An Operator-Splitting Method for Advection-Diffusion-Reaction Problems

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1. INTRODUCTION

In this paper we consider a time-splitting algorithm for solving coupled systems of nonlinear advection-diffusion-reaction problems of the following form:

\[-\nabla \cdot (k(x)\nabla p) \equiv \nabla \cdot u = q, \quad x \in \Omega, \quad t \in J,\]

\[\phi_i \frac{\partial c_i}{\partial t} \nabla \cdot D(u) \nabla c_i + u \cdot \nabla c_i = \nabla (\tilde{c}_i - c_i) q + \phi_i R_i(c_1, c_2, \ldots, c_N),\]

\[x \in \Omega, \quad t \in J, \quad i = 1, 2, \ldots, N,\]

\[c_i(x, 0) = c_{io}(x), \quad x \in \Omega, \quad i = 1, 2, \ldots, N,\]

where \(\Omega\) is a bounded domain in \(\mathbb{R}^2\), \(J = (0, T]\), and \(q = \max \{q, 0\}\) is nonzero at source points only. The \(R_i\) are nonlinear reaction terms and \(D(u)\) is a tensor and velocity-dependent. Furthermore, \(\tilde{c}_i\) is specified at injection sources and \(\tilde{c}_i = c_i\) at production sources.

Boundary conditions one frequently encounters are of the following form, with \(\partial \Omega\), the boundary of \(\Omega\), and \(\partial \Omega = \Gamma_1 \cup \Gamma_2\) and \(n\) the outer normal,

\[u \cdot n = (D(u)\nabla c_i - u c_i) \cdot n = 0, \quad x \in \Gamma_1, \quad t \in J,\]

\[p = p' \text{ on } \Gamma_2, \quad t \in J,\]

and \(c_i\) satisfying an inflow or an outflow boundary condition on \(\Gamma_2\). Systems of p.d.e.'s of the form (1.1) occur frequently in many engineering applications; in particular the modeling of contaminant transport in groundwater.

Contamination of aquifers from sources such as improperly disposed toxic wastes, leaking storage tanks and seepage from polluted streams and
ponds is meeting with increasing public concern. Microbial biodegradation, the decomposition of contaminants by microorganisms, is an important natural process that can be accelerated to protect a potable water supply. This procedure is physically and chemically complex, involving transport and interaction of various hydrocarbons and microbes as well as water movement within the aquifer.

For many of these problems, the flow is advection-dominated and the time scales for reactions and advection-dispersion are quite different. Reactions occur much faster than advection. For more details, see [2]. Thus, to solve these nonlinear equations simultaneously would be very costly in computer time.

To avoid the above difficulties we propose solving the problem in a sequential fashion, using a numerical method which is particularly suited to each piece of the computation. First, accurate velocities are calculated using a mixed finite element procedure. A time-splitting algorithm is then employed for treating the advection-dispersion and reaction terms. Namely, the reaction terms are separated from the advection-dispersion terms. The latter is treated using a modified method of characteristics. This method was first formulated in one space variable by Douglas and Russell [5] and then extended by Russell [11, 12] to two and three spatial dimensions. In this scheme one combines the time derivatives and the advection term as a directional derivative. In other words the procedure involves time-stepping along the characteristics, allowing one to use large accurate timesteps. An algorithm combining the mixed finite element method and the modified method of characteristics was first applied to the miscible displacement problem in porous media by Ewing, Russell and Wheeler [8,9]. This paper uses many of the theoretical tools developed in [5, 9, 11].

In our time-splitting algorithm the reaction terms become a system of nonlinear ordinary differential equations. Computationally we found the second order Runge-Kutta explicit method to be adequate.

In summary, we first perform one advection-dispersion time step using a finite element modified method of characteristics. Subsequently we compute reactions using a second-order Runge-Kutta method for many small time steps. The approximation to the solution at the last small time step is then used as initial data for the next advection-dispersion step.

This time-splitting sequential approach is ideal for parallel computation. The advection-dispersion step can be solved simultaneously on different processors. Moreover, the backward tracking of the characteristics is not vectorizable, but can be easily implemented in a parallel fashion. Clearly the reaction o.d.e.'s can be done in parallel over as many processors as are available. For applications of this time-splitting scheme to microbial biodegradation the reader is referred to [3, 4, 14].

The remaining sections are developed in the following fashion. Preliminaries and notation are established in Section 2. The scheme is formally defined in the subsequent section. In Section 3 a priori error estimates, $L^\infty(L^2)$ are derived. For convenience, we have simplified our discussion by
assuming that the velocity vector \( u \) is given and no flow boundary conditions are prescribed, i.e. \( \Gamma_1 = \partial \Omega \). The additional complexity of analyzing a computed \( u \) obtained by a mixed finite element procedure can be handled in a standard technical fashion; see [9] for instance. Similar remarks hold for more general boundary conditions.

Some computational results for the microbial biodegradation problem are briefly described in Section 4. Concluding remarks are given in the last section.

