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Accuracy of Operator Splitting for Advection-Dispersion-Reaction Problems

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An operator-splitting approach is often used for the numerical solution of advection-dispersion-reaction problems. Operationally, this approach advances the solution over a single time step in two stages, one involving the solution of the nonreactive advection-dispersion equation and the other the solution of the reaction equations. The first stage is usually solved with a finite difference, finite element, or related technique, while the second stage is normally solved with an ordinary differential equation integrator. The only generally published guidelines on numerical accuracy suggest that the discretization errors associated with each stage must be small in order to achieve high accuracy of the overall solution. However, in this note we demonstrate that there is an inherent mass balance error present in the operator-splitting algorithm for problems involving continuous mass influx boundary conditions. The mass balance error does not exist for instantaneous mass input problems. These conclusions are based upon analysis of a simple first-order decay problem for which each stage of the calculation can be performed analytically (i.e., without discretization error). For this linear decay problem we find that the product of the first-order decay coefficient (k) times Δt must be less than approximately 0.1 in order for the mass balance error to be less than 5%. We also present a variant of the normal operator-splitting algorithm in which the order of solving the advection-dispersion and reaction operators is reversed at each time step. This modification reduces the mass balance error by more than a factor of 10 for a wide range of $k\Delta t$ values.

INTRODUCTION

Groundwater contamination problems have motivated extensive research into numerical techniques for accurate and efficient solution of the equations governing the transport of reactive pollutants in porous media. The governing transport equation, called the advection-dispersion-reaction equation (ADRE), can be written as

$$\frac{\partial c}{\partial t} = \nabla \cdot (\mathbf{D} \cdot \nabla c - \mathbf{v}c) + R(c, t) \qquad (1)$$

where c is the solute concentration, $\mathbf{D}$ is the hydrodynamic dispersion tensor, $\mathbf{v}$ is the pore water velocity, and $R(c, t)$ is the net production rate due to reaction. Many recent transport models have adopted the operator-splitting (OS) approach promoted by Wheeler, Dawson, and coworkers [*Wheeler and Dawson*, 1987; *Chiang et al.*, 1989; *Wheeler et al.*, 1987; *Rifai and Bedient*, 1990; *Kinzelbach et al.*, 1991]. The OS method can be viewed as an approximate technique to integrate (1) over an arbitrary time interval Δt. In the notation of *Tompson and Dougherty* [1990], this integration can be written as

$$\Delta c = c(\mathbf{x}, t + \Delta t) - c(\mathbf{x}, t) = \int_t^{t+\Delta t} \nabla \cdot (\mathbf{D} \cdot \nabla c - \mathbf{v}c)\, dt + \int_t^{t+\Delta t} R\, dt \qquad (2)$$

In OS, the above integration is split into two stages. The first stage entails solution of the first integral containing the advective and dispersive operators to find a "trial" solution $c^*(\mathbf{x}, t + \Delta t)$; the second stage entails using this trial solution as the initial condition for solution of the second integral, which contains only reaction terms.

The OS strategy has several attractive features for solving (1). Each stage can be solved using a different numerical technique that is specially suited to achieve high accuracy for each integral in (2). Solution of the first integral is usually accomplished with a finite difference, finite element, or related technique, while an ordinary differential equation integrator is normally used for solution of the second integral. For example, *Chiang et al.* [1989] use a finite element technique plus a modified method of characteristics for the first stage, and a second-order explicit Runge-Kutta method for the second stage. *Tompson and Dougherty* [1990] use a random walk particle-tracking algorithm for the first stage. Since any nonlinearity in (1) usually is confined to the reaction term, OS is computationally efficient because it converts the original nonlinear partial differential equation into a linear partial differential equation plus a nonlinear ordinary differential equation. Since the time scale of reaction is often much smaller than that of advection and dispersion, OS permits solution of the nonlinear second integral in (2) using time steps much smaller than Δt, which is typically the time step size selected for accurate solution of the first integral. On the practical side, the two-stage splitting can lead to a flexible modular code that can easily be extended to handle coupled reactions and alternative reaction submodels for the $R(c, t)$ term [*Odencrantz et al.*, 1990]. Other features of OS, including its implementation on parallel computers, have been discussed by *Wheeler and Dawson* [1987] and *Wheeler* [1988].

