

A numerical method for solving a scalar advection-dominated transport equation with concentration-dependent sources

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Abstract

A numerical scheme, upstream biased Eulerian algorithm for transport equations with sources (UpBEATES), is developed for solving a scalar advective-dominated transport equation with concentration-independent and -dependent source terms. A control-volume method is used for spatial discretization. Time integration is invoked to yield a discrete system of integrated-flux-integrated-source form equations. The Bott's upstream-biased Eulerian advection scheme [Moneatry and Weakly Review 117 (1989a) 1006; Moneatry and Weakly Review 117 (1989b) 2633] is employed for approximating advective fluxes. A two-level time weighting scheme is employed for the dispersive fluxes. An upstream-biased Eulerian algorithm is proposed for the concentration-dependent source term. Flux and source limiters are developed to ensure non-negative evolution of the scalar concentration field. Numerical experiments were presented to illustrate its performance in comparison with theoretical solutions and those of conventional methods. The proposed scheme is mass-conservative, produces non-negative concentration values, exhibits low numerical dispersion, and is efficient for advection-dominated problems with concentration-dependent source terms. Like other Eulerian schemes, the Courant–Friedrich–Levy (CFL) stability criterion has to be met.

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1. Introduction

The fate and transport of a chemical species through porous media is often subject to one or more of the following processes: chemical and biological reactions such as utilization and growth, adsorption, decay, death, external forcing such as injection and extraction (withdrawals). Mathematical description of such a problem generally leads to an advection–dispersion equation with reactive or source terms. In many cases, the transport is advection-dominated.

Numerical solution of a homogeneous scalar advection equation using conventional methods (i.e. forward-in-time, central-difference-in-space scheme, and the first-order upstream scheme) is well known to be plagued with difficulties (Noorishad, Tsang, Perrochet & Musy, 1992). The difficulties are two-fold: non-

physical oscillation (wiggles, ripples, over- or under-shooting) associated with the central-difference-in-space schemes, and excessive numerical dispersion associated with the first-order upstream scheme. In the absence of background concentration values, oscillation manifests itself into non-physical negative values, which should be prohibited. Excessive numerical dispersion always leads to underestimation of peak concentration values, and overestimation of extent of concentration plume, the consequence of which could be a serious one.

Although the approximation of the advective term by the first-order upstream scheme is seemingly a step-down in accuracy from the second-order center difference scheme, it proves to be in the right direction (Noorishad et al., 1992). Upstream biased numerical schemes, of which the first-order upstream scheme is one, are characterized by the fact that the approximation of advective mass flux across an interface between two neighboring computational cells is more closely

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related to the concentrations in cells upstream of the interface than those downstream of the interface. This makes sense from a physical point of view. Upstream biased, higher-order-accurate schemes, it then seems, would provide the desired solution to the problems associated with the conventional advection schemes. This is partly true because upstream biased, higher-order advection schemes are much less diffusive. Examples are the fourth-order-accurate scheme of Crowley (1968) and the third- and higher-order-accurate schemes of Tremback, Powell, Cotton and Pielke (1987), which use the method of polynomial fitting to represent the local distribution of a dependent variable inside a computational cell. However, the increase in the order of approximation in the upstream direction often introduces dispersive oscillations and negative concentrations, which are typical of both centered or upstream biased second- and higher-order accurate schemes for advection-dominated problems.

Non-physical oscillation is closely related to a local mass balance problem, albeit not a global one. Over-shooting in the solution results, indirectly or directly, from overestimation of fluxes into a nodal point (in finite element method) or computation cell (in finite volume method), while under-shooting is a result of underestimation of fluxes out of a nodal point or computational cell. Excessive numerical dispersion, however, is caused by the low order approximation of the first-order spatial derivative of the associated numerical schemes. Thus, remedies for non-physical oscillation should be directed towards avoiding over- and under-estimation of fluxes into or out of a nodal point or a computational cell, whereas efforts for reducing numerical dispersion should focus on increasing the order of approximation of the first-order spatial derivative of the scalar concentration field.

The flux-corrected transport (FCT) method, developed by Boris and Book (1973) and generalized by Zalesk (1979) for multidimensional cases, was designed for eliminating unphysical oscillations associated with higher-order advection schemes. It involves the following two steps (Thuburn, 1996). First, the first-order upstream scheme, which is oscillation-free but diffusive, is used to advect the concentration field. Then, an anti-diffusive correction is applied. Through carefully constraining or limiting the anti-diffusive fluxes, the scheme as a whole can be made to be oscillation-free.

Another conceptually similar approach for eliminating oscillations is to employ a single stage in which the full fluxes are carefully constrained using a flux limiter. An example of this approach is an upstream biased, area-preserving advection scheme proposed by Bott (1989a,b). The flux from a grid box or cell is computed using an extension of the integrated flux-form of Tremback et al. (1987) along with area-preserving polynomial fitting for local variation of the scalar concentration

field. Because of the fitting of higher-order polynomials, oscillations and negative concentrations are often produced. To ensure non-negative evolution of concentration field, these fluxes are then limited by lower and upper bounds. The scheme is forward in time, explicit, conservative, does not produce negative scalar concentration values, exhibits very low numerical dispersion, and is computationally efficient. Modifications to this scheme have been presented by Bott (1992), Easter (1992) and Chlond (1994).

Most of the schemes mentioned earlier were exclusively developed for homogeneous advection problems. Some of the higher-order schemes, when extended to cases involving sources or strong biological/chemical reactions often lose their higher-order of accuracy due to their first-order approximation to these terms. For heterogeneous advection-dominated problems associated with water flooding of petroleum reservoirs, Douglas and co-workers have developed a modified method of characteristics with adjusted advection (MMOCAA) that conserves mass and is a significant improvement over previous MMOC simulations (Douglas, Pereira & Yeh, 2000). Nguyen and Dabdub (2001) recently developed the quintic spline Taylor-series expansion (QSTSE) based on a two-level time-marching scheme. QSTSE uses quintic splines to compute the space derivatives. QSTSE is an Eulerian type of scheme, whereas as the upstream biased Eulerian algorithm for transport equations with sources (UpBEATES) is a Lagrangian one. In comparison to QSTSE's fifth-order polynomial fit, our method uses a fourth-order interpolation between data points for flux. However, higher-order polynomials can be used just as efficiently because of the explicit nature of our approach. For most problems, fourth-order interpolation is sufficient. Bott's scheme is a satisfactory compromise between the very accurate, but computationally costly ASD method and the very fast, but less accurate Galerkin finite element techniques. The UpBEATES scheme pays special attention to the handling of concentration dependent biological and chemical reaction terms in advection-dominated transport. It applies limiters to both fluxes and source terms to avoid nonphysical oscillations and negative concentrations. In general, first-order upstream methods, even for pure advection transport problems, suffer from excessive dispersion. The UpBEATES scheme is very efficient and avoids such problems associated with advection-dominated problems in general, and advection-dominated transport with strong chemical/biological reactions in particular. Neither the MMOCAA nor QSTSE approaches address strong chemical/biological reactions in the advection transport equation, which is part of the focus of this work.

It is the purpose of this paper to extend Bott's (1989a,b) area-preserving, positive definite Eulerian advection scheme to include dispersion and source

terms. For simplicity and illustrative purposes, we shall restrict ourselves to a one-dimensional advection-dominated transport equation with sources that are dependent on scalar concentration in a nonlinear fashion. The presentation of this paper is divided into four parts. Firstly, a background for the present study is presented. This includes a review of Bott's advection scheme for a homogeneous advective transport equation. Next, the extension of Bott's numerical method for solving an advection-dominated transport equation with sources is presented. Thirdly, the performance of the newly proposed scheme will be examined using a series of numerical experiments, and compared with that of the analytical solutions and the conventional methods. And finally, we present the major conclusions of this paper and discuss possible extensions of the proposed method to more complicated cases.

2. Background

2.1. A pure advection problem

We first consider the advective transport of a scalar concentration under one-dimensional flow described by:

$$\frac{\partial C}{\partial t} + \frac{\partial vC}{\partial x} = 0, \quad (1)$$

subject to appropriate initial and boundary conditions. Here C is a scalar concentration, v the velocity that may vary in both space and time. The Lagrangian form of (1) is:

$$\frac{DC}{Dt} = 0, \quad (2)$$

where $D/Dt = \partial/\partial t + v\partial/\partial x$, and $dx/dt = v$ represents the so called characteristic curves. Here we have employed an implicit assumption that the flow field satisfies $\nabla \cdot \vec{v} = 0$, which is the case for incompressible flow through porous media. Given two points on a characteristic curve, (x_0, t_0) and (x, t) we integrate (Eq. (2)) from (x_0, t_0) to (x, t) to obtain the relationship between concentrations at these two points:

$$C[x, t] = C[x_0, t_0]. \quad (3)$$

Eq. (1) represents the shape-preserving movement of an initial distribution of the scalar variable C .