2. PRELIMINARIES AND NOTATION

On \( \Omega \), we define the Sobolev spaces and norms:

\[
L^2(\Omega) = \left\{ f : \int_\Omega |f|^2 \, dx \, dy < \infty \right\}, \quad ||f||^2 = \int_\Omega |f|^2 \, dx \, dy,
\]

\[
L^\infty(\Omega) = \left\{ f : \text{ess sup}_\Omega |f| < \infty \right\}, \quad ||f||_{L^\infty} = \text{ess sup}_\Omega |f|,
\]

\[
H^m(\Omega) = \left\{ f : \frac{\partial^{|\alpha|} f}{\partial x^\alpha} \in L^2(\Omega) \text{ for } |\alpha| \leq m \right\},
\]

\[
||f||_m = \sum_{|\alpha| \leq m} ||\frac{\partial^{|\alpha|} f}{\partial x^\alpha}||, \quad m \geq 0,
\]

\[
W^m_\infty(\Omega) = \left\{ f : \frac{\partial^{|\alpha|} f}{\partial x^\alpha} \in L^\infty(\Omega) \text{ for } \alpha \leq m \right\},
\]

\[
||f||_{W^m_\infty} = \max_{|\alpha| \leq m} ||\frac{\partial^{|\alpha|} f}{\partial x^\alpha}||_{L^\infty}, \quad m \geq 0.
\]

The inner product on \( L^2(\Omega) \) is denoted by \((\cdot, \cdot)\).

We also use the following spaces that incorporate time dependence. Let \([a, b] \subset J\) and let \( X \) be any of the above \( L^p \) or Sobolev spaces. For \( f(x, t) \) suitably smooth on \( \Omega \times [a, b] \) we let

\[
H^m(a, b; X) = \left\{ f : \int_a^b \| \frac{\partial^\alpha f(\cdot, t)}{\partial t^\alpha} \|_X^2 \, dt < \infty, \quad \alpha \leq m \right\},
\]

\[
||f||_{H^m(a, b; X)} = \left[ \sum_{\alpha=0}^m \frac{1}{\alpha!} \int_a^b \| \frac{\partial^\alpha f(\cdot, t)}{\partial t^\alpha} \|_X^2 \, dt \right]^\frac{1}{2}, \quad m \geq 0,
\]
Similarly, \( W^m_{\infty}(a,b;\mathcal{X}) \) and the norm \( ||f||_{W^m_{\infty}(a,b;\mathcal{X})} \) are defined. If \([a,b]=\mathcal{I}\), we simplify our notation and write \( L_{\infty}(W^1_{\infty}) \) for \( L_{\infty}(0,T;W^1_{\infty}(\Omega)) \). For details regarding Sobolev spaces, see Adams [1].

We make the following regularity assumptions on the components \( c_i, p, \) and \( u \), i.e.

\[
c \in L_{\infty}(H^{s+1}) \cap H^1(H^{s+1}) \cap L_{\infty}(W^1_{\infty}) \cap H^2(L^2),
p \in L_{\infty}(H^1),\]
\[
u \in L_{\infty}(W^1_{\infty}) \cap W^1_{\infty}(L^\infty) \cap H^2(L^2),
\]

where \( s \geq 0 \). In addition, we require the following assumptions on the coefficients. Let \( k_s, k^{**}, \phi_s, \phi^{*}, D_s, \) and \( K^* \) be positive constants such that

\[
0 < k_s \leq k(x) \leq k^{**}, \quad 0 < \phi_s \leq \phi_i(x) \leq \phi^{*}, \quad 0 < D_s \leq D(x, u),
\]
\[
\left| \nabla \phi_i(x) \right| + \left| \frac{\partial D}{\partial u_j}(x, u) \right| + |q(x, t)| + \left| \frac{\partial q}{\partial t}(x, t) \right| + \left| \frac{\partial R_i(c)}{\partial c_j} \right| + \left| R_i(c', t^n) \right|_{H^{s+1}} \leq K^*.
\]

Furthermore, \( R \) must satisfy the following condition, which we will refer to in later sections as

**Condition A:** For each \( i = 1, \ldots, N \), \( R_i(s) \) is twice differentiable and \( R_i \) and all first and second derivatives of \( R_i \) with respect to \( s \) are bounded over a set \( \mathcal{B} = \{s \in \mathcal{R}^n / ||| s ||| \leq Y^* \} \), where \( Y^* \) satisfies

\[
e^{K^* T} \left[ \max_{0 \leq t \leq T} \sup_{\Delta x, \Delta t \to 0} \left( \max_{n} \sup_{\Delta t} \left| C(x, t^n) \right| \right) \right] + \frac{e^{K^* T}}{K^*} \left| ||| R(0) ||| \right| \leq Y^*.
\]

Here \( C \) is our approximate solution to \( c \) and \( ||| \cdot ||| \) is the \( l^1 \) vector norm, i.e. \( ||| c(x, t) ||| = \sum_{i=1}^{N} |c_i(x, t)| \).

For convenience, we have assumed that the \( q \) are smooth functions. Our arguments could however be modified to establish convergence for the point source case, see [6] and [7].

3. **TIME-SPLITTING PROCEDURE**

Let \( h > 0 \) and \( M_h \) be a finite dimensional subspace of \( H^1(\Omega) \). We further assume that \( M_h \) has a nodal basis \( \{u_k\} \) and that the following approximation properties hold. There exists an integer \( k^* \geq 0 \) such that
\[
\inf_{x \in M_h} \{ ||f - x|| + h ||f - x||_1 + ||f - x||_{L^\infty} + h ||f - x||_{W_1^1} \}
\]

\[
\leq K_0 h^l ||f||_t, \quad 2 \leq l \leq k^* + 1,
\]

\[
||x||_{W_1^1} \leq K_0 h^{-1} ||x||_1, \quad ||x||_{L^\infty} \leq K_0 h^{-1} ||x||_1,
\]

\[
||x||_1 \leq K_0 h^{-1} ||x||, \quad x \in M_h,
\]

where \( K_0 \) is independent of \( h \). It is well known that these properties are valid for continuous piecewise polynomials of degree \( \leq k^* \) on a quasi-uniform mesh of diameter \( \leq h \).

