國 立 交 通 大 學

環 境 工 程 研 究 所

碩 士 論 文

地下水二維污染歷程重建：未來連續正規化法

Two-dimensional Groundwater Contamination Source Reconstruction： Future Sequential Regularization Method

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中 文 摘 要

當一個污染源釋放污染物進入地下水中，經由傳流及延散作用，會造成地下水污染。當一個場址發現地下水有污染，且其已知污染源位置上曾更替過數個工廠或工廠的經營者時，污染源釋放歷程的重建，可以幫助我們得知地下水中，污染源釋放的濃度歷程，並可釐清各可能責任團體之責任歸屬問題。目前許多地下水污染源歷程重建的方法，只能求得由指數函數所代表的歷程，在重建激變性型態如三角形或階梯形的釋放歷程會產生顯著的誤差。

本研究利用未來連續正規化法(Future-sequential regularization method, FSRM)，針對一個地下水的污染場址作採樣分析，結合地下水污染傳輸控制方程式之基本解，可以重建污染釋放歷程。FSRM可將污染傳輸方程式，由病態的問題(ill-posed problem)轉換成小康構成問題(well-posed problem)，使分析結果滿足穩定狀態且有單一解。我們利用在一個監測井所量得的濃度時間分佈數據，逆推過去文獻提及的地下水二維污染案例；此外，也重建三角形及階梯形的

釋放歷程案例。

為了模擬現地可能之情形，本研究分析的案例，除了時間性數據的二維面源傳輸案例，另外含水層可以為有限或無限寬度。本研究除了分析三角及階梯型態的污染源對重建結果的影響，同時也針對幾個問題進行探討，分別是非等間距時間的採樣數據、採樣濃度量測誤差、及其他方法重建歷程結果之比較等。

Two-dimensional Groundwater Contamination Source Reconstruction： Future Sequential Regularization Method.

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ABSTRACT

As a site is found to have groundwater contamination, the reconstruction of the source release history can provide helpful forensic information to identify the responsible parties at a known source location since the owner of the contaminated source changes several times. The objective of this study is to use a full-estimation technique and Future-sequential regularization method (FSRM) incorporated with a fundamental solution of the groundwater transport equation to recover the source release history of a groundwater contamination. This method can transform the plume release function from the ill-posed problem into a well-posed one with a solution satisfying the unique and stable conditions. A lectured two-dimensional (2-D) groundwater contamination case is used to assess the performance of the source identification. In addition, we used two different source release functions

(namely the triangle function and the step function) to evaluate the effectiveness of FSRM in recovering the release history.

The FSRM is capable of recovering a release history based on the concentration measurements sampled from a monitoring well. With an appropriate value of regularization parameter, FSRM is robust in recovering the optimal release history in terms of the triangle or step source release function. In order to have better representation to the field conditions, the problems of two dimensional plumes are considered to originate from an area source and the aquifer can be of finite or infinite width. Besides, this thesis also investigates the problems of observation data with non-uniform time intervals, data with measurement errors, and comparisons with the solutions obtained by other inverse methods.

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毓婷　謹致於

交通大學環境工程研究所

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TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

NOTATION

a_j	The release strength of the plume
b_j	The measurement of the spread of the release function
B	Width of the aquifer [L]
B_1	Beginning coordinate of the source in the y-direction
B_2	Ending coordinate of the source in the y-direction
C	Concentration
$\partial C/\partial t$	The change in solute concentration with time $[ML^{-3}T^{-1}]$
$C(x, y, z, t)$	The contaminant concentration in the groundwater $[ML^{-3}]$
$C_{ext}(x_n,T)$	The exact concentration at location x_n at time T
$C_{meas}(x_n,T)$	The measured concentration at location x_n at time T
C_{in}	Contaminant source release function $[ML^{-3}]$
C_{ini}	The ith contaminant source release function
D	The hydraulic dispersion coefficient tensor $[L^2T^{-1}]$
D_x	x-component of the dispersion tensor
D_y	y-component of the dispersion tensor
D_z	z-component of the dispersion tensor
F	A kernel function defined by Eq.(3)
h_{i-1}	the width of ith interval
H	Depth of the aquifer [L]
H_1	Beginning coordinate of the source in the z-direction
H_2	Ending coordinate of the source in the z-direction
k	kernel function
L_1	Beginning coordinate of the source in the x-direction
L_2	Ending coordinate of the source in the x-direction
N	The numbers of recovered data
r	Regularization parameter
s	Time
S_i	Second derivative at the point (x_i, y_i)
t	Time
t_j	The release times of the plume
T	Sampling time
u	Release history

v	Average linear velocity vector [LT^{-1}]
x	Longitudinal coordinate
x_i	The x coordinates of the ith plume source
x_s	x-coordinate of a point source
y	Transfer coordinate
y_i	The y coordinates of the ith plume source
z	Vertical coordinate
z_i	The z coordinates of the ith plume source
δ_n	The random number from a Gaussian standard population
ε	The error magnitude
τ	Time
Δ_i	$\Delta_i \equiv \int_0^{t_1} k(t_i - s)ds$
χ_i	The characteristic function defined by $\chi_i(t) = 1$ for $t_{i-1} < t < t_i$, and $\chi_i(t) = 0$ otherwise

CHAPTER 1 INTRODUCTION

1.1 Background

Recently, many soil and groundwater contamination events have been reported in Taiwan. These reports reveal that people's health may be impaired if living near the contaminated sites. Therefore, an effort should be made to investigate the contaminant source and assess the remedial measures. Generally speaking, groundwater contaminants may originate from the disposal of wastewater for various purposes. All sources and causes of contamination can be classified into two categories: point sources and non-point sources. Point sources, characterized by the presence of identifiable sources, include storage tanks, pipeline releases, and chemical manufacturing locations. Non-point sources are referred to as larger-scale and more diffuse contamination originated from many smaller sources; for example, the agricultural fertilizers leaching through soil and finally affecting aquifers (Chen and Yeh, 2006).

The remediation of groundwater contamination may be expensive, and the responsible party rather than the public should pay the costs. In addition, the assessment of the remediation needs to know the total contaminant mass before groundwater remediation. This information could be estimated while the source release history, including the release concentration and release time, is reconstructed.

Groundwater contamination is a water quality problem which may affect the utility of an aquifer. To minimize the potential hazardous effect of the contamination, the contaminant concentrations for some crucial species in the aquifer must be rectified to the regulated acceptable levels. The advection and dispersion are the main mechanisms affecting the transport of a contaminant in a groundwater flow system. The recovery of a contaminant release history portrays the temporal distribution of the source concentration when entering the groundwater system. The recovery of the release history from a known contamination source can provide forensic information to identify parties responsible for groundwater contamination.

The reconstruction of contaminant release history can help us understand the temporal distribution of the source concentration when entering the groundwater system. As a site is found to have groundwater contamination, the reconstruction of the source release history can provide helpful forensic information to identify the responsible parties at a known source location since the owner of the contaminated source changes several times. Utilizing these concentration data in an inverse model with responsible estimates of the transport parameters can reconstruct the release history from the plume source.

1.2 Literature Review

Groundwater transport mainly contains advection and dispersion processes, which are irreversible. Therefore, modeling the contaminant transport using reversed time is an ill-posed problem. The implications of this problem are twofold. First, the ill-posed problem is extremely sensitive to errors in the input data, so small errors in the measurement of existing plume may drastically change the recovered source release history. Second, the ill-posed problem results in unstable numerical schemes making it impossible to run transport models with reversed time and obtain an accurate contamination history (Skaggs and kabala, 1994).

Various methods were proposed in literature to solve the problem of source identification in the past two decades. Atmadja and Bagtzoglou (2001) reviewed the methods that had been developed to identify the contaminant source location and recover the time-release history. They classified the contaminant transport inversion methods into four categories. They are: direct approaches, analytical solution and regression approaches, probabilistic and geo-statistical simulation approaches, and optimization approaches.

1.2.1 Direct approaches

Various methods are also applied to solve the Fredholm integral equation in the mathematical field. Amato and Hughes (1991) used a regularization method by minimizing the functional of the Fredholm integral equation of the first kind numerically. Conditioning on the data and the regularization parameter, this procedure was shown to be a correct regularization method. Several numerical experiments were given and comparisons with Tikhonov regularization (TR) schemes were also presented. Hansen (1992) reviewed several numerical tools that can be applied for the analysis and solution of systems of linear algebraic equations originated from Fredholm integral equations of the first kind. Those tools were developed on the basis of the singular value decomposition (SVD) and the generalized SVD which can be used to study many details of the integral equation. Lamm (1995) generalized the idea of Beck (1985) in solving the heat flow problem and viewed that method as one in a large class of regularization methods. The solution of an ill-posed first kind Volterra equation is converted to be the limit of a sequence of well-posed second kind Volterra equations.

Skaggs and Kabala (1994) used Tikhonov regularization to solve the solute transport equations reversely and recover the spatial release history of the contaminant plumes in a one-dimensional (1-D), homogeneous system. Perhaps, TR is the most widely used technique for regularizing discrete ill-posed problems (Aster et al., 2005). Basically, TR is to transfer the ill-posed problem to a well-posed minimization problem and find the best value of the regularization parameter via the method of Lagrange multipliers. In addition, Skaggs and Kabala (1995) also applied the quasi-reversibility (QR) method to the same problem solved by TR and employed a Monte Carlo methodology to recover the release history of an arbitrary plume in a medium with dispersive properties. Woodbury and Ulrych (1996) used minimum relative entropy (MRE) approach to recover the release history of a pollutant for 1-D transport with constant known velocity and dispersivity system. Fundamentally, MRE is an information-theoretic method in solving the problems. They showed that MRE method yields exact expressions for the expected values of the linear inverse problem and the posterior probability density function (pdf) if given prior information of an upper and lower bounds, a prior bias, and constraints in terms of measured data. Woodbury et al. (1998) extended the MRE method to recover the source release history of a three-dimensional plume. They pointed out that the relative entropy measure can indicate the reduction in uncertainty between the posterior and prior pdfs if the new information provided by the physical constrains and data.

