**EULERIAN-LAGRANGIAN LOCALIZED ADJOINT
METHODS FOR REACTIVE TRANSPORT IN GROUNDWATER**

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EULERIAN-LAGRANGIAN LOCALIZED ADJOINT METHODS FOR REACTIVE TRANSPORT IN GROUNDWATER*

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Abstract. In this paper, we present Eulerian-Lagrangian localized adjoint methods (ELLAM) to solve convection-diffusion-reaction equations governing contaminant transport in groundwater flowing through an adsorbing porous medium. These ELLAM schemes are developed for various combinations of boundary conditions. The derived schemes do conserve mass. Numerical results are presented and discussed.

§1. INTRODUCTION.

In recent years, the contamination and pollution of groundwater resources have made it increasingly more important to understand underground flows of contaminant fluids and to predict them effectively. However, mathematical models are, in general, strongly convection-dominated partial differential equations, which may be solved analytically for only a limited number of special cases. More general solutions require numerical approximations to the governing equations. The purpose of this paper is to develop some effective numerical methods to simulate contaminant transport with adsorption in groundwater.

First, let us review the physical and mathematical background of this problem. We consider the transport of a solute, labeled α , in a fluid phase F flowing through a porous medium. The fluid phase may consist of many molecular species, such as water and dissolved minerals. We use the letter β to index all of these species. We think of the specific species α as a soluble contaminant in the fluid. The porous medium is composed of a rock phase, which we index by R , and which also can consist of many molecular species. We are especially interested in transfers of material α between the fluid and rock phases, which can occur when some of the contaminant adsorbs onto the rock as it travels through the porous medium.

From the species mass balance [1,19], for the solute α in the fluid phase F , we have

$$(1.1) \quad \frac{\partial}{\partial t} (\phi_F \rho_F^\alpha) + \nabla \cdot (\mathbf{v}_F^\alpha \phi_F \rho_F^\alpha) = r_F^\alpha,$$

where ϕ_F is a volume fraction, ρ_F is the mass of the fluid per unit volume of fluid; ρ_F^α is the mass of the solute in the fluid phase per unit volume of fluid, and $\omega_F^\alpha = \rho_F^\alpha / \rho_F$. The quantity $\mathbf{v}_F^\alpha$ is the velocity of the solute in the fluid phase, and r_F^α is the rate of

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all transfers of mass from other constituents, including the species α in other phases, into the solute α in the fluid phase.

Similarly, for the solute α in the rock phase R , we have

$$(1.2) \quad \frac{\partial}{\partial t}(\phi_R \rho_R^\alpha) + \nabla \cdot (\mathbf{v}_R^\alpha \phi_R \rho_R^\alpha) = r_R^\alpha,$$

where the definitions of variables are similar to those in equation (1.1).

Let $\mathbf{v}_F = (\sum_\beta \rho_F^\beta \mathbf{v}_F^\beta) / \rho_F$ be the barycentric velocity of the fluid; $\nu_F^\beta = \mathbf{v}_F^\beta - \mathbf{v}_F$ be the diffusion velocity of constituent β ; and $\mathbf{j}^\beta = \omega_F^\beta \nu_F^\beta$ the diffusive flux of species β . Here β can be any constituent in the fluid. We assume that we know the Darcy velocity $\mathbf{v} = \phi_F \mathbf{v}_F$ of the fluid in the rock. Also we denote ρ_F^α by u . Then equation (1.1) can be rewritten as

$$(1.3) \quad \frac{\partial}{\partial t}(\phi_F u) + \nabla \cdot (\mathbf{v} u) + \nabla \cdot (\phi_F \rho_F \mathbf{j}^\alpha) = r_F^\alpha.$$

Now we consider the diffusive flux $\mathbf{j}^\alpha$. For actual groundwater systems $\mathbf{j}^\alpha$ can be very complicated. A common model [1,19] for this variable, called hydrodynamic dispersion model, is $\phi_F \rho_F \mathbf{j}^\alpha = -\mathbf{D} \nabla u$, where $\mathbf{D}$ is the diffusion tensor. Mathematically, $\mathbf{D}$ is a symmetric and positive definite matrix whose entries depend on the Darcy velocity $\mathbf{v}$, $\mathbf{x}$, and t .

For this problem, we make following assumptions:

1. $\phi_F + \phi_R = 1$. That is, we only have two phases, fluid and rock. [1,19] also discuss multiphase case.
2. $r_F^\alpha + r_R^\alpha = -Ku$, for some coefficient $K \geq 0$. In other words, the solute can transfer between the fluid and rock phases by adsorbing and desorbing, and the solute decays to another molecular species by a first-order chemical reaction with rate K . When $K = 0$, net reaction is zero.

Because the rock is stationary, in (1.2), $\mathbf{v}_R^\alpha = \mathbf{0}$. Adding (1.2) to (1.3) and using these assumptions, we get

$$(1.4) \quad \frac{\partial}{\partial t}[(1 - \phi_F) \rho_R \omega_R^\alpha + \phi_F u] + \nabla \cdot (\mathbf{v} u) - \nabla \cdot (\mathbf{D} \nabla u) = -Ku.$$

While adsorption in nature can exhibit tremendous variation depending on the chemistry of the materials involved, there are a few relatively simple functional forms that often appear in mathematical models [1]. In this paper, we assume the following linear form:

$$(1.5) \quad \omega_R^\alpha = \mu u,$$

that is often reasonable for groundwater systems. Here, μ is a nonnegative constant. Then (1.4) can be rewritten as

$$(1.6) \quad \frac{\partial}{\partial t}(\Phi u) + \nabla \cdot (\mathbf{v} u) - \nabla \cdot (\mathbf{D} \nabla u) = -Ku.$$

where $\Phi = (1 - \phi_F) \rho_R \mu + \phi_F$.

These strongly convection-dominated problems, which also arise in the numerical simulation of oil reservoirs and a multitude of other applications, often present serious

numerical difficulties [1,19]. Conventional methods usually exhibit some combination of nonphysical oscillation and excessive numerical diffusion [1,19,25]. Because of the Lagrangian nature of advective transport, Eulerian-Lagrangian methods (ELM) have been successfully applied to these problems [14,17,18,27,32]. The principal drawbacks of ELM are their failure to conserve mass and the difficulty of formulating them for general boundary conditions.

Celia, Russell, Herrera and Ewing have recently developed Eulerian-Lagrangian localized adjoint methods (ELLAM) [7] to solve convection-diffusion problems. ELLAM are formulated to maintain mass conservation and to treat general boundary conditions. Thus, ELLAM overcome the two principal shortcomings of ELM while maintaining their numerical advantages. In this paper, we develop ELLAM schemes to solve convection-diffusion-reaction problems. We carefully treat various combinations of inflow and outflow boundary conditions in this paper. Numerical results are presented, compared, and discussed.

We first briefly describe these methods. The ELLAM formulation was motivated by localized adjoint methods (LAM) [3,5,6]. Let

$$(1.7) \quad Lu = f, \quad x \in \Omega \text{ or } (x, t) \in \Omega,$$

denote a partial differential equation in space or space-time. Integrating against a test function w , we obtain the weak form

$$(1.8) \quad \int_{\Omega} Lu \, w \, d\Omega = \int_{\Omega} fw \, d\Omega .$$

If we choose test functions w to satisfy the formal adjoint equation $L^*w = 0$, except at certain nodes or edges denoted by l_i on Ω , then integrating by parts (the divergence theorem in higher dimensions) yields

$$(1.9) \quad \sum_i \int_{l_i} u \, L^*w \, ds = \int_{\Omega} fw \, d\Omega .$$

By choosing various test functions w in (1.9), we can focus upon different types of information. Herrera has built an extensive theory around this concept [22,23]. Within this framework, we can also obtain optimal spatial methods and general characteristic methods [7,20,28,29]. We will discuss this further in Section 2.