Let \( \Delta t > 0 \) and \( \Delta t_e = \Delta t/M \), where \( M \) is a positive integer. Set \( t^n = n \Delta t \) and \( t^{j,n} = t^n + j \Delta t_e, \quad 0 \leq j \leq M \). Let \( f^n = f(t^n) \) and \( f^{j,n} = f(t^{j,n}) \). Also let \( t^{N_e} = T \). Furthermore, let \( f_k = f(x_k) \) for \( x_k \) a node in \( \Omega \).

Our convergence analysis will use a technique based on comparing our time-splitting, finite element approximation to an elliptic projection; see [13, 9]. Define \( C_i(\cdot, t) \in M_h \) by

\[
(D(u)\nabla \bar{c}_i, \nabla \chi) + (\bar{c}_i, \chi) + (q \bar{c}_i, \chi) = -(\phi_i \chi, \chi) + (c_i, \chi) + (q c_i, \chi) + (q c_i, \chi)
\]

where \( \chi \in M_h \), \( t \in J \), \( i = 1, 2, \ldots, N \).

Before defining our time-splitting procedure we comment on the modified method of characteristics applied to the single advection-diffusion equation

\[
\phi \frac{\partial c}{\partial t} + u \cdot \nabla c - \nabla \cdot D \nabla c = q.
\]

The basic idea is to think of the hyperbolic part of this equation, namely \( \phi \frac{\partial c}{\partial t} + u \cdot \nabla c \), as a directional derivative. Let \( \tau \) denote the unit vector in the direction \( (u_1, u_2, \phi) \) in \( \Omega \times J \) and set

\[
\psi = \left[ |u|^2 + \phi^2(x) \right]^{1/2}.
\]

Then one obtains

\[
\psi \frac{\partial c}{\partial \tau} - \nabla \cdot D \nabla C = q,
\]

which has the form of the heat equation. We further note that

\[
\frac{\partial c^n}{\partial \tau} = \frac{c^n(x) - c^{n-1}(x - \frac{u(x, t^n)}{\phi(x)} \Delta t)}{\Delta t \sqrt{1 + |u|^2/\phi^2(x)}} \]  

and if we let
\[ \dot{x} = x - (u(x, t^n)/\phi(x))\Delta t, \quad (3.6) \]

then

\[ \psi \frac{\partial c^n}{\partial t} = \phi \frac{c^n - c^{n-1}(\dot{x})}{\Delta t}. \quad (3.7) \]

The time-split procedure is a collection of maps

\[ C_i: \{ t^0, t^1, \ldots, t^{N^*} = T \} \rightarrow M_h \text{ defined by} \]

\[ (\phi_i \frac{C_i^n - \overline{C}_i^{n-1}}{\Delta t}, x) + (D(u^n) \nabla C_i^n, \nabla x) = (q^n(\dot{c}_i^n - C_i^n), x), \quad (3.8) \]

\[ x \in M_h, \quad n \geq 1, \quad i = 1, 2, \ldots, N, \]

where

\[ \overline{C}^0_i(x) = \overline{C}_i(\dot{x}, 0), \quad n = 1, \quad (3.9a) \]

and for \( n > 1 \), \( \overline{C}^{n-1}_i = \overline{C}^{M,n-1}_i \) where

\[ \overline{C}^{M,n-1}_i = \sum_k \left[ C_i^{0,n-1} + \Delta t \sum_{j=0}^{M-1} R_i(C_i^{j,n-1} + \frac{\Delta t}{2} R(C_i^{j,n-1})) \right] \]

\[ \times \, u_k(\dot{x}). \quad (3.9b) \]

Here for \( i = 1, 2, \ldots, N, \)

\[ C_i^{0,n-1} = C_i^{n-1}, \quad (3.10a) \]

\[ C_i^{j+1,n-1} = C_i^{j,n-1} + \Delta t \, R_i(C_i^{j,n-1} + \frac{\Delta t}{2} R(C_i^{j,n-1})), \quad (3.10b) \]

\[ j = 0, 1, 2, \ldots, M-1. \]

We note that (3.8) is the discretization of the advection step using the modified method of characteristics as the basic numerical scheme. Also, equation (3.10b) corresponds to taking \( M \) time steps of size \( \Delta t \) with an explicit second-order Runge-Kutta scheme applied to the system of o.d.e.'s

\[ \overline{c}_i(x_k) = R(\overline{c}(x_k)), \quad t^{n-1} < t \leq t^n \]

\[ \overline{c}(x_k, t^{n-1}) = C^{n-1}(x_k), \]

where \( x_k \) is a mesh point in \( \Omega \). Equation (3.9b) is then obtained by spatially interpolating the approximations to the values \( \overline{C}_i(x_k, t^{M,n-1}) \) and evaluating this interpolate at \( \dot{x} \).

In the analysis that follows \( K \) will denote a generic constant. We will also assume that \( l = \min(s,k^*) \). See (2.1) and (3.1)-(3.3).

Let
\[ \alpha^{i,n-1}(x) = C^{i,n-1}(x) + \frac{\Delta t}{2} \mathcal{R}(C^{i,n-1}(x)), \quad x \in \Omega, \]

where \( C^{i,n-1} \) is defined by (3.10). Similarly with \( c_i^{i,n-1} \) defined recursively by (3.10) and \( c_i^{0,n-1} = c_i^{n-1} \), let

\[ \gamma^{i,n-1}(x) = c^{i,n-1}(x) + \frac{\Delta t}{2} \mathcal{R}(c^{i,n-1}(x)). \]

