exact and approximate solutions at three different times for test case 1. In this case, the agreement between the exact model and the approximations is excellent. In addition to the excellent matching, these results reproduce the expected step concentration profile for a continuous input source.

Figure 5 shows a plot of the concentration profile for exact and approximate solutions at three different times for test case 2. Again, the agreement between the exact model and the approximations is excellent. This case represents transport with Peclet number (xV/D) of 100 at x = 1 ft.

Figure 6 shows a plot of the concentration profile for exact and approximate solutions at three different times for test case 3. The agreement between the exact model and the approximations is also excellent. This case represents transport with Peclet number (xV/D) of 10 at x = 1 ft.

The maximum relative error for all cases occurred at x = 0. Table 2 shows the maximum relative errors for three cases. A second measure of relative errors for models was obtained from the Mean Relative Prediction Errors (MRPE) which is

$$MRPE = \sum \frac{ABS(\text{Approximation} - \text{Exact})_i}{\sum (\text{Exact})_i} 100\% . \tag{44}$$

Equation (44) is to provide a comparative measure of how well the models matches the exact solutions over the entire simulation domain. The form of the denominator in the MPRE is chosen to prevent division by zero when the domain includes uncontaminanted positions. Table 3 lists the MRPEs for one-dimensional model testing.

The maximum relative error for all cases was 2.5%, with the approximation having slightly higher total mass (expressed as the integral of the concentration profile) and the maximum error always occurring in the earliest time profiles. Generally these results indicate that the approximate models are valid and useful models for an exponentially decaying input source, when the length and time scales are sufficiently large; and that even at small length and time scales the approximations are good.

Mass conservation was tested in Figure 6. The area compassed by the concentration profile curves at $t = 10$ days and $t = 20$ days are 5,000 units and 5,000 units, respectively, which means that mass is conserved.

Table 2. The Maximum Relative Errors for One-Dimensional Model Testing

Test Case	Time, day	Exact Model	Appr. no.1	Appr. no.2	Max.Error
no.1	T=100	975.0	1000.0	1000.0	2.5%
	T=10	992.0	1000.0	1000.0	0.8%
	T=1	997.0	1000.0	1000.0	0.3%
no.2	T=100	0.044	0.045	0.045	2.3%
	T=10	365.0	368.0	368.0	0.8%
	T=1	903.0	905.0	905.0	0.2%
no.3	T=20	0.0	0.0	0.0	0.0%
	T=10	0.045	0.045	0.045	0.0%
	T=1	368.0	368.0	368.0	0.0%

Note: Error = [(Exact - Approximation) / Exact] x 100%

Table 3. MRPEs for One-Dimensional Model Testing

Time day	Test Case 1, %		Test Case 2, %		Test Case 3, %	
	Appx.no.1	Appx.no.2	Appx.no.1	Appx.no.2	Appx.no.1	Appx.no.2
1	0.22	0.22	1.10	1.10	0.32	0.27
10	0.10	0.10	0.32	0.27	0.21	0.14
20					0.19	0.12
100	0.05	0.05	0.21	0.14		
Average	0.12	0.12	0.54	0.50	0.24	0.18

Table 4 lists the results of convergence testing for Gaussian Quadrature method to evaluate convolutions. The range of the argument was divided into 256, 512, 1024, 2048, 4096 and 8192 elements respectively, and then parameters of one-dimensional model testing (case 1 when t = 100 days and x = 0 ft) were used to calculate the concentrations. Results show that Gaussian Quadrature method is convergent.

Table 4. Convergence Testing of Quadrature for Convolutions

Number of Quadrature Points	$C_i(0, 100)$	$\Delta_i = C_{i+1}-C_i$	Δ_{i+1}/Δ_i
256	680.65		
512	846.67	166.02	
1024	923.97	77.30	0.50
2048	962.06	38.09	0.50
4096	981.04	18.98	0.50
8192	990.52	9.48	0.50

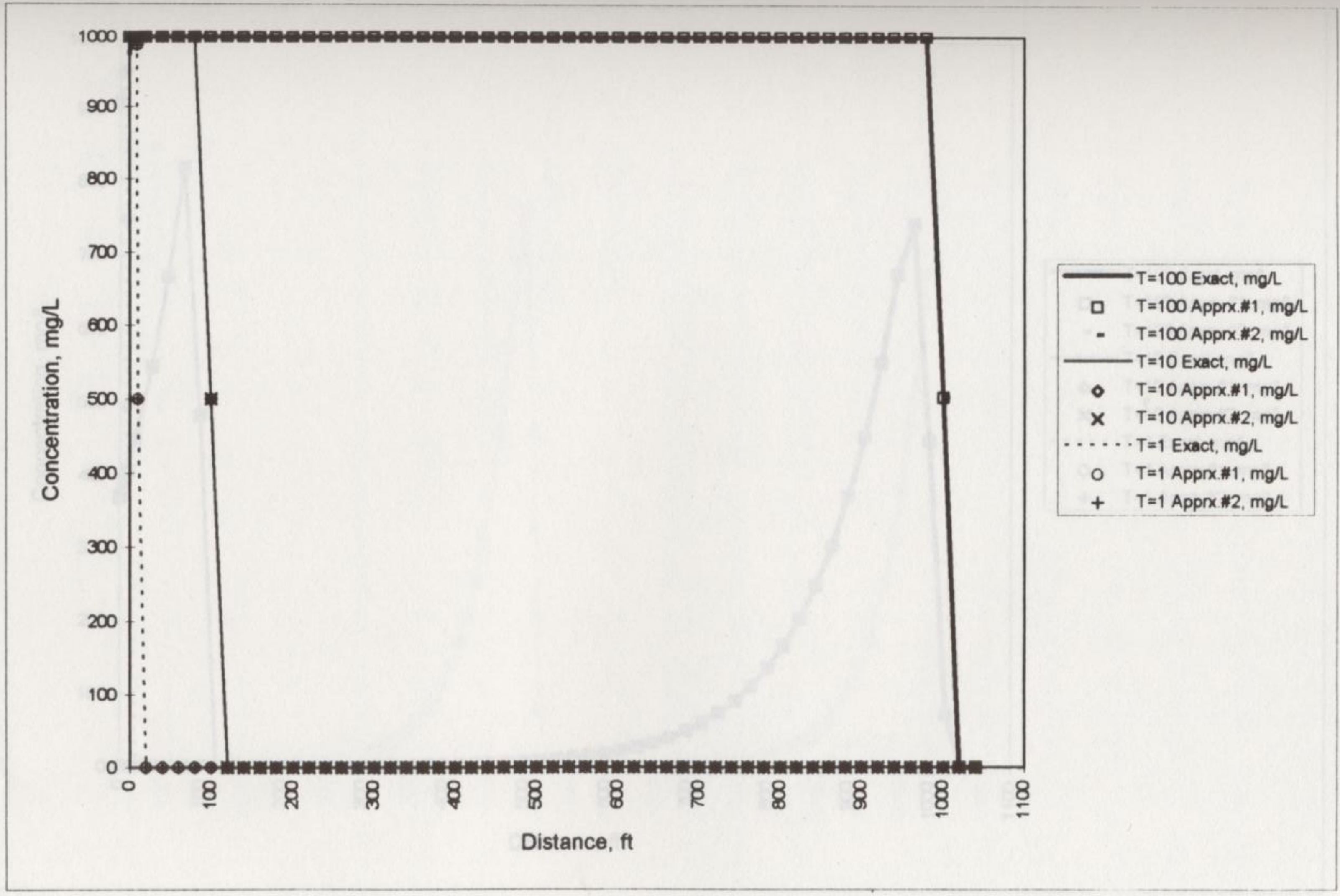

Figure 4. Model Testing for Test Case 1 for One-Dimensional Flow

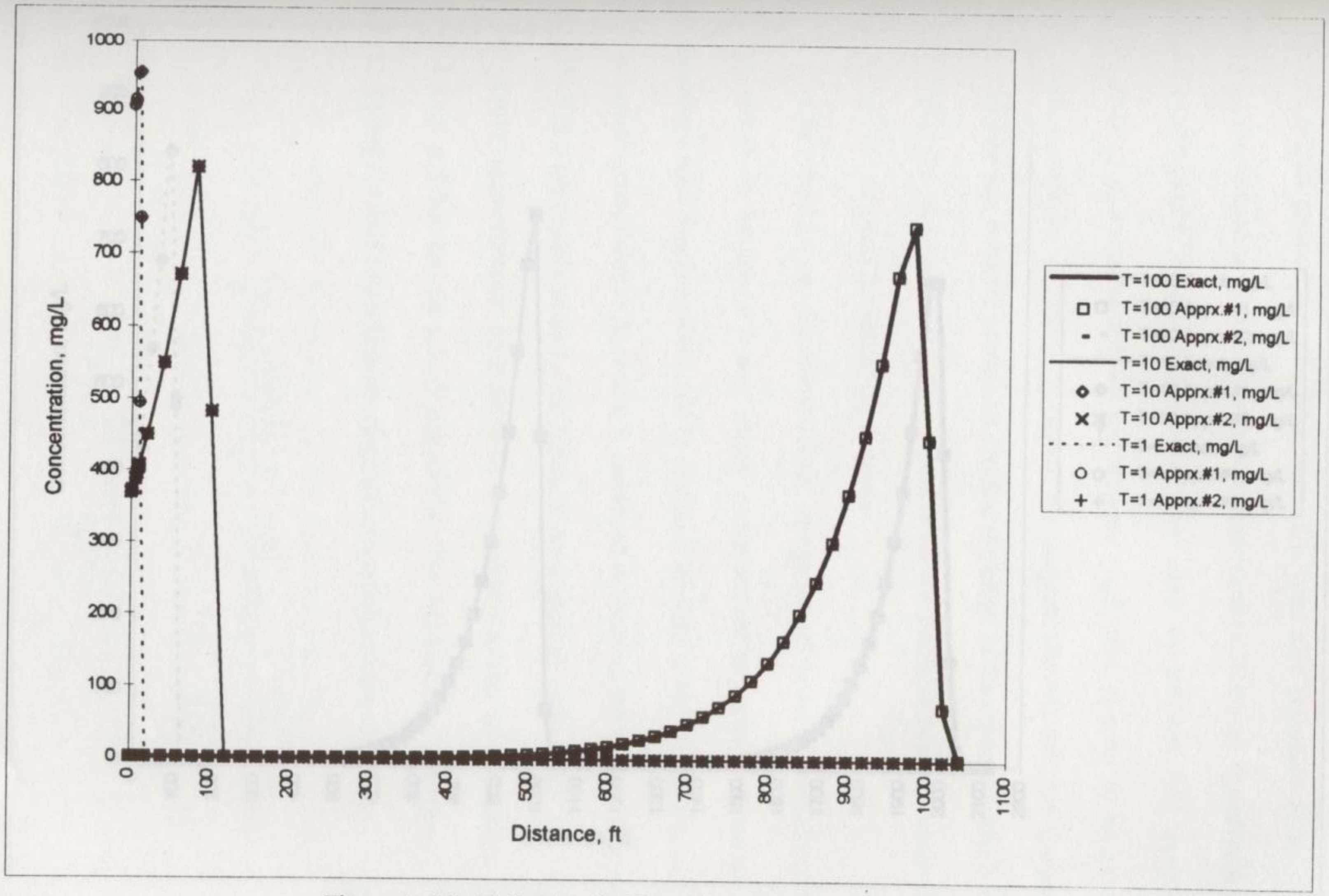

Figure 5. Model Testing for Test Case 2 for One-Dimensional Flow

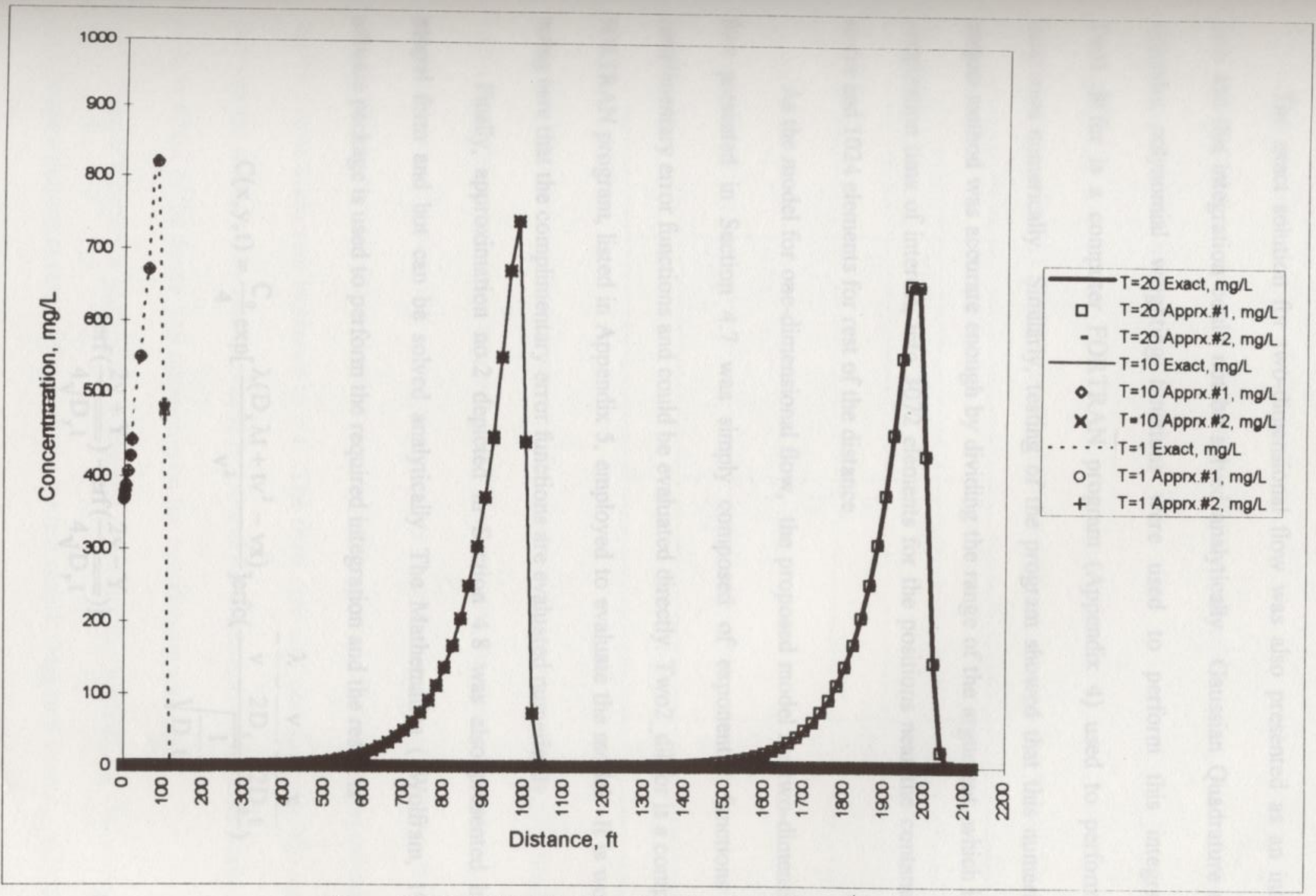

Figure 6. Model Testing for Test Case 3 for One-Dimensional Flow

5.2 Model Testing for Two-Dimensional Flow

The exact solution for two-dimensional flow was also presented as an integral form and this integration could not be solved analytically. Gaussian Quadrature using Legendre polynomial weighting functions were used to perform this integration. Two1_dll.for is a computer FORTRAN program (Appendix 4) used to perform the integration numerically. Similarly, testing of the program showed that this numerically integral method was accurate enough by dividing the range of the argument, which is the computation time of interest, into 3072 elements for the positions near the contaminant source and 1024 elements for rest of the distance.

As the model for one-dimensional flow, the proposed model for two-dimensional flow presented in Section 4.7 was simply composed of exponential functions and complimentary error functions and could be evaluated directly. Two2_dll.for is a computer FORTRAN program, listed in Appendix 5, employed to evaluate the model. It is worthy noting here that the complimentary error functions are evaluated numerically.

Finally, approximation no.2 depicted in Section 4.8 was also presented in an integral form and but can be solved analytically. The Mathematica (Wolfram, 1994) software package is used to perform the required integration and the result is

$$C(x,y,t) = \frac{C_0}{4}\exp[\frac{\lambda(D_x\lambda t + tv^2 - vx)}{v^2}]\mathrm{erfc}(\frac{-\frac{\lambda}{v} - \frac{v}{2D_x} + \frac{x}{2D_x t}}{\sqrt{\frac{1}{D_x t}}})$$

$$[\mathrm{erf}(\frac{2y+Y}{4\sqrt{D_y t}}) - \mathrm{erf}(\frac{2y-Y}{4\sqrt{D_y t}})]. \qquad (45)$$

Then a computer FORTRAN program was coded to evaluate the above expressions. See Appendix 6 for a listing of Two3_dll.for.

The model was tested in three cases and the numerical values of the parameters used in the model are shown in Table 5.

Table 5. Parameters Used for Two-Dimensional Model Testing

Parameters	Test Case 1	Test Case 2	Test Case 3
C_0, mg/L	1000	1000	1000
V, ft/day	10	10	100
D_x	0.1	10.0	20.0
D_y	0.01	1.0	2.0
Y, ft	100	100	100
λ, 1/day	0.0	0.1	1.0

The first test case was to compare the results of the approximations with the exact results when the source decay rate was zero. This case was the closest that corresponded to Domenico's original model and was equivalent to a constant source at $x = 0$. The second test case was similar to the first case with dispersion coefficients increased tenfold and the source decay rate increased to 0.1. The third case was also similar to the second case with the source decay rate increased to 1.0 and the dispersion coefficients doubled to show the effect of the decay and dispersion on the contaminant transport.