1.2.2 Analytical solution and regression approaches

Lawson and Hanson (1995) proposed the least squares (LS) and Stark and Parker (1995) used the bounded valuables least squares (BVLS) for recovering the release history. Aster (2005) also applied both LS, BVLS to the inverse problems and gave an example for the illustration of the recovery of the release history. The problem of solving for a least squares solution with LS and BVLS includes the minimizing or maximizing a linear function to bounds constraints and that solutions to this problem can be estimated. Sun et al. (2006) formulated a new variant of the robust least squares (RLS), called constrained robust least squares (CRLS) and allowed for imposing nonnegativity constraints, for identifying the contaminant source release histories. Originated in the field of robust identification, the RLS estimator considers the errors arising from model uncertainty and reduces the sensitivity of the optimal solution to perturbations in model and data. The authors demonstrated the use of CRLS in solving one- and two-dimensional test problems in the ill-conditioned and uncertain system and showed that CRLS gave much better performance than its classical counterpart, the nonnegative least squares.

1.2.3 Probabilistic and geostatistical simulation approaches

Butera and Tanda (2003) utilized a geo-statistical approach to identify the probability of the source location for the same problem solved by TR. Their applications focused on the case of non-point and multiple sources in a 2-D groundwater flow system of an infinite domain. Boano et al. (2005) also applied geo-statistical method to identify the contaminant sources in the river pollution problems.

1.2.4 Optimization approaches

Sayeed and Mahinthakumar (2005) developed a parallel simulation-optimization framework including genetic algorithms and several local search approaches for solving PDE-based inverse problems. Their hybrid optimization algorithms were demonstrated to recover the groundwater contaminant source release history successfully. Newman et al. (2005) applied a hybrid method based on the simulated annealing and minimum relative entropy to estimate the magnitude and transverse spatial distribution of mass flux through a plane. When applying to a numerically generated test problem and a tracer experiment, the results demonstrated that the hybrid method is a very effective tool in inferring the contaminant mass flux probability density function, expected flux values, and confidence limits. Chen and Yeh (2006) used simulated annealing (SA) in incorporating with an exponential type of source release function and a fundamental solution of the groundwater transport equation to recover the release history of a groundwater contamination. The SA generates trial values for the parameters in the assumed release function expressed in terms of exponential functions. The simulated concentrations are then obtained from the fundamental solution with the trial source release function. While minimizing the sum of square errors between the simulated and sampling concentrations, SA can determine the optimal parameters of the assumed release function.

1.3 Objectives

Although various methods for solving the release history recovery problem can be found in groundwater literature, most of them focused only on the case of the source release pattern expressed in terms of the exponential function. The case that the source release history is in a form of triangle or step function, which may pose the problem of numerical oscillation in the inversion process, has not yet been addressed.

The objective of this thesis is to design a novel approach capable of solving the source release history recovery problem in an easy and effective way and to demonstrate that the proposed method is applicable to point source and non-point source cases as well. Using the FSRM recovers the source release history in the form of the triangle or step function. Note the FSRM in solving the inverse problem requires that the observed data are of a fixed time interval. Thus, cubic spline is adopted to interpolate the observed data of non-uniform time intervals into uniformly distributed ones. Such an interpolation approach enable the FSRM to recover the release history in the case that the observed data have non-uniform time intervals.

CHAPTER 2 METHODS

2.1 Advection-Dispersion Equation

Advection and hydrodynamic dispersion are the main mechanisms that make the dissolved contaminant migrate and spread in groundwater. Advection, the most significant mass transport process that the contaminant carried by the flowing groundwater, results from the gradient in fluid head. Hydrodynamic dispersion, a microscopic phenomenon, is caused by a combination of mechanical dispersion and molecular diffusion. Mechanical dispersion causes contaminant to spread out, owing to the variation of flow path and velocity in the groundwater movement. Molecular diffusion is the process in which the contaminants move from high concentration area to low concentration area due to concentration gradient.

The advection-dispersion equation for a conservative contaminant in a steady uniform flow field can be written as (Yeh, 1981):

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} - v\frac{\partial C}{\partial x} \qquad (1)$$

where $\partial C/\partial t$ is the change in solute concentration with time [$ML^{-3}T^{-1}$]; D_x and D_y are the hydraulic dispersion coefficient [L^2T^{-1}] in the x and y direction, respectively; v is the average linear velocity vector[LT^{-1}] in the x direction.

For the problem of recovering the release history of a contaminant, the source location is generally treated as a known. The release history of a groundwater contamination from a known site may be written as

$$C(x_s, y_s, t) = C_{in}(t) \tag{2}$$

where x_s and y_s, are the x- and y- coordinates of the plume source [L], respectively, and $C_{in}(t)$ represents the contaminant source release function [ML^{-3}].

Contaminant transport is a dispersive and irreversible process; as a result, modeling groundwater contaminant transport with reversed time is an ill-posed problem whose solution does not satisfy general condition of uniqueness or stability. Accordingly, the strategy of the proposed method is to avoid solving the ill-posed problem directly. Instead, a relative well-posed problem is formulated and solved.

2.2 Analytical model

Analytical model is easy to employ as a preliminary site assessment tool in predicting contaminant transport. The analytical solutions for the transient, 1-, 2-, and 3-D models (AT123D) given by Yeh (1981) can be used to simulate the spatial-temporal concentration distribution of a contamination in a groundwater system.

Assume that the aquifer is isotropic and homogeneous, the flow is steady and uniform and the release of contaminant from the source is continuous. The concentration distribution of the contamination plume may be written as (Skaggs and kabala, 1994):

$$C(x,y,z,T)=\int_0^T C_{in}(\tau)F(x,y,z,T-\tau)d\tau \quad (3)$$

where $C(x, y, z, T)$ is the plume concentration in the groundwater [ML^{-3}], T is the sampling time, $C_{in}(\tau)$ is the contaminant source release function [ML^{-3}], and $F(x,y,z,T-\tau)$ is the kernel function which is the fundamental solution of Eq. (1) and depends on the source geometry and the aquifer configuration (Yeh, 1981). Note that the left-hand side of Eq. (3) is dimensionless if $C_{in}(\tau)$ is represented by a dimensionless source release function.

For the case of two-dimensional transport, $F(x, y, T-\tau)$ may be represented as (Yeh, 1981):

$$F(x,y,T-\tau)=X_iY_j \quad (4)$$

where X and Y express the area source in x and y direction, respectively, and the subscripts i and j denote the type of the source geometries and the aquifer configurations. The selection of fundamental function depends on the source geometry and aquifer condition. Once $F(x, y, T-\tau)$ is selected, the distribution of a groundwater plume concentration can be simulated by applying the Gaussian quadrature to estimate Eq. (3) with a given source release function, $C_{in}(\tau)$, and sampling time.

Three types of source geometries and two kinds of aquifer configurations are considered herein as examples. The source geometry is point, area, or volume sources and the aquifer configuration is of finite width or infinite width. Hence, the functions X_i, Y_j, and Z_k, are given as follows for some specific cases, according to Yeh (1981). Once $F(x,y,z,T-\tau)$ is selected for an appropriate source geometry and aquifer configuration, the distribution of plume concentration can be simulated by applying the Gaussian quadrature to Eq. (1) with a given source release function, $C_{in}(\tau)$, and sampling time.

If, for example, a conservative contaminant released from an area source in an aquifer of infinite width with a steady uniform flow, then the kernel function in Eq. (3) is equal to X_2Y_4 (Yeh, 1981), that is:

$$F(x,y,T-\tau)=\frac{1}{4}\left[erf\left(\frac{x-L_1-v(T-\tau)}{\sqrt{4D_x(T-\tau)}}\right)-erf\left(\frac{x-L_2-v(T-\tau)}{\sqrt{4D_x(T-\tau)}}\right)\right] \cdot \left[erf\left(\frac{y-B_1}{\sqrt{4D_y(T-\tau)}}\right)-erf\left(\frac{y-B_2}{\sqrt{4D_y(T-\tau)}}\right)\right] \quad (5)$$

where B is the width of the aquifer [L], L_1, B_1 and L_2, B_2 are the beginning of the x-, y- and the end of the x-, y- coordinates of the area source [L], respectively.

2.3 Source release functions

A commonly-used release function expressed in a dimensionless exponential form is, given by Skaggs and Kabala (1994),

$$C_{in}(t)=\sum_{j=1}^{n} a_j \quad \exp\left(-\frac{(t-t_j)^2}{2b_j^{\ 2}}\right) \quad (6)$$

where t_j is the source release time; b_j is the measurement of the spread of the release function; a_j is the release strength of source.

Two cases of the source release histories in terms of triangle and step functions are considered. The triangle release history function represents the contaminant concentration increasing linearly from zero to a certain value and then decreasing linearly to zero, while the step release history function represents the contaminant source released suddenly and maintained a constant concentration for a certain period of time. Both two cases occur very likely in the real world.

A dimensionless triangle source release function can be expressed as

$$C_{in}(t) = \begin{cases} \dfrac{(t - t_0)}{t_1 - t_0}, & for \quad t_0 \le t < t_1 \\ \dfrac{(t_2 - t)}{t_2 - t_1}, & for \quad t_1 \le t \le t_2 \\ 0, \quad for \quad t < t_0 \ \ and \ \ t > t_2 & \end{cases} \tag{7}$$

where the source release begins at (time) t_0 and ends at t_2 and the peak concentration occurs at t_1. The dimensionless unit step release history function can be written as

$$C_{in}(t) = \begin{cases} 0, & t < t_1 \\ 1, & t_1 \le t \le t_2 \\ 0, & t > t_2 \end{cases} \tag{8}$$

The source releases at a constant rate from t_1 to t_2 and there is no release at other times.

2.4 Contamination concentration

Based on Eq. (3), the concentration distribution of a contaminant plume can be estimated if the aquifer configuration and the source location, geometry, and release history are known. In other words, once the $C_{in}(t)$ and $F(x, y, z, T-\tau)$ are determined, the contamination concentration can be predicted by Eq. (3). Conversely, if the contaminant concentrations are obtained from field measurements, one might treat the $C_{in}(t)$ as an unknown and solve Eq. (3) as an inverse problem.