Set \( \psi_i = c_i - \tilde{C}_i \) and \( \zeta_i = C_i - \tilde{C}_i \). Then subtracting (3.4) from (3.9), we obtain after some manipulation

\[
\frac{1}{\Delta t}(\phi_i(\zeta_i^n - \zeta_{i-1}^n), \chi) + (D(u^n) \nabla \zeta_i^n, \nabla \chi)
\]

\[ = \left[ (\phi_i \frac{\partial c_i^n}{\partial t} + u^n \cdot \nabla c_i^n) - \phi_i \frac{c_{i-1}^n - c_{i-1}^{n-1}}{\Delta t}, \chi \right] + \left( \phi_i \frac{\xi_i^n - \xi_{i-1}^n}{\Delta t}, \chi \right) \]

\[ - (\xi_i^n, \chi) - (q^n \zeta_i^n, \chi) - (\phi_i \frac{\xi_{i-1}^n - \xi_{i-1}^{n-1}}{\Delta t}, \chi) \]

\[ + (\phi_i \frac{\xi_{i-1}^{n-1} - \xi_{i-1}^{n-1}}{\Delta t}, \chi) + \left[ -(\phi_i R_i(c^n), \chi) + (\phi_i \frac{\Delta t}{\Delta t} \sum_{j=0}^{M-1} \sum_{k} R_i(\alpha_k^{i,n-1}) \psi_k^{n-1}, \chi) \right]. \]

(3.11)

Here \( \tilde{f}(x) = f(\bar{x}) \), where \( \bar{x} \) is given by (3.6).

For an \( L^2 \) estimate of \( \zeta_i \), choose \( \chi = \zeta_i^n \) as a test function and denote the resulting terms on the right-hand side as \( T_1, T_2, T_3, \ldots, T_7 \), i.e.

\[
\frac{1}{2\Delta t} \left[ (\phi_i \zeta_i^n, \zeta_i^n) - (\phi_i \zeta_{i-1}^n, \zeta_{i-1}^n) \right] + (D(u^n) \nabla \zeta_i^n, \nabla \zeta_i^n)
\]

\[ \leq T_1 + T_2 + \cdots + T_7. \]

(3.12)

Terms \( T_1, T_2, \ldots, T_6 \) were estimated in Ewing et al. and we briefly indicate appropriate bounds. That is,

\[
T_1 = \left| \left( \phi_i \frac{\partial c_i^n}{\partial t} + u^n \cdot \nabla c_i^n - \phi_i \frac{c_{i-1}^n - c_{i-1}^{n-1}}{\Delta t}, \zeta_i^n \right) \right|
\]

\[ \leq K || \frac{\partial^2 c_i^n}{\partial t^2} ||_{L^2(t_{i-1}, t_i; L^2)} \Delta t + K || \zeta_i^n ||^2, \]

(3.13)

\[ T_2 = \left| \left( \phi_i \frac{\xi_i^n - \xi_{i-1}^n}{\Delta t}, \zeta_i^n \right) \right|
\]

\[ \leq K(\Delta t)^{-1} || \frac{\partial \xi_i}{\partial t} ||_{L^2(t_{i-1}, t_i; L^2)} + K || \zeta_i^n ||^2 \]

\[ \leq K(\Delta t)^{-1} K^{2(i+1)} || c_i ||^2_{H^1(t_{i-1}, t_i; H^{i+1})} + K || \zeta_i^n ||^2. \]

(3.14)
\[ T_3 = |(\xi_i^n, \xi_j^n)| \leq Kh^{2(l+1)} ||c_i||_{L^H}^2 + K ||\xi_i^n||^2, \quad \text{and} \quad (3.15) \]

\[ T_4 = |(q^n\xi_i^n, \xi_j^n)| \leq K ||\xi_i^n||^2. \quad (3.16) \]

The terms \( T_5 \) and \( T_6 \) have the form \( |(\phi_i \frac{\hat{f} - f}{\Delta t}, \xi_j^n)| \). Using duality they are bounded by

\[ ||\frac{\hat{f} - f}{\Delta t}||_{H^{-1}} ||\phi_i \xi_j^n||_{H^1}. \]

A detailed estimate of \( ||\frac{\hat{f} - f}{\Delta t}||_{H^{-1}} \) is derived in [9] and behaves like \( ||f||_{L^2}. \) Thus

\[ T_5 + T_6 = \left( \phi_i \frac{\hat{\xi}_i^{n-1} - \xi_i^{n-1}}{\Delta t}, \xi_j^n \right) + \left( \phi_i \frac{\hat{\xi}_i^{n-1} - \xi_i^{n-1}}{\Delta t}, \xi_j^n \right) \]

\[ \leq Kh^{2(l+1)} + \epsilon ||\xi_j^n||_{H^{-1}}^2 + K ||\xi_j^n||^2. \quad (3.17) \]

We have estimates for all the terms except the last term (enclosed in brackets) on the right-hand side of (3.11). For convenience we drop the subscript \( i \) in bounding this term. We write

\[ T_7 = - \left( \phi R(\xi^n), \xi^n \right) - \left( \phi \frac{\Delta t}{\Delta t} \sum_{j=0}^{M-1} \sum_k R(\alpha_k^{j,n-1}) \hat{v}_k, \xi^n \right) \]

\[ = S_1 + S_2 + S_3 + S_4, \quad (3.18) \]

where

\[ S_1 = \left( \phi \frac{\Delta t}{\Delta t} \sum_{j=0}^{M-1} \sum_k (R(\alpha_k^{j,n-1}) - R(\gamma_k^{j,n-1})) \hat{v}_k, \xi^n \right), \quad (3.19) \]

\[ S_2 = \left( \phi \sum_k \left[ \left( \sum_{j=0}^{M-1} \frac{\Delta t}{\Delta t} (R(\gamma_k^{j,n-1}) - R(\gamma_k^{j,n-1})) \right) \hat{v}_k, \xi^n \right) \right), \quad (3.20) \]

\[ S_3 = \left( \phi \sum_k (R(c_k^n)(\hat{v}_k - v_k)), \xi^n \right), \quad (3.21) \]

and

\[ S_4 = \left( \phi \sum_k (R(c_k^n)(\hat{v}_k - v_k)), \xi^n \right). \quad (3.22) \]