Figure 7 shows a plot of the centerline concentration profiles for the exact and approximate solutions at three different times for test case 1. Figure 8 shows a plot of off-

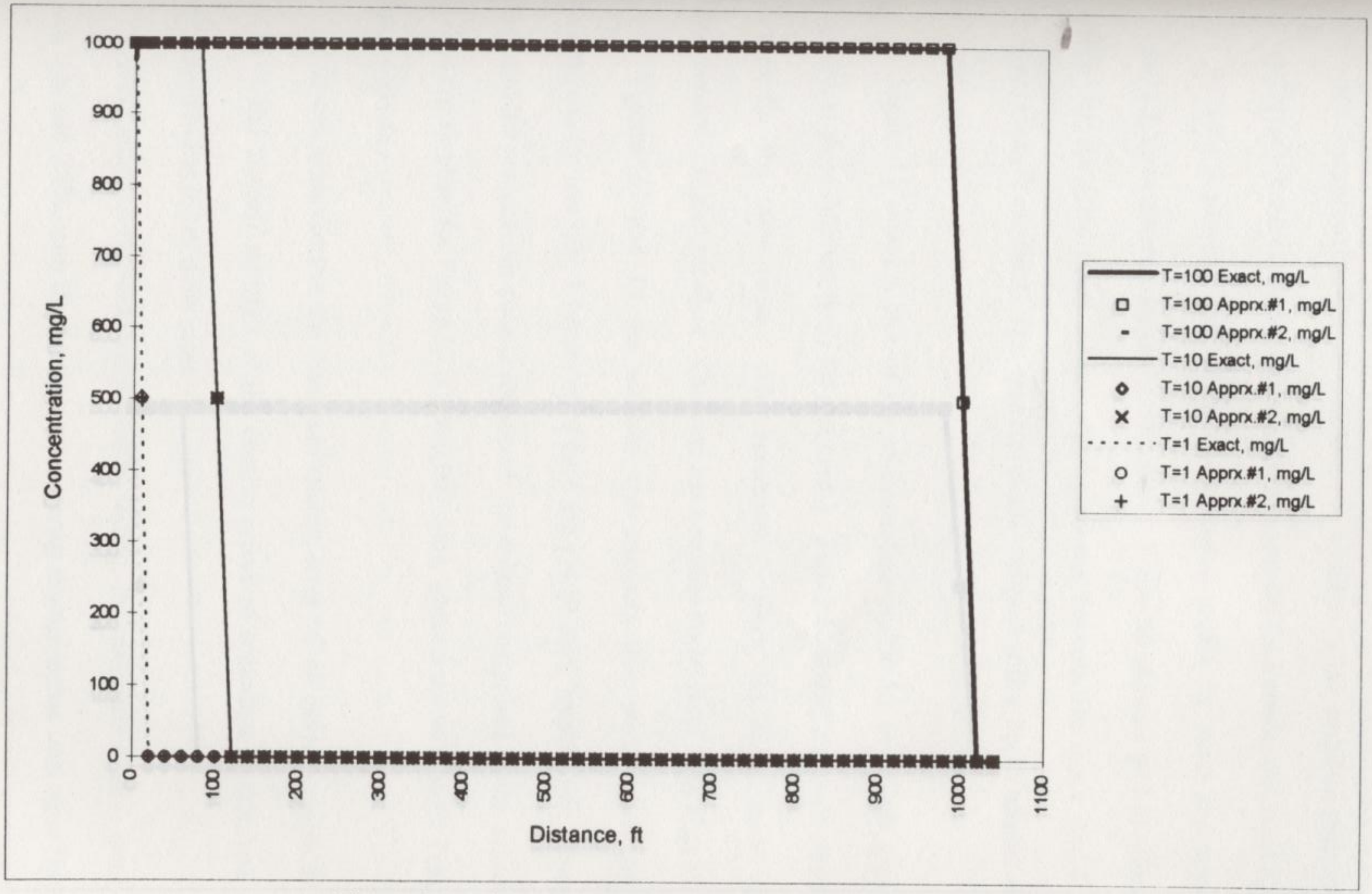

Figure 7 Model Testing for Test Case 1 for Two-Dimensional Flow
Centerline Concentration Profiles

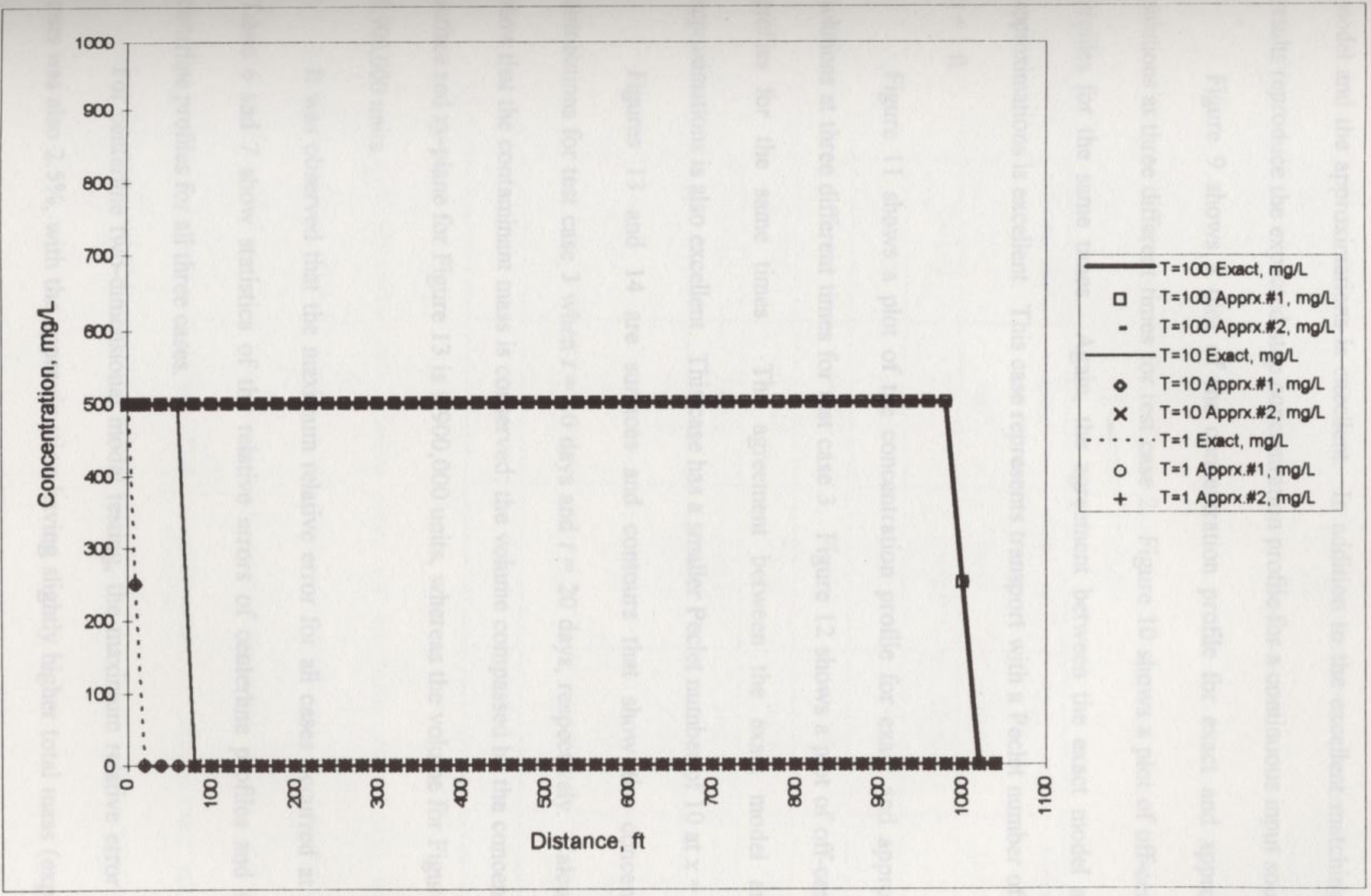

Figure 8 Model Testing for Test Case 1 for Two-Dimensional Flow
Off-Centerline Concentration Profiles (y=50 ft)

centerline profiles for the same times. In this case, the agreement between the exact model and the approximations is excellent. In addition to the excellent matching, these results reproduce the expected step concentration profile for a continuous input source.

Figure 9 shows a plot of the concentration profile for exact and approximate solutions at three different times for test case 2. Figure 10 shows a plot of off-centerline profiles for the same times. Again, the agreement between the exact model and the approximations is excellent. This case represents transport with a Peclet number of 100 at $x = 1$ ft.

Figure 11 shows a plot of the concentration profile for exact and approximate solutions at three different times for test case 3. Figure 12 shows a plot of off-centerline profiles for the same times. The agreement between the exact model and the approximations is also excellent. This case has a smaller Peclet number of 10 at $x = 1$ ft.

Figures 13 and 14 are surfaces and contours that show the concentration distributions for test case 3 when $t = 10$ days and $t = 20$ days, respectively. Calculations show that the contaminant mass is conserved: the volume compassed by the concentration surface and xy-plane for Figure 13 is 9,900,000 units, whereas the volume for Figure 14 is 9,900,000 units.

It was observed that the maximum relative error for all cases occurred at $x = 0$. Tables 6 and 7 show statistics of the relative errors of centerline profiles and of off-centerline profiles for all three cases.

For centerline two-dimensional model testing, the maximum relative error for all cases was also 2.5%, with the approximation having slightly higher total mass (expressed as the integral of the concentration profile) and the maximum error always occurring in the earliest time profiles. Generally these results indicate that the approximate models are valid, and useful models for an exponentially decaying input source.

Table 6. The Maximum Relative Errors for Two-Dimensional Model Testing (Centerline Profile)

Test Case	Time, day	Exact mg/L	Appr. no.1 mg/L	Appr. no.2 mg/L	Maximum Error, %
no.1	T=100	975.0	1000.0	1000.0	2.5
	T=10	992.0	1000.0	1000.0	0.8
	T=1	997.0	1000.0	1000.0	0.3
no.2	T=100	0.044	0.045	0.045	2.3
	T=10	365.0	368.0	368.0	0.8
	T=1	903.0	905.0	905.0	0.2
no.3	T=20	0.0	0.0	0.0	0.0
	T=10	0.045	0.045	0.045	0.0
	T=1	368.0	368.0	368.0	0.0

Once again the maximum relative error for all cases was 2.5%, with the approximation having slightly higher total mass (expressed as the integral of the concentration profile) and the maximum error always occurring in the earliest time profiles. Generally these results indicate that the approximate models are valid, and useful models for an exponentially decaying input source.

Table 7. The Maximum Relative Errors for Two-Dimensional Model Testing (Off-Centerline Profile)

Test Case	Time, day	Exact Model mg/L	Appr. no.1 mg/L	Appr. no.2 mg/L	Maximum Error, %
no.1	T=100	975.0	1000.0	1000.0	2.5
	T=10	992.0	1000.0	1000.0	0.8
	T=1	997.0	1000.0	1000.0	0.3
no.2	T=100	0.0	0.0	0.023	
	T=10	0.0	0.0	184.0	
	T=1	903.0	905.0	905.0	0.2
no.3	T=20	0.0	0.0	0.0	0.0
	T=10	0.0	0.0	0.023	
	T=1	0.0	0.0	184.0	

Table 8 lists the MRPEs for the Two-Dimensional Model Testing.

Table 8. MRPEs for Two-Dimensional Model Testing

Time day	Test Case 1, %.				Test Case 2, %				Test Case 3, %			
	Appx. no.1		Appx. no.2		Appx. no.1		Appx. no.2		Appx. no.1		Appx. no.2	
	Center	Off-Center	Center	Off-Center	Center	Off-Center	Center	Off-Center	Center	Off-Center	Center	Off-Center
1	0.46	0.46	0.46	0.46	14.9	14.7	6.8	6.7	0.54	0.53	0.42	0.42
10	0.14	0.14	0.14	0.14	2.12	2.04	1.51	1.45	0.38	0.38	0.25	0.25
20									0.34	0.35	0.22	0.22
100	0.05	0.05	0.05	0.05	1.48	1.48	0.85	0.84				
Ave.	0.22	0.22	0.22	0.22	6.16	6.06	3.05	3.0	0.42	0.42	0.30	0.30

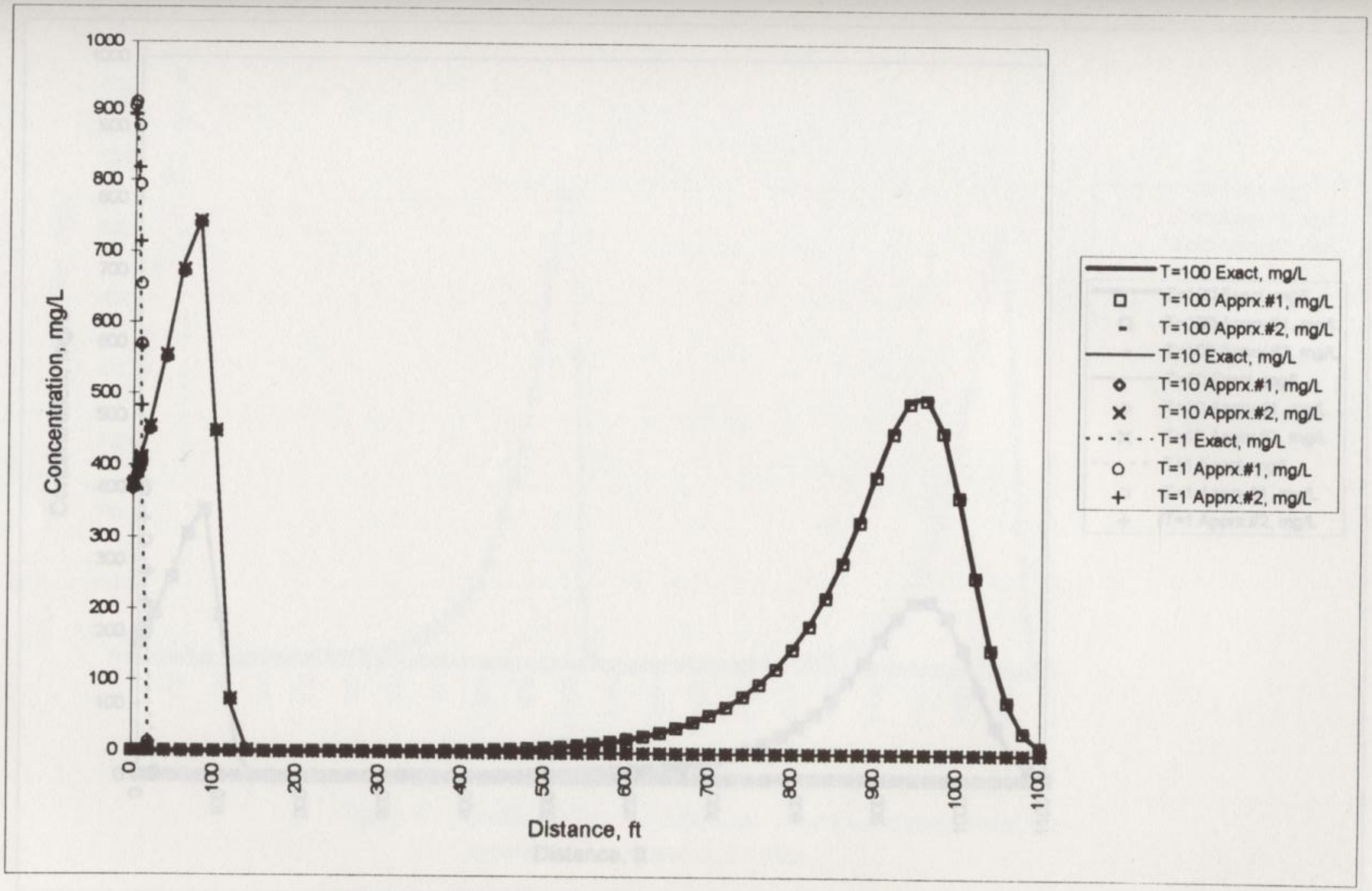

Figure 9 Model Testing for Test Case 2 for Two-Dimensional Flow Centerline Concentration Profiles

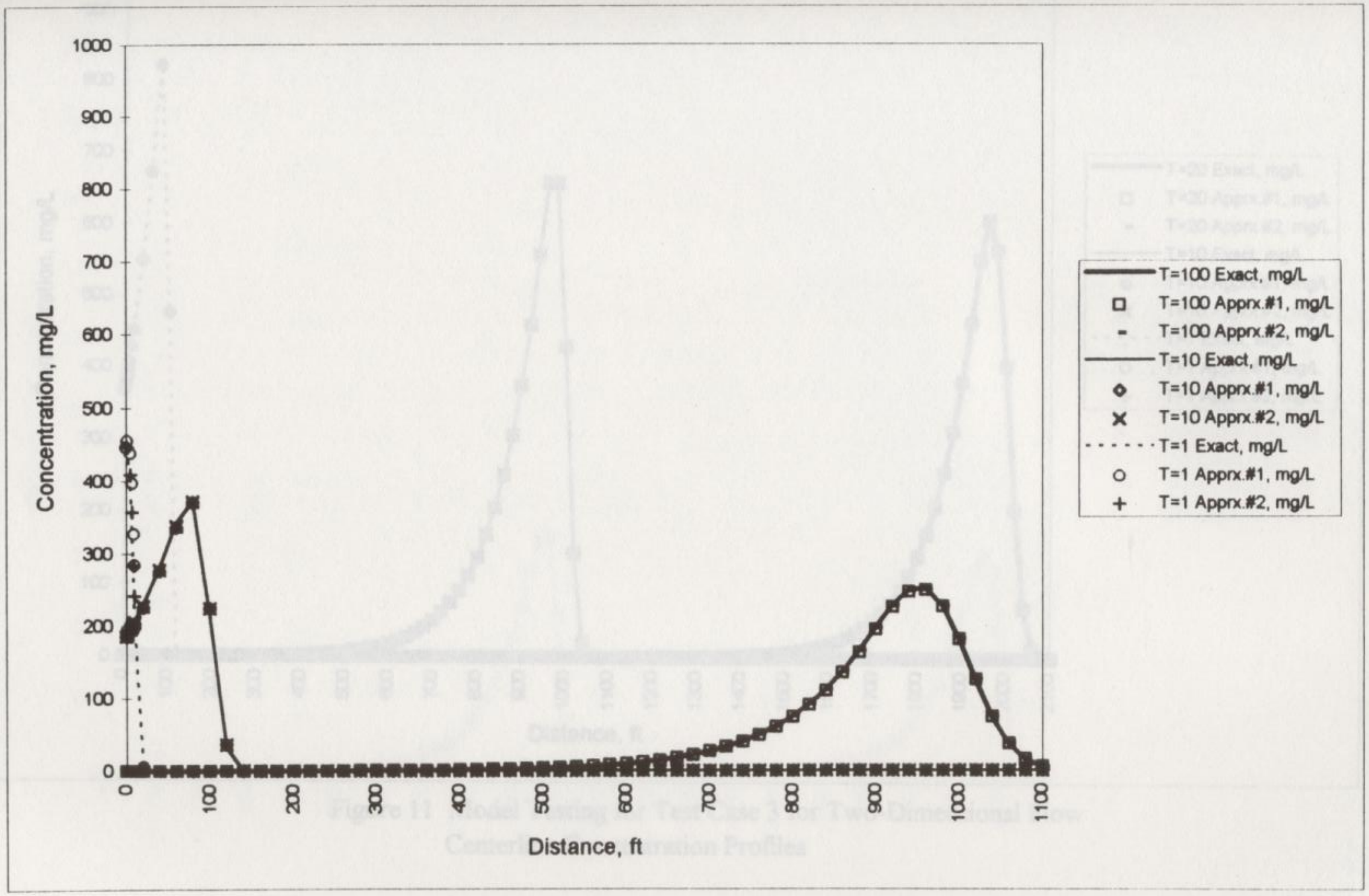

Figure 10 Model Testing for Test Case 2 for Two-Dimensional Flow Off-Centerline Concentration Profiles (y=50 ft)

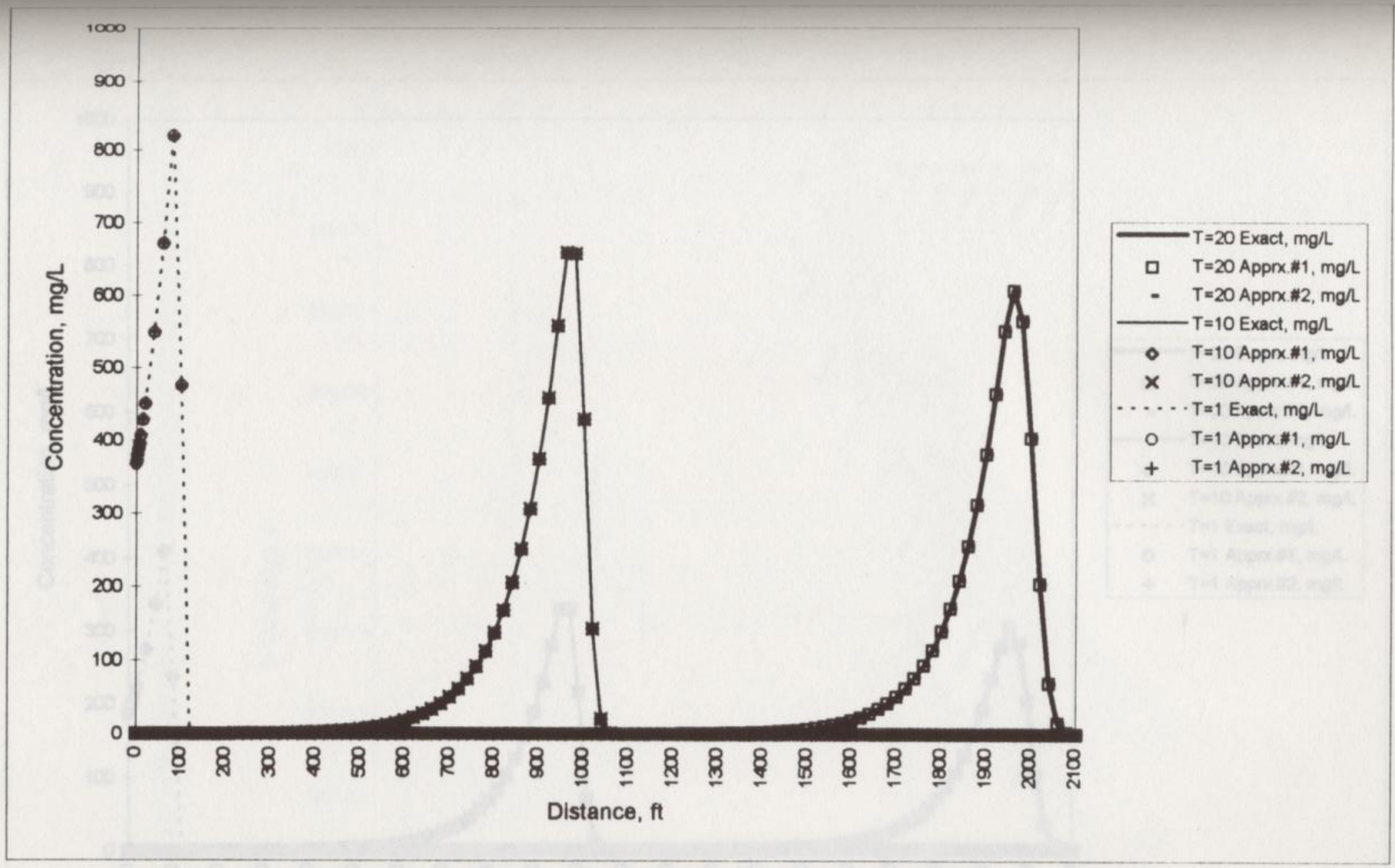

Figure 11 Model Testing for Test Case 3 for Two-Dimensional Flow Centerline Concentration Profiles