2.5 Future-Sequential Regularization Method

In fact, Eq. (3), which involves definite integral with a constant lower limits and a variable upper limit dependent on the time T, is the Volterra integral equation of the first kind (Press et al., 1992). If the upper limit of integration is also a constant; then Eq. (3) can be characterized as the Fredholm equation. The solution of Eq. (3) is extremely sensitive to arbitrarily small perturbations of the system. The development of stable and reliable numerical methods particularly suited for the solution of Eq. (3) has therefore always been a challenge.

A reasonable way to compute a meaningful 'smooth' solution to Eq. (3), i.e., a solution which has some useful properties in common with the exact solution to the underlying and unknown-unperturbed problem, is to somehow filter out the high-frequency components associated with the small singular values. The classical way to filter out the high-frequency components associated with the small singular values is to apply regularization to the problem. It is standard terminology today to classify any method that seeks to compute a 'smooth' solution as a regularization method and regularization is commonly applied directly to solve the Volterra integral equation of the first kind (Hansen, 1992).

The follows introduce how the FSRM solves Eq. (3) inversely. Lamm (1995) extended the theoretical context of the FSRM developed by Beck (1985) to solve the inverse heat conduction problem. For the application of FSRM in solving the groundwater plume source identification problem, Eq. (3) can be expressed as a first-kind Volterra equation with convolution kernel *k* and given data *f*. That is

$$\int_0^t k(t-s)u(s)ds = f(t), \; t \in [0, t] \tag{9}$$

where *u(s)* is an unknown contaminant release history function. If an extra unknown function occurs on the left-hand side of Eq. (9), it is known as the Volterra equation of the second kind. That is

$$u(t) + \int_0^t k(t-s)u(s)ds = f(t), \; t \in [0, t] \tag{10}$$

The right-hand side *f(t)* and the kernel function *k* are assumed to be known (Linz, 1985).

Lamm (1995) used a very effective stabilization method to analyze the inversion of linear Volterra operators of convolution type. The FSRM is a special case in a class of regularization methods in which the solution of an ill-posed, first-kind Volterra equation is found to be the limit of a sequence of solutions of well-posed, second-kind Volterra equation. A physical problem is considered as well-posed if there exists a unique solution that depends continuously on the non-uniform data.

With the Volterra integral operator A, the solution of Eq. (9) starts with the following collocation equation

$$Au(t_i) = f(t_i) \tag{11}$$

for $i = 1,2,\ldots,N$ and N is the number of data points. One has $u = \sum_{i=1}^{N} c_i \chi_i$ for some real c_i, which are the unknown contaminant release history and χ_i is the characteristic function defined by $\chi_i(t) = 1$ for $t_{i-1} < t < t_i$, and $\chi_i(t) = 0$ otherwise. Thus, Eq. (11) is reduced to

$$Au(t_j) = \sum_{i=1}^{j} c_i \int_0^{t_1} k\left(t_{j-i+1} - s\right) ds \tag{12}$$

By defining $\Delta_i \equiv \int_0^{t_1} k\left(t_i - s\right) ds$ for $i = 1,2,\ldots,$ Eq. (12) can thus be expressed as a matrix form. In fact, the ill-posed original problem leads to poor conditioning of the lower-triangular matrix A^N, especially as Δ_1 gets to zero. Therefore, there are errors introduced in calculating c_1, c_2, and so on. The nature of a Volterra equation is such that the output of c at time t is only influenced by the input data f at times prior to t. It is common for stabilizing the inversion process to impose additional constraints that bias the solution, a process referred to as regularization. Therefore, it makes sense to use future data $f(t_{i+1})$, $f(t_{i+2})$,…in computing c_i. To illustrate, suppose that r has been fixed, and select c_1 minimizing the least squares fit to data J_1 as

$$J_1(c_1) = \left|Ac_1\chi_1(t_1) - f(t_1)\right|^2 + \left|Ac_1(\chi_1 + \chi_2)(t_2) - f(t_2)\right|^2 + \cdots$$
$$+ \left|Ac_1(\chi_1 + \chi_2 + \cdots \chi_r)(t_r) - f(t_r)\right|^2 \tag{13}$$

In Equation (13) the solution c_1 is influenced from $f(t_1)$ to $f(t_r)$, and from t_1 to t_r, where the function c_1 is the optimal solution at the time period. For the c_2, the period from t_2 to t_{r+1} overlaps the function c_1, thus the process amends the solutions and regularizes in the presence of data error to get the optimal solutions. After estimating the solution of c_1, and hold c_1 fixed, then the optimal solution of c_2 is chosen by the same way based on minimizing the least square and so on. For this approach, when $J_i(c_i)$=0, each c_i is determined as the optimal value.

After a series of mathematical manipulation, Eq. (9) could be written as the regularized equation

$$\int_0^t \left(\sum_{i=1}^{r} s_i k(t + (i-1)\Delta t - s) \right) u(s)ds + u(t)\left(\sum_{i=1}^{r} s_i \tilde{\Delta}_{i-1} \right)$$
$$= \sum_{i=1}^{r} s_i f\left(t + (i-1)\Delta t\right) \tag{14}$$

with $\tilde{\Delta}_i = \Delta_1 + \Delta_2 + ... + \Delta_i$ and $s_i = \tilde{\Delta}_i / \tilde{\Delta}_1$ for $i = 1,2,\ldots,r$ where r is a regularization parameter. Equation (14) is a well-posed, second-kind integral equation. The unknown u in Eq. (14) has to be solved sequentially with the lower-triangular matrix and appropriate regularization parameter r. Note that required total numbers of sampling data when applying the FSRM is N+r-1 and the recovered concentration is still N.

2.6 Choice of regularization parameter in FSRM

The choice of the value of *r* is important. If *r* is too small, the solution will have numerical oscillation. In contrast, larger *r* gives a dispersed solution. Different kinds of source release history may use different value of *r*, which actually may depend on the location of monitoring well, dispersion coefficient, average linear velocity, and the sampling time period. However, an appropriate value of *r* is usually found by trial-and-error. For recovering the source release history, Eq. (14) is solved in matrix form using the observed concentrations. The solution of FSRM depends strongly on the value of the regularization parameter *r*, where *r* may equal 1, 2, …. This method uses no regularization if $r = 1$ and some regularization as *r* increases. One may start with $r = 2$ for recovering the release history. If the recovered release history exhibits obvious oscillation, then *r* should be increased until the oscillation is significantly diminished. When *r* gets larger, the curve of recovered history becomes dispersed or stabilized. FSRM utilizes future observed data if $r \geq 2$ in recovering the release history. The value of $r-1$ represents the numbers of future measured data used in the analysis. In other words, a larger value of *r* requires more future sampled concentration data. Nevertheless, the number of *r* required to perform well in recovering the release history depends on the shape of the release pattern and source geometry.

2.7 Cubic spline

Field observed concentration data were usually not sampled uniformly. The implementation of FSRM requires that the time interval for sampling the temporal plume concentration data should be fixed. Therefore, a piecewise polynomial approximation such as the cubic spline can be used to interpolate the observation data from a non-uniform time interval into a uniform one.

Consider a set of third-degree polynomials, y_i, between each pair of contiguous data points from x_i to x_{i+1}. The cubic spline constructs an interpolating polynomial that is smooth in the first derivative, and continuous in the second derivative, both within an interval and at its boundaries. A general expression for cubic spline is

$$h_{i-1}S_{i-1} + 2(h_{i-1} + h_i)S_i + h_i S_{i+1} = 6\left(\frac{y_{i+1} - y_i}{h_i} - \frac{y_i - y_{i-1}}{h_{i-1}}\right) \quad (15)$$

where $h_i = x_{i+1} - x_i$ represents the width of ith interval and S_i denotes the second derivative at the point (x_i, y_i). Leng and Yeh (2003) used Eq. (15) to generate the interpolated data successfully for the observed drawdown data of non-uniform time intervals in order to facilitate the application of the Extend Kalman filter.

2.8 Measurement errors

Field sampled concentration data inevitably contains measurement errors. A multiplicative error model is used to generate random measurement error on the sample data. The multiplicative error model is expressed as

$$C_{meas}(x_n, T) = C_{ext}(x_n, T) + \varepsilon \delta_n C_{ext}(x_n, T) \tag{16}$$

where $C_{meas}(x_n, T)$ denotes the measured concentration at location x_n at time T, $C_{ext}(x_n, T)$ represents the exact concentration (or simulation concentration) at location x_n at time T, x_n is the location of the nth sample, ε is the error level, δ_n is the nth random deviate from a Gaussian standard population (standard normal), and the product $\varepsilon\delta_n C_{ext}$ is equal to the measurement error at x_n.

CHAPTER 3 CONCENTRATION DATA

3.1 Measured concentrations

Recovering the source release history of a groundwater contamination needs to be inferred from the plume concentration measurements. Therefore, to asses the performance of FSRM in recovering the source release history, the measured concentrations are generated by Eq. (3) using hypothetical release functions. Consider an area contaminant source which has the dimensions of 5m × 5m. The concentration distribution is simulated based on Eq. (5) with v = 1 m/day, D_x = 0.5 m^2/day, and D_y = 0.05 m^2/day for a two dimensional contaminant transport. The monitoring well is installed at (x, y) = (30, 6) near the source of contaminant, which is located at the origin (0, 0).

3.2 Sampling concentration data

Previously, Skaggs and Kabala (1994) used 1-D spatial concentration data to recover the release history. The plumes generated by the source history function, i.e., Eq (3), were given at time T = 300 day and 25 different locations for the distance x = [0.01 m, 25.05 m, 50 m, … , 250 m, 275 m, 300 m] with a 10 m interval for x ranging from 50 to 250 m. Therefore, a total of 25 spatial concentration data were used in the recovery of source release history. After that, most articles in recovering the release history adopts their concentration data set for case studies.

In addition, Woodbury and Ulrych (1996) also used 1-D spatial concentration data sampled at the downstream of source ranging from 5 m to 300 m with a 5 m interval and thus a total of 60 data points were used in the recovery of source release history. In principle, the sampling data should cover the whole range of plume concentration in order to recover the entire release history.