Before deriving bounds for the above terms, we wish to make the following observations. Namely if \( f_j \) is a piecewise polynomial interpolate of a continuous function \( f \), then
\[ \|f_1\| \leq K \|f\| . \]  

(3.23)

Also by considering the map \( G: \mathbb{R}^2 \to \mathbb{R}^2 \) given by
\[
G(x) = \hat{x} = x - \frac{u^n(x)}{\phi(x)} \Delta t ,
\]

one can show that
\[
\int_{\Omega} (F(G(x)))^2 \, dx \leq \text{const} \int_{\Omega} (F(x))^2 \, dx, \quad \text{i.e.}
\]
\[ \|F(G)\| \leq K \|F\| \quad (3.24) \]

where \( K \) is a constant independent of \( h \). For details the reader is referred to [9].

Using (3.24) and (3.23), we have that
\[
|S_1| \leq \|\phi\|_{L^\infty} \frac{\Delta t^2}{\Delta t} \sum_{j=0}^{M-1} \|\sum_i (R(\alpha^{i,n-1}) - R(\gamma^{i,n-1})) \hat{e}_k\| \|s^n\|
\]
\[
\leq K \|\phi\|_{L^\infty} \Delta t \sum_{j=0}^{M-1} \|\sum_i (R(\alpha^{i,n-1}) - R(\gamma^{i,n-1})) v_k\| \|s^n\|
\]
\[
\leq K \|\phi\|_{L^\infty} \Delta t \sum_{j=0}^{M-1} \|(R(\alpha^{j,n-1}) - R(\gamma^{j,n-1}))\| \|s^n\| .
\]

By the Lipschitz continuity assumption on \( R \), we further obtain
\[
|S_1| \leq \|\phi\|_{L^\infty} \frac{\Delta t^2}{\Delta t} K(K^\ast(N+1))
\]
\[
\times \sum_{i=1}^N \sum_{j=0}^{M-1} \|C_t^{i,n-1} - c_t^{i,n-1}\| \|s^n\| . \quad (3.25)
\]

Consider the initial value problems
\[
s_t = R(s), \quad t^{n-1} < t \leq t^n ,
\]
\[
s(t^{n-1}) = c^{n-1}, \quad (3.26)
\]
and
\[
\tilde{s}_t = R(\tilde{s}), \quad t^{n-1} < t \leq t^n ,
\]
\[
\tilde{s}(t^{n-1}) = \tilde{c}^{n-1} . \quad (3.27)
\]

Thus,
Next we estimate the second term in the bracket in (3.28). Subtracting (3.27) from (3.26), taking the inner product of the result with $s - \overline{c}$ and integrating, we see that

$$\int_{\Omega} (s - \overline{c}) : (s - \overline{c}) \, dxdy = \int_{\Omega} (R(s) - R(c)) : (s - \overline{c}) \, dxdy.$$  

Thus,

$$\frac{1}{2} \frac{d}{dt} \| s - \overline{c} \|_{L^2}^2 \leq K^* \| s - \overline{c} \|_{L^2}^2$$

or

$$\| s - \overline{c} \|_{L^2}^2(t^n-1 + \tau) \leq e^{2K^*} \| s - \overline{c} \|_{L^2}^2(t^n-1), \quad 0 \leq \tau \leq \Delta t,$$

$$= e^{2K^*} \| \xi_{i,n} - c_{n-1} \|_{L^2}^2$$

$$\leq \sum_{i=1}^{N} K \left( \| \xi_{i,n} \|_{L^2}^2 + \| \xi_{i,n} \|_{L^2}^2 \right)$$

$$\leq \sum_{i=1}^{N} K \left( \| \xi_{i,n} \|_{L^2}^2 + \Delta t \xi_{i,n} \right).$$

Before estimating the first and third terms above, we state the following lemma, which can be found in Henrici [10].

**Lemma 3.1.** Let $y = (y_1, y_2, \ldots, y_N), f(y) = (f_1(y), \ldots, f_N(y))$ satisfy

$$y'(t) = f(y(t)), \quad a \leq t \leq b,$$

$$y(a) = \eta.$$

Let $y^m$ denote the explicit second-order Runge-Kutta approximation to $y(a + m \Delta t_s) = y(t^m), \Delta t_s > 0$, which is given by

$$y^m = \eta + \Delta t_s \sum_{i=1}^{m-1} f(y^i + \frac{\Delta t_s}{2} f(y^i)).$$

Let $\| \cdot \|$ denote the $l^1$ vector norm and assume $f$ is Lipschitz continuous. Then

$$\| y^m - y(t^m) \| \leq N \Delta t_s^2 K(M)$$

where $K(M)$ is a constant which depends on $M = \Delta t / \Delta t_s$. Here

$$N \leq M_2 + D_2 M_0^2,$$
\[ M_2 = \max_{\|y\| \leq Y} \|f'''(y)\|, \] (3.32)

\[ D_2 = \max_{1 \leq i, j, s \leq N} \|f^{i,j,s}(y)\|, \] (3.33)

\[ M_0 = \max_{\|y\| \leq Y} \|f(y)\|, \] (3.34)

\[ Y = e^{L_{b-a}}\|\eta\| + \frac{e^{L_{b-a}}-1}{L} ||f(0)|| \] (3.35)

where \( L \) involves the Lipschitz constant for \( f \), and

\[ f'''(y) = \sum_{i,j,k=1}^{N} \left[ \frac{\partial^2 f}{\partial y_j \partial y_k} f_j \cdot f_k + \frac{\partial f}{\partial y_j} \frac{\partial f_j}{\partial y_k} f_k \right], \] (3.36)

\[ f^{i,j,s}(y) = \left\{ \frac{\partial^2 f_1}{\partial y_{j_1} \partial y_{j_2}}, \ldots, \frac{\partial^2 f_N}{\partial y_{j_1} \partial y_{j_2}} \right\} \cdot \] (3.37)