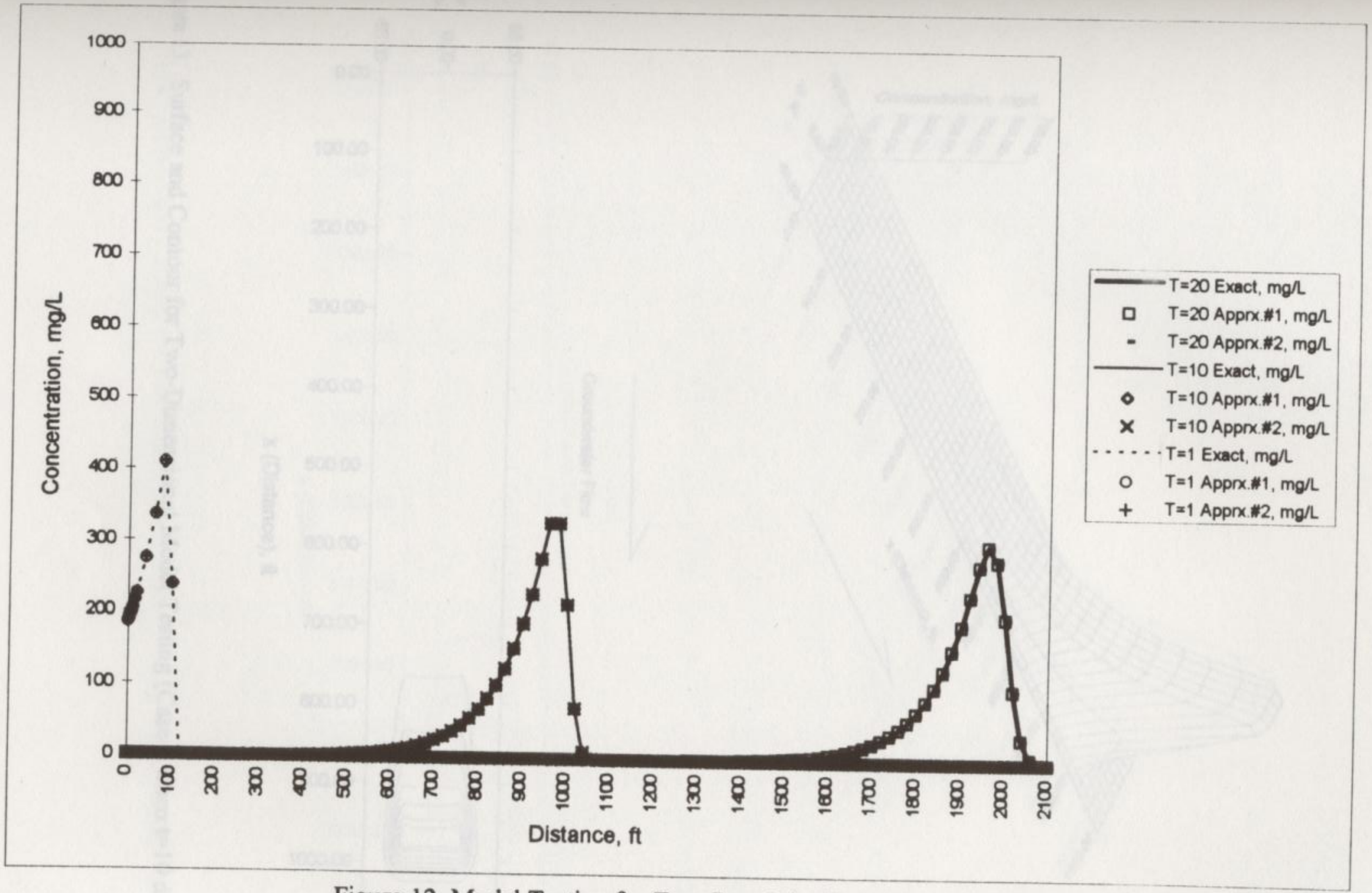

Figure 12 Model Testing for Test Case 3 for Two-Dimensional Flow Off-Centerline Concentration Profiles (y=50 ft)

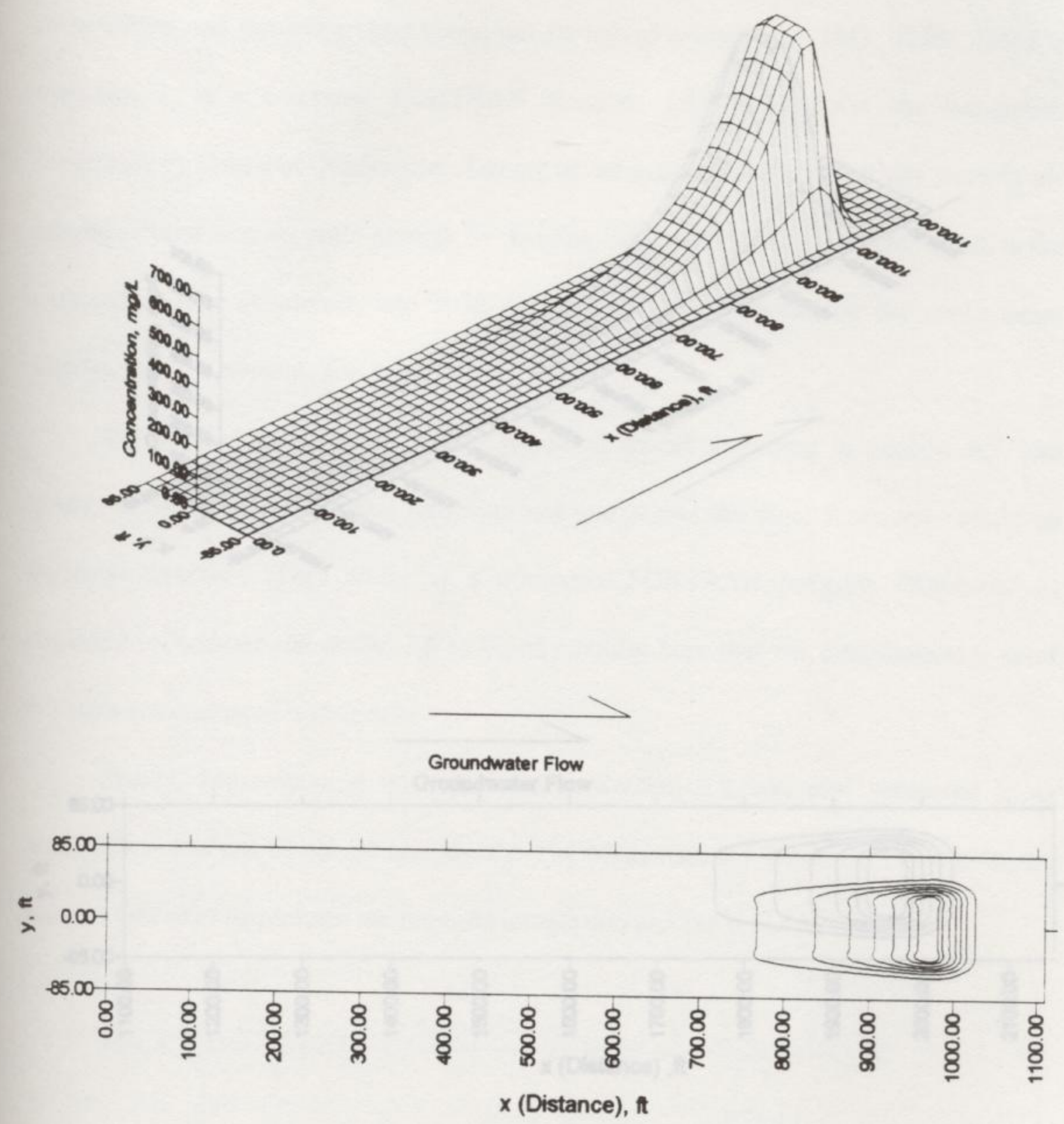

Figure 13. Surface and Contour for Two-Dimensional Model Testing (Case 3 when t=10 days)

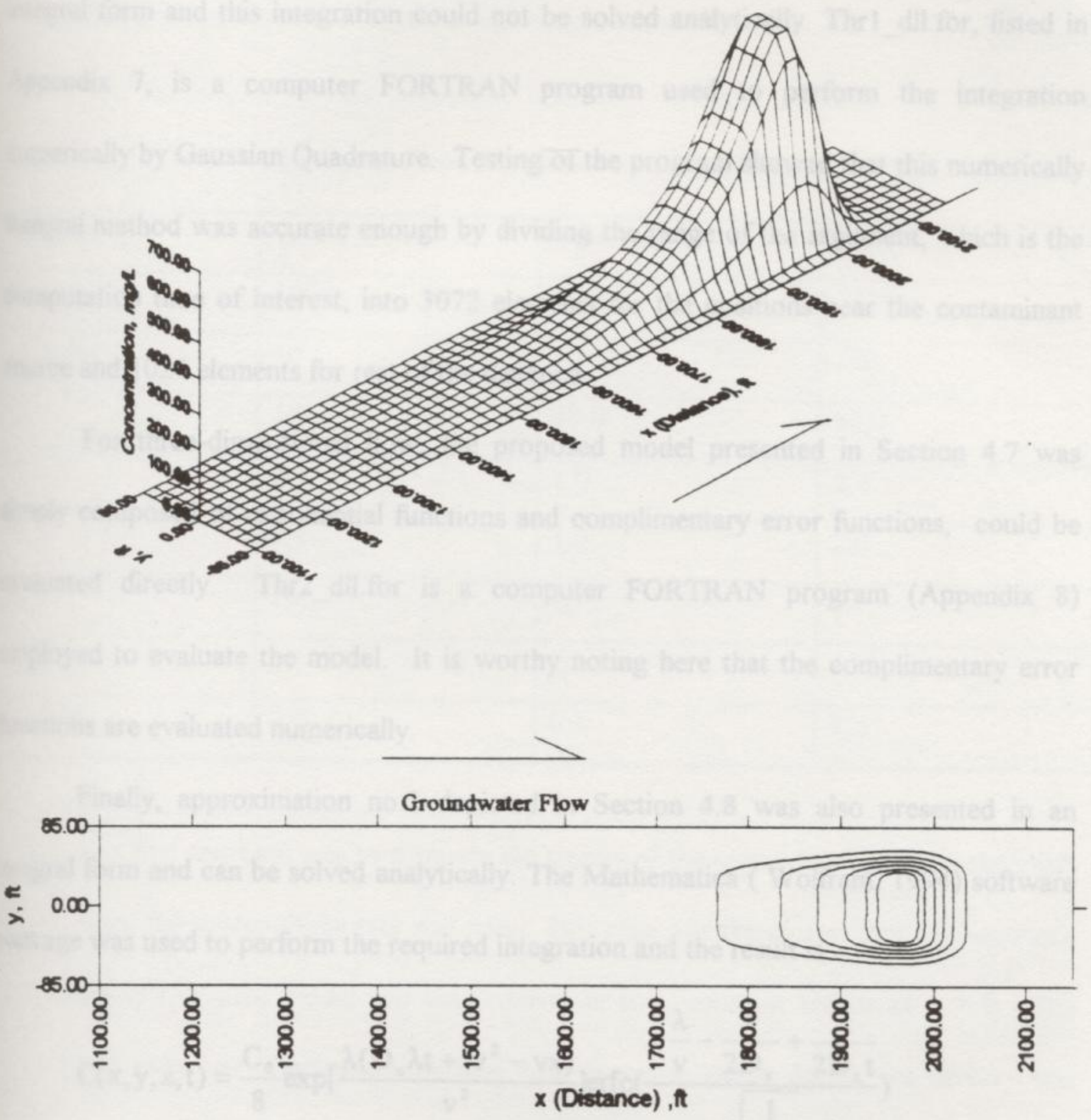

Figure 14. Surface and Contour for Two-Dimensional Model Testing (Case 3 when t=20 days)

5.3 Model Testing for Three-Dimensional Flow

Once again, the exact solution for three-dimensional flow was presented as an integral form and this integration could not be solved analytically. Thr1_dll.for, listed in Appendix 7, is a computer FORTRAN program used to perform the integration numerically by Gaussian Quadrature. Testing of the program showed that this numerically integral method was accurate enough by dividing the range of the argument, which is the computation time of interest, into 3072 elements for the positions near the contaminant source and 1024 elements for rest of the distance.

For three-dimensional flow, the proposed model presented in Section 4.7 was simply composed of exponential functions and complimentary error functions, could be evaluated directly. Thr2_dll.for is a computer FORTRAN program (Appendix 8) employed to evaluate the model. It is worthy noting here that the complimentary error functions are evaluated numerically.

Finally, approximation no.2 depicted in Section 4.8 was also presented in an integral form and can be solved analytically. The Mathematica (Wolfram, 1994) software package was used to perform the required integration and the result is

$$C(x,y,z,t) = \frac{C_0}{8}\exp[\frac{\lambda(D_x\lambda t + tv^2 - vx)}{v^2}]\mathrm{erfc}(\frac{-\frac{\lambda}{v} - \frac{v}{2D_x} + \frac{x}{2D_x t}}{\sqrt{\frac{1}{D_x t}}})$$

$$[\mathrm{erf}(\frac{2y+Y}{4\sqrt{D_y t}}) - \mathrm{erf}(\frac{2y-Y}{4\sqrt{D_y t}})][\mathrm{erf}(\frac{2z+Z}{4\sqrt{D_z t}}) - \mathrm{erf}(\frac{2z-Z}{4\sqrt{D_z t}})]. \quad (46)$$

Then a computer FORTRAN program was coded to evaluate the expressions. See Appendix 9 for the listing of Thr3_dll.for. The model was tested for three cases and Table 9 lists the parameters used to test three-dimensional models.

Table 9. Parameters Used for Three-dimensional Model Testing

Parameters	Test Case 1	Test Case 2	Test Case 3
C_0, mg/L	1000	1000	1000
V, ft/day	10	10	100
D_x	1.0	10.0	20.0
D_y	0.1	1.0	2.0
D_z	0.1	1.0	2.0
Y, ft	10	10	10
Z, ft	10	10	10
λ, 1/day	0.0	0.1	1.0

The first test case was to compare the results of the approximations with the exact results when the source decay rate was zero. This case was the closest that corresponded to Domenico's original model and was equivalent to a constant source at x = 0. The second test case was identical to the first case except a source decay rate of 0.1 was imposed. The third case was also identical to the first case except a source decay rate of 1.0 was imposed. The numerical values of the parameters used in the model are shown in Table 9. No particular length or time scale was considered, so these numerical values must be viewed as generic values all in appropriate units.

Figure 15 shows a plot of the centerline concentration profiles for the exact and approximate solutions at three different times for test case 1. Figure 16 shows a plot of off-centerline profiles for the same times. In this case, the agreement between the exact model and the approximations is excellent. In addition to the excellent matching, these results reproduce the expected step concentration profile for a continuous input source.

Figure 17 shows a plot of the concentration profile for exact and approximate solutions at three different times for test case 2. Figure 18 shows a plot of off-centerline profiles for the same times. Again, the agreement between the exact model and the approximations is excellent. This case represents transport with a Peclet number of 100 at $x = 1$ ft.

Figure 19 shows a plot of the concentration profile for exact and approximate solutions at three different times for test case 3. Figure 20 shows a plot of off-centerline profiles for the same times. The agreement between the exact model and the approximations is also excellent. This case has a smaller Peclet number of 10 at $x = 1$ ft and the effect of dispersion is evident in the profiles.

Figure 21 is a density rendering that shows the concentration clouds for test case 3 when $t = 10$ days and $t = 20$ days, respectively. The red color indicates high concentration, purple low. The spatial volume occupied by the contaminant at $t = 10$ days is smaller than the spatial volume occupied by the contaminant at $t = 20$ days, because the contaminant is more concentrated at the earlier time point. The contaminant mass is conserved. It was observed that the maximum relative error for all cases occurred at $x = 0$. Tables 10 and 11 show statistics of the relative errors of centerline profiles and of off-

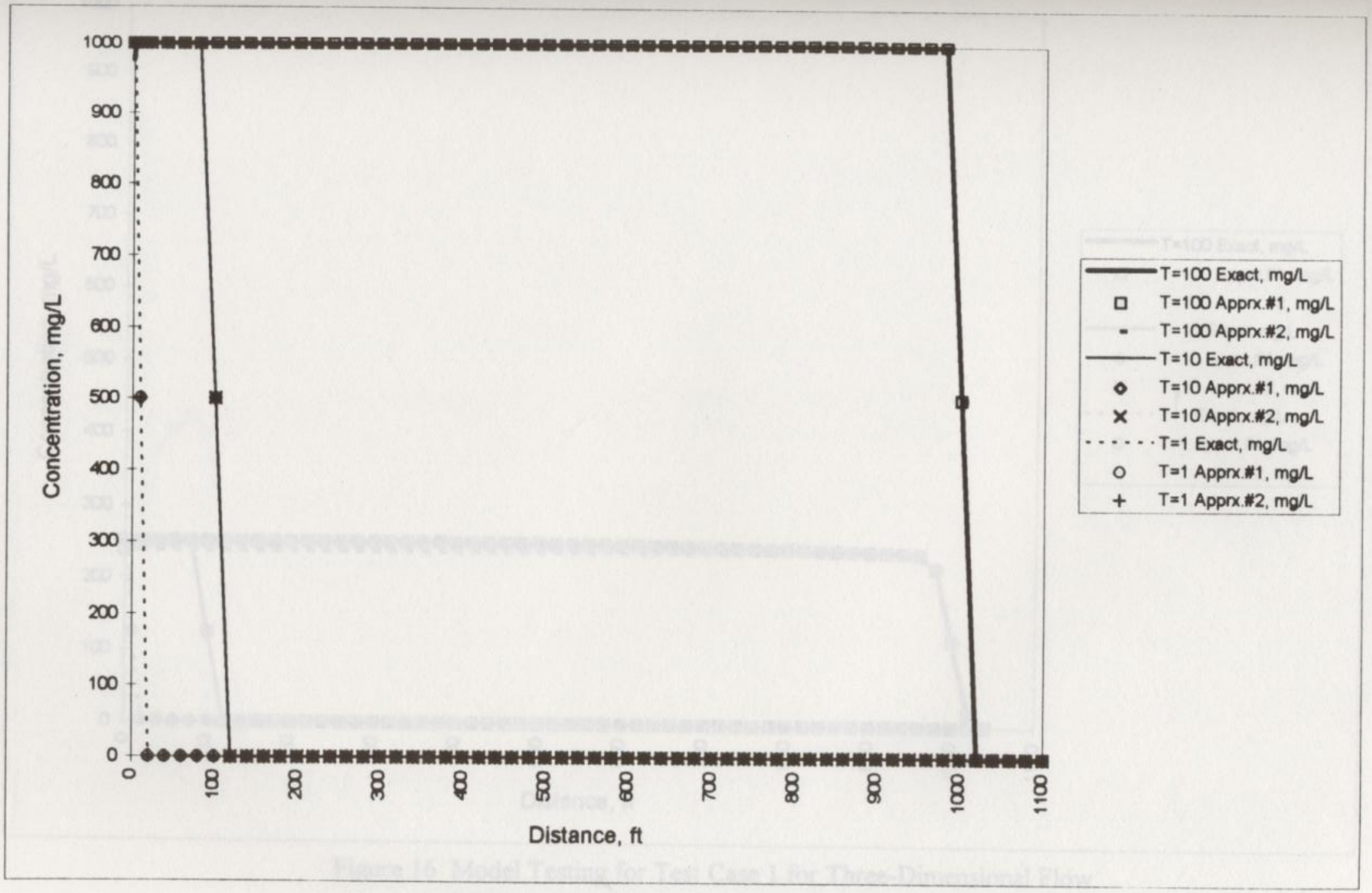

Figure 15 Model Testing for Test Case1 for Three-Dimensional Flow Centerline Concentration Profiles

