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A Space-Time Accurate Method for Solving Solute Transport Problems

SHU-GUANG LI, FENG RUAN, AND DENNIS MCLAUGHLIN

Ralph M. Parsons Laboratory, Department of Civil Engineering, Massachusetts Institute of Technology, Cambridge

Solute transport studies frequently rely on numerical solutions of the classical advection-diffusion equation. Unfortunately, solutions obtained with traditional finite difference and finite element techniques typically exhibit spurious damping or oscillation when advection dominates. Recently developed variants of these techniques such as the finite analytic method (Chen and Li, 1979; Chen and Chen, 1984) and the optimal test function method (Celia et al., 1989a, b, c) perform well for steady state problems. Extensions of these methods to the transient case have, however, not been successful, primarily because of inadequate approximations of the temporal derivative. The new numerical method proposed in this paper avoids this difficulty by taking the Laplace transform of the transient equation. The transformed expression behaves like a steady state advection-diffusion equation with a first-order decay term. This expression can be solved with either the finite analytic or optimal test function method and the time dependence recovered with an efficient inverse Laplace transform algorithm. The result is an accurate and robust transient solution which performs well over a very wide range of Peclet numbers. We demonstrate this approach by applying the finite analytic method to a Laplace transformed one-dimensional model problem. A comparison with other competing techniques shows that good approximations are required in both space and time in order to obtain accurate solutions to advection-dominated problems. A good space approximation combined with a poor temporal approximation (or vice versa) does not give satisfactory results. The method we propose provides a balanced space-time approximation which works very well for one-dimensional problems. Extensions to multiple dimensions are conceptually straightforward and briefly discussed.

INTRODUCTION

Most studies of solute transport through the natural environment rely on some version of the classical advection-diffusion equation, which we write here in its one-dimensional form as

$$\frac{\partial c}{\partial t} + u(x)\frac{\partial c}{\partial x} = \frac{\partial}{\partial x} D(x)\frac{\partial c}{\partial x} - K(x)c + s(x, t), \quad (1)$$

with the following initial and boundary conditions

$$c(x, 0) = f(x);\ c(0, t) = g_0(t);\ c(l, t) = g_l(t), \quad (2)$$

where c is the dependent variable (e.g., solute concentration); x is the spatial coordinate ($0 \le x \le l$); t is time ($t > 0$); u is a steady state velocity; K is a first-order decay coefficient; $s(x, t)$ is a source-sink term; $f(x)$, $g_0(t)$ and $g_l(t)$ are, respectively, initial and boundary functions; and l is the length of the solution domain.

Although analytical solutions of this equation are available for certain special cases, many problems of practical interest (e.g., transport through a heterogeneous velocity field) must be solved numerically. Numerical solutions of the advection-diffusion equation can be surprisingly difficult, even though it is linear and has a simple mathematical form. Solutions based on conventional finite difference or finite element discretizations are, for example, almost always plagued with either spurious oscillations or excessive numerical diffusion when the advective term becomes dominant. Most traditional solution algorithms are forced to make compromises between these two types of undesirable behavior.

The structure of the advection-diffusion equation suggests the use of "operator splitting" techniques which treat the advective (hyperbolic) and diffusive (parabolic) terms differently. This approach leads to numerical algorithms which combine Eulerian and Lagrangian solution methods [*Gray and Pinder*, 1976; *Holly and Preissmann*, 1977; *Neuman*, 1981; *Neuman and Sorek*, 1982; *Baptisa et al.*, 1984; *Cheng et al.*, 1984; *Wheeler and Dawson*, 1988; *Chiang et al.*, 1989; *Yeh*, 1990; *Celia et al.*, 1990; *Yang and Hsu*, 1991; *Li and Venkataraman*, 1991]. When the advective portion of the equation is solved with an Lagrangian (or characteristic-based) method Courant and grid Peclet number stability requirements can be significantly relaxed. The performance of such method is, however, critically dependent on the accuracy of the backward trajectory-tracking and concentration interpolation [*Holly and Preissmann*, 1977; *Li and Venkataraman*, 1991]. Linear interpolation [*Neuman*, 1981; *Neuman and Sorek*, 1982; *Douglas and Russell*, 1982; *Wheeler and Dawson*, 1988; *Chiang et al.*, 1989] can lead to excessive numerical diffusion [*Roache*, 1972; *Huffenus and Khaletzky*, 1981]. Quadratic interpolation [*Douglas and Russell*, 1982; *Baptisa et al.*, 1984] reduces numerical damping somewhat but can introduce spurious oscillations [*Roache*, 1972; *Huffenus and Khaletzky*, 1981]. Higher-order interpolation techniques based on more interpolating nodes [*Martin*, 1975] can reduce numerical diffusion further but may introduce even more severe oscillations [*Holly and Preissmann*, 1977]. *Holly and Preissmann* [1977] proposed a Hermite interpolation technique (also see *Fischer* [1977]) which achieves good accuracy at the expense of increased computational effort, particularly for multidimensional problems [*Huffenus and Khaletzky*, 1981]. Although the operator splitting concept clearly has considerable potential it also has limitations which must be recognized when it is applied to practical problems.

