Advances in Water Resources 75 (2015) 80–92

Contents lists available at ScienceDirect

Advances in Water Resources

journal homepage: www.elsevier.com/locate/advwatres

On different numerical inverse Laplace methods for solute transport problems

Quanrong Wang [a], Hongbin Zhan [b,a,*]

[a] School of Environmental Studies, China University of Geosciences, Wuhan, Hubei 430074, PR China

[b] Department of Geology and Geophysics, Texas A& M University, College Station, TX 77843-3115, USA

ARTICLE INFO

Article history:
Received 22 April 2014
Received in revised form 27 October 2014
Accepted 1 November 2014
Available online 7 November 2014

Keywords:
Numerical Laplace inversion methods
Solute transport problems
Numerical accuracy and efficiency

ABSTRACT

Numerical inversion is required when Laplace transform cannot be inverted analytically by manipulating tabled formulas of special cases. However, the numerical inverse Laplace transform is generally an ill-posed problem, and there is no universal method which works well for all problems. In this study, we selected seven commonly used numerical inverse Laplace transform methods to evaluate their performance for dealing with solute transport in the subsurface under uniform or radial flow condition. Such seven methods included the Stehfest, the de Hoog, the Honig–Hirdes, the Talbot, the Weeks, the Simon and the Zakian methods. We specifically investigated the optimal free parameters of each method, including the number of terms used in the summation and the numerical tolerance. This study revealed that some commonly recommended values of the free parameters in previous studies did not work very well, especially for the advection-dominated problems. Instead, we recommended new values of the free parameters for some methods after testing their robustness. For the radial dispersion, the de Hoog, the Talbot, and the Simon methods worked very well, regardless of the dispersion-dominated or advection-dominated situations. The Weeks method can be used to solve the dispersion-dominated problems, but not the advection-dominated problems. The Stehfest, the Honig–Hirdes, and the Zakian methods were recommended for the dispersion-dominated problems. The Zakian method was efficient, while the de Hoog method was time-consuming under radial flow condition. Under the uniform flow condition, all the methods could present somewhat similar results when the free parameters were given proper values for dispersion-dominated problems; while only the Simon method, the Weeks method, and the de Hoog method worked well for advection-dominated problems.

1. Introduction

Advection–dispersion equation (ADE) has been widely used to describe the solute transport processes like the contaminant or tracer transport in the porous media [1], heat transport in geothermal reservoirs [2,3], and so on. To investigate the behaviors of such substances transport in the subsurface either under a uniform or radial flow field, the Laplace transform method becomes one of the most powerful tools. However, the analytical inverse Laplace transform is generally too difficult to carry out in the closed-from fashion, because of the complicated forms of the solutions in the Laplace domain. Alternatively, the numerical method is called in to conduct the inverse Laplace transform.

For the solute transport in a radial flow field (radial dispersion), one unique feature is that the Peclet number (Pe) is greatest around the injecting (or pumping) well screen and decreases with radial distance from such a well, where Pe is defined as the ratio of the rate of advection of a physical quantity by the flow to the rate of dispersion of the same quantity driven by the gradient. Moench and Ogata [4], and Chen [5,6] applied the Stehfest method [7,8] to numerically invert the solutions of radial transport in the Laplace domain, and found that the Stehfest method was suitable for solving such problems. Subsequently, Chen [6] and Moench [9] pointed out that the Stehfest algorithm could not perform well for solute transport problems with large Pe. This is because ADE becomes a hyperbolic equation from the parabolic equation when advection is dominating. Chen [10,11], Chen et al. [12], Chen et al. [13], and Liu et al. [14] introduced the Crump technique [15] for the inverse Laplace transform. This method employed the epsilon algorithm to calculate the real part of the complex Fourier series when conducting the integral of the inverse Laplace transform.

* Corresponding author at: Department of Geology and Geophysics, Texas A& M University, College Station, TX 77843-3115, USA.

E-mail addresses: wqr88@126.com (Q. Wang), zhan@geos.tamu.edu (H. Zhan).

http://dx.doi.org/10.1016/j.advwatres.2014.11.001
0309-1708/© 2014 Elsevier Ltd. All rights reserved.

Nomenclature

a_j	Taylor coefficient [dimensionless]	N	number of terms used in the summation [dimensionless]
g	scale factor [dimensionless]	Pe	Peclet number [dimensionless]
a_f	free constant parameter [dimensionless]	Q	injection rate (positive) [L^3/T]
Ai	Airy function	r	radial distance from the center of the well [L]
B	vertical aquifer thickness [L]	r_w	radius of the well [L]
C	resident concentration in the aquifer [M/L^3]	s	Laplace variable
C_0	resident concentration at the injection well [M/L^3]	t	time [T]
D_{0a}	effective diffusion coefficient of the aquifer [L^2/T]	$t_{\max}$	largest value of t for which one could evaluate the function of $f(t)$
D_L	longitudinal hydrodynamic dispersion coefficient [L^2/T]	T	time interval in the jth time subsection [T]
D_r	radial dispersion coefficient [L^2/T]	v	flow velocity [L/T]
erfc()	complementary error function	x	distance [L]
$f(t)$	real-time domain function	σ	arbitrary real value greater than the real parts of all the singularities of $F(s)$
$\tilde{f}(t)$	numerical approximation to the exact inverse $f(t)$	σ_0	Laplace convergence abscissa [dimensionless]
$F(s)$	corresponded function of $f(t)$ in Laplace domain	α	free parameter needed to be optimized [dimensionless]
$H(x)$	unit step function	α_r	radial dispersivity of the aquifer [L]
i	$\sqrt{-1}$	θ	porosity of the aquifer [dimensionless]
K	an integer [dimensionless]	τ	numerical tolerance [dimensionless]
$K_{1/3}$	modified Bessel functions of the second kind, 1/3 order		
$L_j()$	jth Laguerre polynomial [dimensionless]		