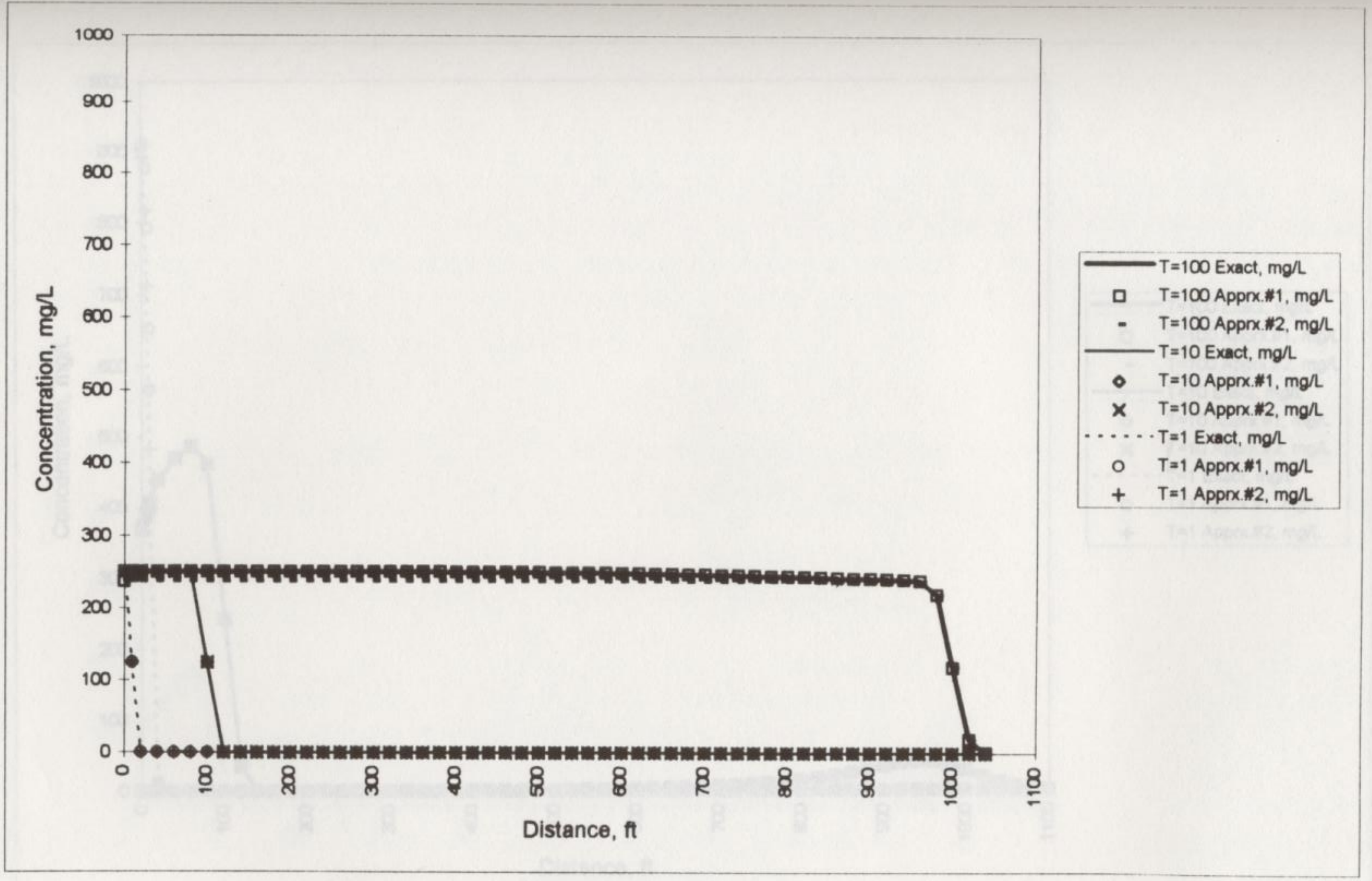

Figure 16 Model Testing for Test Case 1 for Three-Dimensional Flow Off-Centerline Concentration Profiles (y=z=5 ft)

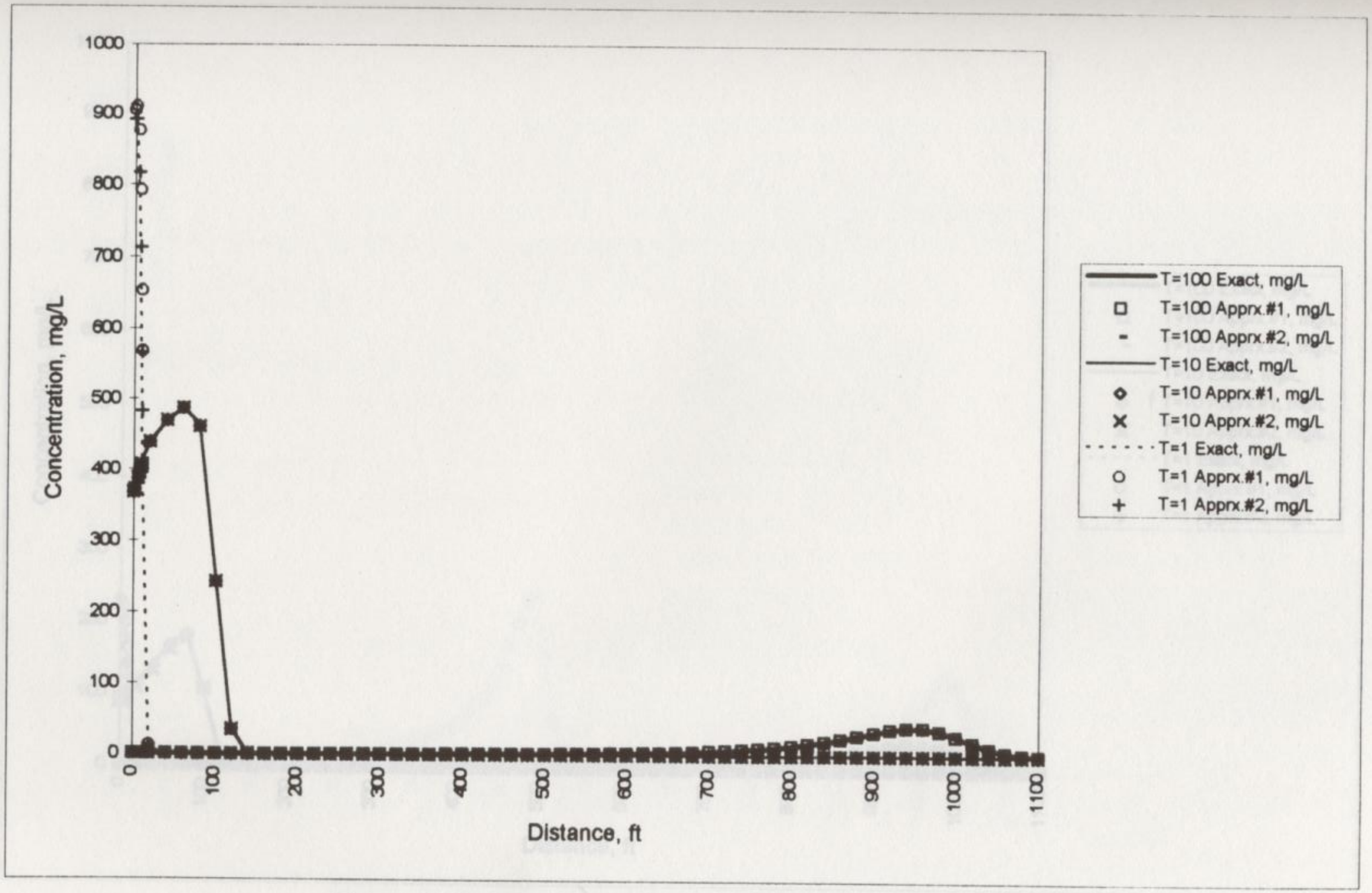

Figure 17 Model Testing for Test Case 2for Three-Dimensional Flow Centerline Concentration Profiles

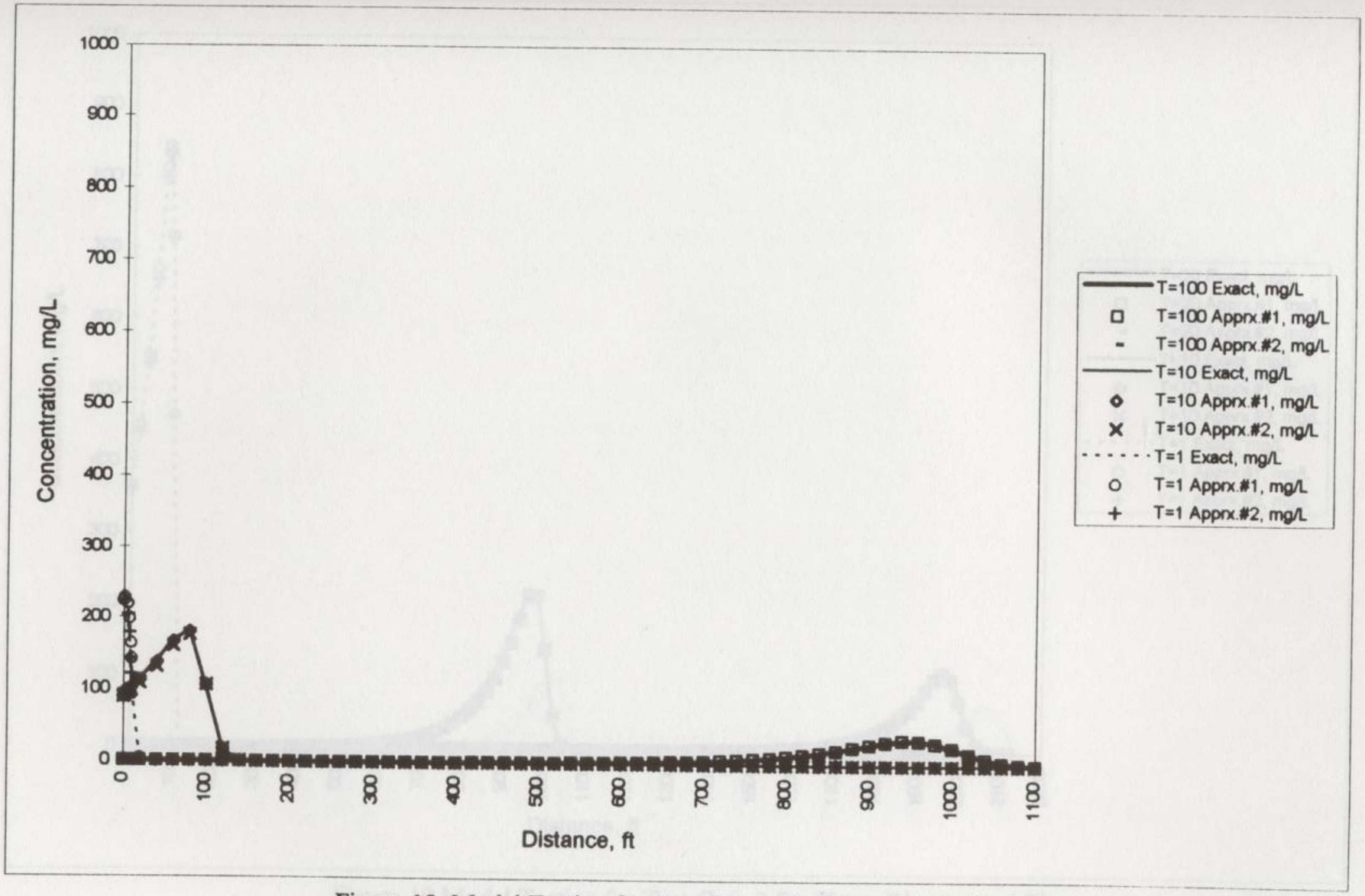

Figure 18 Model Testing for Test Case 2 for Three-Dimensional Flow Off-Centerline Concentration Profiles (y=z=5 ft)

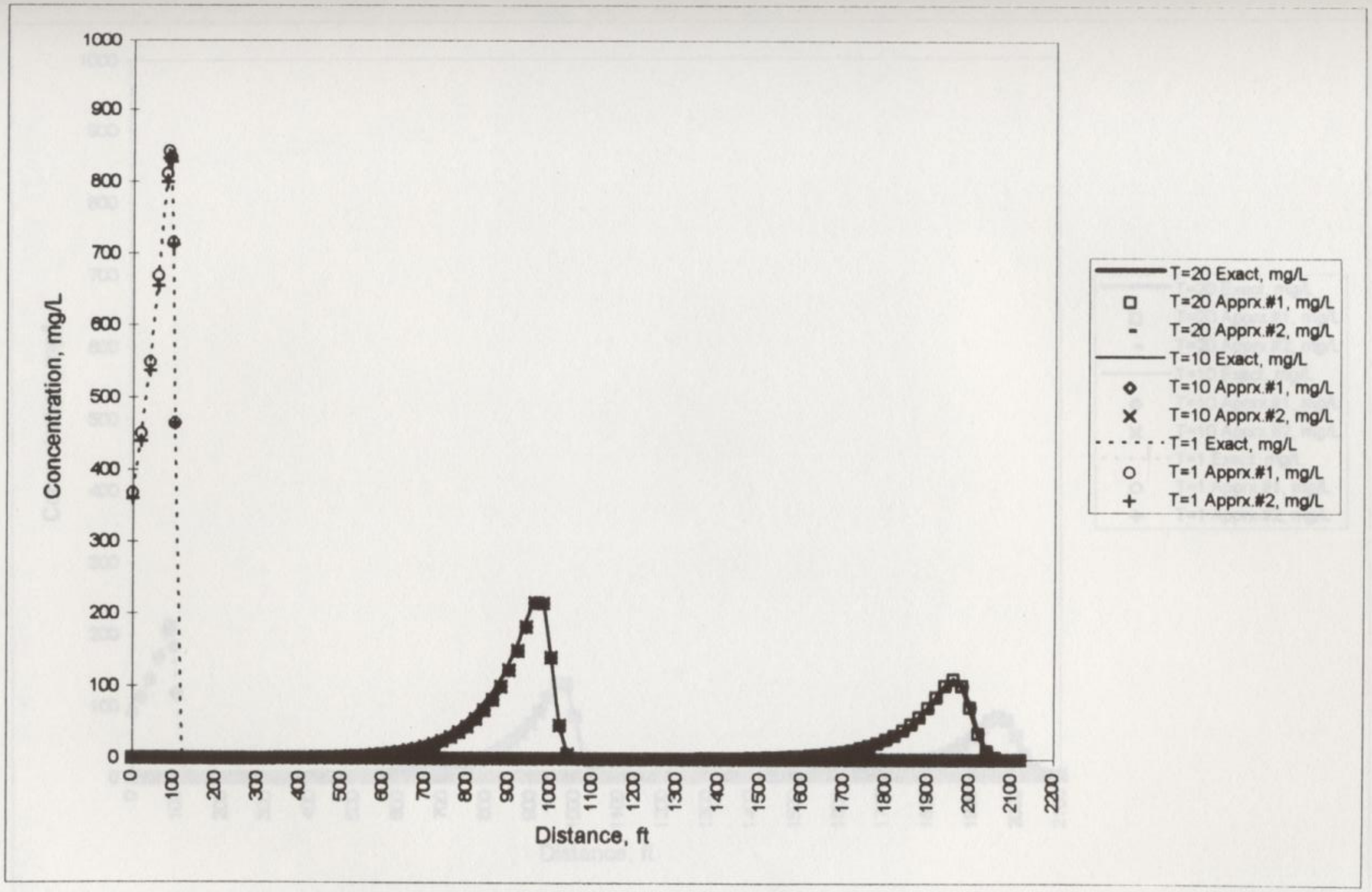

Figure 19 Model Testing for Test Case 3 for Three-Dimensional Flow Centerline Concentration Profiles

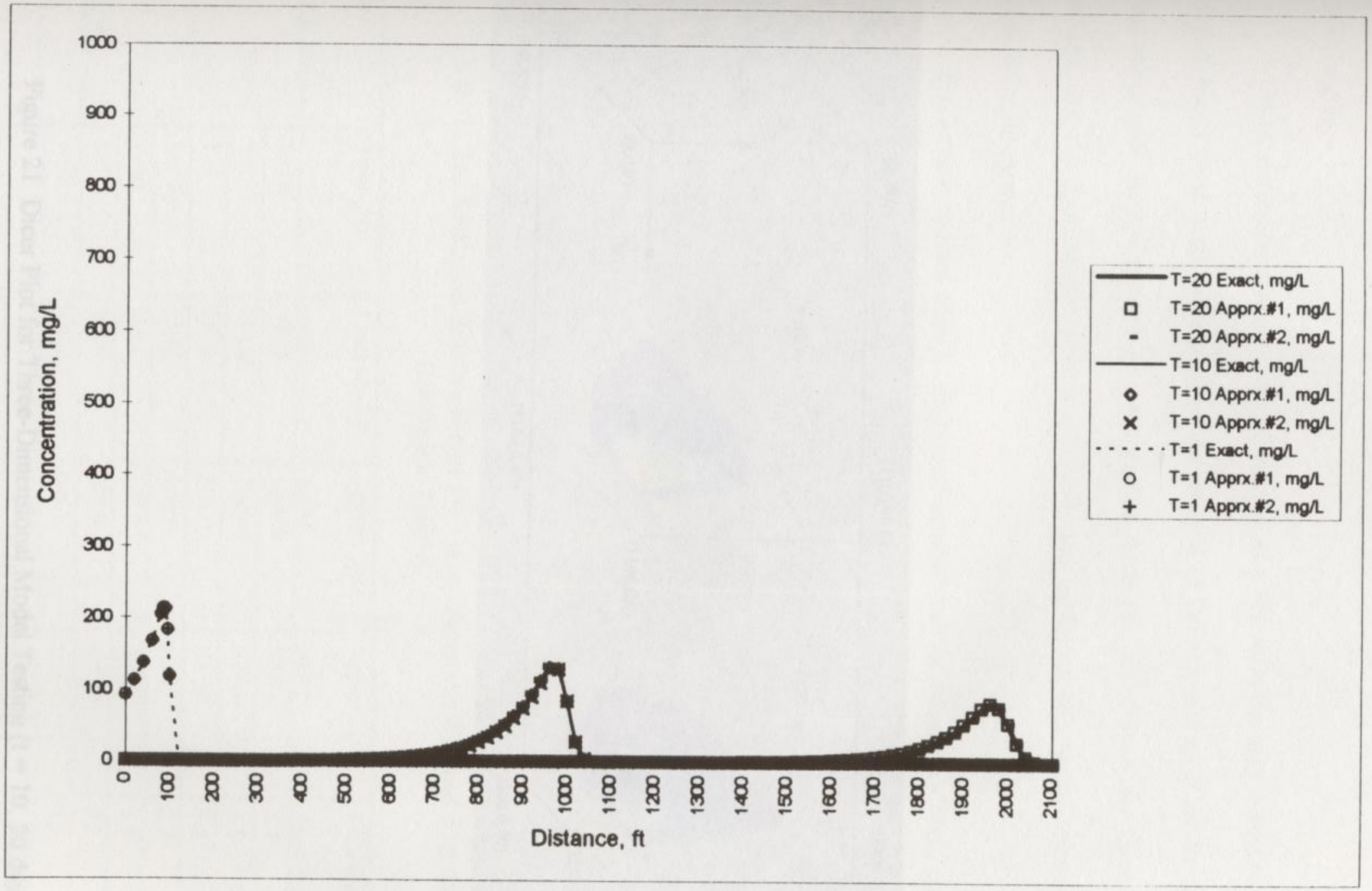

Figure 20 Model Testing for Test Case 3 for Three-Dimensional Flow
Off-Centerline Concentration Profiles (y=z=5 ft)

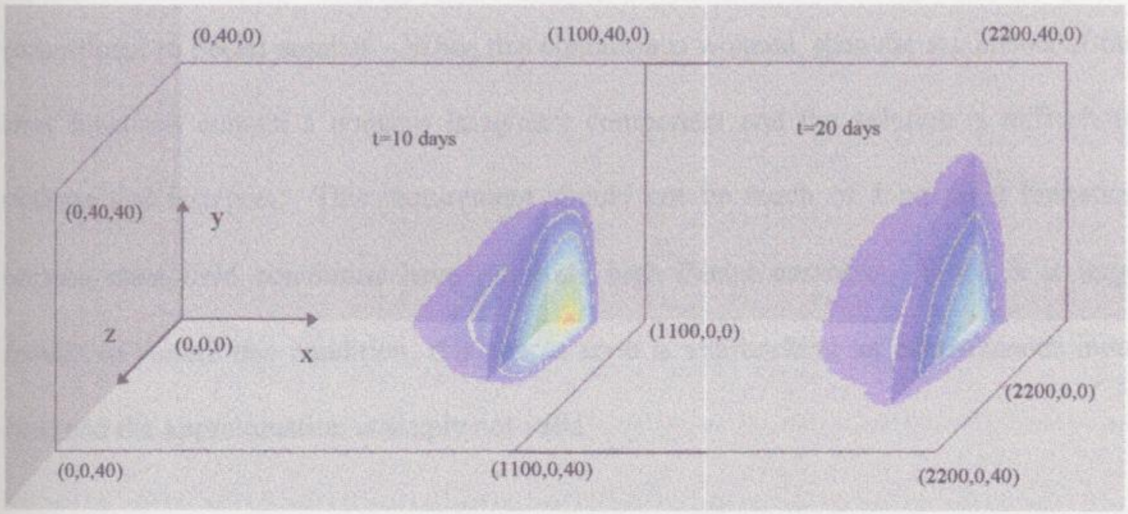

Figure 21 Dicer Plot for Three-Dimensional Model Testing (t = 10, 20 days)

centerline profiles for all three cases. Table 12 lists the MRPEs for three-dimensional model testing.