Wheeler and Dawson [1987] give a formal proof of the convergence of the OS method for solving (1). However, we are not aware of any critical assessment of the accuracy of OS in the groundwater modeling literature. The literature suggests that a necessary condition for accuracy is that each stage of the OS be performed accurately. However, related work on hyperbolic problems in the numerical analysis literature by *Strang* [1968] and *LeVeque and Oliger* [1983]

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shows that time splitting can introduce numerical error for certain classes of operators. In this note we show that there is an error inherent in the splitting of the reaction operator from the advection/dispersion operator; this error exists even if each stage of the OS algorithm is solved exactly. We will demonstrate this by examining a very simple model problem of one-dimensional transport with first-order decay.

MODEL PROBLEM SPECIFICATION

Consider a simplified form of (1) for one-dimensional transport and first-order decay,

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial c}{\partial x} - vc\right) - kc \tag{3}$$

where k is the first-order decay constant (t^{-1}). The following initial and boundary conditions for (3) are assumed:

$$c(x, t = 0) = 0 \tag{4}$$

$$\left(vc - D\frac{\partial c}{\partial x}\right)_{x=0} = vc_0 \tag{5}$$

$$c(x \to \infty, t) = 0 \tag{6}$$

Equation (5) is a third-type boundary condition specifying a continuous input at $x = 0$ of solute at concentration c_0.

Equation (3), subject to conditions (4)–(6), has an exact analytical solution which has been presented by several investigators, including *Javandel et al.* [1984] and *van Genuchten* [1981]. This solution can be used over the first time step to find the exact result for $c(x, \Delta t)$, which will be denoted $c_{ex}(x, \Delta t)$. In applying OS, the first stage entails solution of the nonreactive form of (3) and the second stage entails solution of the simple ordinary differential equation $\partial c/\partial t = -kc$; each stage can be solved exactly to find the approximate OS solution at $t = \Delta t$, which will be denoted $c_{OS}(x, \Delta t)$. In the next section we evaluate the accuracy of OS for the simple one-dimensional problem by comparing $c_{ex}(x, \Delta t)$ and $c_{OS}(x, \Delta t)$.

RESULTS

Analytical Results

The analytical solution of (3), subject to conditions (4)–(6), can be determined in a variety of ways. For example, *van Genuchten* [1981] employed Laplace transforms. For the purposes of this technical note, it is more convenient to represent the solution using a time superposition of the so-called impulse response function, which is the solution for the case of an instantaneous input of mass at $x = 0$. That is, boundary condition (5) is replaced by

$$\left(vc - D\frac{\partial c}{\partial x}\right)_{x=0} = A\delta(t) \tag{7}$$

where A is the total mass input per unit cross-sectional area of void space and $\delta(t)$ is the Dirac delta function. We use the notation $G(x, t)$ to represent the impulse response function. Because the substitution $c'(x, t) = c(x, t)e^{kt}$ will transform (3) into a nonreactive advection-dispersion equation in $c'(x, t)$, we find that the impulse response function can be written as

$$G(x, t) = e^{-kt}G^{NR}(x, t) \tag{8}$$

where $G^{NR}(x, t)$ is the impulse response function of the nonreactive form of (3). $G^{NR}(x, t)$ has been reported by several investigators [e.g., *Jury and Roth*, 1990; *Kreft and Zuber*, 1978] and is

$$G^{NR}(x, t) = A\left\{\frac{1}{(\pi Dt)^{1/2}}\exp\left[-\frac{(x - vt)^2}{4Dt}\right] - \frac{v}{2D}\exp\left(\frac{vx}{D}\right)\operatorname{erfc}\left(\frac{x + vt}{(4Dt)^{1/2}}\right)\right\} \tag{9}$$

