

**A Parallel Numerical Model for
Subsurface Contaminant
Transport with Biodegradation
Kinetics**

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ABSTRACT

In this paper we discuss the formulation of a simulator for groundwater flow and transport with biodegradation kinetics that has been developed at Rice University for massively parallel, distributed memory, message passing machines. The numerical procedures employed are a mixed finite element method for flow and the characteristics-mixed method for transport. Kinetics are treated by time splitting. The linear solvers are based on domain decomposition. Application of this procedure to a bioremediation problem as well as numerical experiments on the INTEL i860 and INTEL Delta are discussed. Results indicate that the procedure is theoretically mass conservative over each grid cell and is approximately so in implementation. Preliminary tests indicate that the procedure is robust and applicable to realistic groundwater problems. Moreover, the numerical model scales almost linearly with the number of processors even for fairly coarse grids.

1. INTRODUCTION

Bioremediation techniques such as microbial biodegradation are part of an innovative, emerging technology for handling subsurface water contamination [5–7,12,23,29,32]. The microbial biodegradation process involves the stimulation of indigenous microorganisms to remove subsurface contaminants. U. S. Environmental Protection Agency studies [31] have shown that this type of restoration strategy can result in complete removal of contaminants, whereas other proposed restoration strategies have not proven as effective.

Biological decontamination is physically and chemically complex. It involves the transport and interaction of hydrocarbons, microbes, oxygen, nitrogen, and various chemical compounds as well as the movement of water within the aquifer. Numerical simulation of these processes is a critical step in understanding and designing

bioremediation applications [1,9,14-16,24,34-36]. Indeed, without computational science, in situ biodegradation of contaminants on a wide scale is impractical.

New parallel supercomputers, allowing simultaneous use of hundreds to thousands of processors, have greatly expanded the potential for building detailed models of these porous media processes. Parallel computing provides the capability of solving larger, more realistic and practical problems faster and more economically. This includes the ability to use an adequately refined discretization mesh, to incorporate complex chemical and physical effects associated with the transport of both hydrocarbons and organic contaminants in porous media, and to employ stochastic or conditional simulation. The latter is essential for simulating a realistic geologic aquifer, since much of the data needed to characterize it cannot be quantified accurately, and since often the chemical and physical processes are not well understood. Conditional simulation is ideally suited to parallel computation.

In this paper we will emphasize modeling of the flow and transport in the saturated zone. Extensions to multicomponent, multiphase models in the unsaturated zone are presently being considered, but because of page limitations, they will not be discussed herein.

The outline of the paper is as follows. In §2 we describe the governing flow and transport equations with biodegradation in a saturated porous medium. For simplicity, we assume linear sorption and aerobic conditions. More general kinetics such as Michaelis-Menton can be treated with the numerical techniques described in this paper.

In §3, we first describe the mixed finite element method for an elliptic flow equation [8,26]. We then formulate the characteristics-mixed method [3]. Theoretical convergence estimates are stated for the characteristics-mixed method. Finally, we briefly discuss the time-splitting scheme employed for treating advection-diffusion-reaction problems.

In §4 we describe the parallel implementation of the procedure, and in §5 we present three dimensional, parallel, bioremediation simulation results. Conclusions and current directions on parallel implementation are given in §6.

2. CONTAMINANT TRANSPORT WITH BIODEGRADATION

The governing equations of transport with biodegradation in a saturated porous medium are described by a coupled, nonlinear advection-diffusion-reaction system consisting of m_s electron donors (substrates) and m_n electron acceptors or nutrients, and a system of m_x ordinary differential equations involving microbial mass. (Transport of microbes can be treated also if one assumes instead a system of advection-diffusion-reaction equations for the microbes.) The governing equation of flow is given by Darcy's Law and the continuity equation.

