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Exact series solutions of reactive transport models with general initial conditions

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SUMMARY

Exact solutions of partial differential equation models describing the transport and decay of single and coupled multispecies problems can provide insight into the fate and transport of solutes in saturated aquifers. Most previous analytical solutions are based on integral transform techniques, meaning that the initial condition is restricted in the sense that the choice of initial condition has an important impact on whether or not the inverse transform can be calculated exactly. In this work we describe and implement a technique that produces exact solutions for single and multispecies reactive transport problems with more general, smooth initial conditions. We achieve this by using a different method to invert a Laplace transform which produces a power series solution. To demonstrate the utility of this technique, we apply it to two example problems with initial conditions that cannot be solved exactly using traditional transform techniques.

1. Introduction

Mathematical models describing the transport and reaction of dissolved solutes in saturated porous media can play an important role in informing our understanding of contaminant fate and transport processes (Bear, 1972; Domenico, 1987; Remson et al., 1971; Wang and Anderson, 1982; Zheng and Bennett, 2002). For some modeling projects, it is relevant to implement a detailed numerical model that can account for multidimensional, multispecies, nonlinear reactive transport processes (Clement et al., 1998; Clement, 2011; Molz et al., 1986; Zheng and Wang, 1999). In other cases, where insufficient data or finances are available to support the use of a detailed numerical model, a simpler approach, based on an analytical solution of a linear partial differential equation (pde) model, could be more relevant (Clement, 2011; Jones et al., 2006).

Several previous researchers have sought to develop exact solutions to systems of coupled linear advection diffusion reaction equations with decay-chain reaction process. In 1971, Cho (1971) presented an exact solution of a one-dimensional model representing the reactive transport of a system with three components describing nitrification processes. van Genuchten and Wierenga (1976) and van Genuchten (1981, 1985) derived similar exact solutions for decay-chain processes with more complicated inlet boundary conditions and for a system that made an explicit distinction between mobile and immobile species (van Genuchten and Wierenga, 1976; van Genuchten, 1981, 1985). All of these studies were based on solving the governing pde using a Laplace transform technique which meant that the approach was only relevant for relatively simple initial conditions. Both Cho (1971) and van Genuchten and Wierenga (1976, 1981, 1985) focused on problems where the domain was initially free of solutes. Building on these previous investigations, Lunn et al. (1996) presented exact solutions of the system studied by Cho (1971) using a Fourier transform method. This approach allowed Lunn to solve the system for more complicated initial conditions including a constant non-zero initial condition, and an exponentially decaying initial condition.

Further developments of exact or semianalytical solutions of coupled linear advection diffusion reaction equations with decay-chain reaction networks have also been reported. These include extensions to any number of species in the reaction network (Clement, 2000), the presence of distinct equilibrium reactions represented by different retardation factors (Srinivasan and Clement, 2008a,b) as well as dealing with reactive transport processes in two- and three-dimensions (Jones et al., 2006; Sudicky et al., 2013; Wexler, 1992). Approaches based on Green's functions (Kreyszig, 2006) have also been used successfully to analyze two-

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and three-dimensional transport problems with persistent source terms (Leij et al., 2000). More recent developments have included semianalytical solutions for mathematical models where the transport coefficients are spatially variable (Suk, 2013). Regardless of these developments, we note that previously-reported solution methods based on an integral transform technique are restricted in the sense that they require a relatively simple initial condition to permit the exact calculation of the inverse transform. For example, van Genuchten and Wierenga (1976) and van Genuchten (1985) considered a solute-free initial condition; Lunn et al. (1996) considered either a spatially constant or exponentially decaying initial condition; and Srinivasan and Clement (2008a,b) focused on an exponentially decaying initial condition. One of the limitations of these previous methods is that they cannot be applied to other kinds of initial conditions. If, for example, we wished to study the reactive transport of a system with some initial distribution of solute that is neither spatially uniform or decaying exponentially with position, it is impossible to use any of these previous methods to provide an exact solution. These restrictions motivated the recent work by Wang et al. (2011) who proposed an approximate superposition method to solve reactive transport pdes with nonzero initial conditions. While this recent work did not provide any exact solutions to the governing pde model, they did provide insight into conditions where their approximation provided useful information (Wang et al., 2011).

In this work we describe and implement a method that provides an exact power series solution for linear reactive transport problems for more general initial conditions. Our method involves a different way of calculating an inverse Laplace transform and this allows us to consider more general, smooth, non-zero initial conditions, such as nonmonotone functions, which have not been dealt with previously in an exact mathematical framework. In addition to presenting the theoretical aspects of our approach, we also present two example calculations. The first example calculation is for a single species reactive transport model where we consider a nonmonotone initial condition for which traditional transform inversion techniques are not applicable. Second, we consider a coupled problem where again we chose a nonmonotone initial condition which means that traditional exact inverse transform techniques are not applicable. For both cases we compare our truncated power series solutions with numerical calculations to confirm that the proposed method produces accurate results. We conclude by pointing out how our method can be implemented in a very straightforward way using symbolic software and we provide Maple code as supplementary material.