In this paper, we develop ELLAM to solve the one-dimensional linear constant-coefficient convection-diffusion-reaction equation,

$$(1.10) \quad Lu \equiv u_t + Vu_x - Du_{xx} + Ku = f(x, t), \quad a < x < b, \quad 0 < t \leq T,$$

subject to one of the following boundary conditions at the inflow boundary $x = a$,

$$(1.11) \quad \begin{aligned} u(a, t) &= g_1(t), & 0 < t \leq T, \\ -Du_x(a, t) &= g_2(t), & 0 < t \leq T, \\ Vu(a, t) - Du_x(a, t) &= g_3(t), & 0 < t \leq T; \end{aligned}$$

one of the analogous conditions at the outflow boundary $x = b$,

$$\begin{aligned}
(1.12) \quad & u(b, t) = h_1(t), \quad 0 < t \leq T, \\
& -Du_x(b, t) = h_2(t), \quad 0 < t \leq T, \\
& Vu(b, t) - Du_x(b, t) = h_3(t), \quad 0 < t \leq T;
\end{aligned}$$

and also subject to the initial condition

$$(1.13) \quad u(x, 0) = u_0(x), \quad a \leq x \leq b,$$

where D and V , which are positive constants, represent diffusion and velocity, respectively. K represents the reaction coefficient.

The remainder of this paper is organized as follows. In Section 2, we derive a variational formulation satisfied by the exact solution of the problem (1.10). In Sections 3, we develop ELLAM schemes based on the formulation obtained in Section 2. In Section 4, we perform various numerical experiments.

§2. AN ELLAM FORMULATION.

In this section, we derive the formulation satisfied by the exact solution of problem (1.10). Let E and N be two positive integers; then define the mesh and the partition of space and time as follows:

$$\begin{aligned}
(2.1) \quad & \Delta x = \frac{b-a}{E}, \quad x_i = a + i\Delta x, \quad i = 0, 1, \dots, E, \\
& \Delta t = \frac{T}{N}, \quad t^n = n\Delta t, \quad n = 0, 1, \dots, N.
\end{aligned}$$

In the numerical scheme, we consider space-time test functions w that vanish outside $[a, b] \times (t^n, t^{n+1}]$ and are discontinuous at each time level t^n , whose exact form will be given below as part of the ELLAM development. With these test functions, we can rewrite (1.8) as

$$\begin{aligned}
(2.2) \quad & \int_a^b u(x, t^{n+1})w(x, t^{n+1})dx + \int_{t^n}^{t^{n+1}} \int_a^b Du_x w_x d\Omega, \\
& + \int_{t^n}^{t^{n+1}} (Vu - Du_x)w \Big|_a^b dt - \int_{t^n}^{t^{n+1}} \int_a^b u(w_t + Vw_x - Kw) d\Omega \\
& = \int_a^b u(x, t^n)w(x, t_+^n)dx + \int_{t^n}^{t^{n+1}} \int_a^b f w d\Omega,
\end{aligned}$$

where $w(x, t_+^n) = \lim_{t \rightarrow t_+^n} w(x, t)$.

The homogeneous adjoint equation for equation (1.10) is:

$$(2.3) \quad \mathcal{L}^* w \equiv -w_t - Vw_x - Dw_{xx} + Kw = 0.$$

As discussed above, the test function $w(x, t)$ is chosen from the solution space of the homogeneous adjoint equation (2.3). The solution space is infinite-dimensional.

Because the objective of the numerical procedure is the derivation of a finite number of algebraic equations, only a finite number of test functions should be chosen. Different choices of test functions lead to different classes of approximations, including optimal spatial methods and characteristic methods [7]. For adjoint equation (2.3), we naturally have the following three operator splittings:

1. We can split the adjoint operator $\mathcal{L}^*$ into a spatial operator and a temporal operator

$$(2.5) \quad \begin{aligned} w_t &= 0, \\ -Vw_x - Dw_{xx} + Kw &= 0. \end{aligned}$$

This splitting leads to a class of optimal spatial methods involving exponential upstream weighting in space [3,5,6]. Numerical solutions with these methods are characterized by significant time truncation errors, numerical diffusion, and some phase errors. The Courant number is generally restricted to be less than or equal to one, and sometimes must be much less than one [3].

2. Recalling the strong Lagrangian nature of this problem, we can split (2.3) in the following way:

$$(2.6) \quad \begin{aligned} w_t + Vw_x &= 0, \\ -Dw_{xx} + Kw &= 0. \end{aligned}$$

The test functions are constants along the characteristics and the reaction term $K u w$ is lumped at time t^{n+1} . This splitting leads to a class of characteristic methods.

3. We can also write (2.3) into the form

$$(2.7) \quad \begin{aligned} w_t + Vw_x - Kw &= 0, \\ -Dw_{xx} &= 0. \end{aligned}$$

The splitting (2.7) determines the test functions that are hat functions at each time level and vary exponentially along the characteristics. In this manner, the test functions. Recalling that the exact solution of problem (1.10) varies exponentially along the characteristics, splitting (2.7) reflects the intrinsic physics of the problem (1.10) naturally.

We now define our test functions $w_i(x, t)$. First, we discuss the expressions of the characteristics. At time t^{n+1} , the characteristic $X(\theta; x, t^{n+1})$, $t^n \leq \theta \leq t^{n+1}$, which emanates backward from (x, t^{n+1}) , is given by

$$(2.8) \quad X(\theta; x, t^{n+1}) - x = V(\theta - t^{n+1}), \quad t^n \leq \theta \leq t^{n+1}.$$

For a given point x at time t^{n+1} , when it is clear from the context, we shall also write $x(\theta)$ in place of $X(\theta; x, t^{n+1})$.

Similarly, at the outflow boundary $\{x = b, t^n \leq t \leq t^{n+1}\}$, the characteristic $X(\theta; x_E, t)$, $t^n \leq \theta \leq t$, emanating backward from (x_E, t) is

$$(2.9) \quad X(\theta; x_E, t) - x_E = V(\theta - t), \quad t^n \leq \theta \leq t.$$

Also, let $x^* = X(t^n; x, t^{n+1})$ or $x_E^*(t) = X(t^n; x_E, t)$ be the foot of the characteristic defined by (2.8) or (2.9); and let $x_i^* = X(t^n; x_i, t^{n+1})$, $i = 0, 1, \dots, E$, or $x_i^* = X(t^n; x_E, t_i)$, $i = E + 1, \dots, E + IC$, where t_i is given in (2.12) below.

Also, let

$$(2.10) \quad \tilde{x} = x + V\Delta t,$$

i.e., $(\tilde{x}, t^{n+1})$ is the head of the characteristic with the foot (x, t^n) . Especially, $\tilde{x}_0$ is the point such that the characteristic traced backward from $(\tilde{x}_0, t^{n+1})$ meets the inflow boundary $x = x_0$ at time level t^n .

In order to discuss the inflow boundary conditions effectively, we define the notation:

$$(2.11) \quad \Delta t(x) = \begin{cases} t^{n+1} - t^n, & \text{if } x \geq \tilde{x}_0, \\ t^{n+1} - t^*(x), & \text{if } x < \tilde{x}_0, \end{cases}$$

where $\tilde{x}_0$ is given in (2.10) with $x = x_0$; $t^*(x)$ refers to the time when the characteristic $x(\theta)$ traced backward from (x, t^{n+1}) meets the inflow boundary; i.e., $x_0 = X(t^*(x); x, t^{n+1}) = x(t^*(x))$; $t_i^* = t^*(x_i)$, $i = 0, 1, \dots, IC$, where $Cu = V\Delta t/\Delta x$ is the Courant number and $IC = [Cu]$ is the integer part of Cu . For later convenience, in addition to the notations t_i^* , $i = 0, 1, \dots, IC$, given above, we also define a notation $t_{IC+1}^* = t^n$. However, we point out that t_{IC+1}^* may not be $t^*(x_{IC+1})$, in general.