Since the model problem is linear, the solution for any arbitrary mass input function at $x = 0$ can be expressed as a time superposition of the impulse response function [*Jury and Roth*, 1990; *Kreft and Zuber*, 1978; *Hunt*, 1978; *Turner*, 1972]. For the continuous mass input function in boundary condition (5), the solution is

$$c_{ex}(x, t) = \frac{c_0 v}{A}\int_0^t G(x, t - t')\,dt' = \frac{c_0 v}{A}\int_0^t e^{-k\tau}G^{NR}(x, \tau)\,d\tau \tag{10}$$

where $\tau = t - t'$. Setting the upper limit of integration in (10) equal to Δt yields $c_{ex}(x, \Delta t)$.

Next we determine the OS solution. The first stage of the OS method corresponds to solution of the nonreactive form of (3) over one time step to yield the trial solution,

$$c^*(x, \Delta t) = \frac{c_0 v}{A}\int_0^{\Delta t} G^{NR}(x, t - t')\,dt' \tag{11}$$

The second stage uses $c^*(x, t)$ from (11) as the initial condition in solving $\partial c/\partial t = -kc$. Therefore,

$$c_{OS}(x, \Delta t) = c^*(x, \Delta t)e^{-k\Delta t} \tag{12}$$

Hence, the final result is

$$c_{OS}(x, \Delta t) = \frac{c_0 v}{A}e^{-k\Delta t}\int_0^{\Delta t} G^{NR}(x, t - t')\,dt' \tag{13}$$

The difference between (10) and (13) is the error in applying operator splitting over one time step. The error is denoted as $e(x, \Delta t)$ and can be written formally as

$$e(x, \Delta t) = c_{ex}(x, \Delta t) - c_{OS}(x, \Delta t) \tag{14}$$

After substituting the results from (10) and (13), (14) becomes

$$e(x, \Delta t) = \frac{c_0 v}{A}e^{-k\Delta t}\int_0^{\Delta t} G^{NR}(x, \Delta t - t')[e^{kt'} - 1]\,dt' \tag{15}$$

Equation (15) shows that the dimensionless parameter $k\Delta t$ will play a key role in controlling the magnitude of the error; however, in general, $e(x, \Delta t)$ will also be a function of the

other parameters (i.e., v and D) present in $G^{NR}(x, t)$. It is interesting to note that (15) is always nonnegative; therefore, the OS solution "lags behind" the exact solution. The analysis simplifies greatly if we just consider the overall integrated error at $t = \Delta t$, which we define as

$$\bar{e}(\Delta t) = \int_0^\infty e(x, \Delta t)\, dx \tag{16}$$

Since it can be demonstrated that (see, for example, *Kreft and Zuber* [1978])

$$\int_0^\infty G^{NR}(x, t)\, dx = A \tag{17}$$

equation (16) simplifies to

$$\bar{e}(\Delta t) = c_0 v \left[\frac{1}{k}(1 - e^{-k\Delta t}) - \Delta t e^{-k\Delta t}\right] \tag{18}$$

Examining (14) and (16), we see that $\bar{e}(\Delta t)$ is related to the difference between the exact and OS mass in the domain. In fact, result (18) could be obtained very simply by integrating the governing equations over all x to derive an ordinary differential equation for $M(t)$, the total mass per unit column cross-sectional pore area, which is defined by

$$M(t) = \int_0^\infty c(x, t)\, dx \tag{19}$$

It can therefore be demonstrated that $\bar{e}(\Delta t) = M_{ex}(\Delta t) - M_{OS}(\Delta t)$. The relative mass error is denoted as $\bar{E}(\Delta t)$ and is defined by

$$\bar{E}(\Delta t) = \frac{\bar{e}(\Delta t)}{M_{ex}(\Delta t)} = 1 - \frac{k\Delta t e^{-k\Delta t}}{1 - e^{-k\Delta t}} \tag{20}$$