Consider three source history patterns, namely the exponential function, the triangle function and the step function. The concentration data generated by those release patterns and measured from a monitoring well, where data points are less than those of used in previous studies, are used to recover the source release histories by FSRM.

CHAPTER 4 CASE STUDIES AND RESULTS

4.1 Two-dimensional source recovery

This study is based on the analytical approach to recover the source release history, each case assumes that the aquifer is isotropic and homogeneous; the flow is steady and uniform; the contaminant is conservative, no decay, and no adsorbed on the aquifer. Various aquifer parameters and the source geometry and location are assumed known. The target of this study is to reconstruct the contaminant release history in the groundwater by FSRM. The method has an advantage that it can be used to reconstruct release history with arbitrary pattern, including smooth curve and non smooth curve. However, FSRM has a limitation that the observed concentration data must be uniform time interval. In this study, cubic spline was used to overcome the problem. For the concentration data with uniform time interval, three source patterns are designed to demonstrate the proposed method in solving the source release history recovery problem.

Three cases are designed to demonstrate the application of FSRM to the cases of two-dimensional area source for three different source release patterns. The aquifer is assumed to be homogeneous, isotropic, and of infinite width and the groundwater flow is steady and uniform. The contaminant is conservative. Case 1 attempts to recover the release history for a release pattern expressed in terms of a combination of exponential functions. Cases 2 and 3 aim to recover the source release history in terms of the triangle and step functions, respectively.

4.2 Scenario 1: Recovering release history with FSRM

4.2.1 Sampling time with a 7 day interval

Figure 1(a) shows the behavior of a "true" source release history generated based on the exponential functions of Eq. (6) with t_j = 130, 150, and 190, b_j = 5, 10, and 7, and a_j = 1, 0.3, and 0.5 and the recovered release histories estimated by FSRM. The value r is chosen to be 3, 4 or 5 to assess the performance of the FSRM in case 1.1. The recovery of the entire release history needs the sampled data covering the full range of plume concentrations in response to the true release history. Note the monitoring well is located at the downstream of the source with a distance of 30m and the average groundwater velocity is 1 m/day. The plume concentration is sampled starting at the time 112 day with a 7 day interval and thus 22 data points are uniformly spaced for an exponential source pattern. For r = 3, the solution of FSRM is divergent as indicated in Fig. 1(a). When r is increased to 4, the recovered release history is in fairly good agreement with the true release history although the peaks of the concentration curve are slightly lower and shifted. For r = 5, FSRM gives a smoother curve with significant lower concentration in the peaks than the true ones.

Figure 1(b) displays the distribution of the "true" source release history with the triangle function of Eq. (7) with $t_0 = 100$, $t_1 = 175$ and $t_2 = 250$ days for case 1.2. For triangle function form, 28 measured data points are uniformly sampled from t = 98 to t = 287 days. The recovered release history for a triangle form gives fairly good match with the assumed release history for FSRM with r = 4, 5, and 6. However, Fig. 1(b) indicates that the shape of the source release history is better recovered for FSRM with r = 5 than that with r = 4 and 6.

The case 1.3 considers that the source release function is a step function, Eq. (8), with $t_1 = 130$ and $t_2 = 225$ days. Twenty eight data points with a fixed time interval are in the range from t = 119 to t = 273 days. Figure 1(c) shows that when r = 4, an obvious oscillation is observed at the beginning of the step function. The recovered release history almost has no oscillation throughout the whole step function when r = 5. Although the release times at the beginning and the end of the step function are not recovered exactly, the percent of error of the release period is about 12%. As r is increased to 6, the time shifting is more obvious. Those results imply that FSRM can recover the release history reasonably well with an appropriate value of parameter r.

4.2.2 Sampling time with 1 day and 3 day interval

The use of smaller time interval, i.e., more sampling data, for the observed data may improve the estimated results of recovering release history. This section intends to investigate the use of of smaller sampling time interval on the estimated results.

For an exponential source release pattern of Eq. (6), the sampling period of the observed data is exactly the same as that used in section 4.2.1, yet, the sampling time intervals are reduced to 1 day and 3 day instead of 7 day. The plume is sampled starting at the time 112 day with 1 day and 3 day intervals and thus resulting 114 data and 48 data points, respectively. For the cases of the time intervals 1 day and 3 day, the solutions of FSRM with r = 5 and r = 3, respectively, are shown in Fig. 2(a). For the case with 1 day time interval, the recovered release history has a very good agreement with the true release history. On the other hand, for the case of 3 day time interval, the solution still matches well with the true one although the first peak of the concentration curve is slightly lower.

For the source release in terms of the triangle function, 158 and 64 measured data points are uniformly sampled from t = 98 days with time intervals 1 day and 3 day, respectively. Fig. 2(b) demonstrates that the FSRM with r = 5 and r = 4 gives fairly good recovered release histories if compared with the true one.

For the step function form, the observed data are sampled from t = 119 with time intervals 1 day and 3 day; and thus the totals of available data are 120 and 52, respectively. Figure 2(c) shows that when r = 5, the release time is recovered reasonably well, although a small oscillation is observed at the beginning of the step function. The recovered release history exhibits no oscillation throughout the whole step function when r = 4 with 3 day time interval. Obviously, those results indicate that the use of smaller time interval will yield better estimations.

4.3 Scenario 2: Nonuniform sample data and Cubic spline interpolation

In reality the concentration measurements may not be sampled with a fixed time interval, which restricts the use of FSRM in recovering the source release history. Under this circumstance, the cubic spline can be chosen to interpolate the nonuniform observed concentration data into uniform ones. A set of 25 concentration data produced by the analytical model for the sampling period from 100 day to 300 day with non-uniform time intervals illustrated in Figure 4 is considered. The interpolated concentrations with 7 day interval by the cubic spline are used for FSRM in recovering the release history. Thus, a total number of temporal concentrations, the same as those used in scenario 1, are used to recover the source release history.

Figure 3(a) shows the interpolated data and recovered release history for the case that the source pattern is of exponential function. The result indicates that the recovered release history with interpolated concentration data by cubic spline is still as good as the one obtained by FSRM with the uniformly spaced data. The recovered history exhibits three peaks clearly with r = 4, though the peaks are slightly lower and the location is lightly shifted. Moreover, the FSRM gives a poor result when $r > 4$.

In the case of a triangle release function, the recovered history using FSRM with interpolated concentration data is almost identical to that with nonuniform observed concentrations for $r = 5$ as indicated in Fig. 3(b). Similarly, the recovered history shown in Figure 3(c) for the case of a step release obtained by FSRM with $r = 5$ and interpolated data is also close to the one obtained with nonuniform observed data.

4.4 Scenario 3: Measurement errors

One of the major advantages of using FSRM in recovering release history is that the solutions are not affected apparently by the measured error. Three cases with different magnitudes of uncertainty representing possible field measurement errors are considered. The error is added to the concentration data generated by Eq. (3) with assumed release history and known aquifer configuration. Cases 3.1 to 3.3 consider that the ε in Eq. (16) are 0.01, 0.05, and 0.1, respectively, representing different level of measurement error. Those data with measurement errors are shown in Fig. 4. Table 1 lists the mean and the standard deviation of the measurement error $\varepsilon\delta_n C_{ext}$ for different error level ε in those three cases. With different values of ε, the recovered histories by FSRM with $r = 4$ for the exponential release function are shown in Fig. 5 (a), with $r = 5$ for the triangular function are shown in Fig. 5 (b), and with $r = 5$ for the step function are shown in Fig. 5 (c). The results indicate that the recovered release histories are very close to those without the measurement error except that the data with larger uncertainty give small fluctuation in the recovered history.

4.5 Scenario 4: Five other methods for the source recovery

Five methods included the least squares (LS), bounded variables least squares (BVLS), minimum relative entropy (MRE), second-order Tikhonov regularization (TR), and simulated annealing (SA) with the exponential function fitting approach are used to recover the release histories for the triangle and step source history functions in this scenario. Except SA and MRE methods, the other four methods are applied to the case of 1-D solute transport with the observed spatial concentrations sampled from 25 monitoring wells at time $T = 300$ day where the data points are given by Skaggs and Kabala (1994). For the MRE method, a total of 60 data points given in Woodbury and Ulrych (1996) are used. The computer codes developed in Aster (2005) for LS, BVLS, MRE, and TR are used to recover the release history for the triangle and step function patterns.

Using the temporal concentration data in scenario 1, SA method with the exponential function fitting approach developed in Chen and Yeh (2006) is applied to recover the release histories. Figures 6 (a) and (b) demonstrates the recovering release histories for the triangle and step functions, respectively, by SA when j is equal to 1, 2, or 3. For the case of triangle function, when j = 1, the solution is the best although the climax of concentration is slightly lower than that of the true one. However, the recovered history has a long tail at very low concentration region which gives poor prediction at the beginning and end periods of the release history in triangle shape. As j is increased to 2, the recovered history deviates from the true one significantly after time T = 225. For j = 3, a spike appears at time T = 125 which reflects that an extra exponential term used in the fitting model gives a poor result. The recovering release histories for various j are shown in Fig. 6(b) exhibit sinuous curves with obvious oscillation when j = 2 and 3. These results imply that the exponential function is not suitable to recover the source release pattern in the form of triangle and step functions

The recovered result by the MRE method for the case of a triangle pattern is shown in Fig. 7(a) which indicates that the recovered release history has obvious fluctuation, especially on the left-hand side of the triangle. In addition, Fig. 7(b) shows the recovered result by the MRE method for the case of the step release function. Similar to the previous case, the recovered history also has some oscillation on the plateau and obvious dispersion at the sharp edges. Figure 8 shows the recovered results by the LS, BVLS and TR methods for the cases of triangle and step release functions. The recovered histories for the triangle pattern exhibited in Fig. 8(a) demonstrates that the LS and TR methods give acceptable results, while the BVLS method yields the result with drastic fluctuation. However, the results in the case of the step function shown in Fig. 8(b) reveal that the recovered release histories exhibit obvious oscillation within the release period by those three methods and obvious dispersion at the sharp edges by the methods of LS and TR. Based on those case studies, the FSRM method does give better reproducibility for the cases of triangle and step release functions than other methods mentioned above.