These equations defined in a one, two, or three dimensional porous medium Ω can be written as:

Electron Donor (Substrate)

$$\phi R_{S_i} \frac{\partial S_i}{\partial t} - \nabla \cdot (D \nabla S_i - u S_i) = \phi \chi_{S_i} + g_{S_i}, \quad i = 1, \dots, m_s, \quad (1)$$

Electron Acceptor

$$\phi R_{N_i} \frac{\partial N_i}{\partial t} - \nabla \cdot (D \nabla N_i - u N_i) = \phi \chi_{N_i} + g_{N_i}, \quad i = 1, \dots, m_n, \quad (2)$$

Microbial Mass

$$\phi \frac{\partial X_i}{\partial t} = \phi \chi_{x_i}, \quad i = 1, \dots, m_x, \quad (3)$$

Darcy's Law and Continuity

$$u = -K \nabla p \quad \text{and} \quad \nabla \cdot u = f. \quad (4)$$

Here $D = D(u)$ is a hydrodynamic diffusion/dispersion tensor, ϕ is porosity, and R_i is a retardation factor for component i due to adsorption. The χ are possibly nonlinear kinetic terms which account for biodegradation of contaminants, utilization of nutrients, and growth and decay of microorganisms. The number and complexity of specific metabolic pathways or chemical reactions varies with the application. The source/sink terms f and g_i represent production and injection wells. The hydraulic conductivity K is a symmetric positive definite tensor. For convenience of exposition, we will assume that

$$u \cdot \nu = 0,$$

$$D \nabla N_i \cdot \nu = D \nabla S_i \cdot \nu = 0,$$

where ν is the outward, unit, normal vector to $\partial\Omega$, the boundary of Ω .

3. THE NUMERICAL ALGORITHMS

Let $\Omega \subset \mathbb{R}^d$, $d = 1, 2$, or 3 . Let $W = L^2(\Omega)$ denote the set of square integrable functions and $H(\Omega; \text{div}) = \{v \in (L^2(\Omega))^d \mid \nabla \cdot v \in L^2(\Omega)\}$. Let $V = H^0(\Omega; \text{div}) = \{v \in H(\Omega; \text{div}) \mid v \cdot \nu = 0 \text{ on } \partial\Omega\}$.

For spatial discretization, we employ the lowest order Raviart-Thomas spaces [26] defined over a rectangular grid of Ω with maximal grid spacing $h > 0$. These finite dimensional spaces consist of $W_h \subset W$ equal to the set of discontinuous functions that are constant in each cell, and $\tilde{V}_h \subset H(\Omega; \text{div})$ equal to the set of vectors $v = (v_1, v_2, v_3)$ (if $d = 3$) such that v_i is continuous, piecewise linear over the grid in the i th direction and discontinuous, piecewise constant over the grid in the other two directions. We also need the subspace $V_h = \tilde{V}_h \cap V$.

We first describe the mixed finite element method for approximating (4). With (\cdot, \cdot) denoting the $L^2(\Omega)$ -inner product, we write (4) in variational form as

$$(K^{-1}u, v) - (p, \nabla \cdot v) = 0, \quad v \in V,$$

$$(\nabla \cdot u, w) = (f, w), \quad w \in W.$$

In the mixed finite element formulation, we seek the pair $(U_h, P_h) \in V_h \times W_h$ satisfying

$$(K^{-1}U_h, v_h) - (P_h, \nabla \cdot v_h) = 0, \quad v_h \in V_h, \quad (5a)$$

$$(\nabla \cdot U_h, w_h) = (f, w_h), \quad w_h \in W_h. \quad (5b)$$

In order to define the characteristics-mixed method for (1) and (2), we consider the following abstract transport equation for some component concentration c :

$$\phi \frac{\partial c}{\partial t} + u \cdot \nabla c - \nabla \cdot D \nabla c = g \quad \text{in } \Omega, \quad t > 0, \quad (6a)$$

$$D \nabla c \cdot \nu = 0 \quad \text{on } \partial\Omega, \quad t > 0, \quad (6b)$$

$$c(x, 0) = c^0(x) \quad \text{on } \Omega, \quad (6c)$$

where u is assumed given and c^0 is the initial concentration.

A numerical method for (6a)–(6c) that has been used with success is the modified method of characteristics (MMOC-Galerkin) [1,9,13–17,19,20,27,28,34–36]. In this scheme, the time derivative and the advection term (i.e., the hyperbolic part of the equation, $\phi \partial c / \partial t + u \cdot \nabla c$) are combined as a directional derivative along the characteristics, and then the equation is treated as in a Galerkin finite element method. Although this method allows one to use large time-step increments and to treat large Peclet numbers, the main drawback of the method is its nonconservative nature and the cost of tracing the characteristics from many points.