The above result shows that the error measure $\bar{E}(\Delta t)$ is a function only of $k\Delta t$. $\bar{E}(\Delta t)$ increases with increasing $k\Delta t$, and $\bar{E}(\Delta t)$ approaches zero as $k\Delta t$ approaches zero. A plot of $\bar{E}(\Delta t)$ versus $k\Delta t$ is given in Figure 1, which shows that the relative mass error is less than about 0.05 if $k\Delta t$ is less than 0.1. The mass balance error will be analyzed further in the discussion section of the paper. It is emphasized that the error defined above exists even in the absence of numerical discretization errors that may be present at each stage of the OS algorithm.

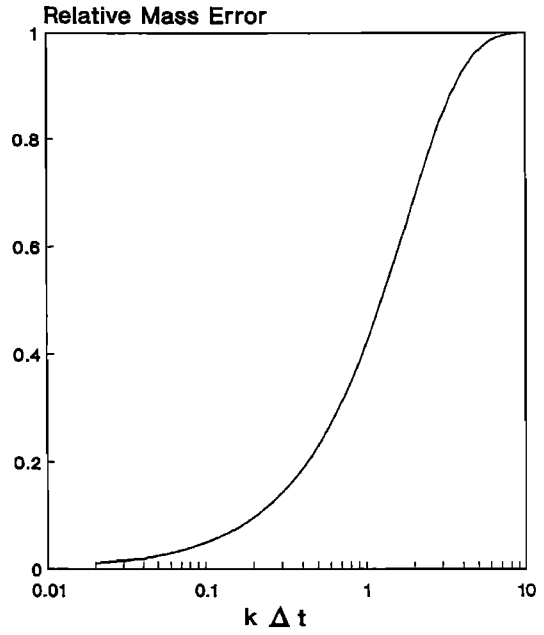

Fig. 1. A plot of (20), which gives the relative mass error over one time step of the normal operator-splitting method, $\bar{E}(\Delta t)$, versus $k\Delta t$.

Numerical Results

The previous analysis considered the OS error over a single time step from $t = 0$ to $t = \Delta t$. Here we present a few numerical results from OS solution of the model problem (3) over many time steps. For solution of the nonreactive advection-dispersion equation in the first stage of OS, we use a standard finite element method based on linear C^0 elements and Crank-Nicolson time differencing [*Pinder and Gray*, 1977]. We use an analytical solution of the first-order decay equation in the second stage of OS. The parameters used in the numerical simulations are $v = 1.0$ m/d, $D = 0.1$ m^2/d, $\Delta x = 0.1$ m, and $\Delta t = 0.05$ d. This discretization yields a grid Courant number ($v\Delta t/\Delta x$) equal to 0.5 and a grid Peclet number ($v\Delta x/D$) equal to 1, which should guarantee that the finite element solution in the first stage is free from numerical dispersion and oscillation [*Daus et al.*, 1985].

Figures 2 and 3 show a comparison between the analytical and OS solution after an elapsed time of 0.5 d for the cases of $k = 0.4$ d^{-1} and 4.0 d^{-1}, respectively. We use the form of the analytical solution reported by *van Genuchten* [1981]. Although the accuracy of OS in the first case ($k\Delta t = 0.02$) is excellent, in the second case ($k\Delta t = 0.2$) it is quite poor. When Δx in the second case is reduced by a factor of 2, the results (not shown) are nearly identical to those in Figure 3. However, when the time step in the second case is reduced