For $i = E, E + 1, \dots, E + IC - 1$, we define:

$$(2.12) \quad t_i = t^{n+1} - \frac{(i - E)\Delta x}{V}, \quad \text{with } t_{E+IC} = t^n.$$

That is, we partition the outflow boundary $\{x = b, t^n \leq t \leq t^{n+1}\}$ according to the magnitude of the Courant number. For $0 < Cu < 2$, we will not partition $[t^n, t^{n+1}]$ further; $[t^n, t^{n+1}]$ has no sub-elements. For $Cu \geq 2$, we further partition $[t^n, t^{n+1}]$ into IC subintervals. The first $IC - 1$ subintervals are of length $\Delta t/Cu$. The last one, which may be up to twice the size of the others, is of length $[(Cu - IC) + 1]\Delta t/Cu$.

Now we define the test functions. For $i = 0, 1, \dots, E$, at current time level t^{n+1} , $w_i(x, t)$ is the standard hat function associated with the node x_i ; for $i = E, \dots, E + IC$, at the outflow boundary $[t^n, t^{n+1}]$, $w_i(x, t)$ is the standard hat function associated with t_i . All $w_i(x, t)$, $i = 0, 1, \dots, E + IC$, vary exponentially along the characteristics and are zero outside $(t^n, t^{n+1}]$ since we want w_i to be localized.

$$(2.13) \quad w_i(x(\theta), \theta) = w_i(x, t^{n+1})e^{-K(t^{n+1}-\theta)}, \quad t^n < \theta \leq t^{n+1}, \quad i = 0, 1, \dots, E;$$

$$w_i(X(\theta; x_E, t), \theta) = w_i(x_E, t)e^{-K(t-\theta)}, \quad t^n < \theta \leq t, \quad i = E, E + 1, \dots, E + IC.$$

Noticing that the test functions satisfy the adjoint equation (2.3), if we put these test functions into (2.2), the last term on the left-hand side of (2.2) vanishes. Let w be any of the test functions defined above. For the second term on the left-hand side of (2.2), if we evaluate temporal integral by a one-point (backward Euler) approximation at t^{n+1} , simple computations yield

$$\begin{aligned}
& \int_{t^n}^{t^{n+1}} \int_a^b Du_x w_x d\Omega \\
&= \int_{t^n}^{t^{n+1}} \int_{x_0}^{x_E(s)} Du_x w_x d\Omega + \int_{t^n}^{t^{n+1}} \int_{x_E(s)}^{x_E} Du_x w_x d\Omega \\
&= \int_{x_0}^{x_E} D \Theta(\Delta t(x)) u_x(x, t^{n+1}) w_x(x, t^{n+1}) dx \\
(2.14) \quad & - \int_{t^n}^{t^{n+1}} D \Theta(t - t^n) u_x(x_E, t) [w_t(x_E, t) - K w(x_E, t)] dt \\
& - \int_a^b \left\{ \int_{t^n}^{t^{n+1}} \left[\int_{\tau}^{t^{n+1}} Du_{\tau x}(x(\theta), \theta) d\theta \right] e^{-K(t^{n+1}-\tau)} d\tau \right\} w_x(x, t^{n+1}) dx \\
& + \int_{t^n}^{t^{n+1}} \left\{ \int_{t^n}^t \left[\int_{\tau}^t D u_{\tau x}(X(\theta; x_E, t), \theta) d\theta \right] e^{-K(t-\tau)} d\tau \right\} \\
& \cdot [w_t(x_E, t) - K w(x_E, t)] dt,
\end{aligned}$$

where

$$(2.15) \quad \Theta(x) = \frac{1 - e^{-Kx}}{K}, \quad x > 0.$$

For the last term on the right-hand side of (2.2), as (2.14), we have

$$\begin{aligned}
& \int_{t^n}^{t^{n+1}} \int_a^b f w(x, t) dx dt \\
&= \int_a^b \Theta(\Delta t(x)) f(x, t^{n+1}) w(x, t^{n+1}) dx \\
(2.16) \quad & + \int_{t^n}^{t^{n+1}} \Theta(t - t^n) f(x_E, t) w(x_E, t) V dt \\
& - \int_a^b \left\{ \int_{t^*(x)}^{t^{n+1}} \left[\int_{\tau}^{t^{n+1}} f_{\theta}(x(\theta), \theta) d\theta \right] e^{-K(t^{n+1}-\tau)} d\tau \right\} w(x, t^{n+1}) dx \\
& - \int_{t^n}^{t^{n+1}} \left\{ \int_{t^n}^t \left[\int_{\tau}^t f_{\theta}(X(\theta; x_E, t), \theta) d\theta \right] e^{-K(t-\tau)} d\tau \right\} w(x_E, t) V dt.
\end{aligned}$$

Putting (2.14) and (2.16) into (2.2), we obtain the formulation satisfied by the solution of problem (1.10) as follows:

$$\begin{aligned}
(2.17) \quad & \int_a^b u(x, t^{n+1}) w(x, t^{n+1}) dx + \int_a^b D \Theta(\Delta t(x)) u_x(x, t^{n+1}) w_x(x, t^{n+1}) dx \\
& + \int_{t^n}^{t^{n+1}} [Vu - Du_x](x_E, t) w(x_E, t) dt - \int_{t^n}^{t^{n+1}} [Vu - Du_x](x_0, t) w(x_0, t) dt \\
& - \int_{t^n}^{t^{n+1}} D \Theta(t - t^n) u_x(x_E, t) [w_t(x_E, t) - Kw(x_E, t)] dt \\
& = e^{-K\Delta t} \int_{\tilde{x}_0}^b u(x^*, t^n) w(x, t^{n+1}) dx + \int_{t^n}^{t^{n+1}} e^{-K(t-t^n)} u(x_E^*(t), t^n) w(x_E, t) V dt \\
& + \int_a^b \Theta(\Delta t(x)) f(x, t^{n+1}) w(x, t^{n+1}) dx \\
& + \int_{t^n}^{t^{n+1}} \Theta(t - t^n) f(x_E, t) w(x_E, t) V dt \\
& - R_x^{n+1}(w(x, t^{n+1})) - R_t^{n+1}(w(x_E, t)),
\end{aligned}$$

where

$$\begin{aligned}
(2.18) \quad & R_x^{n+1}(w(x, t^{n+1})) \\
& = \int_a^b \left\{ \int_{t^*(x)}^{t^{n+1}} \left[\int_{\tau}^{t^{n+1}} Du_{\theta x}(x(\theta), \theta) d\theta \right] e^{-K(t^{n+1}-\tau)} d\tau \right\} w_x(x, t^{n+1}) dx \\
& - \int_a^b \left\{ \int_{t^*(x)}^{t^{n+1}} \left[\int_{\tau}^{t^{n+1}} f_{\theta}(x(\theta), \theta) d\theta \right] e^{-K(t^{n+1}-\tau)} d\tau \right\} w(x, t^{n+1}) dx,
\end{aligned}$$

$$\begin{aligned}
(2.19) \quad & R_t^{n+1}(w(x_E, t)) \\
& = - \int_{t^n}^{t^{n+1}} \left\{ \int_{t^n}^t \left[\int_{\tau}^t D u_{\theta x}(X(\theta; x_E, t), \theta) d\theta \right] e^{-K(t-\tau)} d\tau \right\} \\
& \quad \cdot [w_t(x_E, t) - Kw(x_E, t)] dt \\
& - \int_{t^n}^{t^{n+1}} \left\{ \int_{t^n}^t \left[\int_{\tau}^t f_{\theta}(X(\theta; x_E, t), \theta) d\theta \right] e^{-K(t-\tau)} d\tau \right\} w(x_E, t) V dt.
\end{aligned}$$

§3. ELLAM SCHEMES.

In this section, we develop ELLAM schemes based on the formulation derived in Section 2. First we discuss the choice of the trial functions.