de Hoog et al. [16] improved the Crump method using either the epsilon algorithm or the quotient difference algorithm to compute the full complex Fourier series, and accelerated the convergence of the series. This method was used to conduct the inverse Laplace transform for radial dispersion by Chen et al. [17] and Moench [9]. Moench [18] pointed out that the Talbot [19] algorithm worked very well for Pe smaller than 100, but might become unstable when the function being inverted had a steep front. For the uniform flow field where the Pe is spatially constant, Bullivant and O'Sullivan [20], and Zhan et al. [21,22] employed the Stehfest method to carry out the numerical inverse Laplace transform; Cornaton and Perrochet [23] and Leij et al. [24] used the Crump [15] technique for the inverse Laplace transform; Schwartz et al. [25] used the Weeks method; Leij et al. [24], Leij and van Genuchten [26] and Gao et al. [27] applied the de Hoog algorithm for the inverse Laplace transform.

Actually, except for the Stehfest, the Crump, the de Hoog, and the Talbot algorithms, there are numerous other methods developed for numerical inverse Laplace transform, such as the Post [28,29], the Papoulis [30], the Weeks [31], the Schapery [32], the Zakian [33], the Piessens [34], and so on, which received less attention before in the literature.

In order to figure out the efficiency and accuracy of above mentioned inverse methods, many scientists investigated them through various types of functions, such as Davies and Martin [35], Abate and Whitt [36], Duffy [37], Abate and Whitt [38], Abate et al. [39], Valkó and Abate [40], Cohen [41], Machado [42], Hassanzadeh and Pooladi-Darvish [43] and so on, where the books of Abate et al. [39] and Cohen [41] might be the most comprehensive in the recent studies. One common conclusion was that the numerical inverse Laplace transform was generally an ill-posed problem, and there was no universal method which worked well for all problems [41]. For instance, Hassanzadeh and Pooladi-Darvish [43] thought that the Fourier transform inversion method was the most powerful but also the most computationally expensive one. They showed that the Stehfest method provided accurate results when the solutions behaved like $\exp(-t)$ type of functions where t was time, but failed when the solution was like $\exp(t)$, sinusoid, or wave type of functions [43]. Duffy [37] found that the methods developed by Zakian [33], Honig and Hirdes [44,45], and Talbot [19] could give accurate results, while the application range of the Talbot algorithm was wider since it contained an optimized method for choosing the required free parameters. Abate and Whitt [36] reviewed a few specific variants of the Fourier-series method for calculating cumulative distribution functions and probability mass functions. He pointed out that the Fourier-series method was an excellent candidate for performing numerical transform inversion, and the Weeks method was also a good choice. Abate and Valkó [46] presented two such procedures of inverse Laplace transform, the Gaver–Wynn–Rho algorithm and the fixed Talbot method, and pointed out that both worked very well for inversion when using multi-precision computing. Recently, several studies showed that various numerical inverse Laplace transform methods may be put into the same mathematical framework [47,48]. For example, Abate and Whitt [48] proposed an unified framework and pointed out that the Stehfest algorithm, a version of the Fourier-series method with the Euler summation, and a version of the Talbot algorithm could fit into their unified framework.

Most studies mentioned above reviewed the accuracy of the Laplace transform methods through a standard approach, in which a numerical inversion scheme was tested using some specific functions, whose inverse were known exactly. Although this approach was acceptable to evaluate a new developing scheme, it did not help for some problems when the solution cannot be expressed by the known inverse Laplace transform functions. For example, the closed-form solution cannot be derived easily for most Boundary Value Problems (BVP) concerning the radial dispersion. Chen [49] employed the complex variables to conduct the inverse Laplace transform of a radial dispersion BVP. Such approaches contained integrals, which cannot be determined easily due to the oscillating behavior of the integrands [50,51]. Chiang [52] tested the four inverse Laplace transform methods (Stehfest, Crump, Weeks and Talbot methods) against the semi-analytical solutions by Chen [49], and concluded that the Stehfest method could yield accurate results at early time, but started to generate oscillating (and unrealistic) solutions at late stage. The other three methods worked very well regardless of the early and late stages.

In this study, the numerical accuracy and the computational efficiency of the inverse Laplace transform methods will be tested for the problems related to solute transport either under a uniform or radial flow field. Finite-element numerical solutions will be