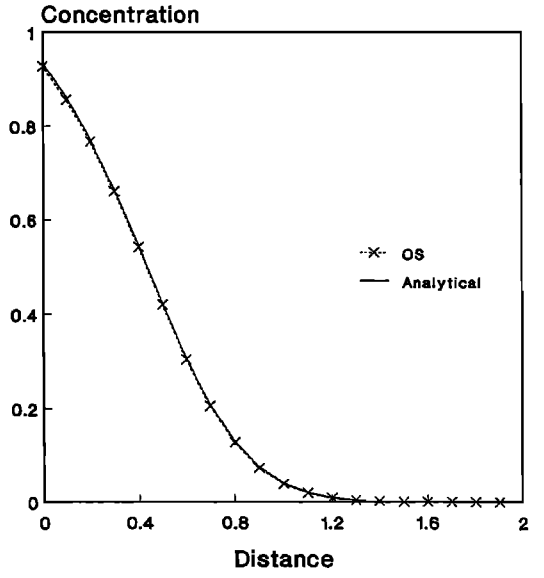

Fig. 2. A comparison between the analytical solution and numerical (operator-splitting) solution after an elapsed time of 0.5 d; the physical and discretization parameters are $v = 1.0$ m/d, $D = 0.1$ m^2/d, $k = 0.4$ d^{-1}, $\Delta t = 0.05$ d, and $\Delta x = 0.1$ m.

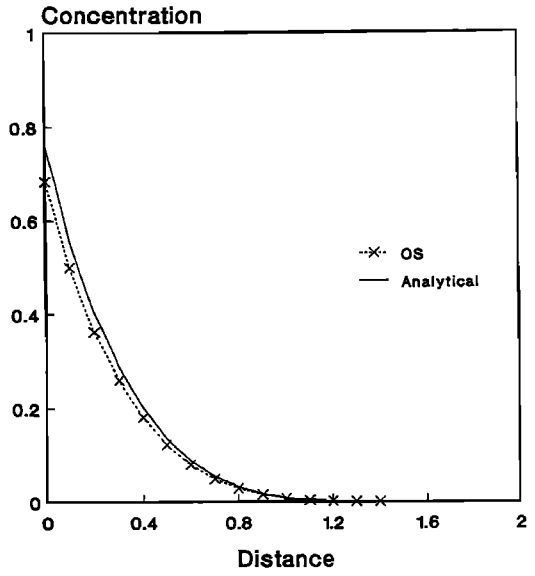

Fig. 3. A comparison between the analytical and numerical solution after an elapsed time of 0.5 d showing the effect of increasing k upon the accuracy of operator splitting; all parameters are identical to Figure 2 except $k = 4.0\ d^{-1}$.

to $\Delta t = 0.005$, thus yielding a $k\Delta t$ value equal to 0.02, the accuracy of OS improves dramatically. This is demonstrated in Figure 4.

Although the numerical simulations have only been performed for a limited range of parameters, they confirm the analytical results presented above. This suggests that the product $k\Delta t$ should be less than about 0.1 in order to guarantee accurate OS solution of reactive transport problems.

Discussion

The analysis leading to definition (20) of the relative mass error indicates that there is too little mass present in the OS solution after one time step. The reason is apparent after examination of the convolution form of the exact analytical solution (10) and the approximate OS solution (13). During some finite time interval Δt, the exact solution states that mass is input into the domain through the boundary at $x = 0$, and that this mass undergoes simultaneous transport and decay; therefore, mass input near the beginning of the time interval will undergo more decay than mass input toward the end. However, the OS formulation states that all of the mass input during the time interval decays for the entire duration Δt; obviously, this will overestimate the amount of mass decayed. It is worth noting that this mass balance error is associated with continuous mass input types of boundary conditions like (5). In the special case of instantaneous mass input (e.g., the boundary condition given by (7)), the OS method would give the exact solution to the model linear problem examined in this paper.