3.1. Trial function. At time t^{n+1} , we use a piecewise-linear trial function. At the inflow boundary, for Neumann or flux boundary conditions, the node values are the known $U(x_0, t^n)$ and the unknown $U(x_0, t^{n+1})$; we do not introduce any extra unknowns. For an inflow Dirichlet boundary condition, $U(x_0, t^n)$ and $U(x_0, t^{n+1})$ are

known. When $Cu \geq 1$, we do not introduce any extra equations; when $Cu < 1$, we introduce one extra unknown at the inflow boundary. We will discuss these in detail in the following subsections. At the outflow boundary $[t^n, t^{n+1}]$, we need to consider two cases. For the outflow Neumann or flux boundary condition, the unknown is the trial function itself. Thus, we use a piecewise-linear approximation at the outflow boundary $[t^n, t^{n+1}]$:

$$(3.1) \quad U(x_E, t) = \sum_{i=E}^{E+IC} U(x_E, t_i) w_i(x_E, t), \quad t^n \leq t \leq t^{n+1}.$$

For the outflow Dirichlet boundary condition, the unknown is the normal derivative of the trial function. Thus, we use a piecewise-constant approximation at the outflow boundary $[t^n, t^{n+1}]$:

$$(3.2) \quad U_x(x_E, t) = \sum_{i=E+1}^{E+IC} U_x(x_E, t_{i-1/2}) \chi_{(t_{i-1}, t_i)}(t), \quad t^n < t \leq t^{n+1},$$

where $\chi_{(t_{i-1}, t_i)}(t)$ is the standard characteristic function that is 1 on (t_i, t_{i-1}) and 0 outside, and $U_x(x_E, t_{i-1/2})$ denotes the constant value of $U_x(x_E, t)$ over (t_i, t_{i-1}) , where $t_{i-1/2} = (t_{i-1} + t_i)/2$.

3.2. Numerical schemes for the interior points. Let U be a piecewise-linear function at time t^{n+1} and $w_i(x, t)$ be the test function defined by (2.13). If we replace u in (2.17) by U and drop the last two terms on the right-hand of (2.17), we obtain our ELLAM scheme at $i = IC + 2, \dots, E - 1$ as follows:

$$(3.3) \quad \int_{x_{i-1}}^{x_{i+1}} U(x, t^{n+1}) w_i(x, t^{n+1}) dx + \int_{x_{i-1}}^{x_{i+1}} D\Theta(\Delta t) U_x(x, t^{n+1}) w_{ix}(x, t^{n+1}) dx \\ = e^{-K\Delta t} \int_{x_{i-1}}^{x_{i+1}} U(x^*, t^n) w_i(x, t^{n+1}) dx + \int_{x_{i-1}}^{x_{i+1}} \Theta(\Delta t) f(x, t^{n+1}) w_i(x, t^{n+1}) dx.$$

When one or more of the characteristics $x_{i-1}(\tau)$, $x_i(\tau)$ or $x_{i+1}(\tau)$ intersects the spatial boundary, the general ELLAM scheme (3.3) should be modified. In this case, inflow or outflow boundary conditions are introduced into the ELLAM schemes. In the next two subsections, we consider ELLAM equations related to inflow and outflow boundaries.

3.3. Numerical schemes for the inflow boundary. In this subsection, we develop ELLAM schemes related to the inflow boundary conditions. Since the approximation of boundary conditions directly affects the approximation in the interior of the domain and also affects the mass conservation property, we need to be very careful. First, we consider the inflow flux boundary condition. Putting the third condition in (1.11) into (2.17), we obtain ELLAM scheme at $i = 0, 1, \dots, IC + 1$ as follows:

$$\begin{aligned}
& \int_{x_{i-1}}^{x_{i+1}} U(x, t^{n+1}) w_i(x, t^{n+1}) dx + \int_{x_{i-1}}^{x_{i+1}} D\Theta(\Delta t(x)) U_x(x, t^{n+1}) w_{ix}(x, t^{n+1}) dx \\
(3.4) \quad & = e^{-K\Delta t} \int_{[x_{i-1}, x_{i+1}] \cap (x \geq \bar{x}_0)} U(x^*, t^n) w_i(x, t^{n+1}) dx \\
& + \int_{x_{i-1}}^{x_{i+1}} \Theta(\Delta t(x)) f(x, t^{n+1}) w_i(x, t^{n+1}) dx + \int_{t_{i+1}^*}^{t_{i-1}^*} g_3(t) w_i(x_0, t) dt,
\end{aligned}$$

where at $i = 0$, the $[x_{i-1}, x_{i+1}]$ and $[t_{i+1}^*, t_{i-1}^*]$ in (3.4) should be replaced by $[x_0, x_1]$ and $[t_1^*, t_0^*] = [t_1^*, t^{n+1}]$, respectively.

For the inflow Neumann boundary condition, if we repeat the above derivation, we obtain the ELLAM scheme at $i = 0, 1, \dots, IC + 1$ as follows:

$$\begin{aligned}
& \int_{x_{i-1}}^{x_{i+1}} U(x, t^{n+1}) w_i(x, t^{n+1}) dx + \int_{x_{i-1}}^{x_{i+1}} D\Theta(\Delta t(x)) U_x(x, t^{n+1}) w_{ix}(x, t^{n+1}) dx \\
& - \int_{t_{i+1}^*}^{t_{i-1}^*} U(x_0, t) w_i(x_0, t) V dt \\
(3.5) \quad & = e^{-K\Delta t} \int_{[x_{i-1}, x_{i+1}] \cap (x \geq \bar{x}_0)} U(x^*, t^n) w_i(x, t^{n+1}) dx \\
& + \int_{x_{i-1}}^{x_{i+1}} \Theta(\Delta t(x)) f(x, t^{n+1}) w_i(x, t^{n+1}) dx + \int_{t_{i+1}^*}^{t_{i-1}^*} g_2(t) w_i(x_0, t) dt.
\end{aligned}$$

Remark 3.1. A negative term involving $U(x_0, t)$ appears on the left-hand side of equation (3.5). We can use constant or linear interpolations along the time direction to approximate this term. However, linear interpolation introduces some nonzero entries in its first column, as does the matrix derived in [7], and so violates the tridiagonal structure of the coefficient matrix. The system derived is more expensive to solve than a tridiagonal system that we expect to have. Constant interpolation can maintain the tridiagonal structure of the system. However, the corresponding numerical solutions are strongly time-dominated. We present some numerical results about this in Section 4. It is the Eulerian nature of the interpolations along the time direction that makes these interpolations inconsistent with the Lagrangian treatment in the interior domain. In order to overcome this difficulty, we combine the last term on the left-hand side of (3.5), translated along the characteristic from $(x_0, t^*(x))$ to (x, t^{n+1}) , with the first term on the left side of (3.5) to get a term $\int_{[x_{i-1}, x_{i+1}] \cap (x \geq \bar{x}_0)} U(x, t^{n+1}) w_i(x, t^{n+1}) dx$. The error involves the first-order derivative of the exact solution along the approximate characteristics, which is much smaller than the interpolation error along the time direction due to the Lagrangian nature of this problem. With this treatment, we still have a tridiagonal coefficient matrix, avoiding the violations of sparsity discussed above. Thus, we use the following scheme for the inflow Neumann boundary condition instead of (3.5). For $i = 0, 1, \dots, IC + 1$, we have

$$\begin{aligned}
& \int_{[x_{i-1}, x_{i+1}] \cap (x \geq \tilde{x}_0)} U(x, t^{n+1}) w_i(x, t^{n+1}) dx \\
& + \int_{x_{i-1}}^{x_{i+1}} D\Theta(\Delta t(x)) U_x(x, t^{n+1}) w_{ix}(x, t^{n+1}) dx \\
(3.6) \quad & = e^{-K\Delta t} \int_{[x_{i-1}, x_{i+1}] \cap (x \geq \tilde{x}_0)} U(x^*, t^n) w_i(x, t^{n+1}) dx \\
& + \int_{x_{i-1}}^{x_{i+1}} \Theta(\Delta t(x)) f(x, t^{n+1}) w_i(x, t^{n+1}) dx + \int_{t_{i+1}^*}^{t_{i-1}^*} g_2(t) w_i(x_0, t) dt.
\end{aligned}$$