2.2. Control-volume discretization

To solve (1) we use a control-volume (or finite-volume) approach. For notational reason we follow Chlond (1994) and define the advective flux $f = vC$. We integrate (1) in space from $x - \Delta x/2$ to $x + \Delta x/2$ and in time from t to $t + \Delta t$ to yield:

$$\frac{\langle C \rangle^{t+\Delta t} - \langle C \rangle^t}{\Delta t} + \frac{\bar{f}_{x+\Delta x/2} - \bar{f}_{x-\Delta x/2}}{\Delta x} = 0, \quad (4)$$

where the angle brackets denote control-volume averages, and an overhead bar indicates a temporal average from t to $t + \Delta t$, i.e.

$$\langle C \rangle^{t+\Delta t} = \frac{1}{\Delta x} \int_{x-\Delta x/2}^{x+\Delta x/2} C[x, t + \Delta t] dx, \quad (5a)$$

$$\begin{aligned} \bar{f}_{x+\Delta x/2} &= \frac{1}{\Delta t} \int_t^{t+\Delta t} f[x + \Delta x/2, t] dt \\ &= \frac{1}{\Delta t} \int_t^{t+\Delta t} v[x + \Delta x/2, t] C[x + \Delta x/2, t] dt, \end{aligned} \quad (5b)$$

The term $\bar{f}_{x+\Delta x/2}$ represents the advective flux across the right boundary of the 1-D control volume defined by $x - \Delta x/2 \leq x' \leq x + \Delta x/2$. A similar definition can be written for $\bar{f}_{x-\Delta x/2}$.

Suppose the computational domain is discretized into M equally spaced computational cells or volumes, with x_i denoting the center of the i th cell ($i = 1, 2, \dots, M$), and $x_{i+1/2} = \Delta x/2$ denotes the nodal point or cell interface. The time is discretized according to $t_{n+1} = t_n + \Delta t$ where $n = 0, 1, 2, \dots$. The discrete versions of (4)–(5) read:

$$C_i^{n+1} = C_i^n - \frac{\Delta t}{\Delta x} (\bar{f}_{i+1/2} - \bar{f}_{i-1/2}), \quad (6)$$

where

$$C_i^{n+1} = \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} \hat{C}[x, t_{n+1}] dx, \quad (7)$$

$$\begin{aligned} \bar{f}_{x+\Delta x/2} &= \frac{1}{\Delta t} \int_t^{t+\Delta t} v[x_{i+1/2}, t_n + \tau] \hat{C}[x_{i+1/2}, t_n + \tau] d\tau \\ &\approx \frac{1}{\Delta t} \int_t^{t+\Delta t} \hat{C}[x_{i+1/2}, t_n + \tau] v_{i+1/2}^{n+1/2} d\tau. \end{aligned} \quad (8)$$

Here C_i^{n+1} is the control-volume average of C in cell i at time t_{n+1} , representing discrete values, \hat{C} denotes a piecewise profile representing the variation of C between discrete locations, $v_{i+1/2}^{n+1/2}$ is the value of v evaluated at the interface between cell i and cell $i+1$ averaged over the time interval $[t_n, t_{n+1}]$, and $\bar{f}_{i+1/2}$ is the integrated advective flux across the interfacial boundary between cells i and $i+1$ and averaged over the time interval $[t_n, t_{n+1}]$.

2.3. Conventional upstream scheme

The essence of any numerically stable and positive-definite scheme for solving (Eq. (1)) lies in its approximation to the integrated advective flux term $C_i^{n+1,0} = C_i^n$ or Eq. (8). A commonly used advection scheme for (1) is the conventional first-order upstream method. Its approximation to (8) can be obtained by (a) using the shape preserving property $\hat{C}[x_{i+1/2}, t_n + \tau] = \hat{C}[x_{i+1/2} - v_{i+1/2}^{n+1/2} \tau, t_n]$; and (b) assuming that $\hat{C}[x, t_n]$ is represented by a step function with constant values in each computational cell. To illustrate, define the Courant number $Cr_{i+1/2}^{n+1/2} = v_{i+1/2}^{n+1/2} \Delta t / \Delta x$. Because $Cr_{i+1/2}^{n+1/2}$ has the same sign as that of the velocity $v_{i+1/2}^{n+1/2}$, it is decomposed according to:

$$Cr_{i+1/2}^{n+1/2} = Cr_{i+1/2}^{n+1/2+} - Cr_{i+1/2}^{n+1/2-},$$

where $Cr_{i+1/2}^{n+1/2+} = \max\{0, Cr_{i+1/2}^{n+1/2}\}$ and $Cr_{i+1/2}^{n+1/2-} = -\min\{0, Cr_{i+1/2}^{n+1/2}\}$ are the non-negative part and the absolute value of the non-positive part of the Courant number $Cr_{i+1/2}^{n+1/2}$, respectively. Invoking the two assumptions (a and b) and making use of the above notations gives the following first-order upstream scheme approximation of Eq. (8) (see also Bott, 1989a):

$$\bar{f}_{i+1/2} = \frac{\Delta x}{\Delta t} (Cr_{i+1/2}^{n+1/2+} C_i^n - Cr_{i+1/2}^{n+1/2-} C_{i+1}^n), \quad (9)$$

for every i . Numerical stability requires that the Courant–Friedrich–Levy (CFL) criterion is met or $Cr_{i+1/2}^{n+1/2+} + Cr_{i+1/2}^{n+1/2-} \leq 1$. The first-order upstream scheme is positive-definite and conserves mass. It yields the exact solution when $|Cr_{i+1/2}^{n+1/2}| = 1.0$ for a uniform velocity field. Because of the poor representation of $\hat{C}[x, t_n]$ by a step function, however, it is only first-order accurate in both space and time (Bott, 1989a). It, therefore, suffers from too much numerical dispersion for $|Cr_{i+1/2}^{n+1/2}| < 1.0$.

2.4. Bott's advection scheme

Bott (1989a,b) recently proposed an upstream-biased Eulerian finite difference advection scheme for solving Eq. (1). The scheme consists of two distinctive steps. In the first step, following Crowley (1968) Tremback et al. (1987), area-preserving polynomials \hat{C} representing the local variations of concentration are fitted to obtain a better representation of the scalar variable between grid points than a simple step function. This is then inserted into Eq. (8) to calculate the integrated fluxes $\bar{f}_{i+1/2}$, across interfaces by making use of the shape-preserving property $\hat{C}[x_{i+1/2}, t_n + \tau] = \hat{C}[x_{i+1/2} - v_{i+1/2}^{n+1/2} \tau, t_n]$. Second, using ideas drawn from the concept of FCT of Boris and Book (1973), specific flux limiters for $\bar{f}_{i+1/2}$, are employed to avoid negative scalar concentration

values. The following provides a review of Bott (1989a,b) scheme (see also Chlond, 1994 for a review).

First we rewrite (8) as:

$$\begin{aligned} \bar{f}_{i+1/2} &= \frac{1}{\Delta t} \int_0^{\Delta t} C(x, t_n + \tau)_{x=x_i+\Delta x/2} v_{i+1/2}^{n+1/2} d\tau \\ &= \frac{1}{\Delta t} \int_0^{\Delta t} \hat{C}(x - v_{i+1/2}^{n+1/2} \tau, t_n)_{x=x_i+\Delta x/2} v_{i+1/2}^{n+1/2} d\tau, \end{aligned} \quad (10)$$

which for now depends only on the concentration profile at time t_n . With the substitution $x' = x - v_{i+1/2}^{n+1/2} \tau$, (10) becomes:

$$\bar{f}_{i+1/2} = \frac{1}{\Delta t} \int_{x_{i+1/2} - v_{i+1/2}^{n+1/2} \Delta t}^{x_{i+1/2}} \hat{C}(x', t_n) dx'. \quad (11)$$

By definition, the advective flux $\bar{f}_{i+1/2}$ should have the same sign as that of $v_{i+1/2}^{n+1/2}$, and it vanishes as $v_{i+1/2}^{n+1/2}$ approaches zero. Following Bott (1989a) we decompose $\bar{f}_{i+1/2}$ into:

$$\bar{f}_{i+1/2} = \bar{f}_{i+1/2}^+ - \bar{f}_{i+1/2}^-, \quad (12)$$

where $\bar{f}_{i+1/2}^+$ and $\bar{f}_{i+1/2}^-$ represent, respectively, the non-negative part and the absolute value of the non-positive part of $\bar{f}_{i+1/2}$. Hence, $\bar{f}_{i+1/2}^+$ and $\bar{f}_{i+1/2}^-$ are contributed by advective flow in the positive and negative x -directions, respectively. To evaluate $\bar{f}_{i+1/2}^+$ and $\bar{f}_{i+1/2}^-$, we first note that the contributing cell to the integral on the right-hand side of (11) is i for $0 \leq Cr_{i+1/2}^{n+1/2} \leq 1.0$, and $i+1$ for $-1 \leq Cr_{i+1/2}^{n+1/2} \leq 0$. Furthermore, we define the normalized coordinates:

$$\begin{aligned} \xi[i] &= (x' - x_i) / \Delta x, \quad \forall 0 \leq Cr_{i+1/2}^{n+1/2} \leq 1.0, \\ \xi[i+1] &= (x' - x_{i+1}) / \Delta x, \quad \forall -1 \leq Cr_{i+1/2}^{n+1/2} < 0. \end{aligned}$$

With these normalized notations, it follows from (Eqs. (10)–(12)) that:

$$\bar{f}_{i+1/2}^{\pm} = \frac{\Delta x}{\Delta t} I_{i+1/2}^{\pm}, \quad (13)$$

where $I_{i+1/2}^+$ and $I_{i+1/2}^-$ are the integrals given by:

$$I_{i+1/2}^+ = \int_{1/2 - Cr_{i+1/2}^{n+1/2+}}^{1/2} \hat{C}[\xi(i), t_n] d\xi(i), \quad (14a)$$

$$I_{i+1/2}^- = \int_{-1/2}^{-1/2 + Cr_{i+1/2}^{n+1/2-}} \hat{C}[\xi(i+1), t_n] d\xi(i+1). \quad (14b)$$