It is possible to modify the OS method to reduce the mass balance error. For example, in the first stage of OS, one could input "extra" mass to compensate for the mass balance error. In the simple linear problem analyzed here, the required extra mass can easily be computed from (20); however, such computation is not possible in more general problems entailing nonlinear reactions. Another possibility we explore here is the implementation of what we call the alternating OS scheme, in which the order of the splitting is reversed at each time step. That is, for the first time step we follow the above procedure with solution of the advection-dispersion operator in the first stage and the reaction operator in the second stage; then, for the second time step, we solve the reaction operator in the first stage and the advection-dispersion operator in the second stage. In the second time step, the alternating OS scheme will underestimate the proper amount of mass decayed, because the reaction stage occurs before the transport stage. Hence, the mass balance errors in the first and second time steps will be counteracting, so that the overall error after two steps may possibly be diminished.

In the appendix we analyze the mass balance error after two steps for both the "normal" and alternating OS methods. The relative mass error for the normal OS scheme, denoted $\bar{E}_N(2\Delta t)$, is given by equation (A6), and that for the alternating OS scheme, denoted $\bar{E}_A(2\Delta t)$, is given by equation (A9). The normal OS scheme underestimates the amount of mass after two time steps, so $\bar{E}_N(2\Delta t)$ is always greater than or equal to zero, whereas the alternating OS scheme overestimates the amount of mass, giving $\bar{E}_A(2\Delta t)$ less than or equal to zero. Figure 5 is a plot of the relative mass error versus $k\Delta t$, which shows that the alternating OS method will have smaller mass balance errors (in absolute value) than the normal OS method for values of $k\Delta t$ less than ≈ 1.5. In order for the absolute value of the relative mass error after two time steps to be less than about 0.05, $k\Delta t$ must be less than 0.4 if the alternating OS scheme is used, and less than 0.1 if the normal OS scheme is used.

In order to demonstrate further the value of the alternating method, we have modified the numerical code previously described in order to implement the alternating OS scheme. We have used this new code to repeat the simulation shown

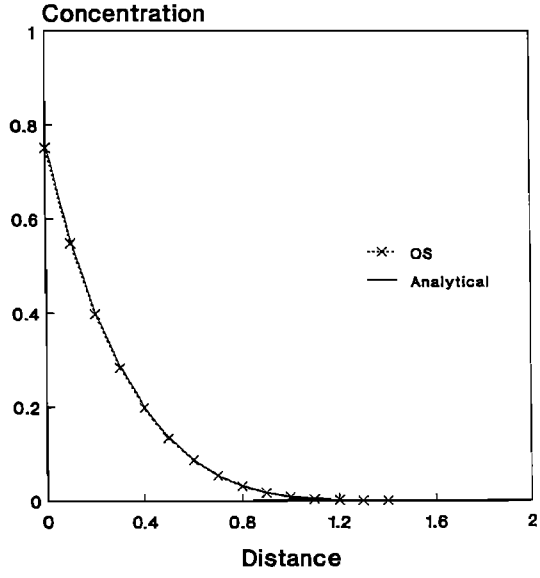

Fig. 4. A comparison between the analytical and numerical solution after an elapsed time of 0.5 d showing the effect of decreasing Δt upon the accuracy of operator splitting; the parameters are $v = 1.0$ m/d, $D = 0.1\ m^2/d$, $k = 4.0\ d^{-1}$, $\Delta t = 0.005$ d and $\Delta x = 0.1$ m.

in Figure 3; the results are shown in Figure 6. Comparing Figures 3 and 6, we see that the results from the alternating OS scheme are significantly better than those from the normal OS scheme. It is emphasized that all discretization parameters are identical in the two simulations. The numerical results corroborate the conclusions drawn from the analysis of the mass balance errors as summarized in Figure 5.

It should be noted that our alternating OS scheme is closely related to the so-called Strang splitting described by *Strang* [1968] and *LeVeque and Oliger* [1983]. These authors demonstrate formally that the Strang splitting has a higher order of accuracy in time than the normal time splitting. Thus, it is not surprising that our results show the superiority of the alternating scheme.