Now, we consider ELLAM schemes related to the inflow Dirichlet boundary condition. If we repeat the derivation for the flux condition, we get an unknown diffusive boundary flux in the ELLAM scheme related to the inflow boundary. If we simply discretize the unknown diffusive flux along the time direction, the algebraic system derived contains the inflow boundary diffusive flux as an unknown. This term may introduce strong time truncation error. The numerical solutions deteriorate and give some oscillations near the inflow boundary. In order to avoid this problem, we approximate the term $-\int_0^T \int_a^b (Du_x)_x w dx dt$ by backward-Euler time integration along the characteristics before integrating by parts in space. This way, we obtain ELLAM scheme at $i = 1, 2, \dots, IC + 1$ as follows [28]:

$$\begin{aligned}
& \int_{x_{i-1}}^{x_{i+1}} U(x, t^{n+1}) w_i(x, t^{n+1}) dx + \int_{x_{i-1}}^{x_{i+1}} D\Theta(\Delta t(x)) U_x(x, t^{n+1}) w_{ix}(x, t^{n+1}) dx \\
& + \int_{[x_{i-1}, x_{i+1}] \cap (x \leq \tilde{x}_0)} \Psi(\Delta t(x)) U_x(x, t^{n+1}) w_i(x, t^{n+1}) dx \\
(3.7) \quad & = e^{-K\Delta t} \int_{[x_{i-1}, x_{i+1}] \cap (x \geq \tilde{x}_0)} U(x^*, t^n) w_i(x, t^{n+1}) dx \\
& + \int_{x_{i-1}}^{x_{i+1}} \Theta(\Delta t(x)) f(x, t^{n+1}) w_i(x, t^{n+1}) dx + \int_{t_{i+1}^*}^{t_{i-1}^*} V g_1(t) w_i(x_0, t) dt,
\end{aligned}$$

where

$$(3.8) \quad \Psi(x) = \frac{De^{-Kx}}{V}, \quad x > 0.$$

Remark 3.2. In order to conserve mass, all test functions should sum to exactly one [7]. Russell [28] chose the test function to be 1 on $[x_0, x_1]$, i.e., replacing w_1 by $w_0 + w_1$ on $[x_0, x_1]$. However, our numerical experiments discussed in next section and our theoretical analysis presented in a subsequent paper show that the ELLAM schemes derived this way only have an asymptotic convergence rate of $O((\Delta x)^{3/2} + \Delta t)$ instead of $O((\Delta x)^2 + \Delta t)$ when Courant number $Cu = V\Delta t/\Delta x$ is very small ($Cu \ll 1$). This is significant if $Cu \ll 1$. Thus, we modify (3.7) in the following way: (1) When $Cu \geq 1$, we choose the test function to be $\tilde{w}_1 = w_0 + w_1 = 1$ on $[x_0, x_1]$ as in [28]. In (3.7), we replace w_i with $\tilde{w}_i$, where $\tilde{w}_i = w_0 + w_1$, if $i = 1$, w_i if $2 \leq i \leq E$. Thus, we do not need any extra equation at $i = 0$. (2) When $Cu < 1$, in order to

maintain second-order convergence in space, we take the test function for $i = 1$ in (3.7) to be w_1 , and we introduce the following ELLAM scheme at $i = 0$ [7]. Noting that $t_1^* = t^n$ in this case:

$$\begin{aligned}
& \int_{x_0}^{x_1} U(x, t^{n+1}) w_0(x, t^{n+1}) dx + \int_{x_0}^{x_1} D\Theta(\Delta t(x)) U_x(x, t^{n+1}) w_{0x}(x, t^{n+1}) dx \\
& + \int_{t_1^*}^{t^{n+1}} DU_x(x_0, t) w_0(x_0, t) dt \\
(3.9) \quad & = e^{-K\Delta t} \int_{[x_0, x_1] \cap (x \geq \bar{x}_0)} U(x^*, t^n) w_0(x, t^{n+1}) dx \\
& + \int_{x_0}^{x_1} \Theta(\Delta t(x)) f(x, t^{n+1}) w_0(x, t^{n+1}) dx + \int_{t_1^*}^{t^{n+1}} V g_1(t) w_0(x_0, t) dt.
\end{aligned}$$

Remark 3.3. This equation solves for the unknown $U_x(x_0, t_{1/2}^*)$ at the inflow boundary, where we regard $U_x(x_0, t)$ as constant on $[t_1^*, t^{n+1}] = [t^n, t^{n+1}]$ with $t_{1/2}^* = (t_1^* + t^{n+1})/2 = (t^n + t^{n+1})/2$ (recall that we only introduce (3.9) when $Cu < 1$, in which case $t_1^* = t^n$). Equation (3.9) also involves $U(x_1, t^{n+1})$. Since $U(x_1, t^{n+1})$ is obtained by solving the equations for $i \geq 1$, which form a closed system, the $i = 0$ equation immediately yields $U_x(x_0, t_{1/2}^*)$ by back substitution. When $Cu \geq 1$, the ELLAM schemes (3.7) derived here are same as those in [28]. When $Cu < 1$, the ELLAM schemes here differ from those in [28] in that $U_x(x_0, t^{n+1})$ is an unknown in (3.9), whereas it was set to $[U(x_1, t^{n+1}) - U(x_0, t^{n+1})]/\Delta x$ in [28]. By doing this, we successfully recover the optimal-order convergence rate $O((\Delta x)^2 + \Delta t)$ when $Cu < 1$. Meanwhile, potential numerical difficulties with the third term on the left-hand side of (3.9), which involves integration of a large function over a small interval if $Cu \ll 1$, are avoided in this way. The equation (3.9) is only needed for the purpose of mass conservation.

3.4. Numerical scheme for the outflow boundary. In this subsection, we develop ELLAM schemes related to the outflow boundary. For outflow Neumann or flux boundary conditions, since the unknowns are $U(x_E, t)$ themselves for various t , we use piecewise-linear trial functions. For the outflow Dirichlet boundary condition, $U(x_E, t)$ is known but $U_x(x_E, t)$ is unknown. We use a piecewise-constant trial function to approximate $U_x(x_E, t)$ [28]. Using the test functions defined in (2.13) and the formulation (2.17), we can obtain the ELLAM schemes at the outflow boundary. For the outflow flux boundary condition, the ELLAM scheme at $i = E+1, \dots, E+IC-1$ is

$$\begin{aligned}
(3.10) \quad & - \int_{t_{i+1}}^{t_{i-1}} \Theta(t - t^n) U(x_E, t) [\hat{w}_{it}(x_E, t) - K \hat{w}_i(x_E, t)] V dt \\
& = \int_{t_{i+1}}^{t_{i-1}} e^{-K(t-t^n)} U(x_E^*(t), t^n) \hat{w}_i(x_E, t) V dt + \int_{t_{i+1}}^{t_{i-1}} \Theta(t - t^n) f(x_E, t) \hat{w}_i(x_E, t) V dt \\
& - \int_{t_{i+1}}^{t_{i-1}} h_3(t) \hat{w}_i(x_E, t) dt - \int_{t_{i+1}}^{t_{i-1}} \Theta(t - t^n) h_3(t) [\hat{w}_{it}(x_E, t) - K \hat{w}_i(x_E, t)] dt,
\end{aligned}$$

where $\hat{w}_i = w_i$ if $E + 1 \leq i \leq E + IC - 2$, $\hat{w}_{E+IC-1} = w_{E+IC-1} + w_{E+IC}$. The scheme at $i = E$ is a combination of both types from (3.3) and (3.10).

Remark 3.4. It is easy to see that (3.10) is indefinite, and this raises questions about the solvability, stability, and convergence properties of these ELLAM schemes. In the subsequent paper, we conclude that this scheme is solvable, and have an optimal-order asymptotic convergence rate. We will discuss and observe the scheme numerically in next section.