By their definitions,

$$Cr_{i+1/2}^{n+1/2-} = \bar{f}_{i+1/2}^- = I_{i+1/2}^- \equiv 0 \quad \forall v_{i+1/2}^{n+1/2} \geq 0, \quad \text{and}$$

$$Cr_{i+1/2}^{n+1/2+} = \bar{f}_{i+1/2}^+ = I_{i+1/2}^+ \equiv 0 \quad \forall v_{i+1/2}^{n+1/2} \leq 0.$$

Following the methodology of Tremback et al. (1987) Bott (1989b) uses area-preserving polynomials of order L ($L = 0, 1, 2, \dots$) with the following form for $\hat{C}(\xi, t_n)$:

$$\hat{C}[\xi(i), t_n] = \sum_{l=0}^L a_{i,l}^n \xi^l(i). \quad (15)$$

The $a_{i,l}^n$ values are determined by requiring the area covered by $\hat{C}[\xi(i), t_n]$ in cell i is equal to $C_i^n \Delta x$. The results are:

$$a_{i,l}^n = \sum_{m=-L/2}^{m=L/2} \beta_{l,m} C_{i\pm m}^n \quad (l = 0, 1, 2, \dots, L). \quad (16)$$

Table 1 lists the values of $\beta_{l,m}$ ($l = 0, 1, 2, \dots, L$; $m = -L/2, -L/2+1, \dots, L/2$) for polynomials of orders $L = 0, 2, 4$, and 6 , respectively (Bott, 1989b; Chlond, 1994; and Table C1 of Holm, 1995). Substitution of Eq. (15) into (14) gives:

$$I_{i+1/2}^+ = \sum_{l=0}^L \frac{a_{i,l}^n}{(l+1)2^{l+1}} [1 - (1 - 2Cr_{i+1/2}^{n+1/2+})^{l+1}], \quad (17a)$$

$$I_{i+1/2}^- = \sum_{l=0}^L \frac{a_{i+1,l}^n}{(l+1)2^{l+1}} (-1)^l \times [1 - (1 - 2Cr_{i+1/2}^{n+1/2-})^{l+1}], \quad (17b)$$

for every i .

The shape-preservation property states that if the scalar variable is initially positive everywhere, it should remain so as it is transported in both space and time. That is, the scheme should be positive definite or preserve signs. Positive definiteness, according to Eq. (6) together with Eq. (12), requires that:

$$C_i^n - \frac{\Delta t}{\Delta x} (\bar{f}_{i+1/2}^+ + \bar{f}_{i-1/2}^-) + \frac{\Delta t}{\Delta x} (\bar{f}_{i+1/2}^- + \bar{f}_{i-1/2}^+) \geq 0, \quad (18)$$

where the third and fourth terms on the left-hand side of Eq. (18) represent the total outgoing and the total incoming fluxes to computational cell i , respectively. Note that $\bar{f}_{i\pm 1/2}^\pm$ should be non-negative everywhere, and $\bar{f}_{i\pm 1/2}^- = 0 \quad \forall \quad v_{i\pm 1/2}^{n+1/2} \geq 0$ and $\bar{f}_{i\pm 1/2}^+ = 0 \quad \forall \quad v_{i\pm 1/2}^{n+1/2} \leq 0$. Making use of these desirable properties, the fact that

only out-fluxes can decrease the value of the left-hand-side of Eq. (18), and substituting Eq. (13) for $\bar{f}_{i\pm 1/2}^\pm$, one obtains the following sufficient condition for Eq. (18):

$$I_{i+1/2}^+ + I_{i-1/2}^- \leq C_i^n. \quad (19)$$

which establishes upper bounds on the integrals $I_{i+1/2}^\pm$. Lower bounds on $I_{i+1/2}^\pm$ are

$$I_{i+1/2}^\pm \geq 0. \quad (20)$$

Conditions (19)–(20) hold if either the order L of polynomials in Eq. (15) is equal to 0 (piece-wise step representation) or 1 (linear interpolation) (Bott, 1989a). The use of polynomials of order $L \geq 2$, however, may result in $\hat{C}[x, t_n]$ values being negative between grid points, particularly near steep concentration fronts (Bott, 1989a,b, 1992). This may result in negative values or exceedingly large values in $I_{i+1/2}^\pm$, depending on values of $Cr_{i+1/2}^{n+1/2\pm}$, which in turn may lead to undesirable evolution of negative scalar concentration values of C . To preserve positive definiteness, Bott (1989a) proposed use of the modified advective fluxes given by

$$\bar{f}_{i+1/2} = \frac{\Delta x}{\Delta t} (\beta_i^n \tilde{I}_{i+1/2}^+ - \beta_{i+1}^n \tilde{I}_{i+1/2}^-), \quad (21)$$

where

$$\beta_i^n = \{1, \quad \forall \quad \tilde{I}_{i+1/2}^+ + \tilde{I}_{i+1/2}^- \leq C_i^n,$$

$$C_i^n / (\tilde{I}_{i+1/2}^+ + \tilde{I}_{i+1/2}^-), \quad \forall \quad \tilde{I}_{i+1/2}^+ + \tilde{I}_{i+1/2}^- > C_i^n,$$

$$\tilde{I}_{i+1/2}^\pm = \max\{I_{i+1/2}^\pm, 0\},$$

for every i . Given discrete cell concentrations C_i^n at time level t_n , the desired cell concentrations C_i^{n+1} are conveniently evaluated using the explicit formula in Eq. (6) following the substitution of Eq. (21). To maintain numerical stability, it is necessary that the CFL criterion $Cr_{i+1/2}^{n+1/2+} + Cr_{i-1/2}^{n+1/2-} \leq 1$ be satisfied at every i for all time.

Because of the use of polynomial fitting for local variations of the scalar concentration field, and application of flux limitations, Bott's scheme conserves mass, is positive definite, accurate, and exhibits very low numerical dispersion. It is also computationally efficient

Table 1

Coefficients $\beta_{l,m}$ ($l = 0, 1, \dots, L$; $m = -L/2, -L/2+1, \dots, 0, L/2-1, L/2$) for polynomials of degrees $L = 0, 2, 4$, and 6

	$L = 0, m = 0$	$L = 2, m = -1, 0, 1$	$L = 4, m = -2, -1, 0, 1, -2$	$L = 6, m = -3, -2, -1, 0, 1, 2, 3$
$\beta_{0,m}$	1			
$\beta_{1,l}$		(-1, 26, -1)/24	(9, -116, 2134, -116, 9)/1920	(-75, 954, -7621, 121 004, -7621, 954, -75)/107 520
$\beta_{2,l}$		(-1, 0, 1)/2	(5, -34, 0, 34, -5)/48	(-259, 2236, -9455, 0, 9455, -2236, 259)/11 520
$\beta_{3,m}$		(1, -2, 1)/2	(-3, 36, -66, 36, -3)/48	(111, -1386, 10 305, -18 060, 10 305, -1386, 111)/11 520
$\beta_{4,m}$			(-1, 2, -2, 1)/12	(7, -52, 83, 0, -83, 52, -7)/288
$\beta_{5,l}$			(1, -4, 6, -4, 1)/12	(-5, 54, -171, 244, -171, 54, -5)/576
$\beta_{6,m}$				(-1, 4, -5, 0, 5, -4, 1)/240
				(1, -6, 15, -20, 15, -6, 1)/720

because it is an explicit scheme. The scheme reduces to the conventional first-order upstream approach if the order L of the polynomial is zero. There have been a number of modified versions of Bott's schemes (Bott, 1992; Easter, 1992; Chlond, 1994), though they all focused on pure advective transport equations without source terms. In the next section, we extend this scheme to a more general advection–dispersion equation with a source term.

3. Theory

In what follows, we will focus on the conservative form of the one-dimensional advection–dispersion equation with source terms described by

$$\frac{\partial C}{\partial t} + \frac{\partial vC}{\partial x} - \frac{\partial}{\partial x} D \frac{\partial C}{\partial x} = q[x, t] + r[C], \quad (22)$$

where $D = D[x, t]$ is the dispersion coefficient; $r[C]$ and $q[x, t]$ are source terms representing, respectively, the concentration-dependent and -independent parts. Other terms are the same as those defined previously in Eq. (1). The decomposition of the source term into these two parts is made because the numerical treatment of these two terms, as will be seen later, will be quite different. In practical applications, for example, $r[C]$, if negative, could represent degradation, decay, irreversible adsorption, withdrawals from wells, and if positive, it could represent growth or irreversible desorption. $q[x, t]$ Represents an external forcing function. If this forcing function is a pulse injection at location x_0 and time t_0 , for example,

$q[x, t]$ is represented by

$$q[x, t] = V_0 C_0 \delta[x - x_0] \delta[t - t_0], \quad (23)$$

where V_0 is the volume of fluid injected per unit cross section area [L^3/L^2], and C_0 is the concentration of this component in the injected fluid.