CONCLUSIONS

In this note we have analyzed the accuracy of an operator-splitting approach to solve a simple one-dimensional problem of transport with first-order decay. Using very elementary mass balance arguments, we have shown that OS exhibits an inherent mass balance error when applied to problems with continuous mass input types of boundary conditions. This error is present even in the absence of numerical discretization errors that may be associated with each stage of the OS algorithm. In practical problems involving multidimensional nonuniform flow, complex domain geometry, nonlinear reactions, etc., each stage of the OS algorithm will be solved by an appropriate approximate numerical technique. Our results suggest that overall accuracy in the OS method requires not only accurate solution of the advection-dispersion and reaction stages, but also a small value of $k\Delta t$. In other words, the maximum permissible Δt will be inversely related to the first-order decay coefficient k, in addition to being restricted by the normal Peclet and Courant criteria arising from numerical approximation of the nonreactive advection-dispersion equation.

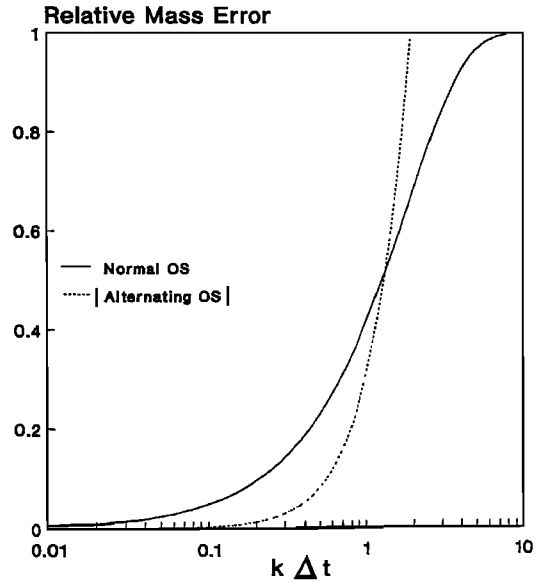

Fig. 5. A plot of the magnitude of the relative mass error over two time steps for the normal and alternating operator-splitting methods versus $k\Delta t$.

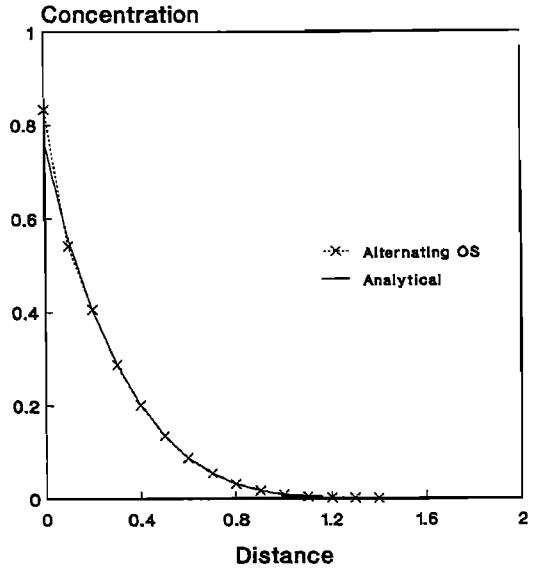

Fig. 6. A comparison between the analytical solution and the numerical solution obtained by the alternating operator-splitting method after an elapsed time of 0.5 d; the parameters are identical to Figure 3.

Although we have analyzed a simple linear decay problem, the general conclusion that there is a time step size restriction related to the reactive time scale is valid for more complex problems involving nonlinear reactions.

Based upon our analysis of the normal OS method in which the advection-dispersion solution is performed in the first stage and the reaction solution in the second stage, we recommend that the time step size be chosen so that the product $k\Delta t$ is less than approximately 0.1. We also introduced a variant of the normal OS method, the alternating OS method, in which the order of solving the advection-dispersion and reaction operators is reversed at each time step. For the model problem we examined, the alternating OS method has mass balance errors more than 10 times smaller than the normal OS method over a reasonable range of $k\Delta t$ values.