CHAPTER 5 CONCLUSIONS

An approach, based on FSRM and a fundamental solution of the groundwater transport equation, is proposed to recover the release history of a contaminant from a known source site. Case studies for the recovery of source release history are demonstrated for contaminant transport in a two-dimensional infinite aquifer system. Three different source release functions, namely the exponential function, triangle function, and step functions are selected to evaluate the performance of FSRM in recovering the release history and other inverse methods such as SA, LS, BVLS, MRE, and TR. The FSRM can only analyze the uniformly distributed temporal concentration data; therefore, the cubic spline is applied to transform the nonuniform data into uniform ones in order to facilitate the use of FSRM in recovering the release history recovery.

The results obtained from the case studies in scenarios 1 and 2 indicate that the proposed approach perform reasonably well in recovering the release history. The following conclusions can be drawn from this study:

1. The proposed method, FSRM, is effective in recovering arbitrary source release history for contaminant transport in one-, two- and three-dimensional domains. Various source geometry and aquifer configuration can be considered if the fundamental solution is chosen from AT123D (Yeh, 1981).

2. Most of existing methods in recovering the release history of a contamination plume requires the use of spatial concentration data which in fact is very costly to obtain from many monitoring wells. In contrast, the FSRM is capable of recovering the release history from the temporal concentration data sampled from only one monitoring well. This implies that the FSRM is a cost-effective method in terms of the number of monitoring wells used in practical applications.

3. The recovered release history is generally sensitive to the measurement error. However, the FSRM perform reasonably well in recovering the source release history if the regularization parameter r is properly chosen. According to this study, the appropriate value of r is 4 for the exponential source pattern and 5 for the release history in terms of triangle function or step function.

4. The FSRM is generally more effective than other existing methods such as SA, LS, BVLS, MRE, and TR in recovering the release histories for the triangle and step source release functions.

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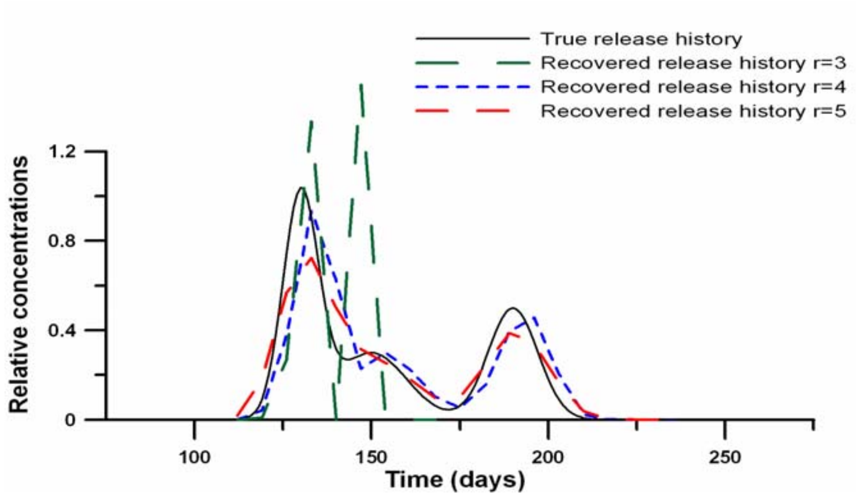
Table 1 The mean and standard deviation of measurement error for different error level ε of three cases.

Error level	Exponential function ($\times 10^{-3}$)		Triangle function ($\times 10^{-3}$)		Step function ($\times 10^{-3}$)	
ε	ME	SDE	ME	SDE	ME	SDE
0.01	1.95	2.73	3.66	5.02	6.90	5.76
0.05	10.26	14.66	21.12	21.24	36.50	35.22
0.1	20.52	29.31	37.02	37.68	73.00	70.43

* ME = mean value

* SDE = standard deviation



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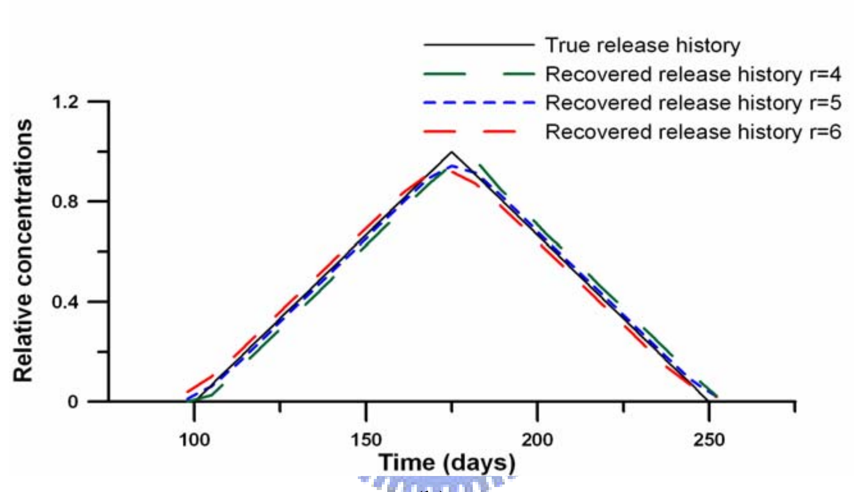

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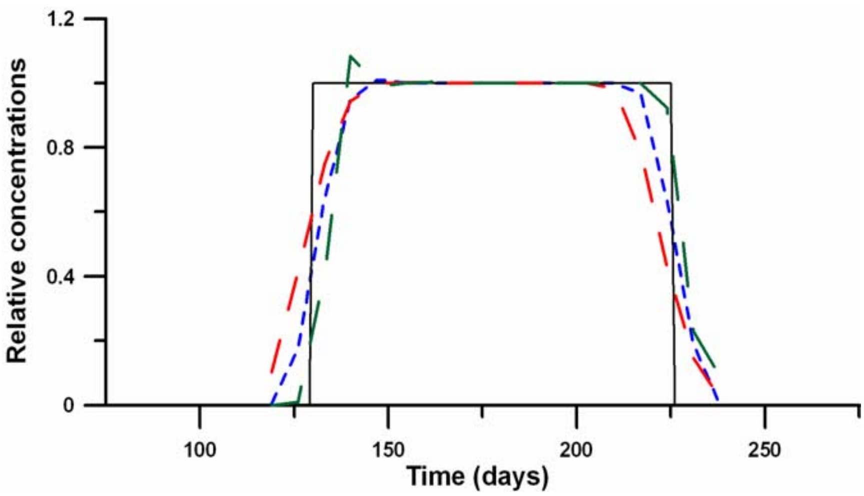
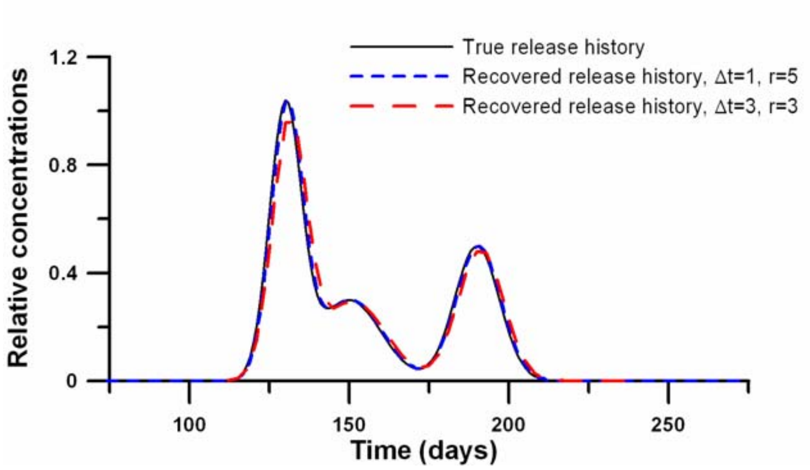
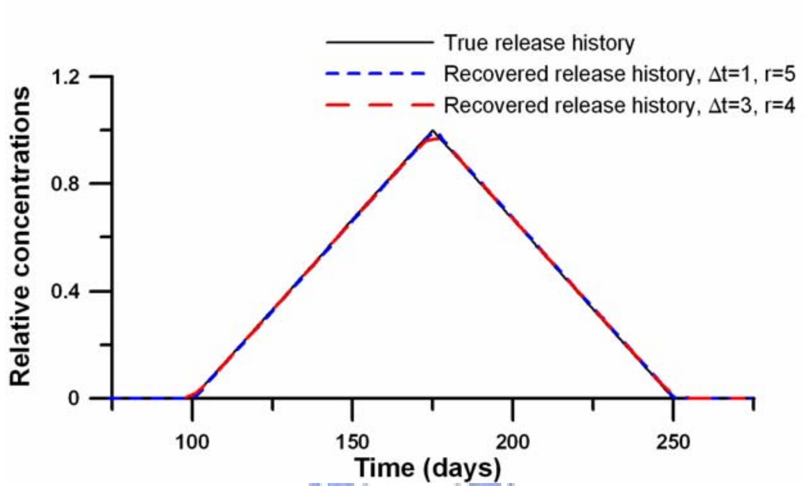


(c)

FIGURE 1 The recovered source release history (a) exponential function for $r = 3, 4, 5$ (b) triangle function for $r = 4, 5, 6$ (c) step function for $r = 4, 5, 6$



(a)