3.1. Control-volume discretization

Applying a control-volume discretization to Eq. (22) in a manner similar to Eq. (1) gives for any finite control-volume i ($i = 1, 2, \dots, M$),

$$\begin{aligned} & \frac{C_i^{n+1} - C_i^n}{\Delta t} + \frac{\bar{f}_{i+1/2} - \bar{f}_{i-1/2}}{\Delta x} - \frac{1}{\Delta x} \\ & \times \left\{ \left(D \frac{\partial C}{\partial x} \right)_{i+1/2} - \left(D \frac{\partial C}{\partial x} \right)_{i-1/2} \right\} \\ & = \bar{q}_i + \bar{r}_i, \end{aligned} \quad (24)$$

where C_i^{n+1} and $\bar{f}_{i+1/2}$ are as defined in Eqs. (7) and (8),

respectively $(\overline{D \partial C / \partial x})_{i+1/2}$ is the time-averaged dispersive flux through the right boundary of cell i , \bar{r}_i and \bar{q}_i are the time- and control-volume-averaged source terms at cell i . The dispersive flux and integrated source terms are given by

$$\left(D \frac{\partial C}{\partial x} \right)_{i+1/2} = \frac{1}{\Delta t} \int_{t_n}^{t_n + \Delta t} \left(D \frac{\partial c}{\partial x} \right)_{x_i + \Delta x/2} dt, \quad (25a)$$

$$\bar{q}_i = \frac{1}{\Delta x \Delta t} \int_{t_n}^{t_n + \Delta t} \int_{x_i - \Delta x/2}^{x_i + \Delta x/2} q[x, t] dx dt, \quad (25b)$$

$$\bar{r}_i = \frac{1}{\Delta x \Delta t} \int_{t_n}^{t_n + \Delta t} \int_{x_i - \Delta x/2}^{x_i + \Delta x/2} r dx dt. \quad (25c)$$

3.2. Integrated advective fluxes

For the sake of comparison, we present two alternatives for approximating the integrated advective fluxes. One is the hybrid approach. The other is Bott's upstream-biased Eulerian advection scheme.

3.2.1. Hybrid scheme

The hybrid approach for approximating integrated advective fluxes switches between the conventional first-order upstream scheme and the time-weighting central difference scheme, depending on the magnitude of the Peclet number defined by $Pe = \text{sfnc}; v_{i+1/2}^{n+1/2} \Delta x \text{sfnc}; / D_{i+1/2}^{n+1/2}$. Here $D_{i+1/2}^{n+1/2}$ is the dispersion coefficient evaluated at the interface between cell i and $i+1$ averaged over the time interval $[t_n, t_n + \Delta t]$. When advection dominates or $Pe \geq 2$, the conventional first-order upstream difference scheme in its explicit form is employed; when dispersion dominates or $Pe < 2$, however, the usual central difference scheme, which is of second-order accuracy, is adopted. A time-weighting central difference scheme is of the form

$$\begin{aligned} \bar{f}_{i+1/2} = v_{i+1/2}^{n+1/2} \left\{ (1 - \omega) \frac{C_{i+1}^n - C_i^n}{\Delta x} \right. \\ \left. + \omega \frac{C_{i+1}^{n+1} - C_i^{n+1}}{\Delta x} \right\}, \end{aligned} \quad (26)$$

where $0 \leq \omega \leq 1.0$ is a weighting factor, with $\omega = 0$ denoting a fully explicit scheme, $\omega = 1$ a fully implicit scheme, with other values of ω denoting a scheme somewhere in between these two.

3.2.2. Bott's upstream-biased Eulerian advection scheme

Because of the presence of dispersion and source terms, the shape preserving property $C[x, t_n + \tau] = C[x - v\tau, t_n]$ invoked by Bott's scheme no longer holds

in the strict sense. Nonetheless, as a local approximation during a small time step and for advection-dominated transport, we assume that this is adequate. Therefore, Bott's advection scheme (12)–(17), can be employed to approximate the integrated advective fluxes $\bar{f}_{i+1/2}$. Flux limiters developed by Bott (1989a) for $\bar{f}_{i+1/2}$ in Eq. (21) are no longer sufficient for preserving signs. Effects from dispersion and sources, however, have to be taken into account. We will discuss this issue later in this section.

3.3. Integrated dispersive fluxes

To approximate the integrated dispersive fluxes, we use the time-weighting scheme

$$\begin{aligned} \left(D \frac{\partial C}{\partial x} \right)_{i+1/2} &= (1 - \omega) D_{i+1/2}^n \frac{C_{i+1}^n - C_i^n}{\Delta x} + \omega D_{i+1/2}^{n+1} \\ &\quad \times \frac{C_{i+1}^{n+1} - C_i^{n+1}}{\Delta x}, \end{aligned} \quad (27)$$

where $D_{i+1/2}^n$ and $D_{i+1/2}^{n+1}$ are the dispersion coefficients evaluated at the interface $x_{i+1/2}$ at time levels t_n and t_{n+1} , respectively; $0 \leq \omega \leq 1$ is the time-weighting factor, with $\omega = 0$ denoting a fully explicit scheme, $\omega = 1$ a fully implicit scheme, and $\omega = 1/2$ the Crank–Nicolson implicit scheme.

3.4. Integrated source terms

The source terms in Eqs. (25b) and (25c) involve control-volume averaging over $[x_{i-1/2}, x_{i+1/2}]$ and time-averaging over $[t_n, t_n + \Delta t]$. We assume that the functional form of $q[x, t]$ is known a priori; hence the evaluation of the concentration-independent part $\overline{\langle q \rangle}_i$ is trivial. Our main focus is, therefore, on evaluation of the integrated concentration-dependent term $\overline{\langle r \rangle}_i$, defined by Eq. (25c). In what follows we present two alternatives for evaluating $\overline{\langle r \rangle}_i$.

3.4.1. A time-weighting method

In the first method we use a time-weighting scheme, i.e.

$$\overline{\langle r \rangle}_i = (1 - \omega) r_i^n + \omega r_i^{n+1}, \quad (28)$$

where r_i^{n+1} is approximated by $r[C_i^{n+1}]$. The use of Eq. (28) will result in a discrete, non-linear system of equations in terms of the unknowns C_i^{n+1} should $\omega \neq 0$ and $r[C]$ vary with C in a non-linear fashion. Should this be the case, linearization has to be performed for Eq. (27). There are, in general, two linearization techniques, Picard iteration and Newton–Raphson iteration.

In the Picard iteration, Eq. (28) is linearized around $C_i^{n+1,m}$ to give

$$\overline{\langle r \rangle}_i = (1 - \omega) r[C_i^n] + \omega r[C_i^{n+1,m}] \quad (29)$$

where m is the current iteration level, and $C_i^{n+1,m}$ is supposedly to have been calculated. The unknown concentrations C_i^{n+1} elsewhere in the discrete transport equation will be replaced by $C_i^{n+1,m+1}$.

When $r[C]$ exhibits strong non-linearity in C , Newton–Raphson iteration may be preferred to that of Picard iteration. Application of this linearization technique for Eq. (28) leads to

$$\begin{aligned} \overline{\langle r \rangle}_i &= (1 - \omega) r[C_i^n] + \omega r[C_i^{n+1,m}] + \omega r'[C_i^{n+1,m}] \\ &\quad \times (C_i^{n+1,m+1} - C_i^{n+1,m}), \end{aligned} \quad (30)$$

which contains the unknown concentrations $C_i^{n+1,m+1}$.

3.4.2. Upstream-biased Eulerian algorithm

The second method for evaluating $\overline{\langle r \rangle}_i$, which will be termed the upstream biased Eulerian scheme, draws ideas from Bott's upstream biased scheme for evaluation of integrated advective fluxes. To proceed we first linearize $r[C]$ around C_i^n , the known concentration in cell i at time level t_n , to obtain

$$\begin{aligned} r[C] &= r[C_i^n] + r'[C_i^n](C - C_i^n) \\ &= r[C_i^n] - r'[C_i^n]C_i^n + r'[C_i^n]C, \end{aligned} \quad (30')$$

where $r'[C_i^n]$ is the first derivative of $r[C]$ evaluated at C_i^n . Assuming that the polynomial (15) has been fitted to describe the local variation of C between grid points, and the shape preserving property $C[x_i, t_n + \tau] = C[x_i - v_i^{n+1/2}\tau, t_n]$ holds, in an approximate sense, locally during the time interval $[t_n, t_{n+1}]$, we substitute Eq. (30) into Eq. (25c) to obtain:

$$\overline{\langle r \rangle}_i = r[C_i^n] - r'[C_i^n]C_i^n + r'[C_i^n]\bar{C}_i, \quad (31)$$

where

$$\bar{C}_i = \frac{1}{\Delta t} \int_0^{\Delta t} \hat{C}[x_i - v_i^{n+1/2}\tau, t_n] d\tau. \quad (32)$$

Here $v_i^{n+1/2}$ is the value of v in cell i averaged over the time interval $[t_n, t_{n+1}]$, which can be estimated by taking the arithmetic average of $v_{i+1/2}^{n+1/2}$ and $v_{i-1/2}^{n+1/2}$. When $v_i^{n+1/2} = 0$, Eq. (32) reduces to C_i^n . Now considering the case $v_i^{n+1/2} \neq 0$, we rewrite Eq. (32) as

$$\bar{C}_i = \frac{1}{v_i^{n+1/2} \Delta t} \int_0^{\Delta t} \hat{C}[x_i - v_i^{n+1/2}\tau, t_n] v_i^{n+1/2} d\tau, \quad (33)$$

which upon the substitution $x' = x_i - v_i^{n+1/2}\tau$ reduces to

$$\bar{C}_i = \frac{1}{v_i^{n+1/2} \Delta t} \int_{x_i - v_i^{n+1/2} \Delta t}^{x_i} \hat{C}[x', t_n] dx'. \quad (34)$$