APPENDIX: DERIVATION OF THE MASS BALANCE ERROR OVER TWO TIME STEPS

The ordinary differential equation for $M_{ex}(t)$, the total mass per unit cross-sectional pore area present in the domain for the exact solution, can be derived by integrating the governing ADRE (3) over all x and applying boundary condition (5). The result is

$$\frac{d}{dt} M_{ex} + kM_{ex} = vc_0 \tag{A1}$$

Solving the above equation subject to the initial condition $M_{ex}(t = 0) = 0$, we find

$$M_{ex}(t) = \frac{vc_0}{k} [1 - e^{-kt}] \tag{A2}$$

In the normal OS scheme, we solve the nonreactive form of (3) in the first stage to compute a trial solution $c^*(x, \Delta t)$, which is used as the initial condition for solving the reaction

ordinary differential equation in the second stage. Integrating the the nonreactive form of (3) over all x yields

$$\frac{d}{dt} M^* = vc_0 \tag{A3}$$

Solving (A3) over one time step subject to the initial condition $M^*(t = 0) = 0$ yields $M^*(\Delta t) = vc_0\Delta t$. Using the solution to the second stage given by (12), we find that the OS mass after one time step is

$$M_{OS}(\Delta t) = M^*(\Delta t)e^{-k\Delta t} = vc_0\Delta t e^{-k\Delta t} \tag{A4}$$

Over the second time step we solve (A3) subject to the initial condition that $M^*(t = \Delta t) = M_{OS}(\Delta t)$ in the first stage. This yields $M^*(t = 2\Delta t) = vc_0\Delta t(1 + e^{-k\Delta t})$. After the second stage we find

$$M_{OS}(2\Delta t) = vc_0\Delta t e^{-k\Delta t}[1 + e^{-k\Delta t}] \tag{A5}$$

Finally we compute $\bar{E}_N(2\Delta t)$, the relative mass error for the normal OS method after two time steps, as

$$\bar{E}_N(2\Delta t) = \frac{M_{ex}(2\Delta t) - M_{OS}(2\Delta t)}{M_{ex}(2\Delta t)}$$

$$= 1 - k\Delta t e^{-k\Delta t} \frac{1 + e^{-k\Delta t}}{1 - e^{-2k\Delta t}} \tag{A6}$$

Next we consider the alternating OS method, in which the reaction equation is solved in the first stage of the second time step and the transport equation is solved in the second stage. The first stage thus entails solution of $\partial c/\partial t = -kc$ using $c_{OS}(x, \Delta t)$ as the initial condition. This gives the trial solution $c^*(x, 2\Delta t) = c_{OS}(x, \Delta t)e^{-k\Delta t}$. Therefore, the trial solution for the mass is

$$M^*(2\Delta t) = M_{OS}(\Delta t)e^{-k\Delta t} \tag{A7}$$

The second stage entails solution of the nonreactive form of (3) using $c^*(x, 2\Delta t)$ as the initial condition. The equation for the total mass is identical to (A3) with M_{OS} replacing M^*. This equation is solved from $t = \Delta t$ to $t = 2\Delta t$ using $M^*(2\Delta t)$ from (A7) as the initial condition. Thus, the final result for the mass after two time steps is

$$M_{OS}(2\Delta t) = vc_0\Delta t[1 + e^{-2k\Delta t}] \tag{A8}$$

Finally, we use (A.2) for $M_{ex}(2\Delta t)$ and (A8) for $M_{OS}(2\Delta t)$ in order to compute $\bar{E}_A(2\Delta t)$, the relative mass error for the alternating OS method after two time steps,

$$\bar{E}_A(2\Delta t) = 1 - k\Delta t \frac{1 + e^{-2k\Delta t}}{1 - e^{-2k\Delta t}} \tag{A9}$$

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