Eulerian solution techniques offer an attractive alternative to Eulerian-Lagrangian methods since they are conceptually simple and easy to implement. In recent years a number of investigators have suggested a series of innovative Eulerian

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numerical algorithms which are based on local analytical solutions of the advection-diffusion equation. Some examples include work by *Spalding* [1972], *Raithby and Torrance* [1974], *Christie et al.* [1976], *Hemker* [1977], *Hughes* [1978], *Chen and Li* [1979], *Hughes and Brooks* [1979], *Wong and Raithby* [1979], *Stubley et al.* [1980], *Chen et al.* [1981], *Hughes and Tezduyar* [1984], *Chen and Chen* [1984], *Barrett and Morton* [1984], *Carey* [1985], *Demkowitcz and Oden* [1986], *Celia and Herrera* [1987], and *Celia et al.* [1989*b*, *c*]. Two analytically based algorithms are of particular interest here: (1) the finite analytic method of Chen [*Chen and Li*, 1979; *Chen et al.*, 1981; *Chen and Chen*, 1984] and (2) the optimal test function method [*Celia et al.*, 1989*a*, *b*, *c*]. Both of these techniques were initially developed for steady state problems and both give exact solutions to the steady state version of (1) when the equation coefficients are constant.

Extensions of the finite analytic and optimal test function techniques to transient problems have typically approximated the time derivative with a finite difference approximation [*Chen and Chen*, 1984; *Hwang et al.*, 1985; *Celia et al.*, 1989*b*, *c*; *Kindred and Celia*, 1989; *Elnawawy et al.*, 1990]. This has the effect of reducing the original transient problem to a series of "steady state" problems defined at successive time steps. Unfortunately, the resulting numerical solutions do not behave optimally. In fact, techniques which combine "optimal" spatial discretization with traditional temporal discretization suffer from the same problems as most other numerical methods when advection dominates. The close interaction between space and time dependence in the advection-diffusion equation requires that both the temporal and spatial derivatives be accurately approximated in order to obtain a satisfactory solution [*Gresho and Lee*, 1981; *Li*, 1988; *Celia et al.*, 1989*b*, *c*; *Celia et al.*, 1990].

This paper proposes a Eulerian numerical technique for solving the transient advection-diffusion equation which is accurate in both space and time. The technique we propose does not explicitly discretize either the space or the time derivatives which appear in the governing equation. Instead, the time derivative is eliminated by taking the Laplace transform of the original equation and the resulting steady state expression is solved with an analytical-based spatial technique such as the finite analytic method or the optimal test function method. The solution in the physical space-time domain is ultimately recovered by using an efficient numerical Laplace inversion algorithm such as the one described by *Crump* [1976] (see *Davies and Martin* [1979] for a review).

Laplace transform methods have been used before in numerical algorithms for solving time-dependent partial differential equations. For example, early finite element theories often eliminated time derivatives with Laplace transformations. This made it possible to identify variational descriptions for the transformed steady state problems [*Gurtin*, 1965; *Javandel and Witherspoon*, 1968]. *Liggett and Liu* [1983] combined a Laplace transform algorithm with the boundary element method to solve the unsteady groundwater flow equation and *Cheng and Liggett* [1984] used a similar approach to solve a soil consolidation problem. Recently, a hybrid Laplace transform/finite element method has been applied to groundwater flow problems by *Moridis and Reddell* [1991] and to solute transport problems by *Yu et al.* [1987] and *Sudicky* [1989]. It is the combination of the Laplace transformation with an analytically based spatial technique that makes our method unique.

The next section of this paper explores in more detail the temporal approximations commonly used to obtain numerical solutions of the advection-diffusion equation. This is followed by a description of our method. We also present a one-dimensional example which provides an instructive comparison with other numerical techniques for solving advection-diffusion equation. We conclude with a discussion of multidimensional extensions and a brief summary of the most important features of our technique.

MORE ON TEMPORAL APPROXIMATIONS

It is well known that numerical solutions of the transient advection diffusion equation are complicated by the first-order spatial derivatives that describe the advective flux. When these derivatives are large it is difficult to obtain an accurate nonoscillatory solution. The emphasis placed on the advective terms in discussions of numerical performance tends to leave one with the wrong impression that the time derivative is straightforward and can be handled with simple methods, such as a traditional finite difference approximation [*Chen*, 1982]. This is, unfortunately, not the case. In fact, the time derivative interacts very closely with the spatial terms and it becomes increasingly important and difficult to approximate as the first-order spatial derivatives become significant.

The difficulties encountered when approximating the time derivative of an advection-dominated transport equation can be clearly seen from the following heuristic analysis [*Li and Venkataraman*, 1991]. Consider the transport by pure advection of a Gaussian hill with an initial standard deviation of σ_x in a uniform flow of constant velocity u_0. The standard deviation σ_x characterizes the spatial variation of the concentration distribution. It is independent of the constant velocity u_0 and remains invariant over time. The temporal concentration profile at a particular location is also Gaussian. The standard deviation of this temporal profile is, however, inversely proportional to the advective velocity u_0:

$$\sigma_t = \frac{\sigma_x}{u_0}, \tag{3}$$

If the computational domain is discretized in space and time, this expression can be rewritten in terms of the Courant number as

$$\frac{\sigma_t}{\Delta t} = \frac{1}{C_r}\frac{\sigma_x}{\Delta x}, \tag{4}$$

where the space and time discretization intervals are Δx and Δt, respectively, and $C_r = u_0 \Delta t/\Delta x$ is the Courant number.