To estimate the first term in (3.28), we recall that for each \( x \in \Omega \), we have an initial value problem of the form (3.26) with initial condition \( C^{n-1} = C^{n-1}(x) \). Applying Lemma 3.1 we obtain

\[ \sum_{i=1}^{N} | C_i^{i,n-1}(x) - s_i(x, t^{i,n-1}) | \leq K \Delta t^2, \] (3.38)

with

\[ K = \bar{K} \cdot K(M), \] (3.39)

where \( \bar{K} \) is of the form (3.31). Hence \( K \) depends on bounds for \( R_i \) and first and second derivatives of \( R_i(s) \) with respect to \( s \), \( i = 1, \ldots, N \), evaluated over all \( s \) contained in a sufficiently large ball \( B(s) \subseteq \mathbb{R}^n \). By (3.32)-(3.35) we can define \( B(s) \) so that its radius is bounded above by

\[ \sup_{x \in \Omega} e^{K^* \Delta t} \| C^{n-1}(x) \| + \frac{e^{K^* \Delta t}-1}{K^*} \| R(0) \| \leq Y^*, \] (3.40)

where \( Y^* \) satisfies (2.3). By Condition A of Section 2, \( K \) is bounded independent of \( \Delta x \) and \( \Delta t \).

By a similar argument applied to the system (3.27) we obtain

\[ \sum_{i=1}^{N} | c^{i,n-1}(x) - \bar{c}_i(x, t^{i,n-1}) | \leq K \Delta t^2. \] (3.41)

Again, \( K \) is of the form (3.39) and depends on bounds for \( R_i \) \( (i = 1, \ldots, N) \) and first and second derivatives of \( R_i \) over a ball \( B(\bar{c}) \subseteq \mathbb{R}^n \). In this case the radius of \( B(\bar{c}) \) is determined by
Hence by Condition A, $K$ is bounded independent of $\Delta z$ and $\Delta t$. (3.38), (3.41) imply

$$\sum_{i=1}^{N} \| C_i^{j,n-1} - s_i(t^{j,n-1}) \| \leq K \Delta t_s^2,$$  (3.43)

and

$$\sum_{i=1}^{N} \| c_i^{j,n-1} - \bar{c}_i(t^{j,n-1}) \| \leq K \Delta t_s^2. \tag{3.44}$$

Therefore by (3.28), (3.29), (3.43), (3.44) and the fact that $\sum_{j=0}^{M-1} \frac{\Delta t_s}{\Delta t} = 1$ we obtain

$$S_1 \leq K \Delta t_s^4 + K \sum_{i=1}^{N} \| s_i^{n-1} \|^2 + K \xi_{t+1}. \tag{3.45}$$

Now,

$$| S_2 | \leq || \phi ||_{L^\infty} \left\{ \sum_{k} \left( \frac{\Delta t_s}{\Delta t} \sum_{j=0}^{M-1} R(\gamma_i^j, n-1) - R(c_k^n) \right) \eta_k \right\} \| s^n \|$$  (3.46)

$$\leq K || \phi ||_{L^\infty} \left\{ \sum_{k} \left( \frac{\Delta t_s}{\Delta t} \sum_{j=0}^{M-1} R(\gamma_i^j, n-1) - R(c_k^n) \right) \eta_k \right\} \| s^n \|$$

$$\leq K || \phi ||_{L^\infty} \left\{ \frac{\Delta t_s}{\Delta t} \sum_{j=0}^{M-1} R(\gamma_i^j, n-1) - R(c_k^n) \right\} \| s^n \|$$

where again we are using (3.24) followed by (3.23).

Consider

$$\| \frac{\Delta t_s}{\Delta t} \sum_{j=0}^{M-1} R(\gamma_i^j, n-1) - R(c^n) \|^2$$

$$= \int \left( \frac{\Delta t_s}{\Delta t} \sum_{j=0}^{M-1} R(\gamma_i^j, n-1(x) + \frac{\Delta t_s}{2} R(c_i^j, n-1(x))) - R(c^n(x)) \right) \| s^n \|^2 dx dy$$
\[
\leq 2\int_0^1 \left| \frac{\Delta t}{\Delta t} \sum_{j=0}^{M-1} R \left( c^{j,n-1}(x) \right) + \frac{\Delta t}{2} R \left( c^{j,n-1}(x) \right) \right|^2 dx dy \\
+ 2\int_0^1 \left| \frac{\varepsilon(x, t^n) - c(x, t^{n-1})}{\Delta t} - R \left( c(x, t^n) \right) \right|^2 dx dy
\]

\[= W_1^2 + W_2^2.\]

Here \( \varepsilon \) is again given by (3.27).

\( W_1 \) can be estimated by applying Lemma 3.1 to the system (3.27), hence

\[ W_1 \leq \frac{K \Delta t}{\Delta t} = K \Delta t. \]

To estimate \( W_2 \) we note that

\[
\left| \frac{\varepsilon(x, t^n) - c(x, t^{n-1}) - R \left( c^n(x) \right)}{\Delta t} \right| \\
= \left| \frac{1}{\Delta t} \int_{t^{n-1}}^{t^n} R \left( \varepsilon(t) \right) dt - R \left( c^n(x) \right) \right| \\
\leq \left| R \left( c(x, t^{n-1}) - R \left( c(x, t^n) \right) \right) \right| \\
+ \Delta t \left| \frac{\partial R}{\partial t} \varepsilon(x, t) \right|_{L^\infty(t^{n-1}, t^n)}
\]

by Taylor's expansion in \( R(\varepsilon(t)) \).