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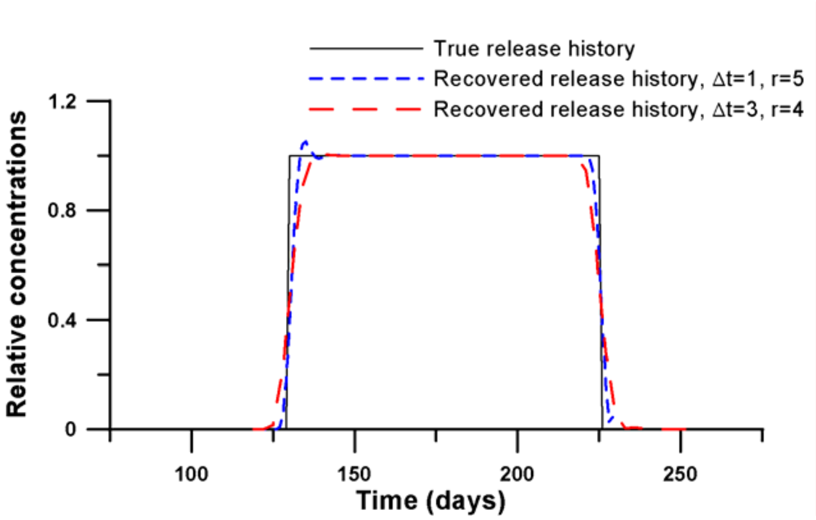
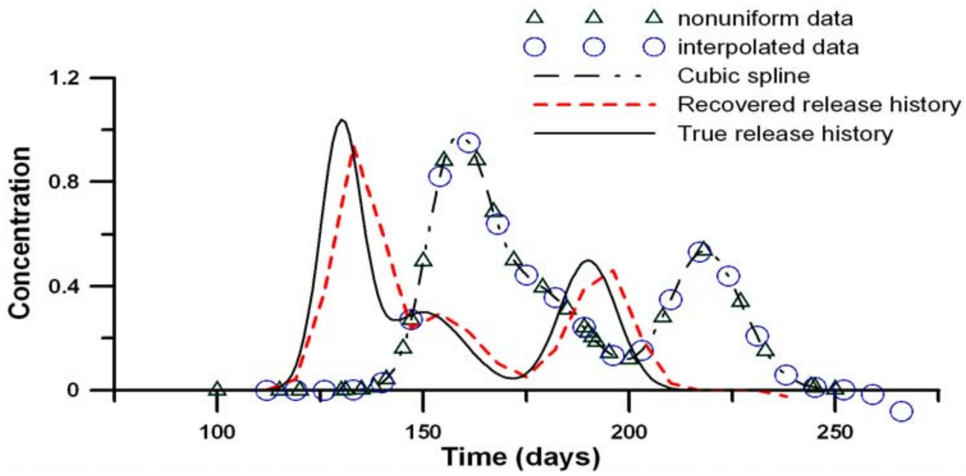


(c)

FIGURE 2 The recovered source release history with time interval 1 day and 3 day (a) exponential function for $r = 5$ and $r = 3$ (b) triangle function for $r = 5$ and $r = 4$ (c) step function for $r = 5$ and $r = 4$



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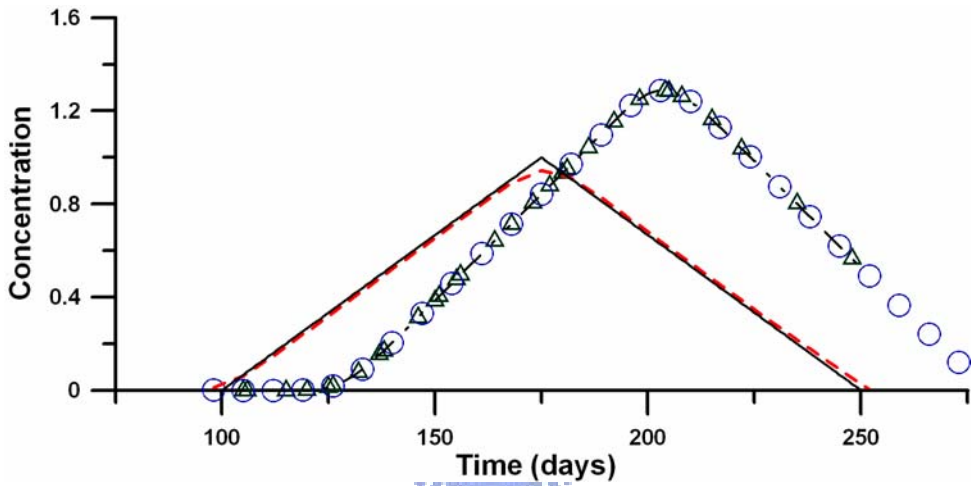

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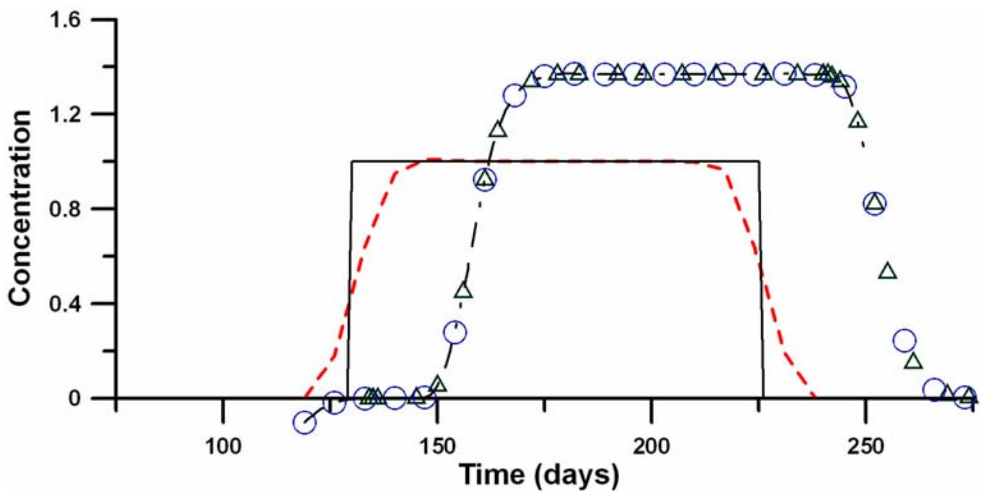
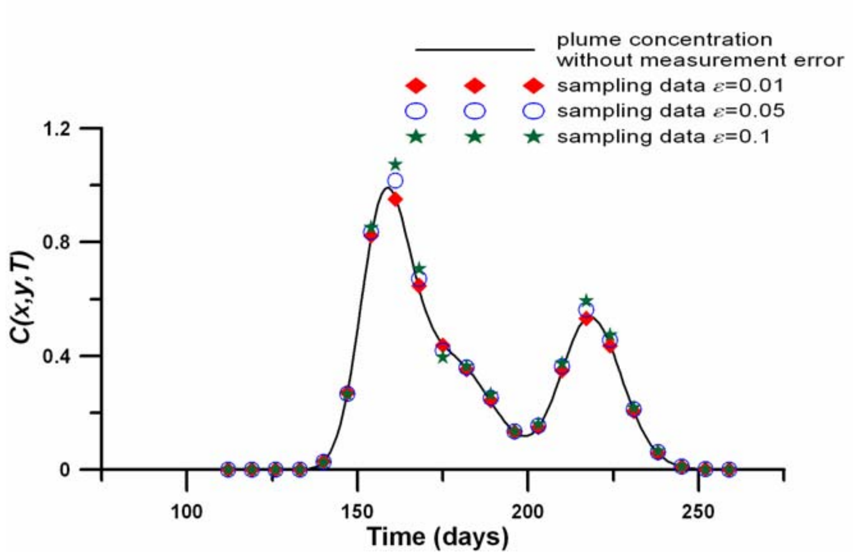
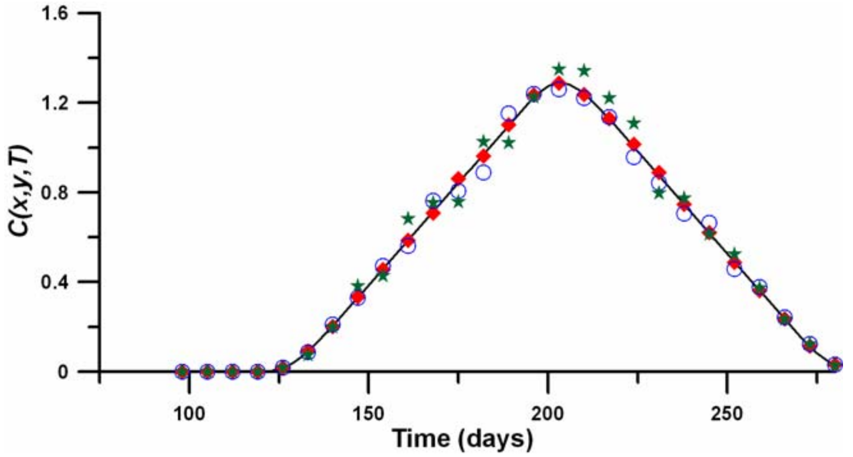


(c)

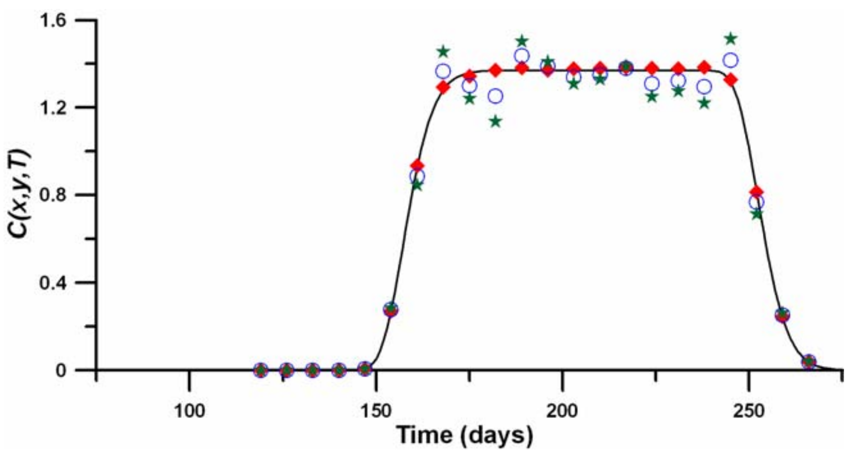
FIGURE 3 Non-uniform observed data, interpolated data, cubic spline, and recovered source release history of (a) exponential function for $r = 4$ (b) triangle function for $r = 5$ (c) step function for $r = 5$



(a)