Equation (4) implies that the relative concentration variability in time, as characterized by $\sigma_t/\Delta t$, is affected by the magnitude of the advective term, as characterized by the Courant number. At low values of the Courant number ($Cr \ll 1$), σ_t is large relative to the time interval so the concentration does not vary much over a single time step. In this case temporal interpolation and time differencing provide good approximations. When the Courant number increases, these approximations break down since $\sigma_t/\Delta t$ de-

creases and the concentration varies more over each single time step. When $C_r \gg 1$, the temporal distribution of concentration becomes practically discontinuous since σ_t approaches zero and the temporal concentration profile approaches a Dirac delta function. In this case, temporal interpolation and time differencing do not provide adequate approximations. This simple analysis clearly shows the difficulties in approximating the time derivative as advection becomes increasingly strong. It also explains why time-dependent extensions of optimal spatial techniques fail when the Courant number is large, even though they perform very well in steady state applications [*Chen*, 1982; *Chen and Chen*, 1984; *Yang*, 1990; *Celia et al.*, 1989*b*, *c*].

A Space-Time Accurate Method

In this section, we describe a new method for solving the transient convective diffusion equation. As mentioned earlier, this method uses the Laplace transform to convert the transient advection-diffusion equation to a steady state expression which can then be solved with an analytical-based spatial technique such as the finite analytic or optimal test function methods. We illustrate the basic idea with a simple one-dimensional transient solute transport problem. In this special case our method is able to reproduce analytical solutions over a very wide range of conditions. The extension to multidimensional problems is conceptually straightforward, although additional approximations must generally be introduced in order to obtain the analytical solutions used in the spatial discretization portion of the algorithm (the multidimensional case is discussed in more detail near the end of the paper). We begin our discussion with a brief review of the Laplace transform and then show how the Laplace transformed advection-diffusion equation can be solved with the finite analytic technique. Finally, we describe the inverse Laplace transformation needed to obtain a solution which depends explicitly on time.

Laplace Transform

The Laplace transform of a generic real-valued function $h(t)$ with $h(t) = 0$ for $t < 0$ is defined as

$$\bar{h}(p) = \int_0^\infty e^{-pt} h(t)\, dt, \tag{5}$$

where $p = \nu + i\omega$ is the complex-valued Laplace transform variable; $h(t)$ is assumed to be at least piecewise continuous and of exponential order λ (i.e., $|h(t)| \leq Me^{\lambda t}$, M being some arbitrary but finite constant), in which case the transform function $\bar{h}(p)$ is well defined for $\nu > \lambda$.

The Laplace transformation provides a convenient tool to solve linear time-dependent differential equations. This transformation is especially useful for solving the transient advection-dominated transport equation since it helps us avoid direct approximation of the time derivative. Taking the Laplace transform on both sides of (1) as well as its boundary conditions, we obtain

$$p\bar{c} + u(x)\frac{\partial \bar{c}}{\partial x} = \frac{\partial}{\partial x} D(x)\frac{\partial \bar{c}}{\partial x} - K(x)\bar{c} + \bar{s}(x, p) + f(x), \tag{6}$$

and the transformed boundary conditions:

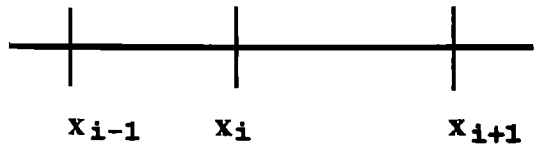

Fig. 1. Local computational element associated with node i.

$$\bar{c}(0, p) = \bar{g}_0(p);\ \bar{c}(l, p) = \bar{g}_l(p), \tag{7}$$

where the accent indicates the complex-valued Laplace transform. Note that the time derivative has been analytically removed and the transient transport equation becomes a complex-valued "steady state" advection-diffusion equation, with the initial condition appearing as a nonhomogeneous source term. This steady state transformed equation can then be solved by one of the analytically based spatial methods.

Optimal Finite Difference Approximation for the Transformed Equation

In order to illustrate our space-time accurate method, we solve the Laplace transformed advection-diffusion equation given in (6) with the finite analytic method described by Chen et al. [*Chen and Li*, 1979; *Chen et al.*, 1981; *Chen and Chen*, 1984]. The finite analytic method decomposes the solution domain into a number of small elements in which local analytic solutions can be obtained due to simple geometry and approximately constant coefficients. When the local analytic solution is evaluated at an interior node, it gives an algebraic equation or, equivalently, a finite difference scheme relating the interior nodal value to the values at the two neighboring nodes.