The first term in (3.49) is bounded by

\[ \Delta t \left| \frac{\partial R}{\partial t} \varepsilon(x, t) \right|_{L^\infty(t^{n-1}, t^n)} \]

Hence

\[ \left| R(c(t^{n-1})) - R(c(t^n)) \right| \leq K \Delta t^{\frac{1}{2}} \left| \frac{\partial R}{\partial t} c(x, t) \right|_{L^2(t^{n-1}, t^n)} \]

\[ \leq K \Delta t^{\frac{1}{2}} \left| c \right|_{H^\infty(t^{n-1}, t^n; L^2)}. \]

To better estimate the second term in (3.49) we note that by (3.27), for \( t^{n-1} \leq t \leq t^n \) and \( x \in \Omega \) we have
\[
\left| \frac{\partial R}{\partial t}(\mathcal{C}(x, t)) \right| = \left| \sum_{i=1}^{N} \frac{\partial R}{\partial c_i} \frac{\partial c_i}{\partial t}(x, t) \right| \\
= \left| \sum_{i=1}^{N} \frac{\partial R}{\partial c_i} R_i(\mathcal{C}(x, t)) \right| \\
\leq K^* ||R(\mathcal{C}(x, t))||_1 .
\]

From o.d.e. theory [10] we have for \( t^{n-1} \leq t \leq t^n \)
\[
||\mathcal{C}(x, t)||_1 \leq e^{\Delta t K^*} ||\mathcal{C}(x, t^{n-1})||_1 + \frac{e^{\Delta t K^*} - 1}{K^*} ||R(0)||_1 \\
\leq Y^* 
\]
where \( Y^* \) is given by (2.3). Hence by Condition A
\[
|| \frac{\partial R}{\partial t}(\mathcal{C}(x, t)) ||_1 \leq K^* \max_{||c|| \leq Y^*} ||R(c)||_1 \\
\leq K \quad \text{for all } x \in \Omega . \tag{3.51}
\]

Combining (3.47), (3.49), (3.50), and (3.51) we obtain
\[
W_2 \leq K \Delta t^2 \left( ||c||_{H^1(t^{n-1}, t^n)}^2 + K \Delta t \max_{||c|| \leq Y^*} ||R(c)||_1 \right) . \tag{3.52}
\]

Hence by (3.46), (3.47), (3.48), and (3.52)
\[
S_2 \leq K \Delta t^2 + K \Delta t \left( ||c||_{H^1(t^{n-1}, t^n)}^2 + ||s^n||^2 \right) . \tag{3.53}
\]

The term \( S_3 \) has the form \( \Delta t (\phi \frac{\hat{f}_n - f}{\Delta t} s^n) \), which we previously considered in treating \( T_5 \) and \( T_6 \), i.e. (3.17). We have then
\[
|S_3| \leq K \||\hat{H}^n - H^n||_{L^2} \||\phi s^n||_{L^2} ,
\]
where
\[
H^n = \sum_k R(c_k^2) v_k ,
\]
Thus
\[
|S_3| \leq K \Delta t \||H^n||_{H^1} \||s^n||_{H^1} \\
\leq K \Delta t^2 ||R^n||^2 + \epsilon ||s^n||^2 . \tag{3.54}
\]

The last term \( S_4 \) involves interpolation theory and is bounded by
Combining (3.11)-(3.18), (3.45), (3.53), (3.54) and (3.55), multiplying by $\Delta t$, summing over $i, i = 1, 2, ..., N$, and $n, n = 1, ..., N^*$, and applying Gronwall's Lemma, we obtain

$$
\sum_{i=1}^{N} \frac{1}{2} \phi_i^2 \zeta_i^{N^*} + \sum_{i=1}^{N} \sum_{n=1}^{N^*} \frac{1}{2} D(u^n)^2 \nabla \zeta_i^n \Delta t 
\leq K ((\Delta t)^2 + h^{2(i+1)}),
$$

where

$$
K = (K^*, ||c||_{H^1(0,T;H^1)}, ||R(c)||_{L^\infty(H^1)}, ||c||_{H^2(0,T;L^2)}),
$$

$$
\max_{||c|| \leq Y^*} ||R(c)||, \max_{||c|| \leq Y^*} ||R''(c)||, \max_{1 \leq i, k \leq N^*} ||R_{ik}(c)||,
$$

with the meanings of the last two terms given by (3.36) and (3.37). From (3.56) and (3.57), we deduce our major result.