The maximum relative error for all cases was 2.5%, with the approximation having slightly higher total mass (expressed as the integral of the concentration profile) and the maximum error always occurring in the earliest time profiles. Generally these results indicate that the approximate models are valid, and useful models for an exponentially decaying input source.

The models require that λ always be smaller than or equal to $v^2/4D_x$, which is proportional to Peclet number . When this condition is violated, then the arguments of the error functions contain a nonzero imaginary component and the solution is difficult to evaluate and interpret. This requirement should not be much of a practical limitation because most field conditions have relatively high Peclet numbers. When λ is large enough to violate this condition, this source term is approaching an instantaneous input case, and the approximation is simply not valid.

Table 10. The Maximum Relative Errors for Three-Dimensional Model Testing (Centerline Profile)

Case	Time, day	Exact Model mg/L	Approx. no.1 mg/L	Approx. no.2 mg/L	Maximum Error, %
no.1	T=100	975.0	1000.0	1000.0	2.5
	T=10	992.0	1000.0	1000.0	0.8
	T=1	997.0	1000.0	1000.0	0.3
no.2	T=100	0.044	0.045	0.045	2.3
	T=10	365.0	368.0	368.0	0.8
	T=1	903.0	905.0	905.0	0.2
no.3	T=20	0.0	0.0	0.0	0.0
	T=10	0.045	0.045	0.045	0.0
	T=1	368.0	368.0	368.0	0.0

Table 11. The Maximum Relative Errors for Three-Dimensional Model Testing (Off-Centerline Profile)

Case	Time, day	Exact Model mg/L	Appr. no.1 mg/L	Appr. no.2 mg/L	Maximum Error, %
no.1	T=100	244.0	250.0	250.0	2.5
	T=10	248.0	250.0	250.0	0.8
	T=1	249.0	250.0	250.0	0.4
no.2	T=100	0.011	0.0	0.011	
	T=10	91.0	0.0	92.0	
	T=1	226.0	0.0	226.0	
no.3	T=20	0.0	0.0	0.0	
	T=10	0.011	0.0	0.011	
	T=1	92.0	0.0	92.0	

Table 12. MRPEs for Three-Dimensional Model Testing

Time day	Test Case 1, %				Test Case 2, %				Test Case 3, %			
	Appx. no.1		Appx. no.2		Appx. no.1		Appx. no.2		Appx. no.1		Appx. no.2	
	Center	Off-Center	Center	Off-Center	Center	Off-Center	Center	Off-Center	Center	Off-Center	Center	Off-Center
1	0.46	0.46	0.46	0.46	14.93	14.85	6.75	6.79	0.47	0.53	1.69	0.49
10	0.14	0.14	0.14	0.14	1.13	2.16	1.13	5.38	8.97	0.21	8..97	4.09
20									0.19	0.20	4.76	3.38
100	0.05	0.05	0.10	0.05	0.91	0.95	11.12	9..54				
Ave.	0.22	0.22	0.23	0.22	5.66	5.99	6..33	7.25	3.21	0.31	5.14	2.65

Chapter 6 Applications and Limitations

In order to show the applicability of the approximate models for exponentially decaying source and the range of input conditions on the solution, four series of model simulations were made. Application of the models was straightforward as all the terms were evaluated using a computer spreadsheet. FORTRAN programs (see Appendices for their listings) were used to evaluate convolution solutions and were called by fifth generation spreadsheets as functions. Some care was required since the FORTRAN programs could not handle large arguments to the exponential functions.

6.1 Application No.1

A mass balance for a source zone leads to the following expression for contaminant leaving the zone,

$$C(t)_{out} = C_{initial} \exp(-\frac{v}{\varepsilon} t), \tag{47}$$

where v is the velocity of fluid, and ε is the source dimension in the velocity direction and is small enough so that complete mixing can be assumed to occur within the source zone.

This expression is exactly the form of the source term in the approximation no.1 models. The models can be applied to determine the concentration profile downstream of the source.

6.2 Application #2

Risk-based corrective action rules require the estimation of concentration (for an exposure assessment calculation) at some receptor downstream a contaminant source. When the source is an exponentially decaying input, the peak concentration is different than that when it is a continuously constant source, or even when the source is a finite "pulse" input with the same total mass as the exponential case.

Figure 22 is a copy of a spreadsheet used to generate three profiles using these three different possible source terms. The continuous source represents a worst-case estimate in terms of peak concentration, the finite "pulse" an intermediate estimate.

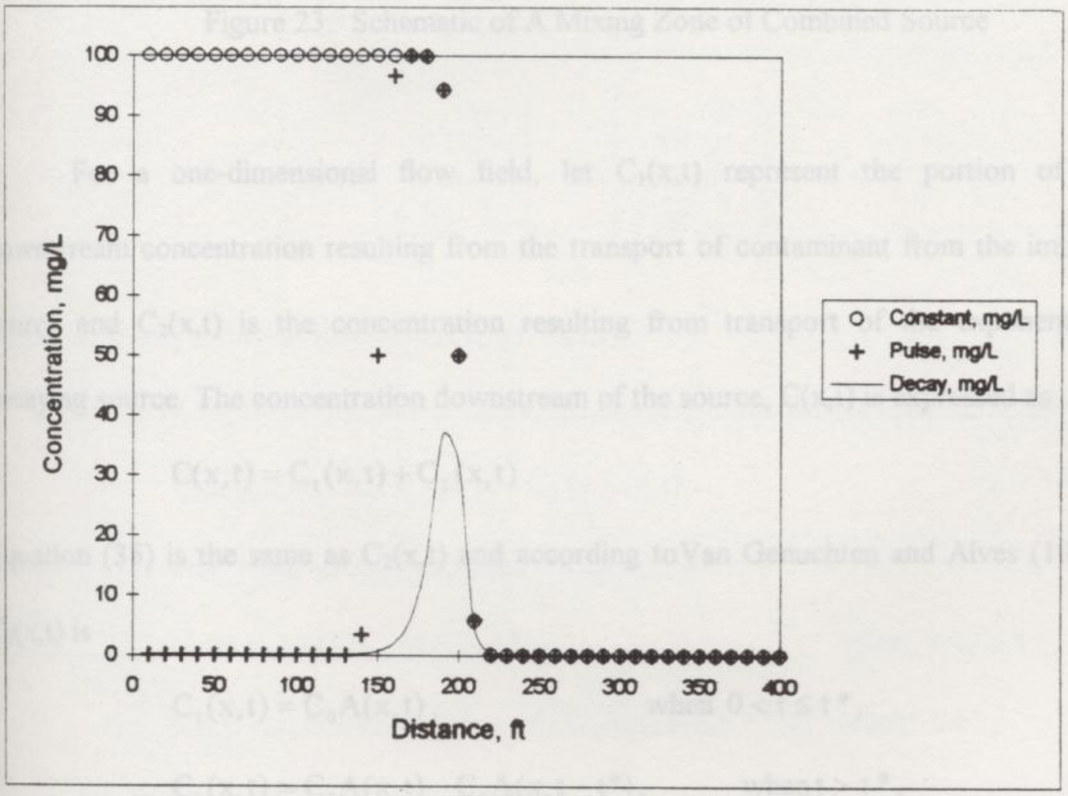

Figure 22. Comparison of Concentration Profiles for Three Sources

6.3 Application No.3

The models can be applied to estimate concentrations downstream of a contaminant source. The source has constant contaminant concentration for a period , followed by exponential decay. Refer to Figure 23 for a schematic of the combined contaminant source system.

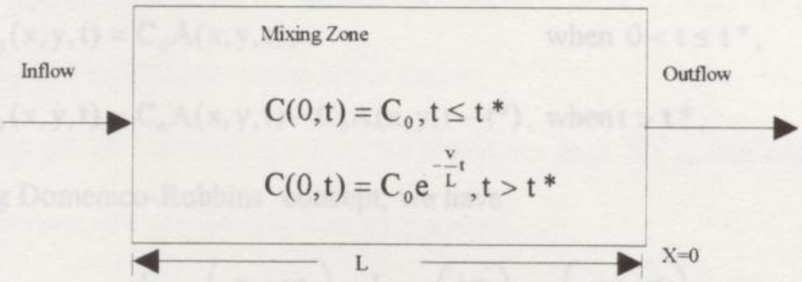

Figure 23. Schematic of A Mixing Zone of Combined Source

For a one-dimensional flow field, let $C_1(x,t)$ represent the portion of the downstream concentration resulting from the transport of contaminant from the impulse source and $C_2(x,t)$ is the concentration resulting from transport of the exponentially decaying source. The concentration downstream of the source, $C(x,t)$ is expressed as

$$C(x,t) = C_1(x,t) + C_2(x,t). \qquad (48)$$

Equation (35) is the same as $C_2(x,t)$ and according toVan Genuchten and Alves (1982), $C_1(x,t)$ is

$$C_1(x,t) = C_0A(x,t), \qquad \text{when } 0 < t \leq t^*,$$

$$C_1(x,t) = C_0A(x,t) - C_0A(x,t-t^*), \qquad \text{when } t > t^*, \qquad (49)$$

where $A(x,t) = \frac{1}{2}\operatorname{erfc}\left(\frac{x - vt}{2\sqrt{D_x t}}\right) + \frac{1}{2}\exp\left(\frac{vx}{D_x}\right)\operatorname{erfc}\left(\frac{x + vt}{2\sqrt{D_x t}}\right)$. (50)

Figure 24 shows this one-dimensional application.

For two-dimensional flow, the concentration downstream the source is

$$C(x,y,t) = C_1(x,y,t) + C_2(x,y,t). \quad (51)$$

Equation (36) is the same as $C_2(x,y,t)$ and $C_1(x,y,t)$ is

$$C_1(x,y,t) = C_0 A(x,y,t), \qquad \text{when } 0 < t \le t^*,$$

$$C_1(x,y,t) = C_0 A(x,y,t) - C_0 A(x,y,t - t^*), \text{ when } t > t^*, \quad (52)$$

where by applying Domenico-Robbins' concept, we have

$$A(x,y,t) = [\frac{1}{4}\operatorname{erfc}\left(\frac{x - vt}{2\sqrt{D_x t}}\right) + \frac{1}{4}\exp\left(\frac{vx}{D_x}\right)\operatorname{erfc}\left(\frac{x + vt}{2\sqrt{D_x t}}\right)]$$

$$[\operatorname{erfc}\left(\frac{y - \frac{Y}{2}}{2\sqrt{D_y \frac{x}{v}}}\right) - \operatorname{erfc}\left(\frac{y + \frac{Y}{2}}{2\sqrt{D_y \frac{x}{v}}}\right)]. \quad (53)$$

Figure 25 shows this two-dimensional application.

Similarly, for three-dimensional flow, the concentration downstream the source is

$$C(x,y,z,t) = C_1(x,y,z,t) + C_2(x,y,z,t). \quad (54)$$

Equation (37) is the same as $C_2(x,y,z,t)$ and $C_1(x,y,z,t)$ is

$$C_1(x,y,z,t) = C_0 A(x,y,z,t), \qquad \text{when } 0 < t \le t^*,$$

$$C_1(x,y,z,t) = C_0 A(x,y,z,t) - C_0 A(x,y,z,t - t^*), \quad \text{when } t > t^*, \quad (55)$$

where by applying Domenico-Robbins' concept, we have

$$A(x,y,z,t) = [\frac{1}{8}\operatorname{erfc}\left(\frac{x - vt}{2\sqrt{D_x t}}\right) + \frac{1}{8}\exp\left(\frac{vx}{D_x}\right)\operatorname{erfc}\left(\frac{x + vt}{2\sqrt{D_x t}}\right)]$$

$$[\operatorname{erfc}\left(\frac{y - \frac{Y}{2}}{2\sqrt{D_y \frac{x}{v}}}\right) - [\operatorname{erfc}\left(\frac{y + \frac{Y}{2}}{2\sqrt{D_y \frac{x}{v}}}\right)]\,[\operatorname{erfc}\left(\frac{z - \frac{Z}{2}}{2\sqrt{D_z \frac{x}{v}}}\right) - \operatorname{erfc}\left(\frac{z + \frac{Z}{2}}{2\sqrt{D_z \frac{x}{v}}}\right)]. \quad (56)$$

Figure 26 shows this three-dimensional application. Table 13 lists the parameters used in one-, two-, and three-dimensional applications.

For Figures 24-28, the leading edges are shallower than the tailing edges due to the effect of the portion of exponentially decaying source.

Table 13. Parameters Used in One-, Two-, and Three-Dimensional Applications

Parameters	One-Dimensional	Two-Dimensional	Three-Dimensional
C_0, mg/L	100	100	100
V, ft/day	1	1	1
λ, 1/day	1	1	1
t, day	40	40	40
t*, day	20	20	20
D_x	0.1	0.1	0.1
D_y		0.01	0.01
Y, ft		10	10
y, ft		5	5
D_z			0.01
Z, ft			5
z, ft			10

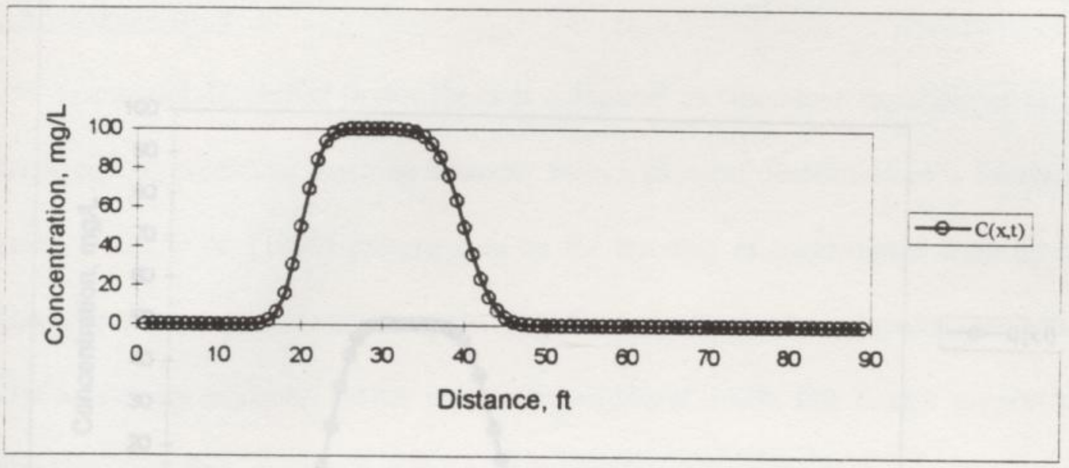

Figure 24. Concentration Profile for One-Dimensional Application (Centerline)

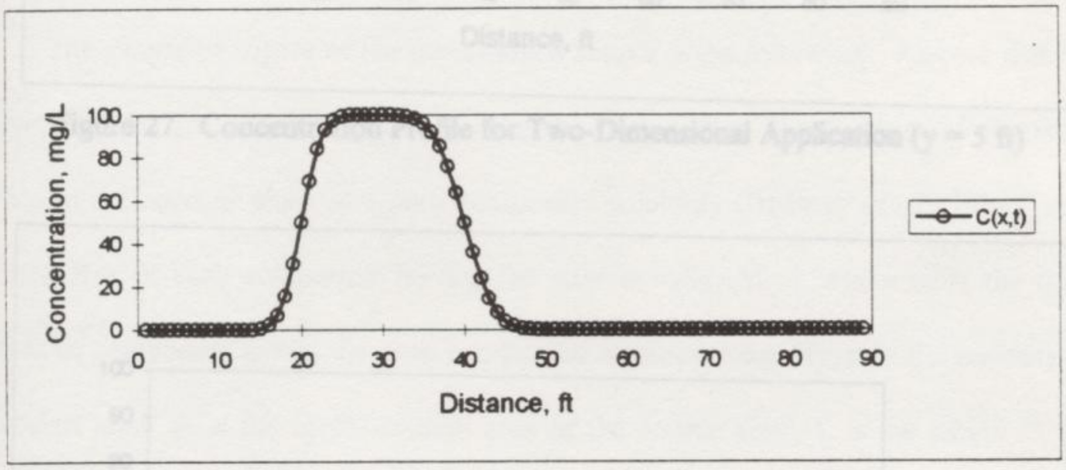

Figure 25. Concentration Profile for Two-Dimensional Application (Centerline)

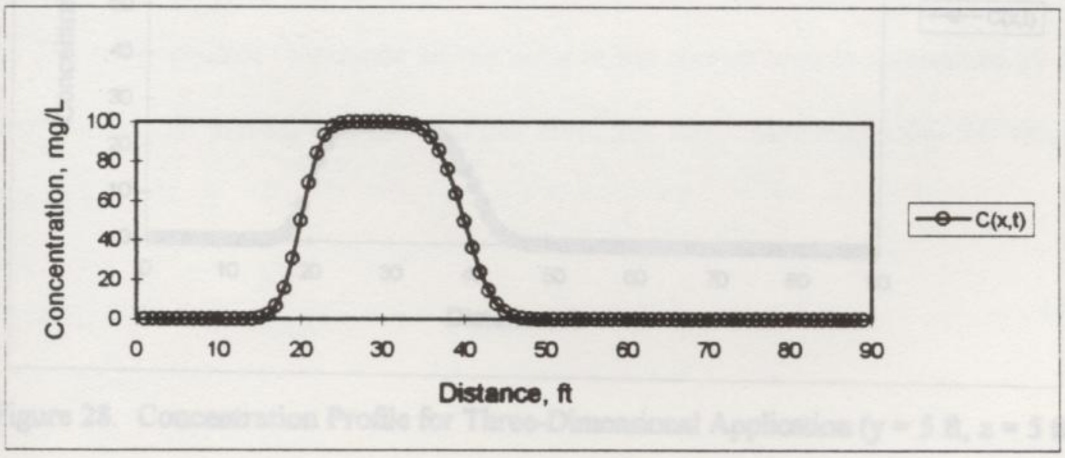

Figure 26. Concentration Profile for Three-Dimensional Application (Centerline)