To evaluate the integral on the RHS of Eq. (34), we follow a similar procedure as that used by Bott (1989a) in evaluating the advective fluxes $\tilde{f}_{i+1/2}$. Let $Cr_i^{n+1/2} = v_i^{n+1/2} \Delta t / \Delta x$ be the Courant number associated with the velocity at x_i . It is then decomposed into a sum of its non-negative and non-positive parts or $Cr_i^{n+1/2} = Cr_i^{n+1/2+} - Cr_i^{n+1/2-}$ with $Cr_i^{n+1/2+} = \max\{0, Cr_i^{n+1/2}\}$ and $Cr_i^{n+1/2-} = -\min\{0, Cr_i^{n+1/2}\}$. In particular, we note that the contributing cell to the integral in Eq. (34) is cell i only for $-1/2 \leq Cr_i^{n+1/2} \leq 1/2$; however, the contributing cells become cells i and $i-1$ for $1/2 < Cr_i^{n+1/2} \leq 1$, and become cells i and $i+1$ for $-1 \leq Cr_i^{n+1/2} < -1/2$. Using these normalized notations and paying attention to the range of integrals we simplify Eq. (34) to:

$$\bar{C}_i = \begin{cases} \frac{I_i^+ + I_i^-}{Cr_i^{n+1/2+} + Cr_i^{n+1/2-}}, & v_i^{n+1/2} \neq 0, \\ C_i^n, & v_i^{n+1/2} = 0, \end{cases} \quad (35)$$

where the integrals I_i^+ and I_i^- are given by:

$$I_i^+ = \int_{\min\{1-Cr_i^{n+1/2+}, 1/2\}}^{1/2} \hat{C}[\xi[i-1], t_n] d\xi[i-1] + \int_{\max\{-Cr_i^{n+1/2+}, -1/2\}}^0 \hat{C}[\xi[i], t_n] d\xi[i], \quad (36a)$$

$$I_i^- = \int_0^{\min\{Cr_i^{n+1/2-}, 1/2\}} \hat{C}[\xi[i], t_n] d\xi[i] + \int_{-1/2}^{\max\{Cr_i^{n+1/2-}, -1/2\}} \hat{C}[\xi[i+1], t_n] d\xi[i+1]. \quad (36b)$$

By definition, $Cr_i^{n+1/2+} = I_i^+ = 0 \quad \forall v_i^{n+1/2} \leq 0$, $Cr_i^{n+1/2-} = I_i^- = 0 \quad \forall v_i^{n+1/2} \geq 0$, I_i^+ and I_i^- are non-negative. The first integral on the RHS of Eq. (36a) vanishes should $Cr_i^{n+1/2+} \leq 1/2$, the second integral on the RHS of Eq. (36b) goes to 0 should $Cr_i^{n+1/2-} \leq 1/2$, and only one of I_i^+ and I_i^- can be nonzero at a time. Substitution of (15) into (36) yields:

$$I_i^+ = \sum_{l=0}^L (-1)^l \frac{a_{i,l}^n}{l+1} (Cr_i^{n+1/2+})^{l+1}, \quad (37a)$$

$$\begin{aligned} & \forall Cr_i^{n+1/2+} \leq 1/2, \\ I_i^+ &= \sum_{l=0}^L \frac{1}{(l+1)2^{l+1}} \\ & \times \{(-1)^l a_{i,l}^n + a_{i-1,l}^n [1 - (2 - 2Cr_i^{n+1/2})^{l+1}]\}, \\ & \forall 1/2 < Cr_i^{n+1/2+} \leq 1, \end{aligned} \quad (37b)$$

$$I_i^- = \sum_{l=0}^L \frac{a_{i,l}^n}{l+1} (Cr_i^{n+1/2-})^{l+1}, \quad \forall Cr_i^{n+1/2-} \leq 1/2, \quad (37c)$$

$$\begin{aligned} I_i^- &= \sum_{l=0}^L \frac{1}{(l+1)2^{l+1}} \\ & \times \{a_{i,l}^n + (-1)^l a_{i+1,l}^n [1 - (2 - 2Cr_i^{n+1/2-})^{l+1}]\}, \\ & \forall 1/2 < Cr_i^{n+1/2-} \leq 1 \end{aligned} \quad (37d)$$

Because the upstream biased Eulerian algorithm is explicit in its approximation to both the advective fluxes and the concentration-dependent source terms, the use of this scheme makes the proposed numerical scheme explicit if the dispersive fluxes can be evaluated explicitly or if dispersion is absent.

3.5. Nonlinear iterations

Nonlinear iterations, when necessary, proceed as follows. During each new time step $n+1$, we set the initial guess value to that at the end of previous time step, or $C_i^{n+1,0} = C_i^n$. Next, the desired approximations to the integrated advective fluxes, dispersive fluxes, and the concentration-dependent source term are substituted into Eq. (23). This usually leads to a discrete, tridiagonal system of algebraic equations that can be rewritten in terms of the incremental concentrations $\delta C_i^{n+1,m+1} (= C_i^{n+1,m+1} - C_i^{n+1,m})$ instead of $C_i^{n+1,m+1}$. The well-known Thomas algorithm is then employed to solve the resulting tridiagonal system of algebraic equations. The iteration continues for $m=0, 1, 2, \dots$, until some norm measure of $\delta C_i^{n+1,m+1}$ or other quantities such as residuals associated with the discrete system of equations is less than a prescribed tolerance level. Upon convergence we set $C_i^{n+1} = C_i^{n+1,m}$. The above procedure is repeated for time steps, $n=1, 2, \dots$, until some maximum simulation time is reached.

3.6. Flux and source limitations

As stated earlier, higher-order schemes for advection-dominated problems often introduce the undesirable non-physical oscillations which manifest as negative concentrations when background concentrations are zero. The concept of flux limitation was first proposed by Boris and Book (1973) as one of the critical steps in their FCT algorithm. It has since been further generalized by Zalesk (1979) for multidimensional cases. The purpose of flux limitation was to ensure that the associated advection schemes produce no oscillation in general, and no negative concentrations in particular. The concept was employed by Bott (1989a,b) to ensure positive definiteness of his advection scheme. Based on the monotone property of pure advection transport, Bott (1992) further developed flux limiters that are capable of eliminating oscillations in general, and

negative concentrations in particular. Drawing ideas from the concept of flux limitation, we propose below the flux and source limiters to preserve positivity of the concentration fields in the presence of dispersion and sources.

To ensure non-negative evolution of the scalar concentration field, it is sufficient that during each time step and in each computational cell, the sum of mass losses through concentration-dependent sources and outgoing advective and dispersive fluxes must be no greater than the mass available at the beginning of the time step. Should this condition be violated, we multiply the mass loss term and outgoing advective and dispersive fluxes by a positive number β ($0 \leq \beta \leq 1.0$) such that the above condition is exactly met, that is, the sum of mass losses and outgoing fluxes is equal to the mass available at beginning of the time step. Note that the limitation of outgoing fluxes from one cell is equivalent to the limitation of incoming fluxes to a neighboring cell. In situations where at least one of the schemes for evaluating advective fluxes, dispersive fluxes, and concentration-dependent source terms are implicit, iterations have to be performed in order to estimate the outgoing fluxes or mass losses through the source terms during a time step. For a detailed derivation of the flux and source limiters, one is referred to [Appendix A](#).

It is important to understand that the flux and source limiters proposed herein cannot guarantee that non-physical oscillations will not be produced when non-zero background concentrations are present. It merely ensures that the associated numerical scheme does not generate negative concentrations. Development of a comprehensive flux and source limiters for eliminating oscillations altogether is a future research topic.

The combination of Bott's upstream biased Eulerian advection scheme (12)–(17) for integrated advective fluxes, the upstream-biased Eulerian integration algorithm (30)–(37) for the integrated concentration-dependent source term, the two-level time-weighting scheme (27) for integrated dispersive fluxes, and flux and source limitations, will be called upstream-biased, Eulerian algorithm for transport equations with sources (UpBEATES) scheme. The combination of hybrid method for advection, two-level time-weighting schemes for both dispersion and the concentration-dependent source term, will be termed the conventional hybrid scheme; which in the absence of dispersion will be reduced to the first-order upstream scheme.

4. Numerical examples

In this section, we present numerical results to examine the performance of the newly proposed numerical scheme UpBEATES in comparison with those given by the conventional schemes. All results will be com-

pared against analytical solutions. We consider two different types of numerical experiments. One is the advective transport of a scalar concentration with a decay source. The other is an advection–dispersion transport of a reactive species through a porous medium subject to equilibrium controlled sorption and an injection source.

4.1. Advective transport with decay source

We first consider an advection problem with decay in a constant velocity field. The domain is 200 m in length. It is discretized into 200 computational cells with $\Delta x = 1$ m. Velocity is $v = 1$ m/day. Since decay is the only source term, it is written $r[C] = -r_0 C$, where r_0 is the first-order decay rate (day^{-1}). In the experiments that follow, decay rates of $r_0 = 0$, 0.005, and 0.01 are considered. To be realistic, we examine the performance of the numerical schemes under three different Courant numbers, $Cr = 0.2$, 0.5 and 0.8. We compare the performance of the UpBEATES scheme (with the order of polynomials equal to $L = 4$) with that of the conventional center-difference (with a time-weighting factor of $\omega = 0.5$) and the upstream schemes. Peclet number $Pe = \infty$ because of the absence of dispersion.

We consider two test problems. One is the transport of a rectangle-shaped plume. The other is a triangle-shaped plume. The analytical solutions for these two types of test problems are easily found to be the translation of the initial plume plus exponential decay in the amplitudes. Free boundary conditions at both boundary points are assumed.

[Fig. 1](#) shows the initial condition (at $t = 0$) and analytical and numerical solutions of the transport and decay of the rectangle-shaped plume at day 50 and 100 for the three decay rates and three Courant numbers. This test problem shows a numerical scheme's capability to handle sharp concentration fronts and Gibbs oscillations that arise in the vicinity of discontinuities ([Chlond, 1994](#)). We observe that the UpBEATES scheme is in general dispersion-free, and does not produce negative concentrations that is typical of other higher-order advection schemes. It is also not sensitive to the values of Courant numbers. This is extremely desirable in cases where the flow field is heterogeneous and one has no control over the Courant numbers. The first-order upstream scheme, though it does not generate oscillation, exhibits high numerical dispersion, especially as the Courant number decreases and time increases. This makes it useless when modeling advection-dominated problems.