For the outflow Neumann boundary condition, the ELLAM scheme at $i = E + 1, \dots, E + IC - 1$ is

$$\begin{aligned}
 (3.11) \quad & \int_{t_{i+1}}^{t_{i-1}} U(x_E, t) \hat{w}_i(x_E, t) V dt \\
 &= \int_{t_{i+1}}^{t_{i-1}} e^{-K(t-t^n)} U(x_E^*(t), t^n) \hat{w}_i(x_E, t) V dt + \int_{t_{i+1}}^{t_{i-1}} \Theta(t - t^n) f(x_E, t) \hat{w}_i(x_E, t) V dt \\
 &\quad - \int_{t_{i+1}}^{t_{i-1}} h_2(t) \hat{w}_i(x_E, t) dt - \int_{t_{i+1}}^{t_{i-1}} \Theta(t - t^n) h_2(t) [\hat{w}_{it}(x_E, t) - K \hat{w}_{it}(x_E, t)] dt.
 \end{aligned}$$

The scheme at $i = E$ is a combination of both types from (3.3) and (3.11).

Remark 3.5. (3.11) is positive definite, so the questions raised in Remark 3.4 for the flux condition do not arise in this case. We will present some numerical experiments for this in next section. We will compare the numerical solutions for the outflow Neumann and flux conditions in the next section.

For the outflow Dirichlet boundary condition, the ELLAM scheme at $i = E + 1, \dots, E + IC - 1$ are as follows:

$$\begin{aligned}
 (3.12) \quad & - \int_{t_{i+1}}^{t_{i-1}} D \Theta(t - t^n) U_x(x_E, t) [\hat{w}_{it}(x_E, t) - K \hat{w}_{it}(x_E, t)] dt - \int_{t_{i+1}}^{t_{i-1}} D U_x(x_E, t) \hat{w}_i(x_E, t) dt \\
 &= \int_{t_{i+1}}^{t_{i-1}} e^{-K(t-t^n)} U(x_E^*(t), t^n) \hat{w}_i(x_E, t) V dt + \int_{t_{i+1}}^{t_{i-1}} \Theta(t - t^n) f(x_E, t) \hat{w}_i(x_E, t) V dt \\
 &\quad - \int_{t_{i+1}}^{t_{i-1}} V h_1(t) \hat{w}_i(x_E, t) dt.
 \end{aligned}$$

Remark 3.6. The equations in (3.12) correspond to the unknowns describing $U_x(x_E, t)$ at the outflow boundary. Because $U(x_E, t^{n+1})$ is known with Dirichlet outflow, the equations for $i \leq E - 1$ decouple and can be solved for the unknowns through $U(x_{E-1}, t^{n+1})$. The equation at $i = E$ relates $U(x_{E-1}, t^{n+1})$ and $U_x(x_E, t^{n+1}) = U(x_E, t_E)$, so can be solved for $U_x(x_E, t_E)$ by forward substitution; the remaining unknowns are obtained similarly. The equations for $i \geq E$ are needed only for the purpose of mass conservation. The analysis for this case uses a lower bound on $(t_{E+IC-1} - t^n)/(t_{E+IC-2} - t_{E+IC-1})$, verifying theoretically the numerical results in [28] that showed the interval $[t^n, t_{E+IC-1}]$ should not be further subdivided.

Remark 3.7. It is easy to see that whether K is positive, zero, or negative, we all

have

$$(3.13) \quad \Theta(\Delta t(x)) \geq 0, \quad \Theta(t - t^n) \geq 0;$$

thus, the ELLAM schemes derived apply to all the cases $K = 0$, $K \geq 0$ and $K < 0$.

Remark 3.8. When $|K|$ is very small, $\Theta(\Delta t(x))$, $\Theta(\Delta t)$, and $\Theta(t - t^n)$ may not be easy to handle numerically. Since in this case $|K| \Delta t$ is small too, we can compute these terms by using their Taylor expansions instead of using their expressions directly: for any $m > 0$,

$$(3.14) \quad \begin{aligned} \Theta(\Delta t(x)) &= \Delta t(x) \left[\sum_{i=0}^m \frac{(-1)^i (K \Delta t(x))^i}{i!} + O((K \Delta t(x))^{m+1}) \right] \rightarrow \Delta t(x), \\ \Theta(t - t^n) &= (t - t^n) \left[\sum_{i=0}^m \frac{(-1)^i (K(t - t^n))^{m+1}}{i!} + O((K(t - t^n))^{m+1}) \right] \rightarrow (t - t^n). \end{aligned}$$

Remark 3.9. From (3.14) and the schemes derived above, we see that these ELLAM schemes for convection-diffusion-reaction problems naturally reduces to the ELLAM schemes for convection-diffusion problems when reaction term vanishes. Conversely, the ELLAM scheme for convection-diffusion problems can be considered as the first-order approximation to the ELLAM schemes for convection-diffusion-reaction problems when $|K|$ is very small.

Remark 3.10. In contrast to the convection-diffusion cases, where the interior ELLAM scheme with backward Euler in time is the same as modified methods of characteristics (MMOC) for the same problem. In the case of convection-diffusion-reaction problem, ELLAM schemes developed in this paper uses the splitting (2.7), while MMOC tend to lump the reaction term at time t^{n+1} and so corresponds to the splitting (2.6). Recalling that the exact solution u of problem (1.1) varies exponentially with rate K along the characteristics, the ELLAM schemes derived in this paper reflect the inherent physics more naturally.

§4. COMPUTATIONAL RESULTS.

In this section, we perform some numerical experiments. We solve the convection-diffusion-reaction equation (1.10) using the ELLAM schemes developed in this paper.

Example 1. In this example, we solve (1.10) with a known solution. Thus, we can compare the numerical solution with the exact one and observe the convergence rate. It is easy to see that

$$(4.1) \quad u(x, t) = \frac{\exp(-Kt) \exp(-\pi(x - Vt)^2 / (0.1 + 4\pi Dt))}{\sqrt{10}\sqrt{0.1 + 4\pi Dt}}.$$

is a solution of problem (1.10) with $f \equiv 0$.

In this example, we choose the parameters in (1.10) as follows: $(a, b) = (0, 1)$, $T = 0.5$, $V = 1$, $D = 0.01$, $K = 0.1$ and $f = 0$. We compute various boundary conditions in (1.11) and (1.12) by using the solution $u(x, t)$. We use $u(x, 0)$ as the initial condition. We then use ELLAM schemes in this paper to solve the problems

with the computed conditions. For each combination of boundary conditions, we perform two kinds of computations. One is to test the convergence rate with respect to Δx , where we pick up small Δt and observe the power α of Δx ; the other is to test the convergence rate with respect to Δt , where we choose small Δx and observe the power β of Δt . We use linear regression to compute α and β from the data. The errors are computed in L^2 norm.

We list the numerical results in the tables at the end of this paper. Tables 1 and 2 are associated with the inflow Dirichlet boundary condition. Table 1 tests factor α , and Table 2 tests β . In each table, we use I, II, III to represent outflow Dirichlet, Neumann, and flux boundary conditions, respectively. Tables 3 and 4 are associated with the inflow flux boundary condition. As above, Table 3 is for α and Table 4 is for β . Cases I, II, III are as defined above. Tables 5 and 6 are associated with the inflow Neumann boundary condition in an analogous manner.

From the numerical results, we see that for all combinations of inflow and outflow boundary conditions, we have second-order convergence in space and first-order convergence in time. We will prove this convergence rate theoretically in the subsequent paper.

From the numerical experiments, we see that the numerical solutions with the inflow Neumann boundary condition are much worse than those with other two inflow boundary conditions. These phenomena are also observed when we use other methods to solve a convection-dominated problem. We discuss this more after Example 5.

Example 2. In Remark 3.1, we discussed the effects of different treatments in the ELLAM schemes for the inflow Neumann boundary condition. In this example, we run some numerical experiments to confirm our expectations. We use (3.5) at $i = 0, 1, \dots, IC + 1$ with a constant interpolation along the time direction to compute the numerical solution. We use the same solution and data as in Example 1. Thus, we can compare these numerical results with those in Example 1. We put the numerical results in Table 7 at the end of this paper. From the numerical results, we can clearly see the strong influence of the time truncation error that makes the numerical solution useless in practice.