In order to illustrate the finite analytic algorithm, we discretize the spatial domain $0 \leq x \leq l$ into N subdivisions: $0 = x_0 < x_1, \cdots, x_{i-1} < x_i < x_{i+1}, \cdots, x_{N-1} < x_N = l$. We define the local element associated with x_i to be the interval $x_{i-1} < x < x_{i+1}$ which spans the three successive computational nodes located at x_{i-1}, x_i, and x_{i+1} (see Figure 1). If the discretized grid is sufficiently fine the various coefficients and source terms in (6) can be approximated as locally constant so

$$u(x) \approx u_i;\ f(x) \approx f_i;\ D(x) \approx D_i;\ \bar{s}(x, p) \approx \bar{s}_i;\ K(x) \approx K_i, \tag{8}$$

where u_i, f_i, D_i, $\bar{s}_i$, and K_i are evaluated at $x = x_i$. When the original coefficients vary over space the discrete values at x_i are assigned to the entire local element so that the Laplace-transformed advection-diffusion equation becomes a locally constant coefficient differential equation. In this case the following analytic solution is easily obtained over the local element:

$$\bar{c}(x, p) = A_1 \exp\left[r_1(x - x_i)/\Delta x_i\right] + A_2 \exp\left[r_2(x - x_i)/\Delta x_i\right] + \frac{\bar{s}_i + f_i}{K_i + p}, \tag{9}$$

where $x_{i-1} \leq x \leq x_{i+1}$, $\Delta x_i = x_i - x_{i-1}$, and r_1 and r_2 are given by

$$r_1 = \frac{Pe_i}{2}\left[1 + \sqrt{1 + \frac{4D_i}{u_i^2}(K_i + p)}\right], \quad (10)$$

$$r_2 = \frac{Pe_i}{2}\left[1 - \sqrt{1 + \frac{4D_i}{u_i^2}(K_i + p)}\right], \quad (11)$$

Here Pe_i is the local Peclet number in element i defined as $u_i\Delta x_i/D_i$ and A_1 and A_2 are two integration constants which can be determined from the following boundary conditions at x_{i-1} and x_{i+1}:

$$\bar{c}(x, p)|_{x=x_{i-1}} = \bar{c}_{i-1}, \quad (12)$$

$$\bar{c}(x, p)|_{x=x_{i+1}} = \bar{c}_{i+1}. \quad (13)$$

Substituting (12) and (13) into (9) and solving for A_1 and A_2 gives

$$A_1 = \frac{e^{r_2\rho_i}\bar{c}_{i-1} - e^{-r_2}\bar{c}_{i+1}}{e^{r_2\rho_i - r_1} - e^{r_1\rho_i - r_2}} - \frac{e^{r_2\rho_i} - e^{-r_2}}{e^{r_2\rho_i - r_1} - e^{r_1\rho_i - r_2}}\frac{\bar{s}_i + f_i}{K_i + p}, \quad (14)$$

$$A_2 = \frac{-e^{r_1\rho_i}\bar{c}_{i-1} + e^{-r_1}\bar{c}_{i+1}}{e^{r_2\rho_i - r_1} - e^{r_1\rho_i - r_2}} + \frac{e^{r_1\rho_i} - e^{-r_1}}{e^{r_2\rho_i - r_1} - e^{r_1\rho_i - r_2}}\frac{\bar{s}_i + f_i}{K_i + p}. \quad (15)$$

Equations (9) through (15) clearly reveal that the concentration $\bar{c}(x, p)$ at any interior point x in the local element is linearly related to the concentrations $\bar{c}(x_{i-1}, p)$ and $\bar{c}(x_{i+1}, p)$ at the two end nodes. In particular, the concentration at the interior node located at x_i can be written in the form of a finite difference algorithm with coefficients that depend on the Laplace variable p:

$$\bar{c}_i = \alpha_i\bar{c}_{i-1} + \beta_i\bar{c}_{i+1} + \gamma_i \quad (16)$$

where $i = 1, 2, \cdots, N-1$, and the coefficients α_i, β_i, and γ_i are given by

$$\alpha_i = \frac{e^{r_2\rho_i} - e^{r_1\rho_i}}{e^{r_2\rho_i - r_1} - e^{r_1\rho_i - r_2}}, \quad (17)$$

$$\beta_i = \frac{e^{-r_1} - e^{-r_2}}{e^{r_2\rho_i - r_1} - e^{r_1\rho_i - r_2}}, \quad (18)$$

$$\gamma_i = 1 + \frac{e^{r_1\rho_i} - e^{r_2\rho_i} - e^{-r_1} + e^{-r_2}}{e^{r_2\rho_i - r_1} - e^{r_1\rho_i - r_2}}\left(\frac{\bar{s}_i + f_i}{K_i + p}\right), \quad (19)$$

where $\rho_i = \Delta x_{i+1}/\Delta x_i$.

Equation (16) defines the desired finite analytic algorithm for solving the Laplace transformed equation given in (6). This algorithm accurately captures the close interactions between advection, diffusion, and reaction which characterize solute transport problems. In particular, it provides gradually varying upwinding as the magnitude of the advection term changes. Spurious oscillations and numerical damping are eliminated in the transformed solution for arbitrarily large Peclet numbers. When the coefficients of (1) are constant and the initial condition $f(x)$ is a simple elementary function, the finite analytic solution to the transformed equation is exact. The finite analytic algorithm remains accurate when the spatial grid spacing becomes nonuniform, so long as the grid captures significant spatial variations in the equation coefficients. Moreover, the solution is analytically differentiable to any desired order without loss of accuracy. These properties represent important improvements over conventional finite difference approaches.