[Fig. 2](#) depicts the performance of the two numerical schemes for a triangle-shaped initial condition. This case should test a numerical scheme's capability to treat sharp peaks and extreme concentrations ([Chlond, 1994](#)). In this case, the UpBEATES scheme performs extremely

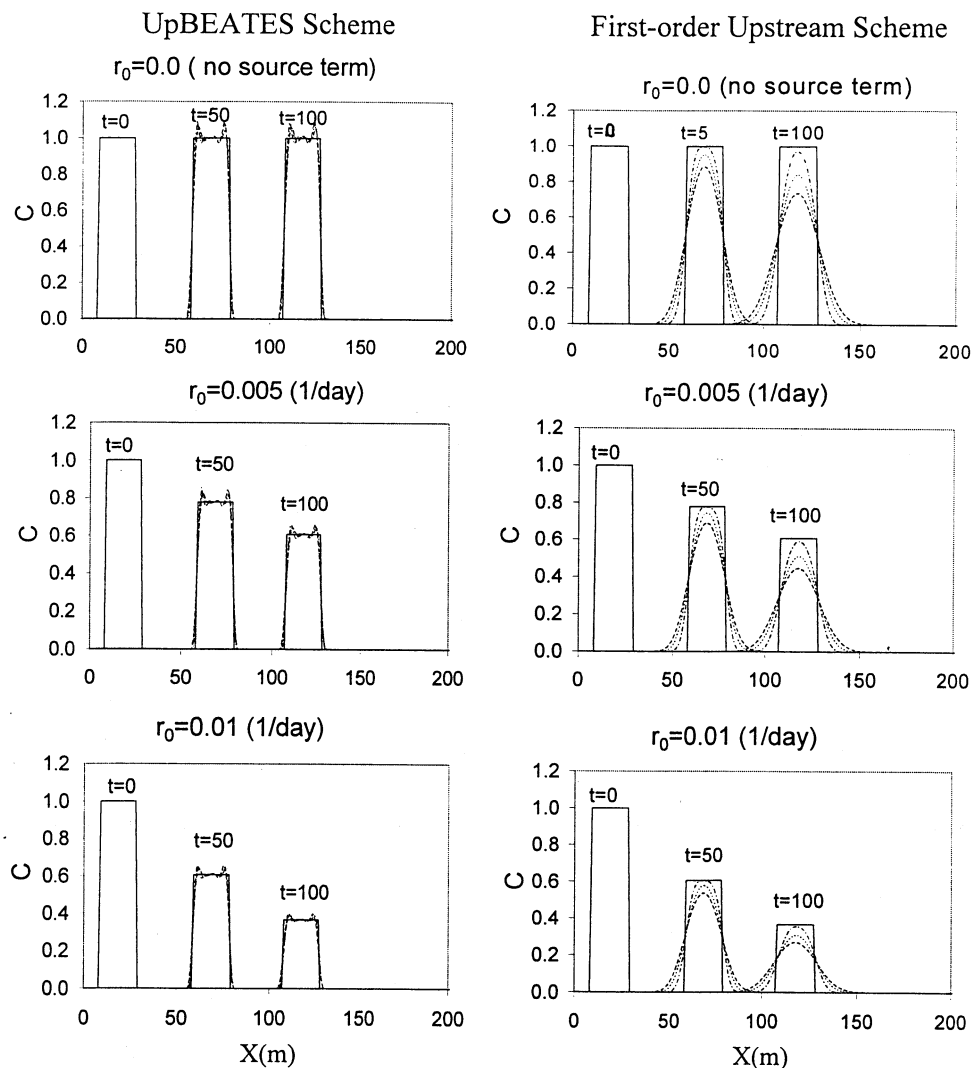


Fig. 1. Solution of the 1-D advection equation with a linear decay term for $v = 1$ m/day and a decay rate r_0 . Initial concentration distribution is a rectangle. Domain is discretized into 200 computational cells, with cell size of 1 m. Shown are the solutions after $t = 50$ and 100 days for decay rates of $r_0 = 0$ (first row), 0.005 (middle row) and 0.01 (third row), and courant numbers $Cr = 0.2$ (long dashed line), 0.5 (dotted line) and 0.8 (dot-dashed line), respectively. Left column is result obtained using UpBEATES scheme (with $L = 4$), while right column is the first-order upstream scheme. Solid lines correspond to the analytical solution.

well. There are essentially no dispersive ripples or oscillation, and no numerical dispersion. Again the scheme is insensitive to magnitudes of the Courant number. The first-order upstream scheme again exhibits too much numerical dispersion, is very sensitive to values of the Courant number, and it does not capture the peak well. The problems manifest themselves through underestimation of the peak concentration, and overestimation of the extent of the concentration plume.

4.2. Advection–dispersion transport with injection, decay and sorption

We now examine an advection–dispersion transport problem subject to decay, injection, and equilibrium-

controlled sorption. The test problem is closely related to an advection–dispersion transport model used by [Harvey and Garabedian \(1991\)](#) in studying bacterial movement through contaminated sandy aquifers. We are primarily interested in their model and analytical solutions rather than the transport behavior of bacterial cells. The modified version of their model is of the form:

$$\frac{\partial \theta R_d C}{\partial t} + \frac{\partial v \theta C}{\partial x} - \frac{\partial}{\partial x} \left(\theta D \frac{\partial C}{\partial x} \right) = -r_0 C + V_0 C_0 \delta[x - x_0] \delta[t - t_0]. \quad (38)$$

In the equation above, θ (porosity) = 0.35; R_d (retardation) varies between 1.0 (no retardation) and 1.3; $v = 0.335$ m/day, $D = 0.737$ m²/day, r_0 (decay rate) varies between 0 and 0.0768825 (day⁻¹) (here we have

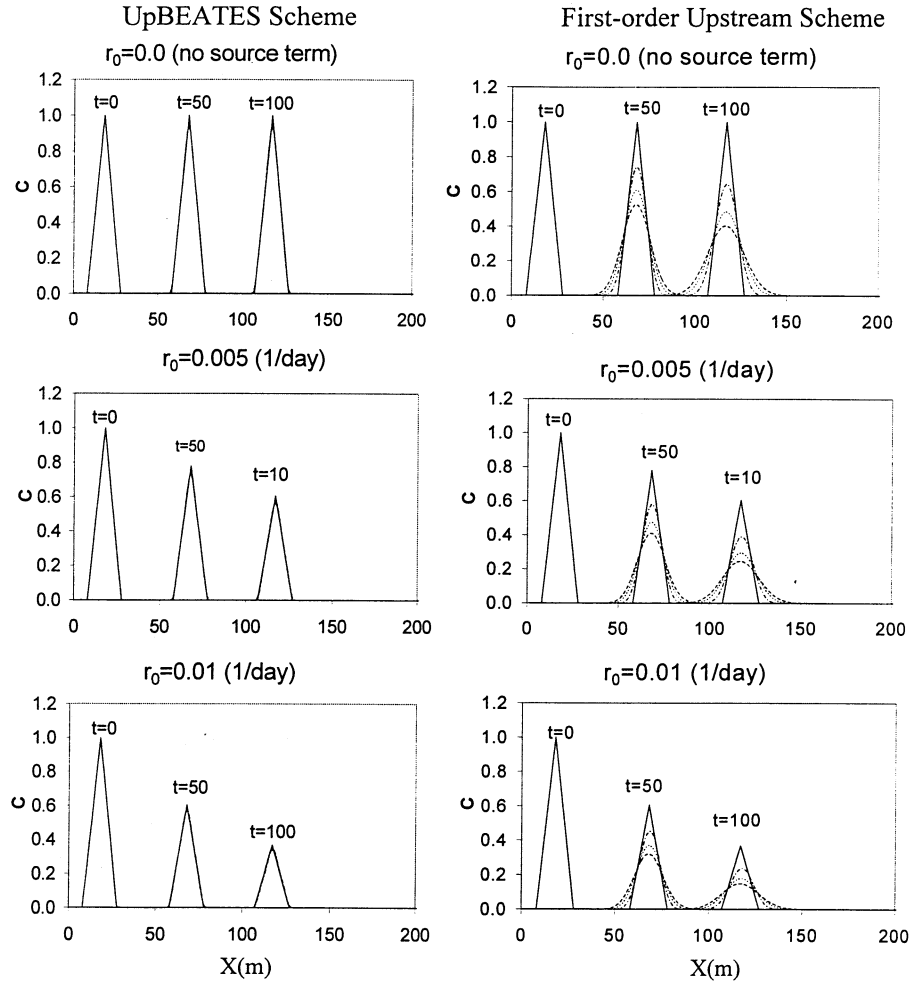


Fig. 2. As in Fig. 1 except that the initial condition is a triangle instead of a rectangle.

interpreted the irreversible filtration in Harvey & Garabedian, 1991 as a decay loss); and $V_0 = 0.17843$ (m^3/m^2). The definitions of other terms are the same as those defined in Eqs. (22) and (23).

The computational domain was chosen large enough to eliminate any effect from boundary conditions. We chose a computational cell size of $\Delta x = 0.1$ m. The time-step size Δt is chosen such that the Courant number $Cr = 0.5$. The Peclet number is $Pe = 4.5$, which indicates advection domination. A two-level time-weighting scheme is adopted for the dispersive flux with a weighting coefficient of $\omega = 0.5$. We are interested in the breakthrough curves 6.8 m downstream of the injection point.