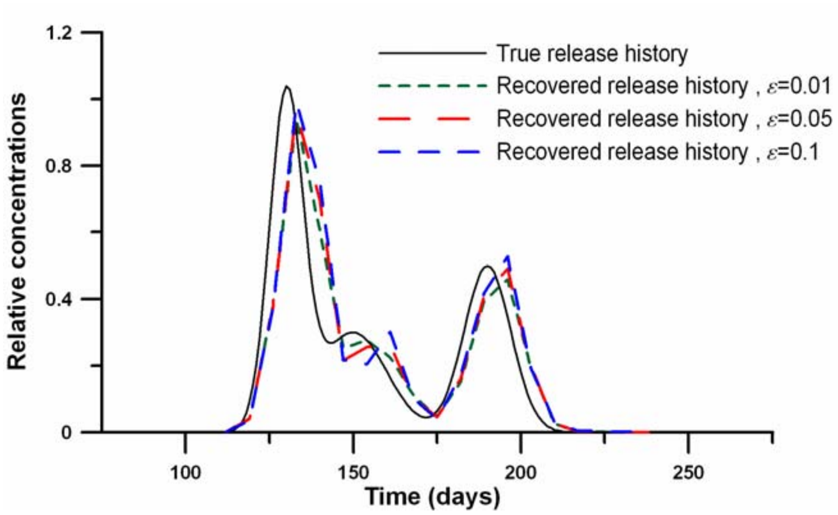


(b)

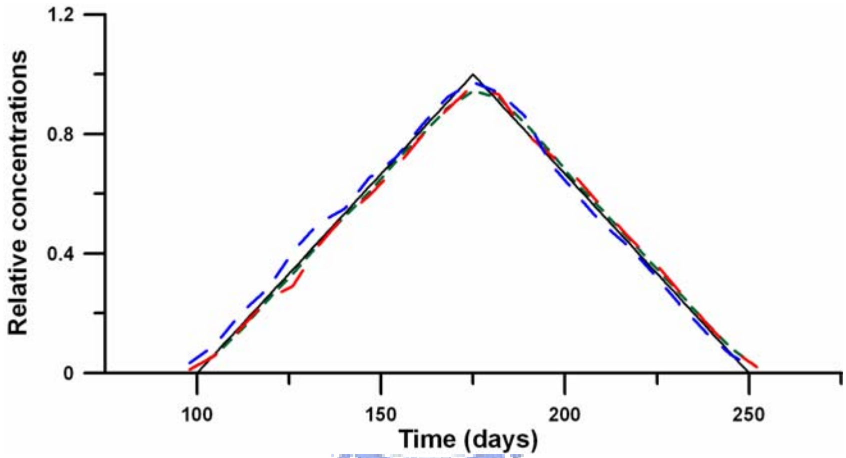


(c)

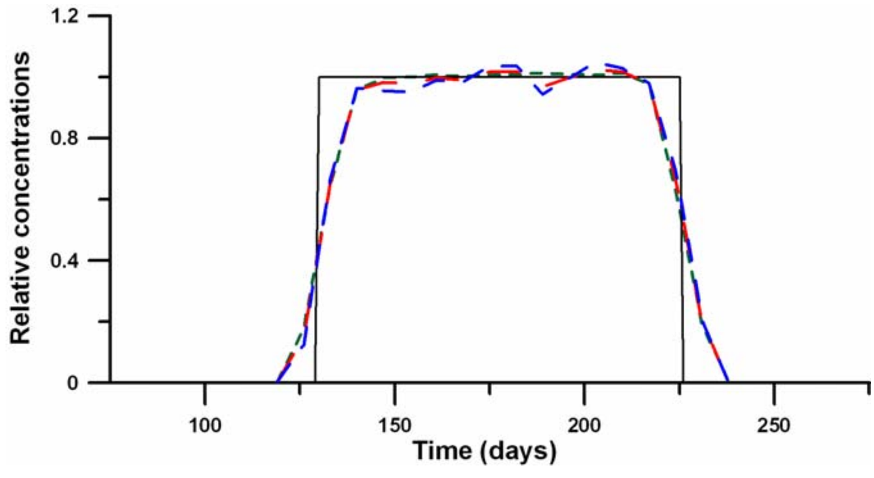
FIGURE 4 The observed data with measurement error $\varepsilon = 0.01$, 0.05, and 0.1
(a) exponential function (b) triangle function (c) step function



(a)

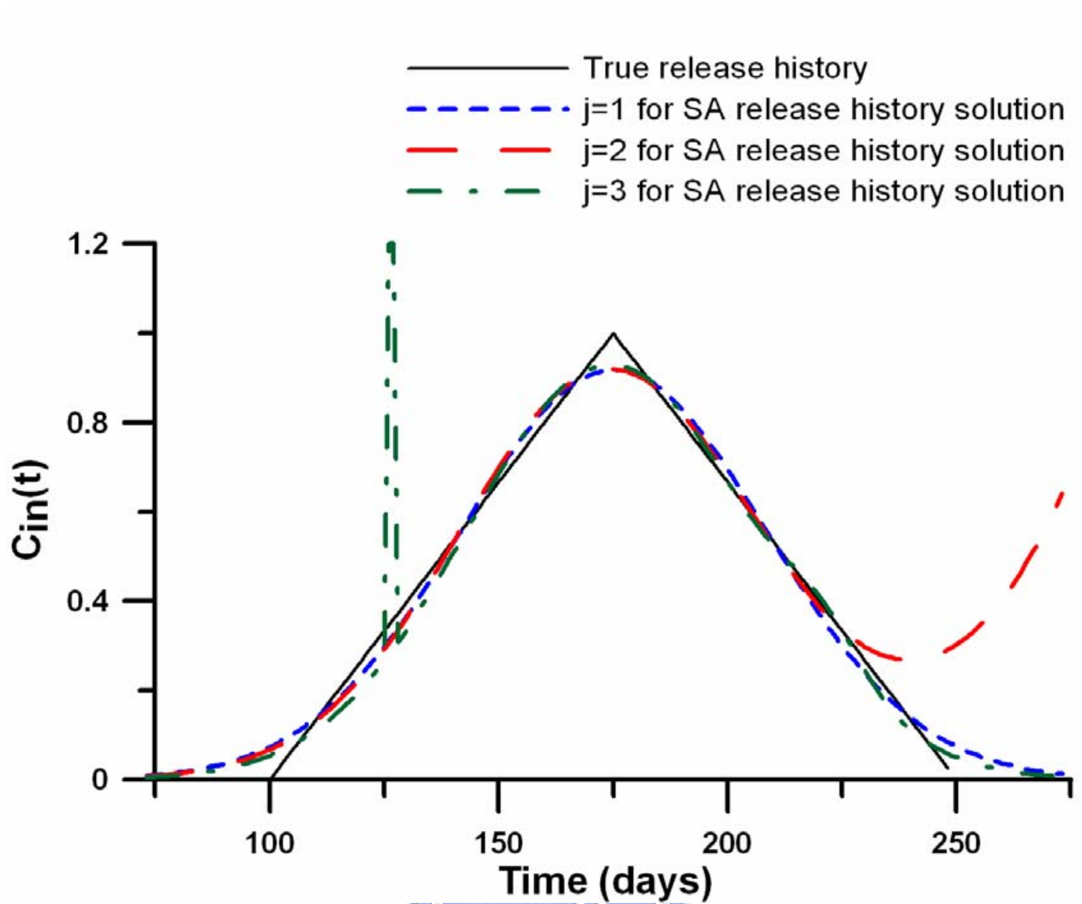


(b)

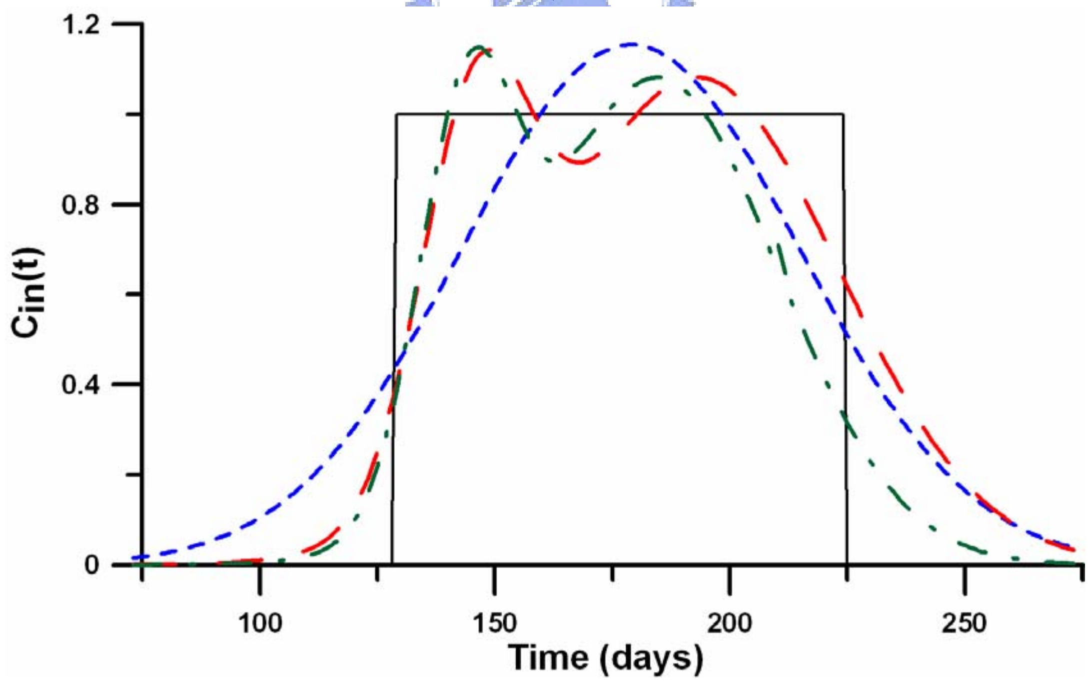


(c)

FIGURE 5 The source release history with measurement error ε = 0.01, 0.05, and 0.1 (a) exponential function (b) triangle function (c) step function