Numerical Inversion of Laplace Transform

In order to obtain the concentration as a function of location and time (rather than of location and the Laplace frequency), we have to invert our solution to (6). The inverse Laplace transform $c(x, t)$ is given by the following well-known inversion formula:

$$c(x, t) = \frac{1}{2\pi j}\int_{\nu - j\infty}^{\nu + j\infty} e^{pt}\bar{c}(x, p)\, dp, \quad (20)$$

or, alternatively,

$$c(x, t) = \frac{e^{\nu t}}{\pi}\int_0^\infty \{\mathrm{Re}\,[\bar{c}(x, p)]\cos\omega t - \mathrm{Im}\,[\bar{c}(x, p)]\sin\omega t\}\, d\omega, \quad (21)$$

where Re and Im denote respectively the real and imaginary parts of their arguments and j is the pure imaginary number, $j = (-1)^{1/2}$. If we discretize (21) using a trapizoidal rule with a step size of π/T, we obtain the following approximation

$$c(x, t) \approx \frac{e^{\nu t}}{T}\left\{-\frac{1}{2}\mathrm{Re}\,[\bar{c}(x, \nu)] + \sum_{m=0}^{N_p}\mathrm{Re}\left[\bar{c}\left(x, \nu + i\frac{m\pi}{T}\right)\right]\cos\frac{m\pi}{T}t - \sum_{m=0}^{N_p}\mathrm{Im}\left[\bar{c}\left(x, \nu + i\frac{m\pi}{T}\right)\right]\sin\frac{m\pi}{T}t\right\}. \quad (22)$$

Equation (22) is the basis of many existing Laplace transform inversion algorithms. Note that the infinite series have been truncated to N_p terms. The summation kernels in these truncated series may be highly oscillatory. One common problem associated with the direct evaluation of (22) lies in the extremely slow convergence of the series expression, with adverse implications for both accuracy and computation time. The value of N_p required for a typical problem is often of the order of 10^3.

Numerous algorithms have been developed in an effort to accelerate the convergence of (22). A comprehensive review on numerical inversion of the Laplace transform based on different accelerating techniques is presented by *Davies and Martin* [1979], who compare fourteen different methods with regard to numerical accuracy, computational efficiency, and ease of implementation. Following *Sudicky* [1989], we use the Crump algorithm to perform the Laplace transform inversion. *Crump* [1976] used the epsilon technique of *Wynn* [1956] to accelerate the convergence of the series summations with excellent results for a wide range of functions. The value of N_p needed for adequate accuracy is dramatically

TABLE 1. Numerical Methods Based on Different Space-Time Approximations

Spatial Approximations	Temporal Approximations	
	Laplace Transform	Fully Implicit
Finite-analytic	finite-analytic/Laplace	central difference/implicit
Central difference	central difference/Laplace	central difference/implicit
Upwinding difference		upwinding difference/implicit

reduced to approximately 15 to 40 for most problems. The Crump algorithm also performs reasonably well for discontinuous functions. Implementation details of the Crump algorithm for transient solute transport simulations can be found in the work by *Sudicky* [1989].

RESULTS AND DISCUSSION

In this section, we use a standard one-dimensional model problem to demonstrate the performance of our space-time accurate method. In this problem we simulate the propagation of a sharp solute concentration front along a line. We assume uniform flow and a conservative solute free of external or internal sources. The initial concentration distribution is a step function with a spatial discontinuity at $x = 0$:

$$c(x, 0) = c_0 \qquad x \le 0 \tag{23a}$$

$$c(x, 0) = 0 \qquad x > 0 \tag{23b}$$

The steep concentration front emanating from this initial condition travels with an asymptotically uniform velocity u_0 and becomes gradually smoother due to diffusion as it moves downstream. The following exact analytical solution is available for this problem:

$$c(x, 0) = \frac{c_0}{2}\left[\operatorname{erfc}\left(\frac{x - u_0 t}{\sqrt{4Dt}}\right) + e^{u_0 x/D}\operatorname{erfc}\left(\frac{x + u_0 t}{\sqrt{4Dt}}\right)\right], \tag{24}$$

where $erfc(\cdot)$ is the complementary error function. This simple model problem provides a stringent performance test on numerical methods for solving the advection diffusion equation, especially in testing their ability to properly track a sharp front.

It is instructive to compare our method to four other numerical techniques which take different approaches to either the temporal or spatial portions of the model problem. Table 1 lists all the techniques considered. Input parameters for the various cases examined are summarized in Table 2 and the simulation results are displayed in Figures 2 through 4. Figure 2 shows the calculated spatial concentration distributions at time $t = 150$ days for four different Peclet numbers ranging from 5 to 500. Our finite analytic/Laplace method clearly stands out in performance. In fact, its filled circles fall on top of the exact curves in every case. Spurious oscillations and artificial damping in the numerical solutions are entirely eliminated.

If a simple time marching scheme such as the fully implicit finite difference technique is used in conjunction with an accurate finite analytic approximation in space, one obtains the finite analytic/implicit method proposed by *Chen* [1982] and *Chen and Chen* [1984]. Figures 1 and 2 clearly show that the performance of the this method degrades significantly at large Peclet numbers. The transient solutions suffer from serious numerical diffusion much like that exhibited by a simple upwinding solution, even though a sophisticated finite analytic approximation is used in space. In fact, the finite analytic/implicit solutions become graphically indistinguishable from the upwinding solutions as the Peclet number becomes increasingly large. This confirms our earlier observation on the importance of an accurate temporal derivative approximation when advection is strong.