Example 3. In Remarks 3.2 and 3.3, we pointed out the treatment for the inflow Dirichlet boundary condition in [28] yields an ELLAM scheme with a convergence rate of $((\Delta x)^{3/2} + \Delta t)$. In this example, we run some numerical experiments to confirm our expectations. We use the scheme in [28] and the schemes (3.7) and (3.9) in this paper to solve problem (1.10). We use the same data as in Example 1 except that the reaction $K = 0$, the solution $u(x, t)$ and the initial condition $u_0(x)$, given in (4.2) below, are translated half units leftward to reflect the effects of the inflow Dirichlet boundary condition more clearly.

$$(4.2) \quad u(x, t) = \frac{\exp(-\pi(x - Vt + 0.5)^2 / (0.1 + 4\pi Dt))}{\sqrt{10}\sqrt{0.1 + 4\pi Dt}},$$

For conciseness, we only present the numerical results with the outflow Dirichlet condition since the results with other two outflow boundary conditions are similar. We

put the numerical results in Table 8. The numerical results confirm our statements. We will theoretically analyse this in the subsequent paper.

We have also performed numerical experiments to observe the effects of inflow or outflow boundary conditions on the numerical solutions. From these experiments, we have the following observations:

1. At the inflow boundary, Dirichlet and flux conditions are “good” conditions. Neumann condition is a “bad” condition. With the same mesh and the analytical solution, the numerical solutions with Dirichlet or flux conditions have negligible approximation errors, and have no phase errors present. The numerical solution with the inflow Neumann boundary has both approximation error and phase error.
2. Physically, inflow Dirichlet or flux conditions specify the concentration or total flux at the inflow boundary, these types of boundary conditions are physically reasonable. Neumann condition specifies only the amount of *diffusive flux* at the inflow boundary. It is not physically reasonable for a convection-dominated problem. Intuitively, for a convection-dominated problem, the diffusive flux only accounts for a small portion of the total flux. It is not reasonable to prescribe its value at the inflow boundary.
3. We now turn to the outflow boundary. At the outflow boundary, the numerical solution with the flux condition presents a little oscillation. While the numerical solution with the Neumann condition is good. The numerical solutions are not affected when Courant number increases. In fact, they are represented more smoothly since we use more spatial points for larger Courant numbers.
4. We point out that the oscillation of the numerical solution with the outflow flux condition is intrinsic in the boundary condition itself, not because of the use of ELLAM scheme. These observations coincide with the fact that the system for Neumann condition is symmetric and coercive at the outflow boundary while the system for the flux condition is indefinite.
5. For the outflow Dirichlet condition, when the “right” value is given at the outflow boundary, the numerical solution is good. Since generally we don’t know the “right” value in advance, a “wrong” value is usually prescribed. It is well-known that the outflow Dirichlet condition usually produces a boundary layer.
6. We now consider the outflow boundary conditions from a physical point of view. A homogeneous Neumann condition means that we just require the fluid flows out of the domain with the same concentration as from the domain. It is physically reasonable. Dirichlet or flux conditions requires that the fluid flows out of the domain with either a prescribed concentration or a prescribed total flux. It is physically unreasonable. This is part of the reason why the solution for this problem usually exhibits some bizzare behavior.
7. At last, we want to point out the following observations. In the case that we given the “right ” for the boundary conditions, the interior numerical solutions are almost independent of whether outflow Neumann or flux boundary conditions are given at the outflow boundary. This corresponds to the facts that in the convection-dominated case, the effects of the outflow boundary conditions on the solution over the interior domain comes from the diffusion, which is very small and negligible

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REFERENCES

- [1] M.B. ALLEN III, G.A. BEHIE, AND J.A. TRANGENSTEIN, *Multiphase flow in porous media*, Lecture Notes in Engineering, Springer-Verlag (1988).
- [2] J.W. BARRETT AND K.W. MORTON, *Approximate symmetrization and Petrov-Galerkin methods for diffusion-convection problems*, Comp. Meth. Appl. Mech. Engrg., 45 (1984), pp. 97–122.
- [3] E.T. BOULOUTAS AND M.A. CELIA, *An analysis of a class of Petrov-Galerkin and optimal test function methods* (M.A. Celia *et al.*, eds.), Proceedings of the Seventh International Conference on Computational Methods in Water Resources (1988), pp. 15–20.
- [4] A. BROOKS AND T.J.R. HUGHES, *Streamline upwind Petrov-Galerkin formulations for convection dominated flows with particular emphasis on the incompressible Navier-Stokes equations*, Comp. Meth. Appl. Mech. Engrg., 32 (1982), pp. 199–259.
- [5] M.A. CELIA, I. HERRERA, AND E.T. BOULOUTAS, *Adjoint Petrov-Galerkin methods for multi-dimensional flow problems*, Proceedings of the Seventh International Conference on Finite Element Methods in Flow Problems, Huntsville, Alabama, (1989), pp. 953–958.
- [6] M.A. CELIA, I. HERRERA, E.T. BOULOUTAS, AND J.S. KINDRED, *A new numerical approach for the advective-diffusive transport equation*, Numerical Methods for PDE's, 5 (1989), pp. 203–226.
- [7] M.A. CELIA, T.F. RUSSELL, I. HERRERA, AND R.E. EWING, *An Eulerian-Lagrangian localized adjoint method for the advection-diffusion equation*, Advances in Water Resources, 13 (1990), pp. 187–206.
- [8] M.A. CELIA AND S. ZISMAN, *An Eulerian-Lagrangian localized adjoint method for reactive transport in groundwater*, Computational Methods in Subsurface Hydrology, Proceedings of the Eighth International Conference on Computational Methods in Water Resources, Venice, Italy, pp. 383–392.
- [9] G. CHAVENT, G. COHEN, AND J. JAFFRE, *Discontinuous upwinding and mixed finite elements for two-phase flows in reservoir simulation*, Comp. Meth. in Appl. Mech. and Eng., 47 (1984), pp. 93–118.
- [10] H.K. DAHLE, *Adaptive characteristic operator splitting techniques for convection-dominated diffusion problems in one and two space dimensions*, IMA Volume 11, Mathematics and Its Applications, Springer Verlag (1988), pp. 77–88.
- [11] H.K. DAHLE, M.S. ESPEDAL, AND R.E. EWING, *Characteristic Petrov-Galerkin subdomain methods for convection diffusion problems* (M.F. Wheeler, ed.), IMA Volume 11, Numerical Simulation in Oil Recovery, Springer-Verlag, Berlin (1988), pp. 77–88.
- [12] H.K. DAHLE, M.S. ESPEDAL, R.E. EWING, AND O. SÆVAREID, *Characteristic adaptive subdomain methods for reservoir flow problems*, Numerical Methods for PDE's (1990), pp. 279–309.
- [13] H.K. DAHLE, R.E. EWING, AND T.F. RUSSELL, *Eulerian-Lagrangian localized adjoint methods for a nonlinear convection-diffusion equation* (to appear).
- [14] C.N. DAWSON, T.F. RUSSELL, AND M.F. WHEELER, *Some improved error estimates for the modified method of characteristics*, SIAM J. Numer. Anal., 26 (1989), pp. 1487–1752.
- [15] L. DEMKOWITZ AND J.T. ODEN, *An adaptive characteristic Petrov-Galerkin finite element method for convection-dominated linear and nonlinear parabolic problems in two space variables*, Comp. Meth. in Appl. Mech. and Eng., 55 (1986), pp. 63–87.
- [16] ———, *An adaptive characteristic Petrov-Galerkin method for convection-dominated linear and nonlinear parabolic problems in one space variable*, J. Comp. Phys. 67 (1986), pp. 188–213.
- [17] J. DOUGLAS, JR. AND T.F. RUSSELL, *Numerical methods for convection-dominated diffusion problems based on combining the method of characteristics with finite element or finite difference procedures*, SIAM J. Numer. Anal., 19 (1982), pp. 871–885.
- [18] M.S. ESPEDAL AND R.E. EWING, *Characteristic Petrov-Galerkin subdomain methods for two-phase immiscible flow*, Comp. Meth. in Appl. Mech. and Eng., 64 (1987), pp. 113–135.