**Theorem 3.1.** Let $c_i, 1 \leq i \leq N$, satisfy (1.1) and assume the regularity and coefficient assumptions (2.1) and (2.2) and Condition A. Let $c_i, 1 \leq i \leq N$ satisfy (3.8)-(3.10). Then there exists a positive constant $K$, whose dependency on $c$ and coefficients is given by (3.57) such that

$$
\sum_{i=1}^{N} \frac{1}{2} \phi_i^2 (C_i - c_i)^2 (T) + \sum_{n=1}^{N^*} \Delta t \frac{1}{2} D(u^n)^2 \nabla (C_i - c_i)^2 
\leq K ((\Delta t)^2 + h^{2(i+1)}).
$$

4. AN APPLICATION: MICROBIAL BIODEGRADATION OF HYDROCARBONS IN GROUNDWATER

In the introduction a brief discussion of the physics of microbial biodegradation of hydrocarbons in groundwater was given. In this section we present some numerical results obtained by an implementation of the splitting scheme of Section 3. The formulation considered was

$$
\frac{dH}{dt} = M_t \cdot \bar{K} \cdot \left( \frac{H}{K_H + H} \right) (\frac{O}{K_O + O}) = R_1(O,H,M_t),
$$

$$
\frac{dO}{dt} = M_t \cdot \bar{F} \cdot \left( \frac{H}{K_H + H} \right) (\frac{O}{K_O + O}) = R_2(O,H,M_t),
$$

and
\[
\frac{dM_t}{dt} = M_t \cdot \bar{k} \cdot Y \cdot \left( -\frac{H}{K_H + H} \right) \left( \frac{O}{K_O + O} \right) + K_c \cdot Y \cdot OC - bM_t
\]

\[= R_2(O, H, M_t) \] (4.1c)

where \( H \) = hydrocarbon concentration, \( O \) = oxygen concentration, \( M_t \) = total microbial concentration, \( \bar{k} \) = maximum hydrocarbon utilization rate per unit mass microorganisms, \( Y \) = microbial yield coefficient, \( K_H \) = hydrocarbon half saturation constant, \( K_O \) = oxygen half saturation constant, \( b \) = microbial decay rate, \( F \) = ratio of oxygen to hydrocarbon consumed, \( K_c \) = first order decay rate of natural organic carbon, and \( OC \) = natural organic carbon concentration.

If (4.1a) and (4.1b) for oxygen and hydrocarbon removal are combined with the advection-dispersion equation for a solute undergoing linear instantaneous adsorption, the following equations are obtained:

\[
\frac{\Phi}{R_H} \frac{\partial H}{\partial t} - \frac{1}{R_H} \nabla \cdot (D \nabla H - uH) = \frac{q}{R_H} \tilde{H} + \frac{\Phi}{R_H} R_1(O, H, M_t),
\] (4.2)

\[
\frac{\Phi}{R_H} \frac{\partial O}{\partial t} - \nabla \cdot (D \nabla O - uO) = \tilde{O} + \Phi R_2(O, H, M_t),
\] (4.3)

\[
u = -\frac{K}{\mu} \nabla p,
\] (4.4)

and

\[
\nabla \cdot u = q,
\]

where \( D \) = dispersion tensor, \( u = (u_1, u_2)^T \) = incompressible Darcy velocities, \( p \) = pressure, \( K/\mu \) = permeability/viscosity, \( R_H \) = retardation factor for hydrocarbons, \( q \) = hydraulic source term, \( \Phi \) = porosity, \( \tilde{H} \) = concentration of hydrocarbon in hydraulic sources, and \( \tilde{O} \) = concentration of oxygen in hydraulic sources. Here \( \tilde{O} \) is specified at injection wells and \( \tilde{O} = 0 \) at production wells.

The movement of naturally occurring microorganisms will be limited by the tendency of the organisms to grow as microcolonies attached to the formation. In most aquifers, greater than 95 percent of the native organisms are attached, and consequently the affinity of microorganisms for solid surfaces will control the transport of the total population. For simplicity, we assume that the exchange of microorganisms between the solid surface and the free solution will be rapid and satisfy \( M_s = \text{constant} \ M_t \), where \( M_s \) = concentration of microbes in solutions. Under this assumption the movement of the microbes can be treated using a simple retardation factor approach [2], i.e.

\[
\frac{\Phi}{R_m} \frac{\partial M_s}{\partial t} - \frac{1}{R_m} \nabla \cdot (D \nabla M_s - uM_s) = \frac{q}{R_m} \tilde{M}_s + \Phi R_3(O, H, M_s),
\] (4.5)
where $R_m = \text{microbial retardation factor}$, $R_m = \frac{M_t}{M_0}$, and $M_0 = \text{concentration of microbes in hydraulic sources}$.

Further details of the equation formulation and parameter selection can be found in Borden and Bedient [2].

In the implementation of the splitting method we used bilinear approximations for the concentrations of oxygen, hydrocarbons and microbes. A mixed finite element procedure was chosen for approximating $(u, p)$ given by (4.4), see [8, 12].

In Figures 4.1-4.3 contour plots of oxygen and hydrocarbon are presented for a heterogeneous permeability media; in (1.1) $k$ varies by two orders of magnitude. For this problem initial conditions were generated by simulating a hydrocarbon spill over a period of five years, assuming background concentrations of oxygen and microbes. Figure 1 represents the initial hydrocarbon plume which we wish to biodegrade. Concentrations are in mg/l.

In the second stage of the simulation injection and production wells are placed with the intention of injecting oxygenated water into the aquifer and producing water with a mixture of oxygen, hydrocarbon, and microbes. Figures 2 and 3 represent, respectively, the hydrocarbon and oxygen contour levels after a period of 3 years. Placement of the wells is given Figure 3.

The mesh used in this study was a nonuniform $31 \times 55$ grid. $\Delta t = 4$ days, and $M = 1000$ ($\Delta t_p = .004$ days) were chosen. The simulations were run on a Cray-XMP supercomputer. The parameters chosen for this case study were identical except in the definition of $k$ to those used in a simulation study presented in [14]. Here we used a highly varying permeability coefficient $k$.

5. CONCLUSIONS

We have formulated a parallel time-splitting algorithm that is accurate, robust, and can be extended to three spatial variables. Theoretical convergence results which yield optimal rates have been derived. In addition this method has been applied to study an important environmental problem, namely groundwater contamination.

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FIGURE 3. OXYGEN-3 YRS.

- Injection well
- Production well
6. REFERENCES