On the other hand, if we achieve temporal accuracy by using the Laplace transformation in time but adopt a conventional central difference approximation in space, we get the finite difference counterpart to the finite element/Laplace transform method of *Sudicky* [1989]. For a small Peclet number of 5 a fairly good match is observed between the exact solutions and the two central difference-based solutions. However, these central difference-based methods soon break down and result in oscillatory solutions for the case of Peclet numbers of 20, 50, and 500, with the spatial extent and amplitude of oscillations increasing as the Peclet number increases. Note that the central difference/implicit method exhibits some numerical diffusion so its associated oscillations are less severe than obtained with the central difference/Laplace transform method. This reflects the dissipative nature of the fully implicit temporal discretization scheme.

Peclet number is not the only factor dictating the perfor-

TABLE 2. Input Parameters for the Model Numerical Example

Parameters	Figure 2				Figure 3		Figure 4	
	Case *a*	Case *b*	Case *c*	Case *d*	Case *a*	Case *b*	Case *a*	Case *b*
Velocity u_0 (m/d)	1	1	1	1	1	1	1	1
Diffusion coefficient D (m^2/d)	1	0.25	0.1	0.01	0.1	1.5	1.0	0.05
Grid spacing Δx (m)	5	5	5	5	1	15	5	5
Peclet number P_e	5	20	50	500	10	10	5	100
Time step Δt (day)	1	1	1	1	1	1	1	1

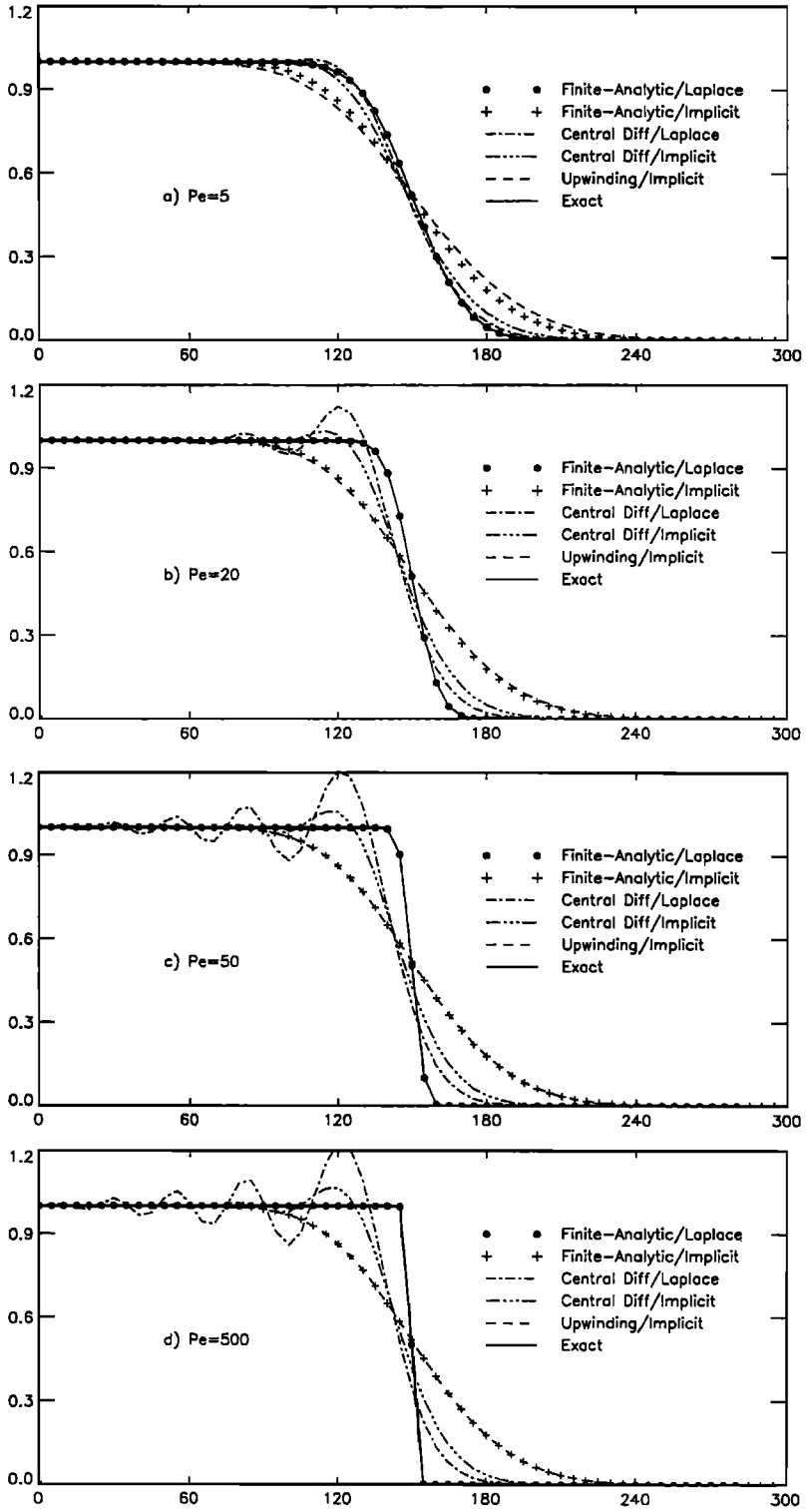

Fig. 2. Spatial concentration distributions at t = 150 days for different Peclet numbers; horizontal and vertical axes are respectively normalized concentration and time in days.