- [19] R.E. EWING, ed., *Research Frontiers in Applied Mathematics*, Vol. 1, SIAM, Philadelphia (1983).
- [20] ———, *Operator splitting and Eulerian-Lagrangian localized adjoint methods for multiphase flow*, Proceedings of Conference on Mathematics of Finite Elements and Applications (MAFELAP), Brunel University, Uxbridge, United Kingdom (to appear).
- [21] R.E. EWING AND H. WANG, *Eulerian-Lagrangian localized adjoint methods for linear advection equations*, Proceedings of International Conference on Computational Engineering Science, Melbourne, Australia (1991), pp. 245–250.
- [22] I. HERRERA, *The algebraic theory approach for ordinary differential equations: highly accurate finite differences*, Numerical Methods for PDE's, 3 (1987), pp. 199–218.
- [23] I. HERRERA, L. CHARGOY, AND G. ALDUNCIN, *Unified formulation of numerical methods*, 3, Numerical Methods for PDE's, 1 (1985), pp. 241–258.
- [24] T.J.R. HUGHES AND A. BROOKS, *A theoretical framework for Petrov-Galerkin methods with discontinuous weighting functions. Applications to the streamline-upwind procedure* (Gallagher, ed.), Finite Elements in Fluids, 4, Wiley (1982).
- [25] C. JOHNSON, *Numerical solutions of partial differential equations by the finite element method*, Cambridge University Press, Cambridge (1987).
- [26] C. JOHNSON AND J. PITKARANTA, *An analysis of the discontinuous Galerkin method for a scalar hyperbolic equation*, Math. Comp. (to appear).
- [27] T.F. RUSSELL, *Time-stepping along characteristics with incomplete iteration for a Galerkin approximation of miscible displacement in porous media*, SIAM J. Numer. Anal., 22 (1985), pp. 970–1013.
- [28] ———, *Eulerian-Lagrangian localized adjoint methods for advection-dominated problems*, Numerical Analysis 1989, Proceedings of the 13th Dundee Conference on Numerical Analysis (D.F. Griffiths and G.A. Watson, eds.), Pitman Research Notes in Mathematics Series, 228, Longman Scientific & Technical, Harlow, U.K. (1990), pp. 206–228.
- [29] T.F. RUSSELL AND R.V. TRUJILLO, *Eulerian-Lagrangian localized adjoint methods with variable coefficients in multiple dimensions*, Computational Methods in Surface Hydrology, Proceedings of the Eighth International Conference on Computational Methods in Water Resources, Venice, Italy (1990), pp. 357–363.
- [30] T.F. RUSSELL AND M.F. WHEELER, *Finite element and finite difference methods for continuous flows in porous media* (R.E. Ewing, ed.), Mathematics of Reservoir Simulation, Frontiers in Applied Math, Philadelphia, Pennsylvania (1983), pp. 35–106.
- [31] V. THOMÉE, *Galerkin finite element methods for parabolic problems*, Lecture Notes in Mathematics, 1054, Springer-Verlag (1984).
- [32] E. VAROGLU AND W.D.L. FINN, *Finite elements incorporating characteristics for one-dimensional diffusion-convection equation*, J. Comp. Phys., 34 (1980), pp. 371–389.

TABLE 1. *Inflow Dirichlet boundary condition, test for factor α .*

Δt	Δx	L^2 error (I)	L^2 error (II)	L^2 error (III)
1/1000	1/10	$1.49424E-2$	$1.49292E-2$	$1.51909E-2$
1/1000	1/20	$3.27526E-3$	$3.27448E-3$	$3.30362E-3$
1/1000	1/40	$7.88156E-4$	$7.88133E-4$	$7.91951E-4$
1/1000	1/80	$1.75615E-4$	$1.75614E-4$	$2.14234E-4$
		$\alpha = 2.13$	$\alpha = 2.13$	$\alpha = 2.05$

TABLE 2. *Inflow Dirichlet boundary condition, test for factor β .*

Δt	Δx	L^2 error (I)	L^2 error (II)	L^2 error (III)
1/20	1/100	$1.59283E-3$	$1.59493E-3$	$1.61248E-3$
1/40	1/100	$7.77086E-4$	$7.77863E-4$	$7.87889E-4$
1/80	1/100	$3.31847E-4$	$3.32139E-4$	$3.38001E-4$
1/160	1/100	$1.22176E-4$	$1.22315E-4$	$1.25394E-4$
		$\beta = 1.23$	$\beta = 1.23$	$\beta = 1.23$

TABLE 3. *Inflow flux boundary condition, test for factor α .*

Δt	Δx	L^2 error (I)	L^2 error (II)	L^2 error (III).
1/1000	1/10	$9.43173E-3$	$9.41098E-3$	$9.81385E-3$
1/1000	1/20	$1.91666E-3$	$1.91534E-3$	$1.96473E-3$
1/1000	1/40	$4.50972E-4$	$4.50931E-4$	$4.57572E-4$
1/1000	1/80	$9.59414E-5$	$9.59373E-5$	$9.66831E-5$
		$\alpha = 2.19$	$\alpha = 2.19$	$\alpha = 2.21$

TABLE 4. *Inflow flux boundary condition, test for factor β .*

Δt	Δx	L^2 error (I)	L^2 error (II)	L^2 error (III).
1/20	1/100	$1.52266E-3$	$1.53486E-3$	$1.54321E-3$
1/40	1/100	$7.50763E-4$	$7.51567E-4$	$7.61940E-4$
1/80	1/100	$3.54362E-4$	$3.54636E-4$	$3.60133E-4$
1/160	1/100	$1.55049E-4$	$1.55159E-4$	$1.57598E-4$
		$\beta = 1.10$	$\beta = 1.10$	$\beta = 1.10$

TABLE 5. Inflow Neumann boundary condition, test for factor α .

Δt	Δx	L^2 error (I)	L^2 error (II)	L^2 error (III).
1/1000	1/10	$1.92754E-1$	$1.92753E-1$	$1.92772E-1$
1/1000	1/20	$4.23847E-2$	$4.23846E-2$	$4.23869E-2$
1/1000	1/40	$9.44468E-3$	$9.44468E-3$	$9.44500E-3$
1/1000	1/80	$1.54254E-3$	$1.54254E-3$	$1.54259E-3$
		$\alpha = 2.31$	$\alpha = 2.31$	$\alpha = 2.31$

TABLE 6. Inflow Neumann boundary condition, test for factor β .

Δt	Δx	L^2 error (I)	L^2 error (II)	L^2 error (III).
1/20	1/100	$4.09166E-2$	$4.09170E-2$	$4.09177E-2$
1/40	1/100	$2.13992E-2$	$2.13993E-2$	$2.13996E-2$
1/80	1/100	$1.06259E-2$	$1.06260E-2$	$1.06261E-2$
1/160	1/100	$4.92285E-3$	$4.92285E-3$	$4.92293E-3$
		$\beta = 1.02$	$\beta = 1.02$	$\beta = 1.02$

TABLE 7. Inflow Neumann boundary condition, test for factor α .

Δt	Δx	L^2 error (I)	L^2 error (II)	L^2 error (III).
1/1000	1/10	$2.07236E-1$	$2.07235E-1$	$2.07253E-1$
1/1000	1/20	$6.39451E-2$	$6.39450E-2$	$6.39466E-2$
1/1000	1/40	$3.33366E-2$	$3.33366E-2$	$3.33367E-2$
1/1000	1/80	$2.63765E-2$	$2.63765E-2$	$2.63765E-2$
		$\alpha = 0.99$	$\alpha = 0.99$	$\alpha = 0.99$

TABLE 8. Comparison of different treatments of inflow Dirichlet boundary condition, test for factor α .

Δt	Δx	L^2 error of scheme in [29]	L^2 error of our scheme
1/1000	1/50	$4.879038E-4$	$3.820066E-4$
1/1000	1/60	$3.774253E-4$	$2.641193E-4$
1/1000	1/70	$3.019386E-4$	$1.931335E-4$
1/1000	1/80	$2.475183E-4$	$1.471224E-4$
		$\alpha = 1.4888$	$\alpha = 2.0957$

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