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Comment on "A space-time accurate method for solving solute transport problems" by S. G. Li, F. Ruan, and D. McLaughlin

Christopher Zoppou
Australian Capital Territory Electricity and Water, Canberra

John H. Knight
Centre for Environmental Mechanics, CSIRO, Canberra

Introduction

Analytical techniques for the solution of the advection-diffusion equation are generally restricted to simple problems with constant coefficients. Practical problems usually involve variable velocity and diffusion coefficients. The solution scheme described by *Li et al.* [1992], based on the Laplace transform, was developed with the capability to solve the advection-diffusion equation with spatially variable coefficients. The Laplace transform is used to evaluate the temporal derivative in the advection-diffusion equation analytically, thereby eliminating the effects of the time derivative on accuracy and stability. Because the temporal derivative is evaluated using the Laplace transform, there is no need for the time-stepping that is associated with more traditional techniques for the solution of the advection-diffusion equation. Therefore it is a potentially more efficient technique.

The authors do not provide numerical simulations involving the spatially variable coefficient advection-diffusion equation. A reason for this might be that there are very few analytical solutions to the advection-diffusion equation with spatially variable coefficients.

The purpose of this discussion is to present what we believe to be a new analytical solution to a particular form of the advection-diffusion equation with spatially variable coefficients and to highlight a potential mass conservation problem that could be encountered with the formulation used by Li et al. The analytical solution can be used to validate schemes for solving the advection-diffusion equation with spatially variable coefficients. The efficiency of the method proposed by Li et al. is demonstrated by comparing its performance for the solution of the advection-diffusion equation with spatially variable coefficients with that of a well-known time-stepping scheme.

Conservative Form of the Advection-Diffusion Equation

Li et al. describe a numerical scheme, based on the Laplace transform, for the solution of the following form of the spatially variable coefficient advection-diffusion equation:

$$\frac{\partial c(x,t)}{\partial t} + u(x)\frac{\partial c(x,t)}{\partial x} = \frac{\partial}{\partial x}\left(D(x)\frac{\partial c(x,t)}{\partial x}\right) - K(x)c(x,t) + S(x,t) \qquad (1)$$

in which $c(x, t)$ is the solute concentration, $D(x)$ is the diffusion coefficient, $K(x)$ is the first-order decay coefficient, $u(x)$ is the fluid velocity, $S(x, t)$ is the sink/source term, x is the spatial coordinate ($0 \le x \le l$), t is the time ($t > 0$), and l is the length of the computational domain.

It will be shown that this equation is, with certain restrictions, mathematically equivalent to the conservative form of the advection-diffusion equation.

Consider the advection-diffusion equation written in conservative form

$$\frac{\partial c(x,t)}{\partial t} + \frac{\partial (c(x,t)u(x))}{\partial x} - \frac{\partial}{\partial x}\left(D(x)\frac{\partial c(x,t)}{\partial x}\right) = 0 \qquad (2)$$

where the sink/source and reaction terms have been neglected.

An analytical solution to (2) will be given for the case when the velocity, $u(x)$, is taken to be a linear function of distance, such that $u(x) = u_0 x$, and the diffusion coefficient a quadratic function of distance, $D(x) = D_0 x^2$, where D_0 and u_0 are constants and $1 \le x \le l$. Equation (2) now becomes

$$\frac{\partial c(x,t)}{\partial t} + u_0\frac{\partial (c(x,t)x)}{\partial x} - D_0\frac{\partial}{\partial x}\left(x^2\frac{\partial c(x,t)}{\partial x}\right) = 0$$

Expanding,

$$\frac{\partial c(x,t)}{\partial t} + (u_0 x - 2D_0 x)\frac{\partial c(x,t)}{\partial x} = D_0 x^2\frac{\partial^2 c(x,t)}{\partial x^2} - u_0 c(x,t) \qquad (3)$$

The last term in this equation is essential for the conservation of mass. The additional term, $2Dx_0$, in the advection term only affects the distribution of the mass.

Comparing (3) with (1) reveals that the form of (1) is sufficiently general, as it accommodates different coefficients (with differing physical interpretation) of (3). It follows from the derivation of (3) that any expression can be used for $u(x)$ and $D(x)$ provided that the concentration profile is smooth and differentiable. It is possible therefore to ensure that (1) conserves mass if in (1)

$$K(x) = \frac{\partial u}{\partial x} + K_p(x)$$

where $K_p(x)$ is the first-order decay coefficient of the physical process being modeled.

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If, in (1), the reaction and sink/source terms were neglected, a naive modeler might use

$$\frac{\partial c(x, t)}{\partial t} + (u_0 x - 2D_0 x) \frac{\partial c(x, t)}{\partial x} = D_0 x^2 \frac{\partial^2 c(x, t)}{\partial x^2} \tag{4}$$

The major difference between this equation and (3) is the omission of the last term in (3), which is necessary for the conservation of mass. This is a nonconservative form of the advection-diffusion equation, and care must be exercised in implementing the algorithm proposed by Li et al. so that conservation of mass is not violated.