mance of advection-diffusion numerical solution techniques. We can alter the grid spacing while keeping P_e constant by adjusting either the diffusion coefficient or the velocity. Figure 3 shows the effect of grid spacing on the computed spatial concentration distributions. Two different Δx values of 5 and 15 m representing a fine and coarse grid are used while keeping $Pe = 5$. The solutions obtained from our finite analytic/Laplace method are again in excellent agreement with the exact solutions for both fine and coarse grids. However, the central difference/Laplace transform solution is accurate only in the case of a fine grid. In this case it is almost indistinguishable from the true solution except for a slight oscillatory bump at the beginning of the sharp front. The performance of the central difference/Laplace transform

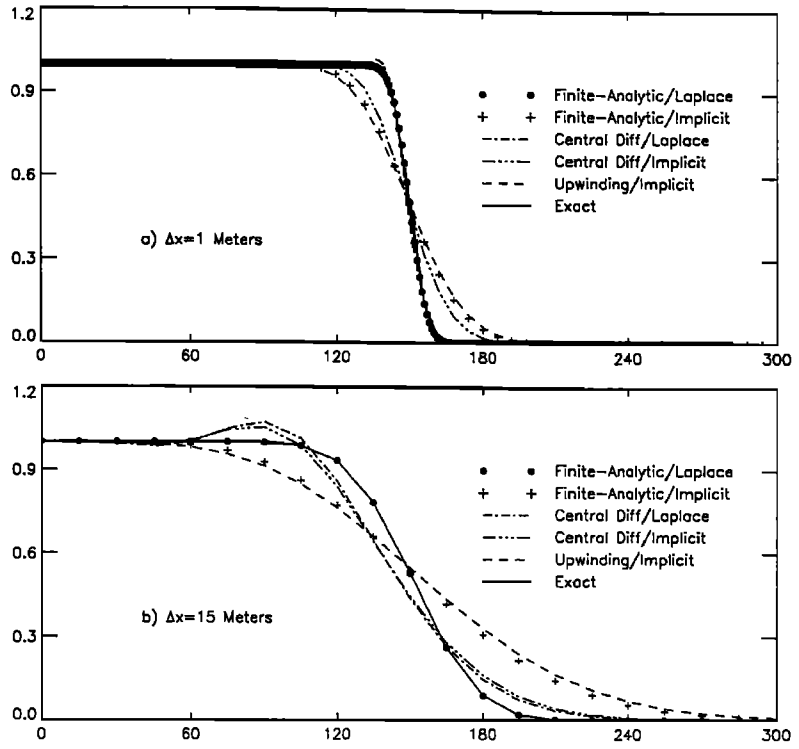

Fig. 3. Spatial concentration distributions at $t = 150$ days for different grid spacing; horizontal and vertical axes are respectively normalized concentration and time in days.

method soon deteriorates as the grid spacing increases, leading to both numerical oscillation and diffusion in the case of a very coarse grid even though the Peclet number is still fairly small and kept unchanged. The finite analytic/implicit method seems less sensitive to grid spacing because of its accurate spatial approximation, but its numerical solutions are consistently highly damped due to the crude temporal approximation. They are only marginally better than simple upwinding solutions, especially for the case of a coarse grid.

The above performance comparisons are based only on snapshots of the spatial concentration distributions at a fixed time. Figure 4 illustrates temporal behavior by plotting concentration solutions obtained between $t = 0$ to $t = 600$ days for two different Peclet numbers ($P_e = 5$ and 100) at a fixed location of $x = 250$ m. The finite analytic/Laplace method is very robust and consistently accurate for all times and for both small and large Peclet numbers. In particular, the sharp temporal front is accurately captured. The other methods, though reasonably good for the low Peclet number case, produce either spurious oscillations or excessive artificial damping for the case of high Peclet number.

This numerical example clearly demonstrates the close interaction between the spatial and temporal derivatives in the advection-diffusion equation. Inappropriate derivative approximation either in space or time can degrade overall solution accuracy no matter how elaborate or accurate the other approximation might be. In effect, the chain is only as strong as its weakest link!

It should be noted that the finite analytic solution for the transformed advection diffusion equation of our model problem is exact and independent of grid spacing because the local approximations made in (8) are all exact when the velocity and the initial concentration are both constant. However, in a more general situation in which flow velocity is nonuniform and initial condition is nonconstant, grid spacing will be dictated by the scales of variability of the flow velocity and initial concentration distribution, as in any other numerical method. Although the grid spacing must be small enough to permit the velocity and initial concentration variations to be resolved, the Peclet number is no longer a constraint.