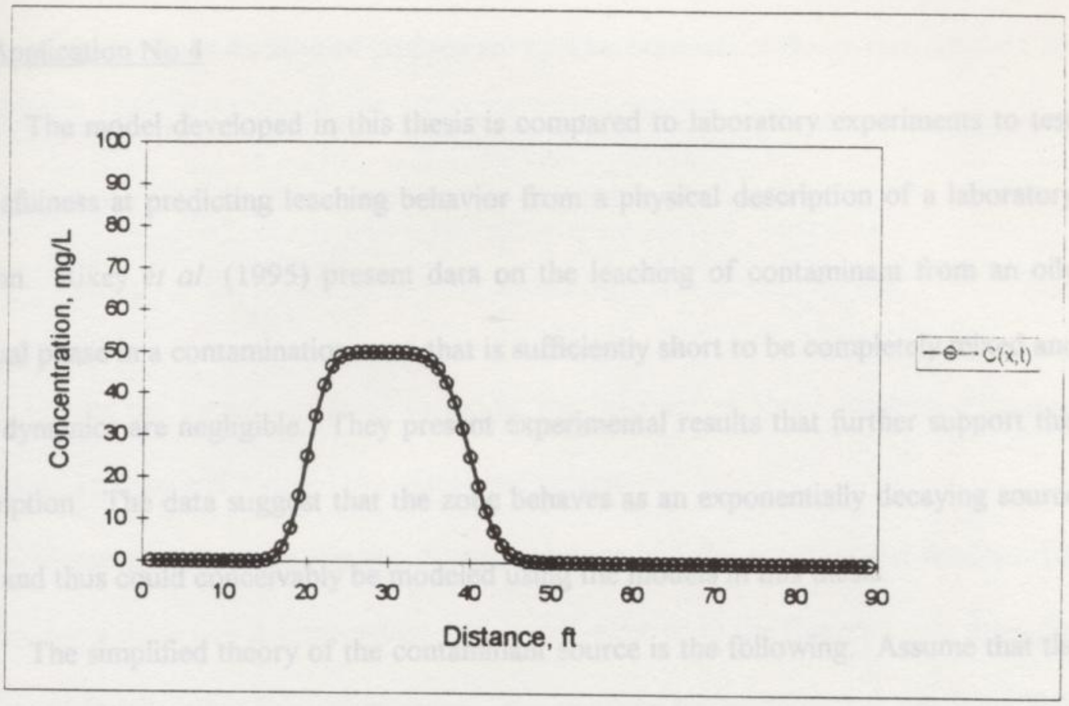

Figure 27. Concentration Profile for Two-Dimensional Application (y = 5 ft)

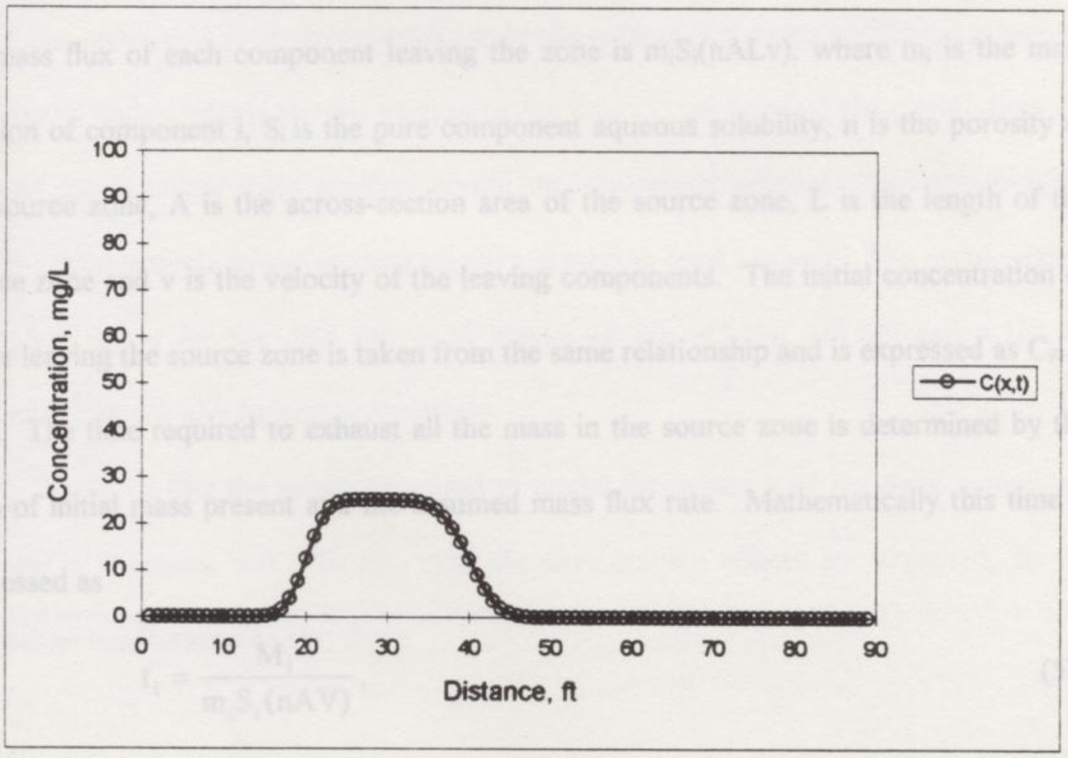

Figure 28. Concentration Profile for Three-Dimensional Application (y = 5 ft, z = 5 ft)

6.4 Application No.4

The model developed in this thesis is compared to laboratory experiments to test its usefulness at predicting leaching behavior from a physical description of a laboratory column. Rixey *et al.* (1995) present data on the leaching of contaminant from an oily residual phase in a contamination zone that is sufficiently short to be completely mixed and zone dynamics are negligible. They present experimental results that further support this assumption. The data suggest that the zone behaves as an exponentially decaying source zone and thus could conceivably be modeled using the models in this thesis.

The simplified theory of the contaminant source is the following. Assume that the concentration in the aqueous phase is roughly expressed as the product of the mass fraction in the residual phase and pure component solubility (Bedient, *et al.*, 1994), then the mass flux of each component leaving the zone is $m_iS_i(nALv)$, where m_i is the mass fraction of component i, S_i is the pure component aqueous solubility, n is the porosity of the source zone, A is the across-section area of the source zone, L is the length of the source zone and v is the velocity of the leaving components. The initial concentration of water leaving the source zone is taken from the same relationship and is expressed as $C_{i0} = m_iS_i$. The time required to exhaust all the mass in the source zone is determined by the ratio of initial mass present and the assumed mass flux rate. Mathematically this time is expressed as

$$t_i = \frac{M_i}{m_iS_i(nAV)}, \quad (57)$$

where, m_i is the mass fraction of component i. The exponential decay rate constant for each species was taken as the ratio of the Peclet number for the column and the exhausting time. Mathematically this decay rate constant is expressed as

$$\lambda_i = \frac{m_i S_i (nA) D_x}{M_i L}. \qquad (58)$$

Table 14 lists the parameters used to model the behavior of three component mixture (Benzene, Toluene and Xylene) in a glass bead column.

Figure 29 shows the simulated concentrations and the experimental results. The column dispersivity was determined by a trial-and -error fit to the Benzene data then used unchanged for the other two components. The required Peclet number is relatively high, which is consistent with the findings of Rixey *et al.* (1995). The results show that the model has reasonable predictive capacity once the column dispersion coefficient is known. The model underpredicts the tail portion of the data curves because the model does not account for changing mass fraction during the dissolution process. Nevertheless, the model would provide useful predictions for a screening level analysis. The mean relative prediction errors for the data shown in Figure 26 are -43.1%, -15.6% and 4.1% for Benzene, Toluene and Xylene, respectively.

Table 15 lists the parameters used to model the behavior of the three component mixture in a natural soil. In this case chromatographic effects are expected, so the retartation coefficient was also fitted.

Table 14. Parameters Used for Model Application in Glass Beads Experiments

	Benzene	Toluene	Xylene
[1]Total Mixture Mass, mg	40	40	40
Component Mass Fraction	0.05	0.05	0.1
[1]Component Mass, mg	2	2	4
Pure Component Solubility, mg/L	1780	515	162
Time to Exhaust Mass, day	4.3805E-05	0.0001514	0.0004813
Initial Flush Concentration, mg/L	89	25.75	16.2
[1]Source Zone Cross-Section Area, cm^2	19	19	19
Source Zone Porosity, n	0.6	0.6	0.6
[1]Velocity, cm/day	45	45	45
Effective Cross-Section Area, cm^2	11.4	11.4	11.4
λ, 1/day	18.2628	5.2839	1.66212
Transport Length, cm	27	27	27
[2]Dispersion Coefficient, cm^2/day	0.972	0.972	0.972

[1] Measurement

[2] Trial-and-Error

Figure 30 shows the simulated concentrations and the experimental results. The column dispersivity was determined by a trial-and-error fit to the Benzene data then used unchanged for the other two components. The required Peclet number is relatively high, which is consistent with the findings of Rixey *et al.* (1995). As the simulation for the glass beads experiments, the results show that the model has reasonable predictive capacity once the column dispersion coefficient is known. The model underpredicts the tail portion of the data curves because the model does not account for changing mass fraction during screening level analysis. The mean relative prediction errors for the data shown in Figure 27 are -72.3%, 24.3% and 58.2% for Benzene, Toluene and Xylene, respectively.

Table 15. Parameters Used for Model Application in Soil Column Experiments

	Benzene	Toluene	Xylene
Total Mixture Mass, mg	40	40	40
Component Mass Fraction	0.05	0.05	0.1
Component Mass, mg	2	2	4
Pure Component Solubility, mg/L	1780	515	162
Time to Exhaust Mass, day	4.3805E-05	0.0001514	0.0004813
Initial Flush Concentration, mg/L	89	25.75	16.2
Source Zone Cross-Section Area, cm^2	19	19	19
Source Zone Porosity, n	0.6	0.6	0.6
Velocity, cm/day	45	45	45
Effective Cross-Section Area, cm^2	11.4	11.4	11.4
λ, 1/day	17.577945	5.08575375	0.6399162
Retardation Coefficient	1.4	1.6	2.5
Transport Length, cm	27	27	27
Dispersion Coefficient, cm^2/day	0.93555	0.93555	0.93555

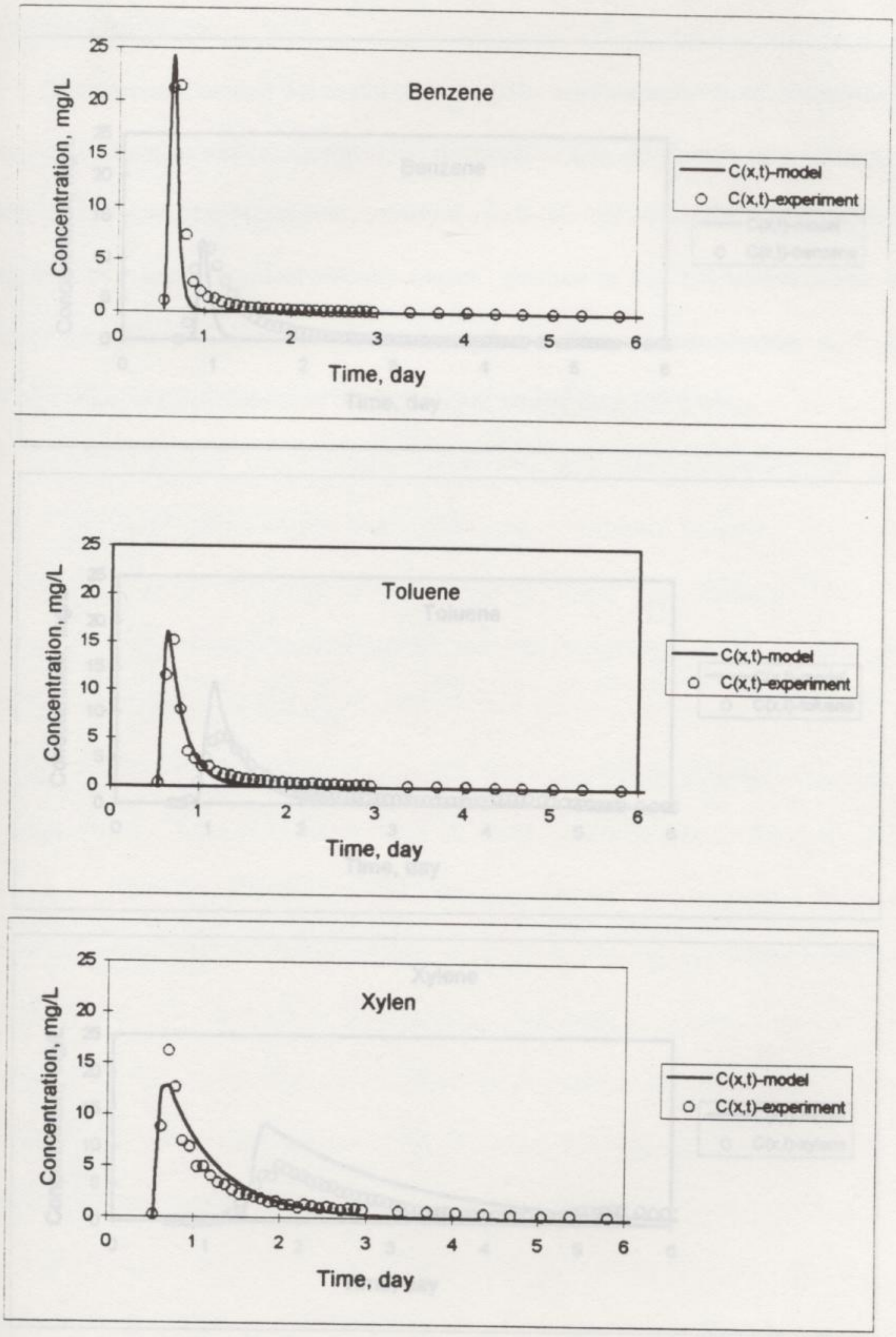

Figure 29. Model Application in Glass Beads Experiments

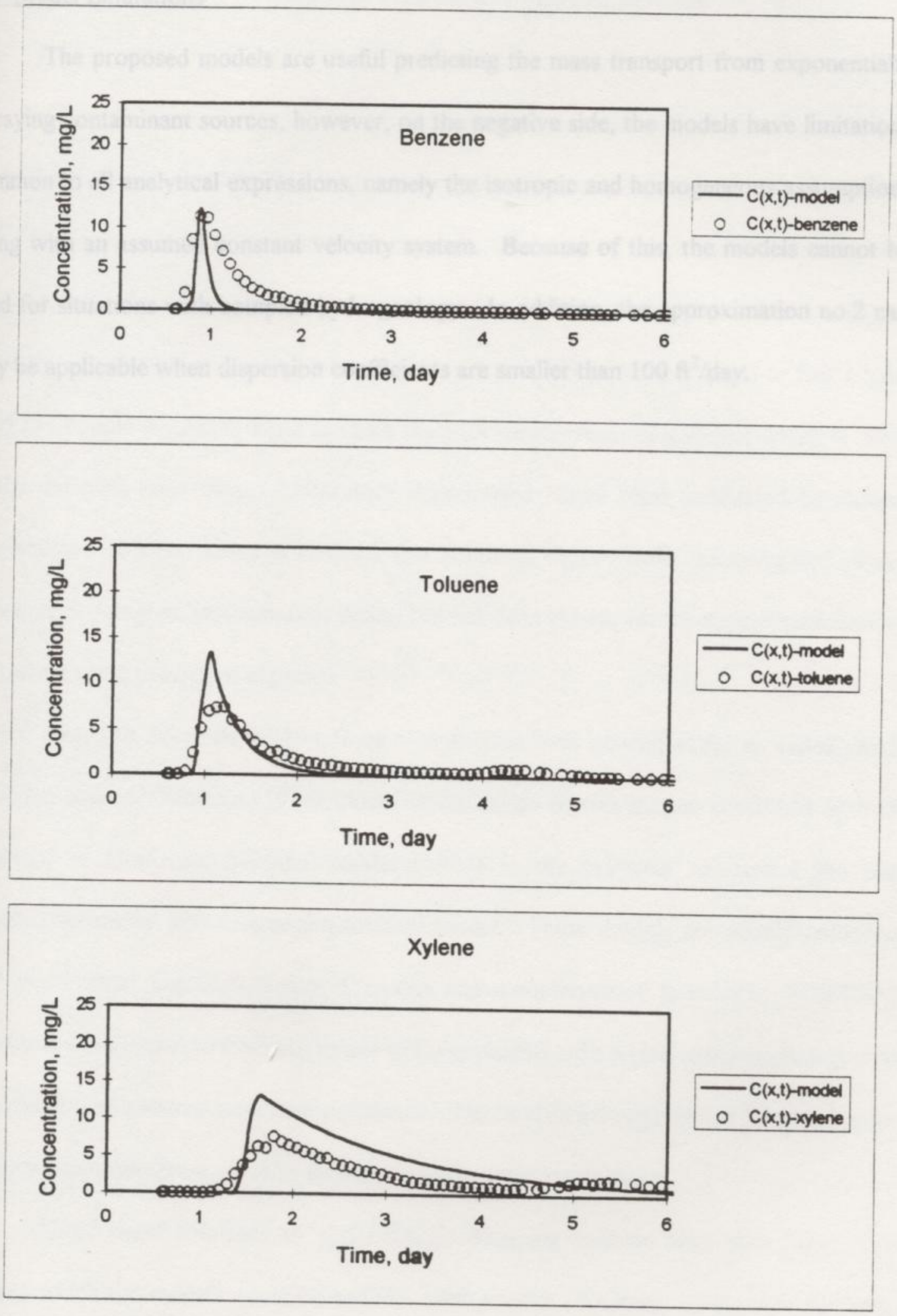

Figure 30. Model Application for Soil Column Experiments

6.4 Model Limitations

The proposed models are useful predicting the mass transport from exponentially decaying contaminant sources, however, on the negative side, the models have limitations common to all analytical expressions, namely the isotropic and homogeneous assumptions along with an assumed constant velocity system. Because of this, the models cannot be used for situations with complex hydrogeology. In addition, the approximation no.2 can only be applicable when dispersion coefficients are smaller than 100 ft^2/day.

Chapter 7 Summary and Conclusions

The literature review shows that, even though a number of analytical models have been developed to simulate the transport of contaminants in subsurface porous media, they are limited to constant concentration sources. A need to have models dealing with exponentially decaying contaminant sources is necessary since time varying are more realistic. To comply with risk-based corrective action rules, industry needs to find a quick way to estimate a concentration at some receptor downstream of a source which is likely to be decaying over time. Laboratory experiments have been conducted to monitor contaminant concentrations in leachate that supports exponentially-decaying-like source, however, a complete mathematical model has not been posed, yet the approximate models do posess some predictive capacity.

Based on previous models, three models have been developed for an exponentially decaying source. Mario's (1974) model is the origin of this model, combined with the concepts in Domenico-Robbins' model (1984) is the principal to extend the one-dimensional model into a three-dimensional model. These models are mainly composed with exponential functions, errors functions and complimentary functions. FORTRAN programs were coded to evaluate values of these models with which concentration profiles downstream of a source were easily obtained. The models are regarded as an approximate solution (approximation no.1) to an exponentially decaying source.

Three exact solutions to exponentially decaying sources have also been found against which the models could be tested. Mathematica (Wolfram, 1994) was employed to perform the required spatial integration and FORTRAN programs used to numerically solve the integration with respect to time. In addition, other solutions to the same source have been obtained and have been tested against the exact solutions. These solutions are also approximate approaches (approximation no.2) and their advantage is that no numerical integration is necessary, thus simplifying the evaluation procedure.