Analytical Solution to a Spatially Variable Advection-Diffusion Equation

An analytical solution to (3) can be obtained using Laplace transforms. This is achieved with the change of variables, $y = \ln(x)$ (see, for example, *Hildebrand* [1962, p. 13]). Equation (3) becomes

$$\frac{\partial c(x, t)}{\partial t} + (u_0 - D_0) \frac{\partial c(x, t)}{\partial y} = D_0 \frac{\partial^2 c(x, t)}{\partial y^2} - u_0 c(x, t) \tag{5}$$

which is in the form of an advection-diffusion equation with constant coefficients and a first-order reaction term. Consider a problem with the following initial and boundary conditions: $c(x, 0) = 0$, $c(1, t) = c_0$ and $c(\infty, t) = 0$, which is similar to the problem used by Li et al. The Laplace transform of (5) is

$$(s + u_0)\bar{c}(y, s) + (u_0 - D_0) \frac{d\bar{c}(y, s)}{dy} = D_0 \frac{d^2\bar{c}(y, s)}{dy^2}$$

in which $\bar{c}(y, s)$ is the Laplace transform of the solute concentration in the Laplace space s. Solving for $\bar{c}(y, s)$,

$$\bar{c}(y, s) = \frac{c_0}{s} \exp\left(\frac{(u_0 - D_0)y}{2D_0} - \frac{y}{D_0^{1/2}}\left[\frac{(u_0 - D_0)^2}{4D_0} + s + u_0\right]^{1/2}\right) \tag{6}$$

Performing the inverse Laplace transform, (3) then has the following analytical solution

$$c(x, t) = \frac{c_0}{2}\left(\frac{1}{x} \operatorname{erfc}\left[\frac{\ln(x) - t(u_0 + D_0)}{2(D_0 t)^{1/2}}\right] + \exp\left(\frac{u_0 \ln(x)}{D_0}\right) \operatorname{erfc}\left[\frac{\ln(x) + t(u_0 + D_0)}{2(D_0 t)^{1/2}}\right]\right) \tag{7}$$

in which erfc is the complementary error function.

Hypothetical Example

Consider an example where $u_0 = 1.0$, $D_0 = 0.005$, $1 \le x \le l = 20$, and $c_0 = 100$, which corresponds to a range of Peclet numbers between $Pe = 40$ and 2, where $Pe = u_0 \Delta x / D_0$ and $\Delta x = 0.2$. The exact concentration profile, given by (7) at $t = 2.5$ for this problem, is illustrated in Figure 1.

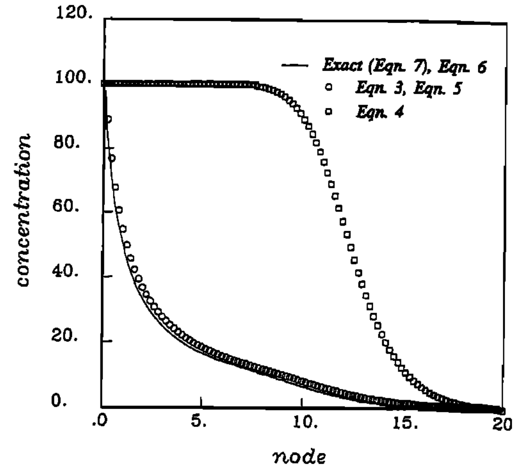

Figure 1. Concentration profile for the spatially variable advection-diffusion coefficient.

Also illustrated in Figure 1 are the simulated profiles using (3), (4), (5), and (6). The finite analytic/Laplace time method proposed by Li et al. was used to solve (3) and (4). In contrast to Li et al., who used the well-known *Crump* [1976] algorithm, the more robust numerical Laplace inversion developed by *de Hoog et al.* [1982] was used.

The results for the numerical inversion of (6) are indistinguishable from the exact results, which indicate that the concentration profile decays exponentially. The results obtained for the solution of (3) using the finite analytic/Laplace time scheme are more accurate than the results obtained using the well-known third-order *Holly and Preissmann* [1977] scheme, which is a time-stepping scheme. To satisfy the Courant criterion, 500 time steps were required for the solution of (5). This scheme required approximately 10 times the computational time required by the finite analytic/Laplace time scheme for the solution of (3).

Conclusions

The solution of the nonconservative form of the advection-diffusion equation, equation (4), produced erroneous results. Mass is not conserved, and the predicted profile bears no resemblance to the analytical solution.

The solution method proposed by Li et al. does not provide any significant advantages over existing methods for the solution of the advection-diffusion equation with constant coefficients. However, for problems involving spatially variable coefficients, it has significant advantages over conventional time-stepping schemes provided care is exercised to ensure conservation of mass.

The analytical solution presented can be used to validate numerical schemes for solving the advection-diffusion equation with variable coefficients. The analytical solution can be readily extended to multidimensional problems.

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J. H. Knight (corresponding author), CSIRO Centre for Environmental Mechanics, GPO Box 821, Canberra, ACT 2601, Australia. (email: knight@enmech.csiro.au)

C. Zoppou, ACT Electricity and Water, GPO Box 366, Canberra, ACT 2601, Australia.

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