It should also be noted that numerical inversion of the Laplace transform generally becomes increasingly difficult or expensive as the temporal concentration gradient increases. Fortunately, the Crump inversion algorithm we use in this example seems to be able to handle steep gradients with a reasonably small number of transform space evaluations. It is important to minimize the number of evaluations N_p while retaining inversion accuracy since we have to solve the transformed convective diffusion equation for every discretized Laplace transform variable p_i, $i = 1, \cdots, N_p$. We have found a value of N_p between 10 and 40 to be adequate in our numerical simulations even though fairly steep gradients exist in most cases. Generally, N_p increases with decreasing diffusion coefficient, which corresponds to an increasing concentration gradient. When the diffusion coefficient is very small and the initial condition is discontinuous, an N_p value of 70 to 100 may be needed for an accurate inversion. Even so, N_p can still be much smaller than the number of time steps required in transport simulations based on standard time-marching schemes. Therefore we believe that our method is not only accurate but also computationally efficient, especially for long time simulations.

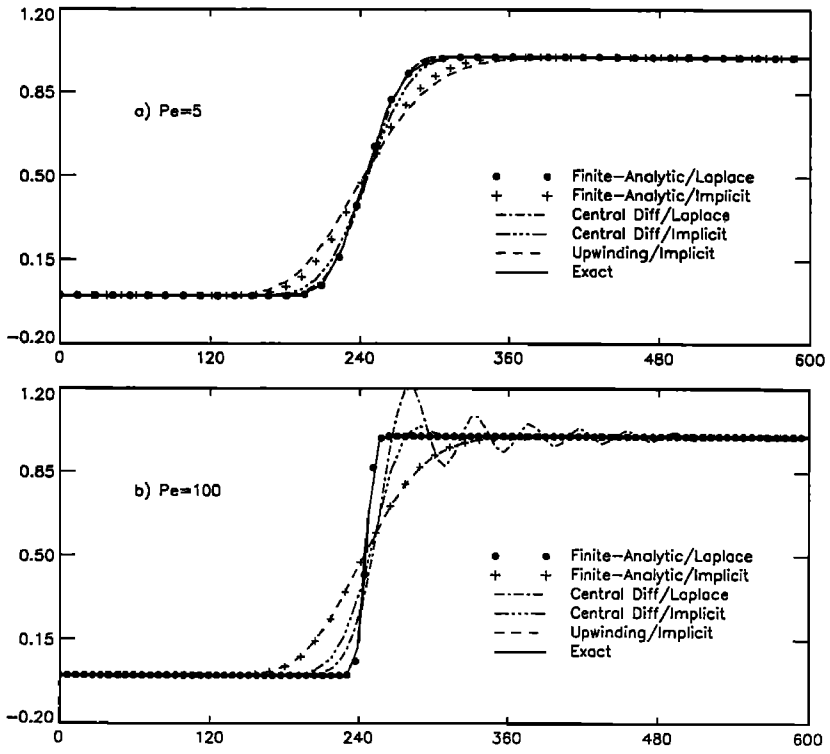

Fig. 4. Temporal concentration distributions at $x = 250$ m for different Peclet numbers; horizontal and vertical axes are respectively normalized concentration and time in days.

EXTENSION TO MULTIDIMENSIONS

The preceding sections describe how our finite analytic/Laplace transform method can be applied to a reasonably general one-dimensional transient advection-diffusion equation. The extension to multidimensional problems is conceptually straightforward since the general principle of consistently accurate space-time approximations always applies, regardless of the problem dimensionality. Therefore the key question is whether or not the optimal spatial method used to solve the Laplace-transformed equation can be extended to multiple dimensions. Both the finite analytic and the optimal test function methods have been extended to multidimensional flow and transport problems [*Chen et al.*, 1981; *Chen*, 1982; *Chen and Chen*, 1984; *Celia*, 1989*a*]. However, such extensions require additional assumptions in order to obtain either local analytical solutions or optimal test functions. So it is unlikely that our method will perform as well in multidimensional applications as it has in the simple one-dimensional example considered here. Nevertheless, we believe that our method represents a significant improvement over existing alternatives, primarily because its balance treatment of temporal and spatial approximations.

CONCLUSIONS

The following points highlight the major findings of this paper:

1. Accurate numerical solution of the transient advection-diffusion equation requires that both the space and time derivatives be carefully considered. An inability to properly approximate either of these derivatives can destroy the overall solution accuracy.

2. In transient applications the finite analytic/implicit technique behaves very much like a simple upwinding scheme, primarily because both approaches share the same crude temporal approximation. Both methods suffer from excessive numerical diffusion unless the Peclet number and Courant number are very small.

3. The central difference/Laplace transform technique performs much like a conventional central difference method, giving solutions which are accurate for small Peclet numbers but which are plagued with serious spurious oscillations for large Peclet numbers.

4. The finite analytic/Laplace method described in this paper is based on a consistently accurate space-time approximation which leads to transient numerical solutions free of spurious oscillations and numerical diffusion for all practical values of Peclet number and for a wide range of grid spacing.

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S.-G. Li, 48-208, Ralph M. Parsons Laboratory, Department of Civil Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139.

D. McLaughlin, 48-209, Ralph M. Parsons Laboratory, Department of Civil Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139.

F. Ruan, 48-420, Ralph M. Parsons Laboratory, Department of Civil Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139.

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