The analytical solution for the breakthrough curve observed at a distance d downstream of the injection point is (Harvey & Garabedian, 1991):

$$\frac{C[x_0 + d]}{C_0} = \frac{V_0}{\theta R_d \sqrt{4\pi D(t - t_0)/R_d}}$$

$$\exp\left[-\frac{(x_0 + d - vt/R_d)^2}{4Dt/R_d} - r_0/R_d\right]. \quad (39)$$

Fig. 3 illustrates breakthrough curves calculated by the UpBEATES scheme (with $L = 4$) and the conventional hybrid scheme for three combinations of retardation factors R_d and decay rates r_0 : (a) $R_d = 1.0$ (no retardation) and $r_0 = 0$ (no decay); (b) $R_d = 1.0$ (no retardation) and $r_0 = 0.0768825$ (day^{-1}); and (c) $R_d = 1.3$ and $r_0 = 0.0768825$ (day^{-1}). The UpBEATES scheme performs very well in all cases, without exhibiting numerical dispersion, and without overshooting and undershooting. The conventional hybrid scheme behaves poorly in all three cases.

5. Conclusions

We have developed a scheme for solving a scalar advection-dominated transport equation with source terms. The method is an extension of Bott's area-preserving, positive definite, integrated flux-form advec-

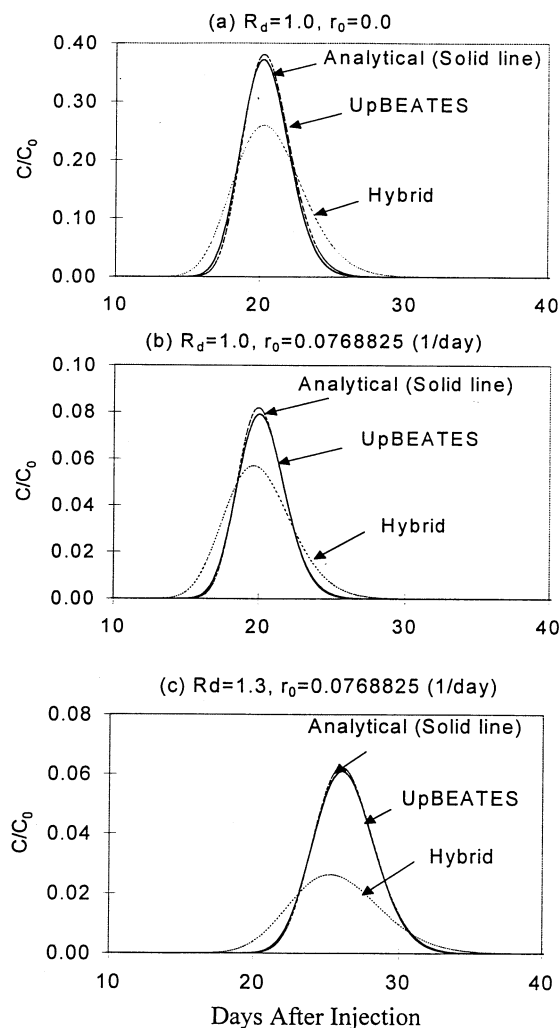


Fig. 3. Solution of an advection–dispersion transport equation subject to decay, equilibrium sorption and pulse injection. Shown are break-through curves at a distance $d = 6.8$ m downstream of the injection location determined using the various numerical schemes as indicated in the figure. $R_d = 0$ corresponds to no sorption. $r_0 = 0$ corresponds to no decay.

tion scheme designed for pure advection equations (Bott, 1989a,b). A control volume approach is used for spatial discretization. Integration over time is then used to obtain a discrete, integrated-flux and integrated-source form conservative equation. Bott's advection scheme is employed to approximate integrated advective fluxes. A time-weighting scheme was proposed for evaluating the integrated dispersive fluxes. Source terms were decomposed into concentration-independent and concentration-dependent parts. An upstream-biased Eulerian algorithm was proposed for evaluating the integrated concentration-dependent source term. A flux and source limitation procedure was developed for ensuring non-negative evolution of the scalar concentration field. The proposed scheme is mass-conservative, produces non-negative concentration values, exhibits

very low numerical dispersion, and is computationally very efficient for advection-dominated problems. It represents a significant improvement over the conventional upstream and hybrid approaches. Numerical experiments also show that the performance of the newly developed scheme matches that of the analytical solution very well for the test problems.

One shortcoming of the proposed UpBEATES scheme is that it cannot avoid non-physical oscillations when extremely steep concentration gradients are involved, as in the case with rectangle-shaped initial concentration. This is because the flux and source limiters were developed to eliminate negative concentrations only. This issue is to be addressed in future research. Douglas and co-workers' MMOCOA procedure is an alternative approach that may also be useful for solving these problems (Douglas et al., 2000).

Although the scheme was developed for a one-dimension advection-dominated equation (with sources and biological/chemical reaction terms), extension to a multidimensional transport equation can be accomplished through operator splitting (Yanenko, 1971). For example, MacQuarrie, Sudicky and Frind, (1990) used an iterative principal direction finite-element method in solving the problems of biodegradation of organic contaminants in groundwater. Efficiency was obtained by decoupling the two-dimensional transport equations into a series of one-dimensional equations. This will work for some 2-D problems with simplified flow conditions. However, the key to this scheme is to track the velocity direction, which is trivial in one dimension, but more challenging in two- or three-dimensions because the characteristic equations are much more difficult to solve. Extension of upstream-biased Eulerian schemes such as this one to multi-dimensional space may not be as straightforward as it seems. As pointed out by LeVeque and Yee (1990) such methods are characterized by the fact that the speed and direction in which the PDVs propagate must be known *a priori* before the interpolation points can be chosen. The interpolation will then be located in the upstream direction where the transported constituent is arriving. In the case of a scalar advection–dispersion equation, the direction the concentration propagates is in line with the sign of the local advective velocity. For multi-dimensional problems, however, the propagating direction and speed of each species may not, in general, agree with that of the corresponding local velocity because of the potential coupling effect through the storage term. Under some general conditions, it can be shown that the direction in which characteristic PDVs propagate are in line with the local advective velocities. For these special situations, the extension to higher order dimensions is more straightforward.

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Appendix A: Derivation of flux and source limiters

To facilitate the derivation of the constraints for non-negative evolution of the concentration field, we linearize the integrated advective fluxes $\bar{f}_{i+1/2}$ around values at the previous iteration m . They are rewritten

$$\bar{f}_{i+1/2} = \bar{f}_{i+1/2}^m + \delta \bar{f}_{i+1/2}^{m+1}, \quad (\text{A.1})$$

where $\bar{f}_{i+1/2}^m$ and $\delta \bar{f}_{i+1/2}^{m+1}$ depend on the kind of advection schemes to be used. If the Bott's upstream biased Eulerian algorithm is used, $\bar{f}_{i+1/2}^m$ is given by Eqs. (12), (13), (14a), (14b), (15), (16), (17a) and (17b), while $\delta \bar{f}_{i+1/2}^{m+1} = 0$. If the hybrid scheme is adopted, and $Pe \geq 2$ (advection domination), $\bar{f}_{i+1/2}^m$ would be given by Eq. (9) and $\delta \bar{f}_{i+1/2}^{m+1} = 0$; however, if $Pe < 2$ (dispersion domination), it follows from Eq. (26) that

$$\bar{f}_{i+1/2}^m = v_{i+1/2}^{n+1/2} \left\{ (1-\omega) \frac{C_{i+1}^n - C_i^n}{\Delta x} + \omega \frac{C_{i+1}^{n+1,m} - C_i^{n+1,m}}{\Delta x} \right\}, \quad (\text{A.2})$$

$$\delta \bar{f}_{i+1/2}^{m+1} = v_{i+1/2}^{n+1/2} \omega \frac{\delta C_{i+1}^{n+1,m+1} - \delta C_i^{n+1,m+1}}{\Delta x}. \quad (\text{A.3})$$

Eq. (A.3) states that the incremental advective flux $\delta \bar{f}_{i+1/2}^{m+1}$ across the interface at $x_i + \Delta x/2$ is linearly related to $\delta C_{i+1}^{n+1,m+1}$ and $\delta C_i^{n+1,m+1}$, the unknown concentration increments associated with the concentrations in the two neighboring cells.

Define $\bar{g}_{i+1/2} = -(D\partial C/\partial x)_{i+1/2}$ as the integrated dispersive fluxes. According to Eq. (27) it can be decomposed into

$$\bar{g}_{i+1/2} = \bar{g}_{i+1/2}^m + \delta \bar{g}_{i+1/2}^{m+1}, \quad (\text{A.4})$$

where

$$\bar{g}_{i+1/2}^m = -D_{i+1/2}^{n+1/2} \left\{ (1-\omega) \frac{C_{i+1}^n - C_i^n}{\Delta x} + \omega \frac{C_{i+1}^{n+1,m} - C_i^{n+1,m}}{\Delta x} \right\},$$

$$\delta \bar{g}_{i+1/2}^{m+1} = -D_{i+1/2}^{n+1/2} \omega \frac{\delta C_{i+1}^{n+1,m+1} - \delta C_i^{n+1,m+1}}{\Delta x}. \quad (\text{A.5})$$

Similarly, the decomposition of the integrated concentration-dependent source term gives

$$\overline{\langle r \rangle}_i = \overline{\langle r \rangle}_i^m + \delta \overline{\langle r \rangle}_i^{m+1} \quad (\text{A.6})$$

where $\overline{\langle r \rangle}_i^m$ and $\delta \overline{\langle r \rangle}_i^{m+1}$ are dependent on the type of integration schemes for sources. For example, if the upstream biased Eulerian algorithm is chosen, $\overline{\langle r \rangle}_i^m$ is given by Eqs. (31)–(35), (36a), (36b), (37a) and (37b), and $\delta \overline{\langle r \rangle}_i^{m+1} = 0$. If, on the other hand, the time-weighting scheme (28) is selected, we have

$$\overline{\langle r \rangle}_i^m = (1-\omega)r[C_i^n] + \omega r[C_i^{n+1,m}], \quad (\text{A.7})$$

and according to Eqs. (29) and (30),

$$\delta \overline{\langle r \rangle}_i^{m+1} = 0 \quad \text{if Picard iteration}, \quad (\text{A.8})$$

$$\delta \overline{\langle r \rangle}_i^{m+1} = \omega r'[C_i^{n+1,m}] \delta C_i^{n+1,m+1} \quad (\text{A.9})$$

if Newton–Raphson iteration.