The model (approximation no.1) and approximation no.2 have been tested against the exact solutions for three test cases. The choosing of the test cases was based on the selection of values of source decay rate, fluid velocity, and dispersion terms. The testing results showed that the agreement between the exact model and the approximations was excellent.

Once the models were set up and tested, they were used for four applications. The first application is to determine a concentration profile downstream of a source which has exactly the form of the source term in the model. The second application is to make an estimation of concentration at some receptor downstream of the source for an exposure assessment calculation. This application could be very practical and useful in determining clean-up strategies because when the source is an exponentially decaying input, the peak concentration is different than that when it is a continuous source. The third application is to predict the mass transport from a source which is a combination of an impulse and exponentially decaying source. Finally, the models were used to predict the output concentrations of a column test for an exponentially-decaying-like source and concentrations simulated by the models were closed to those produced by the real experiments.

So far, based on the work done by the author in this project, the following conclusions have been made:

Accurate approximations for one-, two- and three-dimensional groundwater mass transport are obtained. Solutions are developed for case in which the contaminant source varies exponentially with time. The models presented in this thesis may used as a screening instrument for a preliminary evaluation of the dilution potential of waste sites prior to intensive investigations.

Exact solutions to one-, two- and three-dimensional dispersion equations are presented against which the proposed models have been tested and the agreement is excellent. The proposed models are much easier to use, thus have advantage over the exact solutions. In addition, compared to tedious and time-consuming numerical models, the present models provide a quick and easy way of predicting the concentration distributions downstream of the source.

The models can be used to determine what changes in the source mass and distribution are necessary to ensure that the PORC is less than the MSC at the nearest receptor. Costly information on some potential unknowns could be extracted directly from the concentration distribution using these models. For example, given data at different points in time, field retardation coefficients can be ascertained and incorporated into subsequent calculations.

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Appendix 1 Function One1_dll(T,RX,V,Dx,C,PI,RS)

```
c
c Program to compute semi-analytical solutions of contaminant fate and
c transport for time varying input conditions.
c
c Concept: Numerical convolution of time-varying impulse solutions
c
c Method:  Gaussian Quadrature using Legendre Polynomial weight
c            function
c
c User requirements:  An impulse kernel is supplied.  The user programs
c                     the time-variable input function that
c                     premultiplies the kernel.
c
c Limitations:  High accuracy requires a lot of computations.  A
c               relative error of 10E-7% is default and produces results
c               fairly quickly.
c
      Implicit Real*8 (A-H,O-Z)
      External Funk
c
c Quadrature Integration Routine
c
      TAU=T
      Call Quadr(funk, 0.00000D0,TAU,ANS,
     1          T,RX,V,Dx,C,PI,RS)
      One1_dll=ANS
      RETURN
      End
c
c Kernel Function
c
      Function Pkernel(U,T,RX,V,Dx,C,PI,RS)
      Implicit Real*8(A-H,O-Z)
      W1=(0.5D0*C*V)/(Sqrt(Dx*Pi*(T-U)))
c
      W2=Exp(-RS*U)
c
      w3=(RX-V*(T-U))**2
      w4=4.*Dx*(T-U)
      w5=Exp(-w3/w4)
c
      Pkernel=W1*w2*w5
      Return
      End
c
c Integrand function
c
      Function FUNK(U,T,RX,V,Dx,C,PI,RS)
      Implicit Real*8(A-H,O-Z)
      FUNK=PKernel(U,T,RX,V,Dx,C,PI,RS)
      Return
      End
c
c Gaussian Quadrture Routines
c
      Subroutine Gauleg(X1,X2,X,W,N)
c
c Program computes locations and weights for Quadrture
```

```
c
      Implicit Real*8(A-H,O-Z)
      Dimension X(N),W(N)
      Parameter(EPS=3.D-14)
      M=(N+1)/2
      XM=0.5D0*(X2+X1)
      XL=0.5D0*(X2-X1)
      Do 12 I=1,M
       Z=COS(3.141592654D0*(I-.25D0)/(N+0.5D0))
1         Continue
       P1=1.D0
       P2=0.D0
       Do 11 J=1,N
         P3=P2
         P2=P1
         P1=((2.D0*J-1.D0)*Z*P2-(J-1.D0)*P3)/J
11        Continue
       PP=N*(Z*P1-P2)/(Z*Z-1.D0)
       Z1=Z
       Z=Z1-P1/PP
      If(ABS(Z-Z1).GT.EPS)GOTO 1
       X(I)=XM-XL*Z
       X(N+1-I)=XM+XL*Z
       W(I)=2.D0*XL/((1.D0-Z*Z)*PP*PP)
       W(N+1-I)=W(I)
12    Continue
      Return
      End
c
      Subroutine Quadr(FUNK,A,B,SS,T,RX,V,Dx,C,PI,RS)
c
c Program approximates: Integrate[FUNK[x],{x,a,b}],
c Uses NWT Quadrture points,
c Returns approximation in SS=Sum[W(I)*FUNK[x(I)],{I,1,NWT}]
c
      Implicit Real*8(A-H,O-Z)
      Parameter(NWT=3072)
      Dimension X(NWT),W(NWT)
      External FUNK
      Call Gauleg(A,B,X,W,NWT)
      SS=0.D0
      Do 100 IR=1,NWT
       SS=SS+W(IR)*FUNK(X(IR),T,RX,V,Dx,C,PI,RS)
100   Continue
      Return
      End
```

Appendix 2 Function One2_dll(T,RX,V,Dx,C,RS)

```
c
c  This program is to compute the proposed Model (Approximation #1)
c  for one-dimension case.
c
      Implicit Real*8 (A-H,O-Z)
c
      w2=(RX-T*SQRT(V**2-4*RS*Dx))/(2*SQRT(Dx*T))
      If(w2.LT.0.D0) Then
         Call ERFF(ABS(w2),error)
         w3=ERROR+1
      Else
         Call ERFCC(w2,cerror)
         w3=CERROR
      End If
c
      If(w3.EQ.0.D0) Then
        w1=0.D0
      Else
         w1=(V*RX-RX*SQRT(V**2-4*RS*Dx))/(2*Dx)
      End If
c
      w5=(RX+T*SQRT(V**2-4*RS*Dx))/(2*SQRT(Dx*T))
      If(w5.LT.0.D0) Then
         Call ERFF(ABS(w5),error)
         w6=ERROR+1
      Else
         Call ERFCC(w5,cerror)
         w6=CERROR
      End If
c
      If(w6.EQ.0.D0) Then
         w4=0.D0
      Else
         w4=(V*RX+RX*SQRT(V**2-4*RS*Dx))/(2*Dx)
      End If
c
      w=0.5*C*Exp(-RS*T)*(Exp(w1)*w3+Exp(w4)*w6)
      One2_dll=w
      Return
      End
c
      Subroutine ERFCC(x,cerror)
c
c  Complementary error function approximation
c
      Implicit Real*8 (A-H,O-Z)
      If(x.LT.-4.D0) Then
         Cerror=2.D0
      Else If(x.GT.4.D0)  Then
            Cerror=0.D0
         Else
           z=ABS(x)
           y=1.D0/(1.D0+0.5D0*z)
           CERROR=y*Exp(-z*z-1.26551223D0
     1           +y*( 1.00002368D0
     2           +y*( 0.37409196D0
     3           +y*( 0.09678418D0
     4           +y*(-0.18628806D0
```

```
     5            +y*( 0.27886807D0
     6            +y*(-1.13520398D0
     7            +y*( 1.48851587D0
     8            +y*(-0.82215223D0
     9            +y*( 0.17087277D0)))))))))
      End If
      Return
      End
c
      Subroutine ERFF(x,error)
c
c  Error function approximation
c
      Implicit Real*8 (A-H,O-Z)
      If(x.LT.-4.D0) Then
         error=-1.D0
      Else If(x.GT.4.D0)  Then
            error=1.D0
         Else
      A1=0.0705230784
      A2=0.0422820123
      A3=0.0092705272
      A4=0.0001520143
      A5=0.0002765672
      A6=0.0000430638
      ERROR=1.0-1.0/
     1   (1+x*(A1+x*(A2+x*(A3+X*(A4+x*(A5+x*A6))))))**16
      End If
      Return
      End
```

Appendix 3 Function One3_dll(T,RL,V,D,C,RS)

```
c
c  This program is to compute Approximation #2 for
c  one-dimension case.
c
      Implicit Real*8 (A-H,O-Z)
      w1=RS*(D*RS*T+T*V**2-V*RL)/V**2
c
      w2=(-RS/V-V/(2*D)+RL/(2*D*T))/SQRT(1/(D*T))
      If(w2.LT.0.D0) Then
         Call ERFF(ABS(w2),error)
         w3=ERROR+1
      Else
         Call ERFCC(w2,cerror)
         w3=CERROR
      End If
c
      w=0.5*C*Exp(w1)*(w3)
      One3_dll=w
      Return
      End
c
      Subroutine ERFCC(x,cerror)
c
c  Complementary error function approximation
c
      Implicit Real*8 (A-H,O-Z)
      If(x.LT.-4.D0) Then
         Cerror=2.D0
      Else If(x.GT.4.D0)  Then
            Cerror=0.D0
         Else
           z=ABS(x)
           y=1.D0/(1.D0+0.5D0*z)
           CERROR=y*Exp(-z*z-1.26551223D0
     1           +y*( 1.00002368D0
     2           +y*( 0.37409196D0
     3           +y*( 0.09678418D0
     4           +y*(-0.18628806D0
     5           +y*( 0.27886807D0
     6           +y*(-1.13520398D0
     7           +y*( 1.48851587D0
     8           +y*(-0.82215223D0
     9           +y*( 0.17087277D0)))))))))
      End If
      Return
      End
c
      Subroutine ERFF(x,error)
c
c  Error function approximation
c
      Implicit Real*8 (A-H,O-Z)
      If(x.LT.-4.D0) Then
         error=-1.D0
      Else If(x.GT.4.D0)  Then
            error=1.D0
         Else
      A1=0.0705230784
```

```
      A2=0.0422820123
      A3=0.0092705272
      A4=0.0001520143
      A5=0.0002765672
      A6=0.0000430638
      ERROR=1.0-1.0/
     1     (1+x*(A1+x*(A2+x*(A3+X*(A4+x*(A5+x*A6))))))**16
      End If
      Return
      End
```

Appendix 4 Function Twol_dll(T,RX,RY,V,Dx,Dy,C,PI,RS,WIDTH)

```
c
c This program is to compute semi-analytical solutions of contaminant
fate and
c transport for time varying input conditions.
c
c Concept: Numerical convolution of time-varying impulse solutions
c
c Method:  Gaussian Quadrature using Legendre Polynomial weight
c          function
c
c User requirements:  An impulse kernel is supplied.  The user programs
c                     the time-variable input function that
c                     premultiplies the kernel.
c
c Limitations:  High accuracy requires a lot of computations.  A
c               relative error of 10E-7% is default and produces results
c               fairly quickly.
c
      Implicit Real*8 (A-H,O-Z)
      External Funk
c
c Quadrature Integration Routine
c
      TAU=T
      Call Quadr(funk, 0.00000D0,TAU,ANS,
     1           T,RX,RY,V,Dx,Dy,C,PI,RS,WIDTH)
      Twol_dll=ANS
      RETURN
      End
c
c Kernel Function
c
      Function Pkernel(U,T,RX,RY,V,Dx,Dy,C,PI,RS,WIDTH)
      Implicit Real*8(A-H,O-Z)
      TT=T-(U)
      W1=C*V/(4.*Sqrt(Dx*Pi*TT))
c
      W2=-RS*U
      w3=-(RX-V*TT)**2
      w4=4*Dx*TT
      w5=Exp(w2+w3/w4)
c
      w6=(RY+WIDTH/2)/(2.*Sqrt(Dy*RX/V))
      If(w6.LT.0.D0) Then
       Call ERFF(ABS(w6),error)
       w7=-ERROR
      Else
       Call ERFF(ABS(w6),error)
       w7=ERROR
      End If
      w8=(RY-WIDTH/2)/(2.*Sqrt(Dy*RX/V))
      If(w8.LT.0.D0) Then
       Call ERFF(ABS(w8),error)
       w9=-ERROR
      Else
       Call ERFF(ABS(w8),error)
       w9=ERROR
      End If
```

```
      w10=w7-w9
c
100   Pkernel=W1*w5*w10
      Return
      End
c
c Integrand function
c
      Function FUNK(U,T,RX,RY,V,Dx,Dy,C,PI,RS,WIDTH)
      Implicit Real*8(A-H,O-Z)
      FUNK=PKernel(U,T,RX,RY,V,Dx,Dy,C,PI,RS,WIDTH)
      Return
      End
c
c Gaussian Quadrture Routines
c
      Subroutine Gauleg(X1,X2,X,W,N)
c
c Program computes locations and weights for Quadrture
c
      Implicit Real*8(A-H,O-Z)
      Dimension X(N),W(N)
      Parameter(EPS=3.D-14)
      M=(N+1)/2
      XM=0.5D0*(X2+X1)
      XL=0.5D0*(X2-X1)
      Do 12 I=1,M
       Z=COS(3.141592654D0*(I-.25D0)/(N+0.5D0))
1        Continue
       P1=1.D0
       P2=0.D0
       Do 11 J=1,N
          P3=P2
          P2=P1
          P1=((2.D0*J-1.D0)*Z*P2-(J-1.D0)*P3)/J
11       Continue
       PP=N*(Z*P1-P2)/(Z*Z-1.D0)
       Z1=Z
       Z=Z1-P1/PP
       If(ABS(Z-Z1).GT.EPS)GOTO 1
       X(I)=XM-XL*Z
       X(N+1-I)=XM+XL*Z
       W(I)=2.D0*XL/((1.D0-Z*Z)*PP*PP)
       W(N+1-I)=W(I)
12    Continue
      Return
      End
c
      Subroutine Quadr(FUNK,A,B,SS,T,RX,RY,V,Dx,Dy,C,PI,RS,WIDTH)
c
c Program approximates: Integrate[FUNK[x],{x,a,b}],
c Uses NWT Quadrture points,
c Returns approximation in SS=Sum[W(I)*FUNK[x(I)],{I,1,NWT}]
c
      Implicit Real*8(A-H,O-Z)
      Parameter(NWT=3072)
      Dimension X(NWT),W(NWT)
      External FUNK
      Call Gauleg(A,B,X,W,NWT)
      SS=0.D0
```

```
      Do 100 IR=1,NWT
       SS=SS+W(IR)*FUNK(X(IR),T,RX,RY,V,Dx,Dy,C,PI,RS,WIDTH)
100   Continue
      Return
      End
c
      Subroutine ERFF(x,error)
c
c  Error function approximation
c
      Implicit Real*8 (A-H,O-Z)
      If(x.LT.-4.D0) Then
       error=-1.D0
      Else If(x.GT.4.D0)  Then
         error=1.D0
       Else
      A1=0.0705230784
      A2=0.0422820123
      A3=0.0092705272
      A4=0.0001520143
      A5=0.0002765672
      A6=0.0000430638
      ERROR=1.0-1.0/
     1    (1+x*(A1+x*(A2+x*(A3+X*(A4+x*(A5+x*A6))))))**16
      End If
      Return
      End
```

Appendix 5 Function Two2_dll(T,RX,RY,V,Dx,Dy,C,RS,WIDTH)

```
c
c  This program is to compute Approximation #1 for
c  two-dimension case. (6/2/95 Dan)
c
      Implicit Real*8 (A-H,O-Z)
c
      w2=(RX-T*SQRT(V**2-4*RS*Dx))/(2*SQRT(Dx*T))
      If(w2.LT.0.D0) Then
         Call ERFF(ABS(w2),error)
         w3=ERROR+1
      Else
         Call ERFCC(w2,cerror)
         w3=CERROR
      End If
c
      If(w3.EQ.0.D0) Then
         w1=0.D0
      Else
         w1=(V*RX-RX*SQRT(V**2-4*RS*Dx))/(2*Dx)
      End If
c
      w5=(RX+T*SQRT(V**2-4*RS*Dx))/(2*SQRT(Dx*T))
      If(w5.LT.0.D0) Then
         Call ERFF(ABS(w5),error)
         w6=ERROR+1
      Else
         Call ERFCC(w5,cerror)
         w6=CERROR
      End If
c
      If(w6.EQ.0.D0) Then
         w4=0.D0
      Else
         w4=(V*RX+RX*SQRT(V**2-4*RS*Dx))/(2*Dx)
      End If
c
      w7=(RY+WIDTH/2)/(2*Sqrt(Dy*RX/v))
      If(w7.LT.0.D0) Then
         Call ERFF(ABS(w7),error)
         w8=-ERROR
      Else
         Call ERFF(ABS(w7),error)
         w8=ERROR
      End If
c
      w9=(RY-WIDTH/2)/(2*Sqrt(Dy*RX/v))
      If(w9.LT.0.D0) Then
         Call ERFF(ABS(w9),error)
         w10=-ERROR
      Else
         Call ERFF(ABS(w9),error)
         w10=ERROR
      End If
c
      w=0.25*C*Exp(-RS*T)*(Exp(w1)*w3+Exp(w4)*w6)
     1  *(w8-w10)
      Two2_dll=w
      Return
```

```
      End
c
      Subroutine ERFCC(x,cerror)
c
c  Complementary error function approximation
c
      Implicit Real*8 (A-H,O-Z)
      If(x.LT.-4.D0) Then
        Cerror=2.D0
      Else If(x.GT.4.D0)  Then
          Cerror=0.D0
        Else
         z=ABS(x)
         y=1.D0/(1.D0+0.5D0*z)
         CERROR=y*Exp(-z*z-1.26551223D0
     1           +y*( 1.00002368D0
     2           +y*( 0.37409196D0
     3           +y*( 0.09678418D0
     4           +y*(-0.18628806D0
     5           +y*( 0.27886807D0
     6           +y*(-1.13520398D0
     7           +y*( 1.48851587D0
     8           +y*(-0.82215223D0
     9           +y*( 0.17087277D0)))))))))
      End If
      Return
      End
c
      Subroutine ERFF(x,error)
c
c  Error function approximation
c
      Implicit Real*8 (A-H,O-Z)
      If(x.LT.-4.D0) Then
         error=-1.D0
      Else If(x.GT.4.D0)  Then
          error=1.D0
        Else
      A1=0.0705230784
      A2=0.0422820123
      A3=0.0092705272
      A4=0.0001520143
      A5=0.0002765672
      A6=0.0000430638
      ERROR=1.0-1.0/
     1 (1+x*(A1+x*(A2+x*(A3+X*(A4+x*(A5+x*A6))))))**16
      End If
      Return
      End
```

Appendix 6 Function Thr3_dll(T,RX,RY,V,Dx,Dy,C,RS,WIDTH)

```
c
c  This program is to compute Approximation #2 for
c  two-dimension case. (6/3/95 Dan)
c
      Implicit Real*8 (A-H,O-Z)
      w1=(1/8)*C*Exp(RS*(Dx*RS*T+T*V**2-V*RX)/V**2)
c
      w2=(-RS/V-V/(2*Dx)+RX/(2*Dx*T))/SQRT(1/(Dx*T))
      If(w2.LT.0.D0) Then
       Call ERFF(ABS(w2),error)
       w3=ERROR+1
      Else
       Call ERFCC(w2,cerror)
       w3=CERROR
      End If
c
      w4=(2*RY+WIDTH)/(4*Sqrt(Dy*T))
      If(w4.LT.0.D0) Then
       Call ERFF(ABS(w4),error)
       w5=-ERROR
      Else
       Call ERFF(ABS(w4),error)
       w5=ERROR
      End If
c
      w6=(2*RY-WIDTH)/(4*Sqrt(Dy*T))
      If(w6.LT.0.D0) Then
       Call ERFF(ABS(w6),error)
       w7=-ERROR
      Else
       Call ERFF(ABS(w6),error)
       w7=ERROR
      End If
c
      w=w1*w3*(w5-w7)
      Two3_dll=w
      Return
      End
c
      Subroutine ERFCC(x,cerror)
c
c  Complementary error function approximation
c
      Implicit Real*8 (A-H,O-Z)
      If(x.LT.-4.D0) Then
       Cerror=2.D0
      Else If(x.GT.4.D0)  Then
          Cerror=0.D0
       Else
         z=ABS(x)
         y=1.D0/(1.D0+0.5D0*z)
         CERROR=y*Exp(-z*z-1.26551223D0
     1           +y*( 1.00002368D0
     2           +y*( 0.37409196D0
     3           +y*( 0.09678418D0
     4           +y*(-0.18628806D0
     5           +y*( 0.27886807D0
     6           +y*(-1.13520398D0
```

```
     7          +y*( 1.48851587D0
     8          +y*(-0.82215223D0
     9          +y*( 0.17087277D0)))))))))
      End If
      Return
      End
c
      Subroutine ERFF(x,error)
c
c  Error function approximation
c
      Implicit Real*8 (A-H,O-Z)
      If(x.LT.-4.D0) Then
       error=-1.D0
      Else If(x.GT.4.D0)  Then
         error=1.D0
       Else
      A1=0.0705230784
      A2=0.0422820123
      A3=0.0092705272
      A4=0.0001520143
      A5=0.0002765672
      A6=0.0000430638
      ERROR=1.0-1.0/
     1    (1+x*(A1+x*(A2+x*(A3+X*(A4+x*(A5+x*A6))))))**16
      End If
      Return
      End
```