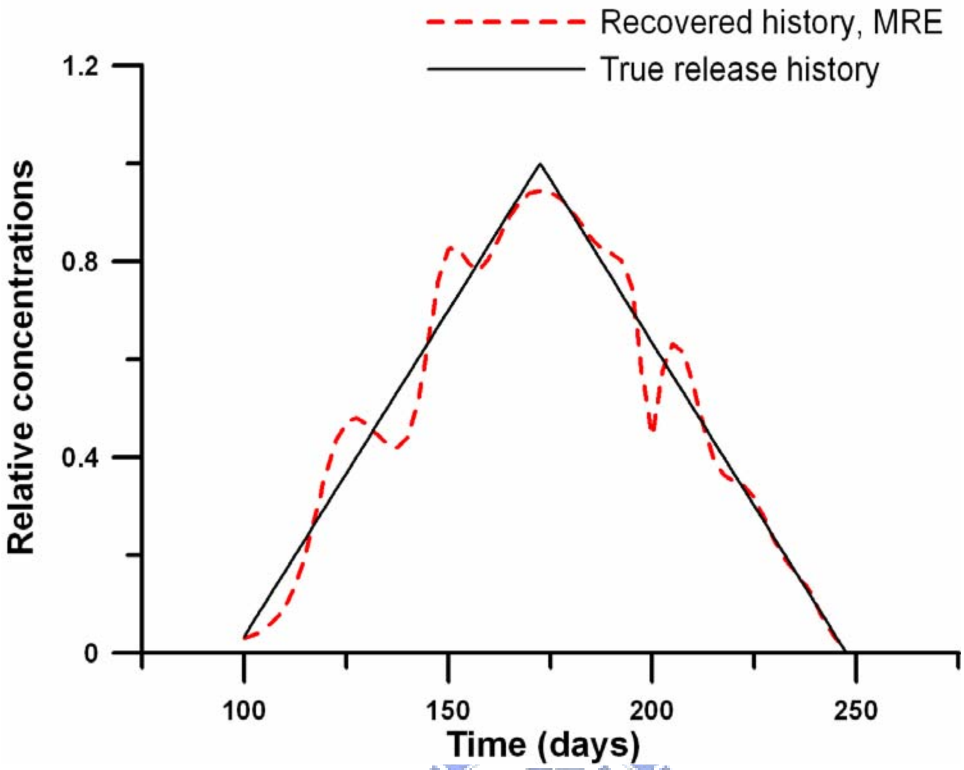


(a)

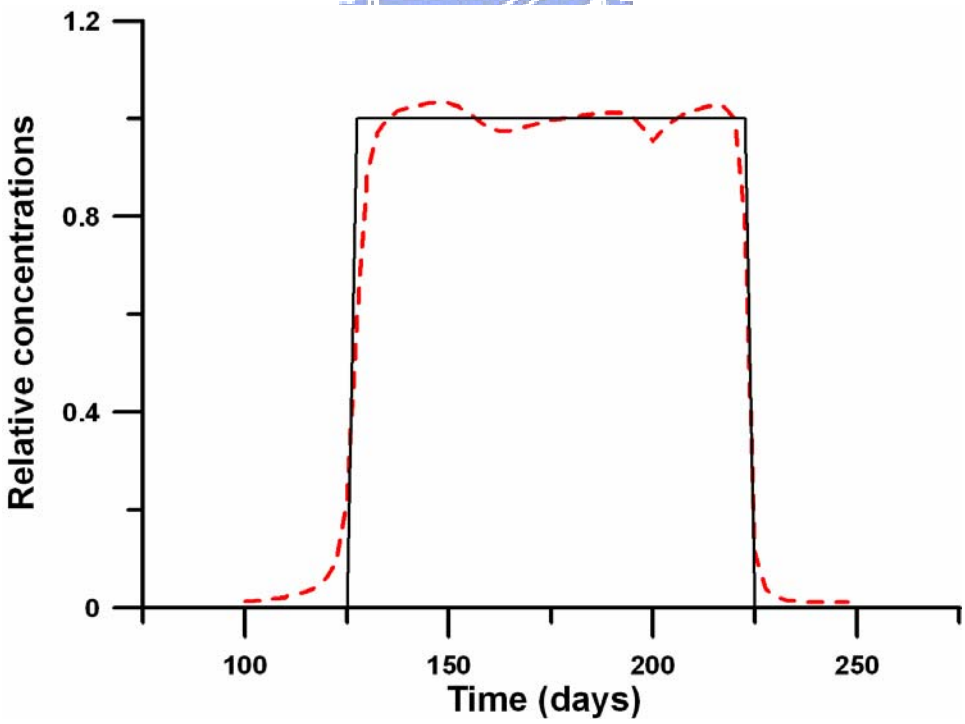


(b)

FIGURE 6 (a) SA method for triangle function source history solution (b) SA method for step function source history solution

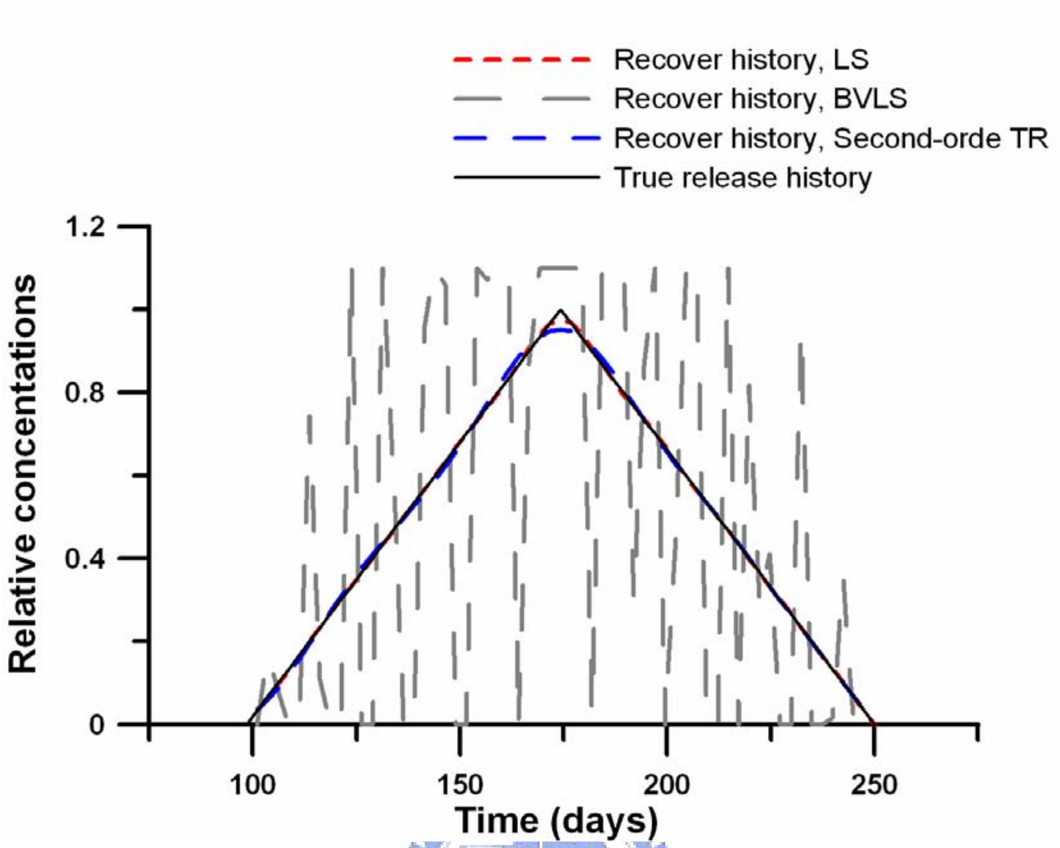


(a)

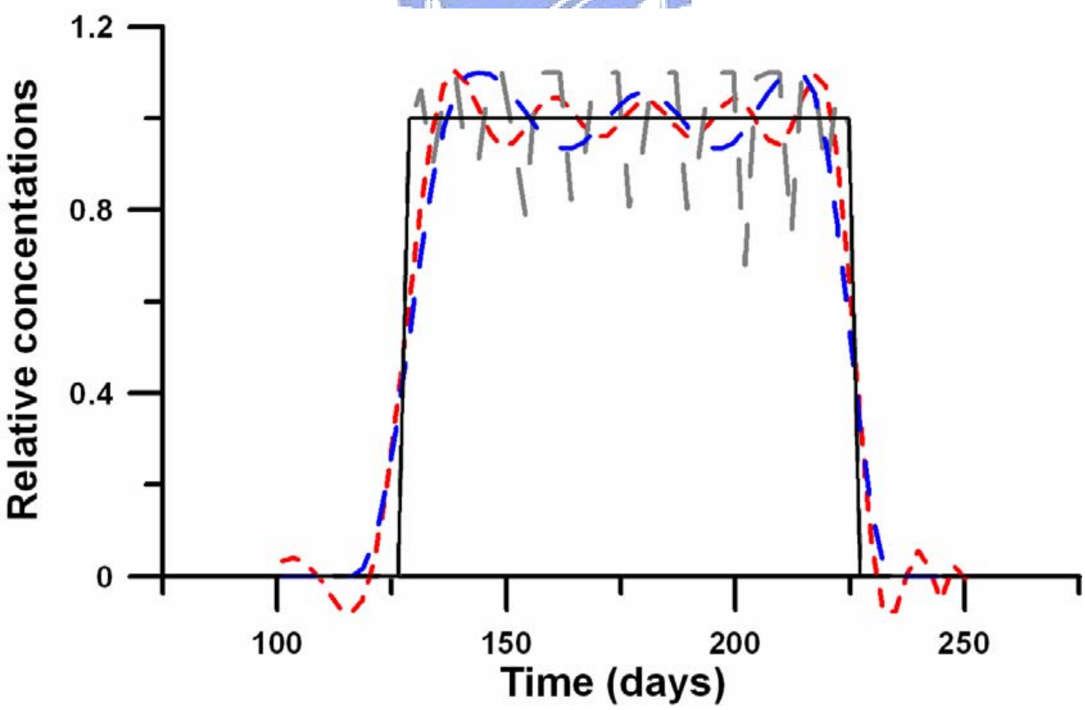


(b)

FIGURE 7 (a) MRE method for triangle function source history solution (b) MRE method for step function source history solution



(a)



(b)

FIGURE 8 LS, BVLS and TR methods for source history solution
(a) triangle function form (b) step function form

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