When iteration converges, $\delta \bar{f}_{i+1/2}^{m+1} = \delta \bar{g}_{i+1/2}^{m+1} = \delta \overline{\langle r \rangle}_i^{m+1} \approx 0$. Under this condition $\bar{f}_{i+1/2}^m$ and $\bar{g}_{i+1/2}^m$ would be the advective and dispersive fluxes, respectively, across the interface at $x_i + \Delta x$ averaged over the time interval $[t_n, t_n + \Delta t]$, and $\overline{\langle r \rangle}_i^m$ would be the time-averaged c-dependent source term; otherwise, they are simply the estimates of those averaged values.

Assume that C_i^n the cell concentrations at the previous time level are non-negative in every computational cell. To avoid negative evolution of the scalar concentration field, it is sufficient, according to mass balance for cell i at iteration level m , that

$$\begin{aligned} C_i^n + (\overline{\langle q \rangle}_i + \overline{\langle r \rangle}_i^m) \Delta t - \frac{\Delta t}{\Delta x} (\bar{f}_{i+1/2}^m - \bar{f}_{i-1/2}^m) - \frac{\Delta t}{\Delta x} \\ \times (\bar{g}_{i+1/2}^m - \bar{g}_{i-1/2}^m) \\ \geq 0. \end{aligned} \quad (\text{A.10})$$

To proceed, we first decompose the advective fluxes according to

$$\bar{f}_{i+1/2}^m = \bar{f}_{i+1/2}^{m+} - \bar{f}_{i+1/2}^{m-}, \quad (\text{A.11})$$

where $\bar{f}_{i+1/2}^{m+}$ and $\bar{f}_{i+1/2}^{m-}$ are the positive and non-negative parts of the estimated advective fluxes $\bar{f}_{i+1/2}^m$ across the interface between cell i and $i+1$ averaged over the time interval $[t_n, t_n + \Delta t]$. Similar decomposition can be made about the dispersive flux $\bar{g}_{i+1/2}^m$,

$$\bar{g}_{i+1/2}^m = \bar{g}_{i+1/2}^{m+} - \bar{g}_{i+1/2}^{m-}. \quad (\text{A.12})$$

Note that $\bar{f}_{i+1/2}^{m+}$ and $\bar{g}_{i+1/2}^{m+}$ are the advective and dispersive fluxes out of cell i , respectively; while $\bar{f}_{i+1/2}^{m-}$ and $\bar{g}_{i+1/2}^{m-}$ are the absolute values of advective and dispersive fluxes into cell i .

Since $r[C]$ represents either growth (if positive) or degradation/decay/withdrawals/irreversible adsorption (if negative) or sum of these processes, it is decomposed into

$$r[C] = r^+[C] - r^-[C] \quad (\text{A.13})$$

where r^+ is the sum of non-negative parts (such as growth or irreversible desorption) of r and r^- is the absolute value of the non-positive parts (such as degradation/decay/withdrawals/irreversible adsorption) of r . It then follows from Eq. (A.13) that

$$\overline{r}_i^m = \overline{r^+}_i^m - \overline{r^-}_i^m. \quad (\text{A.14})$$

(Note that the signs $+/-$ are placed inside the brackets instead of being placed after m). By definition both $\overline{r^+}_i^m$ and $\overline{r^-}_i^m$ should remain non-negative; otherwise they shall be set to zeros.

Making use of Eqs. (A.11), (A.12), (A.13) and (A.14), noting the fact that the concentration-independent source term q is assumed to be positive, and the fact that only outgoing fluxes and mass loss can decrease the value of the left-hand-side of Eq. (A.10), we simplify Eq. (A.10) to

$$C_i^n - \overline{r^-}_i^m \Delta t - \frac{\Delta t}{\Delta x} (\bar{f}_{i+1/2}^{m+} + \bar{f}_{i-1/2}^{m-}) - \frac{\Delta t}{\Delta x} \times (\bar{g}_{i+1/2}^{m+} + \bar{g}_{i-1/2}^{m-}) \geq 0. \quad (\text{A.15})$$

Eq. (A.15) is now the (approximate) sufficient condition ensuring the non-negative evolution of the scalar concentration field. It states that during each time step, the initial mass storage minus total mass loss and total outgoing mass fluxes has to be nonnegative. If it is violated, we seek to limit the mass loss and outgoing fluxes by choosing a positive number $\beta_i^{n+1/2,m}$ ($0 \leq \beta_i^{n+1/2,m} \leq 1$), which is iteration-dependent, such that

$$C_i^n - \beta_i^{n+1/2,m} \left\{ \overline{r^-}_i^m \Delta t + \frac{\Delta t}{\Delta x} (\bar{f}_{i+1/2}^{m+} + \bar{f}_{i-1/2}^{m-}) + \frac{\Delta t}{\Delta x} \times (\bar{g}_{i+1/2}^{m+} + \bar{g}_{i-1/2}^{m-}) \right\} \geq 0. \quad (\text{A.16})$$

We choose $\beta_i^{n+1/2,m}$ according to

$$\beta_i^{n+1/2,m} = \frac{C_i^n}{\overline{r^-}_i^m \Delta t + \frac{\Delta t}{\Delta x} (\bar{f}_{i+1/2}^{m+} + \bar{f}_{i-1/2}^{m-}) + \frac{\Delta t}{\Delta x} (\bar{g}_{i+1/2}^{m+} + \bar{g}_{i-1/2}^{m-}) + \eta}, \quad (\text{A.17})$$

where η is a small positive number (such as 10^{-15}) chosen to avoid the situation where the denominator in Eq. (A.17) vanishes.

The limited advective and dispersive fluxes, and the limited source terms \overline{r}_i^m

$$\bar{f}_{i+1/2}^{m*} = \beta_i^{n+1,m} \bar{f}_{i+1/2}^{m+} - \beta_{i+1}^{n+1,m} \bar{f}_{i+1/2}^{m-}, \quad (\text{A.18})$$

$$\bar{g}_{i+1/2}^{m*} = \beta_i^{n+1,m} \bar{g}_{i+1/2}^{m+} - \beta_{i+1}^{n+1,m} \bar{g}_{i+1/2}^{m-}, \quad (\text{A.19})$$

$$\overline{r}_i^{m*} = \overline{r^+}_i^m - \beta_i^{n+1,m} \overline{r^-}_i^m. \quad (\text{A.20})$$

Substitution of Eqs. (A.18), (A.19) and (A.20) with $\bar{f}_{i+1/2}^m$, $\bar{g}_{i+1/2}^m$, and \overline{r}_i^m being replaced by their respective limited versions into Eq. (24) yields a linear, discrete system of equations in terms of the incremental concentrations $\delta C_i^{n+1,m+1}$,

$$\begin{aligned} & \frac{\delta C_i^{n+1,m+1}}{\Delta t} + \frac{\delta \bar{f}_{i+1/2}^{m+1}}{\Delta x} - \frac{\delta \bar{f}_{i-1/2}^{m+1}}{\Delta x} + \frac{\delta \bar{g}_{i+1/2}^{m+1}}{\Delta x} - \frac{\delta \bar{g}_{i-1/2}^{m+1}}{\Delta x} \\ & - \delta \overline{r}_i^{m+1} \\ & = \overline{q}_i + \overline{r}_i^{m*} - \frac{C_i^{n+1,m} - C_i^n}{\Delta t} - \frac{\bar{f}_{i+1/2}^{m*} - \bar{f}_{i-1/2}^{m*}}{\Delta x} \\ & - \frac{\bar{g}_{i+1/2}^{m*} - \bar{g}_{i-1/2}^{m*}}{\Delta x}. \end{aligned} \quad (\text{A.21})$$

Since $\delta \bar{f}_{i\pm 1/2}^{m+1}$ and $\delta \bar{g}_{i\pm 1/2}^{m+1}$ in general can be expressed in terms of $\delta C_i^{n+1,m+1}$ and $\delta C_{i\pm 1}^{n+1,m+1}$, and $\delta \overline{r}_i^{m+1}$ in terms of $\delta C_i^{n+1,m+1}$, Eq. (A.21) can be simplified to

$$\mathbf{A} \delta C_i^{n+1,m+1} = \mathbf{b}, \quad (\text{A.22})$$

where \mathbf{A} is at most a $N \times N$ tridiagonal matrix (where N is the total number of computational cells) that is contributed by all the terms on the LHS of Eq. (A.22), and \mathbf{b} is a vector of length N containing the RHS of Eq. (A.21). The tridiagonal matrix \mathbf{A} reduces to a diagonal one should both $\delta \bar{f}_{i\pm 1/2}^{m+1}$ and $\delta \bar{g}_{i\pm 1/2}^{m+1}$ vanish, in which case Eq. (A.22) can be solved by direct substitutions.

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