2. Theory

To demonstrate our approach, we first outline how our method allows us to recover a simple function from its Laplace transform without the use of mathematical tables or calculating the inverse transform numerically (e.g., De Hoog et al., 1982). We begin by considering some function $f(t)$, and the Laplace transform of that function, which can be written as

$$\mathcal{L}\{f(t)\} = \int_0^\infty f(t)\mathrm{e}^{-st}\,\mathrm{d}t, \tag{1}$$

where s is the Laplace transform parameter chosen such that the improper integral converges (Beerends et al., 2003; Debnath and Bhatta, 2007; Kreyszig, 2006; Zill and Cullen, 1992). For suitable choices of $f(t)$, such that $\lim_{t\to\infty}\left[\frac{\mathrm{d}^n f(t)}{\mathrm{d}t^n}\mathrm{e}^{-st}\right] = 0$ for all n, repeated application of integration by parts to Eq. (1) gives us

$$\mathcal{L}\{f(t)\} = \frac{1}{s}\left[f(0) + \frac{1}{s}\frac{\mathrm{d}f(0)}{\mathrm{d}t} + \frac{1}{s^2}\frac{\mathrm{d}^2 f(0)}{\mathrm{d}t^2} + \frac{1}{s^3}\frac{\mathrm{d}^3 f(0)}{\mathrm{d}t^3} + \dots\right]. \tag{2}$$

Eq. (2) leads to the initial value theorem (Beerends et al., 2003; Debnath and Bhatta, 2007; Ellery et al., 2013)

$$\lim_{s\to\infty}[s\mathcal{L}\{f(t)\}] = f(0), \tag{3}$$

allowing us to calculate the initial value of the function, $f(0)$, directly from $\mathcal{L}\{f(t)\}$ without needing to explicitly invert the Laplace transform. We may extend the initial value theorem by making a change of variables, let $g(t) = \frac{\mathrm{d}^n f(t)}{\mathrm{d}t^n}$, so that we have $\lim_{s\to\infty}[s\mathcal{L}\{g(t)\}] = g(0)$. Re-stating this result in terms of the original variables gives us

$$\lim_{s\to\infty}\left[s\mathcal{L}\left\{\frac{\mathrm{d}^n f(t)}{\mathrm{d}t^n}\right\}\right] = \frac{\mathrm{d}^n f(0)}{\mathrm{d}t^n}, \tag{4}$$

which means that if we know the Laplace transform of the nth derivative of a function, we can evaluate the nth derivative of that function at $t = 0$ without explicitly inverting the transform. Since we know that the Laplace transform of the nth derivative of a function (Beerends et al., 2003, Debnath and Bhatta, 2007, Kreyszig, 2006 and Zill and Cullen, 1992) is given by

$$\mathcal{L}\left\{\frac{\mathrm{d}^n f(t)}{\mathrm{d}t^n}\right\} = s^n\mathcal{L}\{f(t)\} - \sum_{k=1}^{n}\frac{\mathrm{d}^{k-1}f(0)}{\mathrm{d}t^{k-1}}s^{n-k}, \tag{5}$$

we can re-express Eq. (4) as

$$\frac{\mathrm{d}^n f(0)}{\mathrm{d}t^n} = \lim_{s\to\infty}\left[s^{n+1}\mathcal{L}\{f(t)\} - s\sum_{k=1}^{n}\frac{\mathrm{d}^{k-1}f(0)}{\mathrm{d}t^{k-1}}s^{n-k}\right], \tag{6}$$

which means that given $\mathcal{L}\{f(t)\}$, we can calculate all the derivatives of $f(t)$ at $t = 0$. With this information we may then construct a Maclaurin series

$$f(t) = \sum_{i=0}^{\infty}\frac{\mathrm{d}^i f(0)}{\mathrm{d}t^i}\frac{t^i}{i!}. \tag{7}$$

Therefore, for a particular function $f(t)$, for which we can calculate the Laplace transform, $\mathcal{L}\{f(t)\}$, we may reconstruct the function using Eqs. (6) and (7). The reconstruction of $f(t)$ does not depend on calculating the inverse transform. For the practical implementation of the Maclaurin series representation of $f(t)$, we must truncate Eq. (7) after I terms. We will show, by example, that it is often straightforward to obtain reasonably accurate solutions with a relatively modest value of I.

To demonstrate how we might make use of this result, let us consider the straightforward case of $f(t) = \mathrm{e}^{at}$, for which the Laplace transform is $\mathcal{L}\{f(t)\} = 1/(s-a)$, with $s > a$ (Kreyszig, 2006; Zill and Cullen, 1992). Using Eq. (6) we rapidly see that we have

$$\frac{\mathrm{d}f}{\mathrm{d}t}(0) = a,\ \frac{\mathrm{d}^2 f}{\mathrm{d}t^2}(0) = a^2,\ \frac{\mathrm{d}^3 f}{\mathrm{d}t^3}(0) = a^3,\ \frac{\mathrm{d}^4 f}{\mathrm{d}t^4}(0) = a^4, \dots \tag{8}$$

which, using Eq. (7), allows us to reconstruct the well-known Maclaurin series for the exponential function

$$\mathrm{e}^{at} = 1 + at + \frac{(at)^2}{2!} + \frac{(at)^3}{3!} + \frac{(at)^4}{4!} + \dots. \tag{9}$$

In summary, Eq. (6) gives us an alternative method for inverting a Laplace transform. Instead of using mathematical tables (Kreyszig, 2006; Zill and Cullen, 1992) or numerical inversion (De Hoog et al., 1982), if we have an explicit formula for $\mathcal{L}\{f(t)\}$, even without any knowledge of $f(t)$, we can recover the Maclaurin series representation of $f(t)$ without difficulty, provided that the function is sufficiently smooth. We note that power series solutions have been used previously to study several practical problems of interest in subsurface hydrology (Philip, 1957a; Philip, 1957b), chemical engineering (Ellery and Simpson, 2011) and bioengineering (Simpson and Ellery, 2012). Although we aim to demonstrate the