Appendix 7 Function Thrl_dll(T,RX,RY,RZ,V,Dx,Dy,Dz,C,PI,RS,WIDTH,HEITH)

```
c
c This program is to compute semi-analytical solutions of contaminant
fate and
c transport for time varying input conditions.
c
c Concept: Numerical convolution of time-varying impulse solutions
c
c Method:  Gaussian Quadrature using Legendre Polynomial weight
c          function
c
c User requirements:  An impulse kernel is supplied.  The user programs
c                     the time-variable input function that
c                     premultiplies the kernel.
c
c Limitations:  High accuracy requires a lot of computations.  A
c               relative error of 10E-7% is default and produces results
c               fairly quickly.
c
      Implicit Real*8 (A-H,O-Z)
      External Funk
c
c Quadrature Integration Routine
c
      TAU=T
      Call Quadr(funk, 0.00000D0,TAU,ANS,
     1           T,RX,RY,RZ,V,Dx,Dy,Dz,C,PI,RS,WIDTH,HEITH)
      Thrl_dll=ANS
      RETURN
      End
c
c Kernel Function
c
      Function Pkernel(U,T,RX,RY,RZ,V,Dx,Dy,Dz,C,PI,RS,WIDTH,
     1                 HEITH)
      Implicit Real*8(A-H,O-Z)
      TT=T-(U)
      W1=C*V/(8.*Sqrt(Dx*Pi*TT))
c
      W2=-RS*U
      w3=-(RX-V*TT)**2
      w4=4*Dx*TT
      w5=Exp(w2+w3/w4)
c
      w6=(WIDTH+2.*RY)/(4.*Sqrt(Dy*TT))
      If(w6.LT.0.D0) Then
       Call ERFF(ABS(w6),error)
       w7=-ERROR
      Else
       Call ERFF(ABS(w6),error)
       w7=ERROR
      End If
      w8=(WIDTH-2.*RY)/(4.*Sqrt(Dy*TT))
      If(w8.LT.0.D0) Then
       Call ERFF(ABS(w8),error)
       w9=-ERROR
      Else
       Call ERFF(ABS(w8),error)
       w9=ERROR
```

```
        End If
        w10=w7+w9
c
        w11=(HEITH+2.*RZ)/(4.*Sqrt(Dz*TT))
        If(w11.LT.0.D0) Then
         Call ERFF(ABS(w11),error)
         w12=-ERROR
        Else
         Call ERFF(ABS(w11),error)
         w12=ERROR
        End If
        w13=(HEITH-2.*RZ)/(4.*Sqrt(Dz*TT))
        If(w13.LT.0.D0) Then
         Call ERFF(ABS(w13),error)
         w14=-ERROR
        Else
         Call ERFF(ABS(w13),error)
         w14=ERROR
        End If
        w15=w12+w14
c
        Pkernel=W1*w5*w10*w15
        Return
        End
c
c Integrand function
c
        Function FUNK(U,T,RX,RY,RZ,V,Dx,Dy,Dz,C,PI,RS,WIDTH,
     1              HEITH)
        Implicit Real*8(A-H,O-Z)
        FUNK=PKernel(U,T,RX,RY,RZ,V,Dx,Dy,Dz,C,PI,RS,WIDTH,
     1              HEITH)
        Return
        End
c
c Gaussian Quadrture Routines
c
        Subroutine Gauleg(X1,X2,X,W,N)
c
c Program computes locations and weights for Quadrture
c
        Implicit Real*8(A-H,O-Z)
        Dimension X(N),W(N)
        Parameter(EPS=3.D-14)
        M=(N+1)/2
        XM=0.5D0*(X2+X1)
        XL=0.5D0*(X2-X1)
        Do 12 I=1,M
         Z=COS(3.141592654D0*(I-.25D0)/(N+0.5D0))
1         Continue
         P1=1.D0
         P2=0.D0
         Do 11 J=1,N
            P3=P2
            P2=P1
            P1=((2.D0*J-1.D0)*Z*P2-(J-1.D0)*P3)/J
11        Continue
        PP=N*(Z*P1-P2)/(Z*Z-1.D0)
        Z1=Z
        Z=Z1-P1/PP
```

```
       If(ABS(Z-Z1).GT.EPS)GOTO 1
        X(I)=XM-XL*Z
        X(N+1-I)=XM+XL*Z
        W(I)=2.D0*XL/((1.D0-Z*Z)*PP*PP)
        W(N+1-I)=W(I)
12     Continue
       Return
       End
c
       Subroutine Quadr(FUNK,A,B,SS,T,RX,RY,RZ,
     1                V,Dx,Dy,Dz,C,PI,RS,WIDTH,HEITH)
c
c Program approximates: Integrate[FUNK[x],{x,a,b}],
c Uses NWT Quadrture points,
c Returns approximation in SS=Sum[W(I)*FUNK[x(I)],{I,1,NWT}]
c
       Implicit Real*8(A-H,O-Z)
       Parameter(NWT=3072)
       Dimension X(NWT),W(NWT)
       External FUNK
       Call Gauleg(A,B,X,W,NWT)
       SS=0.D0
       Do 100 IR=1,NWT
        SS=SS+W(IR)*FUNK(X(IR),T,RX,RY,RZ,V,Dx,Dy,Dz,
     1                C,PI,RS,WIDTH,HEITH)
100    Continue
       Return
       End
c
       Subroutine ERFF(x,error)
c
c  Error function approximation
c
       Implicit Real*8 (A-H,O-Z)
       If(x.LT.-4.D0) Then
        error=-1.D0
       Else If(x.GT.4.D0)  Then
          error=1.D0
        Else
       A1=0.0705230784
       A2=0.0422820123
       A3=0.0092705272
       A4=0.0001520143
       A5=0.0002765672
       A6=0.0000430638
       ERROR=1.0-1.0/
     1    (1+x*(A1+x*(A2+x*(A3+X*(A4+x*(A5+x*A6))))))**16
       End If
       Return
       End
```

Appendix 8

```
      Function Thr2_dll(T,RX,RY,RZ,V,Dx,Dy,Dz,C,RS,WIDTH,HEITH)
c
c  This program is to compute Approximation #1 for
c  thr-dimension case. (6/3/95 Dan)
c
      Implicit Real*8 (A-H,O-Z)
c
      w2=(RX-T*SQRT(V**2-4*RS*Dx))/(2*SQRT(Dx*T))
      If(w2.LT.0.D0) Then
         Call ERFF(ABS(w2),error)
         w3=ERROR+1
      Else
         Call ERFCC(w2,cerror)
         w3=CERROR
      End If
c
      If(w2.EQ.0.D0) Then
         w1=0.D0
      Else
         w1=(V*RX-RX*SQRT(V**2-4*RS*Dx))/(2*Dx)
      End If
c
      w5=(RX+T*SQRT(V**2-4*RS*Dx))/(2*SQRT(Dx*T))
      If(w5.LT.0.D0) Then
         Call ERFF(ABS(w5),error)
         w6=ERROR+1
      Else
         Call ERFCC(w5,cerror)
         w6=CERROR
      End If
c
      If(w6.EQ.0.D0) Then
         w4=0.D0
      Else
         w4=(V*RX+RX*SQRT(V**2-4*RS*Dx))/(2*Dx)
      End If
c
      w7=(RY+WIDTH/2)/(2*Sqrt(Dy*RX/v))
      If(w7.LT.0.D0) Then
         Call ERFF(ABS(w7),error)
         w8=-ERROR
      Else
         Call ERFF(ABS(w7),error)
         w8=ERROR
      End If
c
      w9=(RY-WIDTH/2)/(2*Sqrt(Dy*RX/v))
      If(w9.LT.0.D0) Then
         Call ERFF(ABS(w9),error)
         w10=-ERROR
      Else
         Call ERFF(ABS(w9),error)
         w10=ERROR
      End If
c
      w11=(RZ+HEITH/2)/(2*Sqrt(Dz*RX/v))
      If(w11.LT.0.D0) Then
         Call ERFF(ABS(w11),error)
```

```
           w12=-ERROR
        Else
           Call ERFF(ABS(w11),error)
           w12=ERROR
        End If
c
        w13=(RZ-HEITH/2)/(2*Sqrt(Dz*RX/v))
        If(w13.LT.0.D0) Then
           Call ERFF(ABS(w13),error)
           w14=-ERROR
        Else
           Call ERFF(ABS(w13),error)
           w14=ERROR
        End If
c
        w=0.125*C*Exp(-RS*T)*(Exp(w1)*w3+Exp(w4)*w6)
     1  *(w8-w10)*(w12-w14)
        Thr2_dll=w
        Return
        End
c
        Subroutine ERFCC(x,cerror)
c
c  Complementary error function approximation
c
        Implicit Real*8 (A-H,O-Z)
        If(x.LT.-4.D0) Then
           Cerror=2.D0
        Else If(x.GT.4.D0)  Then
              Cerror=0.D0
           Else
             z=ABS(x)
             y=1.D0/(1.D0+0.5D0*z)
             CERROR=y*Exp(-z*z-1.26551223D0
     1          +y*( 1.00002368D0
     2          +y*( 0.37409196D0
     3          +y*( 0.09678418D0
     4          +y*(-0.18628806D0
     5          +y*( 0.27886807D0
     6          +y*(-1.13520398D0
     7          +y*( 1.48851587D0
     8          +y*(-0.82215223D0
     9          +y*( 0.17087277D0)))))))))
        End If
        Return
        End
c
        Subroutine ERFF(x,error)
c
c  Error function approximation
c
        Implicit Real*8 (A-H,O-Z)
        If(x.LT.-4.D0) Then
           error=-1.D0
        Else If(x.GT.4.D0)  Then
              error=1.D0
           Else
        A1=0.0705230784
        A2=0.0422820123
        A3=0.0092705272
```

```
      A4=0.0001520143
      A5=0.0002765672
      A6=0.0000430638
      ERROR=1.0-1.0/
     1    (1+x*(A1+x*(A2+x*(A3+X*(A4+x*(A5+x*A6))))))**16
      End If
      Return
      End
```

Appendix 9 Function Thr3_dll(T,RX,RY,RZ,V,Dx,Dy,Dz,C,RS,WIDTH,HEITH)

```
c
c  This program is to compute Approximation #2 for
c  three-dimension case. (6/4/95 Dan)
c
      Implicit Real*8 (A-H,O-Z)
      w1=0.125*C*Exp(RS*(Dx*RS*T+T*V**2-V*RX)/V**2)
c
      w2=(-RS/V-V/(2*Dx)+RX/(2*Dx*T))/SQRT(1/(Dx*T))
      If(w2.LT.0.D0) Then
       Call ERFF(ABS(w2),error)
       w3=ERROR+1
      Else
       Call ERFCC(w2,cerror)
       w3=CERROR
      End If
c
      w4=(2*RY+WIDTH)/(4*Sqrt(Dy*T))
      If(w4.LT.0.D0) Then
       Call ERFF(ABS(w4),error)
       w5=-ERROR
      Else
       Call ERFF(ABS(w4),error)
       w5=ERROR
      End If
c
      w6=(2*RY-WIDTH)/(4*Sqrt(Dy*T))
      If(w6.LT.0.D0) Then
       Call ERFF(ABS(w6),error)
       w7=-ERROR
      Else
       Call ERFF(ABS(w6),error)
       w7=ERROR
      End If
c
      w8=(2*RZ+HEITH)/(4*Sqrt(Dz*T))
      If(w8.LT.0.D0) Then
       Call ERFF(ABS(w8),error)
       w9=-ERROR
      Else
       Call ERFF(ABS(w8),error)
       w9=ERROR
      End If
c
      w10=(2*RZ-HEITH)/(4*Sqrt(Dz*T))
      If(w10.LT.0.D0) Then
       Call ERFF(ABS(w10),error)
       w11=-ERROR
      Else
       Call ERFF(ABS(w10),error)
       w11=ERROR
      End If
c
      w=w1*w3*(w5-w7)*(w9-w11)
      Thr3_dll=w
      Return
      End
c
      Subroutine ERFCC(x,cerror)
```

```
c
c  Complementary error function approximation
c
      Implicit Real*8 (A-H,O-Z)
      If(x.LT.-4.D0) Then
       Cerror=2.D0
      Else If(x.GT.4.D0)  Then
          Cerror=0.D0
       Else
         z=ABS(x)
         y=1.D0/(1.D0+0.5D0*z)
         CERROR=y*Exp(-z*z-1.26551223D0
     1           +y*( 1.00002368D0
     2           +y*( 0.37409196D0
     3           +y*( 0.09678418D0
     4           +y*(-0.18628806D0
     5           +y*( 0.27886807D0
     6           +y*(-1.13520398D0
     7           +y*( 1.48851587D0
     8           +y*(-0.82215223D0
     9           +y*( 0.17087277D0)))))))))
      End If
      Return
      End
c
      Subroutine ERFF(x,error)
c
c  Error function approximation
c
      Implicit Real*8 (A-H,O-Z)
      If(x.LT.-4.D0) Then
       error=-1.D0
      Else If(x.GT.4.D0)  Then
          error=1.D0
       Else
      A1=0.0705230784
      A2=0.0422820123
      A3=0.0092705272
      A4=0.0001520143
      A5=0.0002765672
      A6=0.0000430638
      ERROR=1.0-1.0/
     1    (1+x*(A1+x*(A2+x*(A3+X*(A4+x*(A5+x*A6))))))**16
      End If
      Return
      End
```

Appendix 10 Interface used to evaluate models: One-Dimensional Solutions

10-1. Definition file for functions

```
; onel_dll.DEF -- Definition file for onel_dll.DLL

LIBRARY onel_dll          ; Must be the same as base filename.
DESCRIPTION 'DLL for VB'
EXETYPE WINDOWS 3.1
CODE PRELOAD MOVEABLE DISCARDABLE
DATA PRELOAD MOVEABLE SINGLE
HEAPSIZE 1024
EXPORTS onel_dll          ; function name
    WEP
```

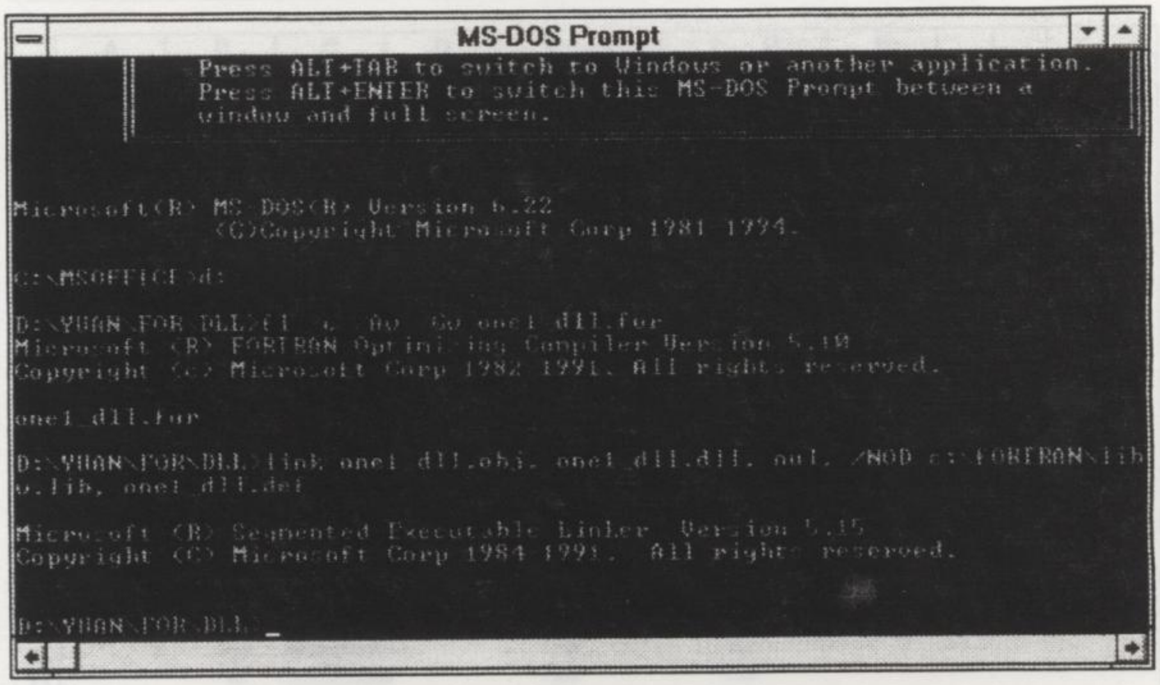
10-2. Compiling file for functions

```
fl /c /Aw /Gw onel_dll.for
```

10-3. Link file for functions

```
link onel_dll.obj, onel_dll.dll, nul, /NOD c:\fORTRAN\lib\ldllfew.lib,
onel_dll.def
```

10-4. Commands to carry out compile and link at DOS prompt



Another way to show the commands on the previous page screen clearly.

```
Microsoft(R) MS-DOS(R) Version 6.22
        (C)Copyright Microsoft Corp 1981-1994.

C:\MSOFFICE>d:

D:\YUAN\FOR\DLL>fl /c /Aw /Gw one1_dll.for
Microsoft (R) FORTRAN Optimizing Compiler Version 5.10
Copyright (c) Microsoft Corp 1982-1991. All rights reserved.

one1_dll.for

D:\YUAN\FOR\DLL>link one1_dll.obj, one1_dll.dll, nul, /NOD c:\fORTRAN\lib\ldllfe
w.lib, one1_dll.def

Microsoft (R) Segmented-Executable Linker  Version 5.15
Copyright (C) Microsoft Corp 1984-1991.  All rights reserved.
```

10-5. A spreadsheet to evaluate models (One-Dimensional)

	A	B	C	D	E	F	G	H	I	J
1	**Title:**	**One-Dimensional Solutions**								
2										
3	**1. Data**									
4	V, ft/day	10	*CALL("d:\yuan\for\dll\one1_dll.dll","one1_dll","beeeeeee",B11,B13,B4,B5,B6,B7,B8)							
5	D	0.1	**CALL("d:\yuan\for\dll\one2_dll.dll","one2_dll","beeeeee",B11,B13,B4,B5,B6,B8)							
6	C, mg/L	1000	***CALL("d:\yuan\for\dll\one3_dll.dll","one3_dll","beeeeee",B11,B13,B4,B5,B6,-B8)							
7	PI	3.14159								
8	RS, 1/day	0								
9										
10	**2. Solutions**									
11	T, day	100								
12		Dist, ft	*Exact, mg/L		**Apprx.#1, mg/L		***Apprx.#2, mg/L			
13		0	974.7126732		1000		1000			
14		1	999.9999999		1000		1000			
15		7	999.9999999		1000		1000			
16		8	999.9999999		1000		1000			
17		9	999.9999999		1000		1000			
18		10	999.9999999		1000		1000			
19		20	999.9999999		1000		1000			
20		40	999.9999999		1000		1000			
21		60	999.9999999		1000		1000			
22		80	999.9999999		1000		1000			
23		100	999.9999999		1000		1000			
24										
25										