The characteristics-mixed method introduced by the authors [3] retains all the advantages of MMOC-Galerkin in addition to being theoretically conservative. As in MMOC-Galerkin, a directional derivative is used to treat the hyperbolic part of (6a), but then a mixed finite element method is applied to treat the diffusion/dispersion.

Before defining the characteristics-mixed method, we write (6a)–(6c) in a saddle point weak formulation. Define $\tilde{V} = (L^2(\Omega))^d$, $\tilde{z} = -\nabla c$, and the dispersive flux as $z = -D \nabla c$. Then (6a) is expressed for $(c, \tilde{z}, z) \in W \times \tilde{V} \times V$ as

$$\left(\phi \frac{\partial c}{\partial t} + u \cdot \nabla c, w \right) + (\nabla \cdot z, w) = (g, w), \quad w \in W, \quad (7a)$$

$$(\tilde{z}, v) = (c, \nabla \cdot v), \quad v \in V, \quad (7b)$$

$$(z, v) = (D \tilde{z}, v), \quad v \in \tilde{V}. \quad (7c)$$

To discretize this equation, we begin with the characteristic approximation. So let $\Delta t > 0$ be the time-step increment and $t^n = n \Delta t$ for $n = 1, 2, \dots$ (Δt could vary with the time-step in practice). The characteristic trace-back along the velocity field u of a point $x \in \Omega$ at time t^n to time t^{n-1} is approximately

$$\check{x}(x, t^{n-1}) = x - \frac{u(x, t^n)}{\phi(x)} \Delta t. \quad (8)$$

As a consequence, the hyperbolic terms in (6a) at time t^n are

$$\phi \frac{\partial c^n}{\partial t} + u^n \cdot \nabla c^n \approx \phi \frac{c^n - \check{c}^{n-1}}{\Delta t}, \quad (9)$$

wherein we use the notation $\psi^n = \psi(t^n)$ for functions of time and $\check{\psi}(x) = \psi(\check{x})$ for functions of space.

The characteristics-mixed algorithm can be stated as follows. First let $C^0 \in W_h$ approximate the initial concentration c^0 . Then for each time level n , find $(C^n, \tilde{Z}^n, Z^n) \in W_h \times \tilde{V}_h \times V_h$ such that

$$\left(\phi \frac{C^n - \tilde{C}^{n-1}}{\Delta t}, w \right) + (\nabla \cdot Z^n, w) = (g^n, w), \quad w \in W_h, \quad (10a)$$

$$(\tilde{Z}^n, v) = (C^n, \nabla \cdot v), \quad v \in V_h, \quad (10b)$$

$$(Z^n, v) = (D\tilde{Z}^n, v), \quad v \in \tilde{V}_h, \quad (10c)$$

$$\tilde{C}^{n-1} = \mathcal{P}(C^{n-1}, \tilde{Z}^{n-1}), \quad (10d)$$

where in (10d) we require the definition (11a)–(11b) below of the post-processing operator \mathcal{P} . (This more general form of the mixed method is analyzed in greater detail in [2].) It is well known that in a single time-step of the mixed method, C^n is convergent to c^n only to the first order in h , and that we can improve this order through various post-processing techniques. Therefore, we apply the post-processing (10d) to the concentration at time t^{n-1} before taking the next time-step. In fact, we should view the post-processed quantity $\tilde{C}^n = \mathcal{P}(C^n, Z^n)$ as our approximate concentration at time t^n . As a consequence, the theorem below shows that we obtain a better overall rate of convergence for the scheme.

We now define \mathcal{P} . Let $\tilde{W}_h \subset W$ denote our post-processing space. This space consists of discontinuous, piecewise linear functions defined over the grid. Define $\mathcal{P} : W \times \tilde{V} \rightarrow \tilde{W}_h$ for $(\omega, v) \in W \times \tilde{V}$ by $\mathcal{P}(\omega, v) = \tilde{\omega} \in \tilde{W}_h$, where over the grid cell R ,

$$(\phi(\tilde{\omega} - \omega), w)_R = 0, \quad w \in W_h, \quad (11a)$$

$$(\nabla \tilde{\omega} + v, \nabla \tilde{w})_R = 0, \quad \tilde{w} \in \tilde{W}_h. \quad (11b)$$

The notation $(\cdot, \cdot)_R$ means that the integration is restricted to R . Note that $w = 1$ gives material balance; in fact, mass is conserved cell by cell over the grid. The following convergence is attained by the scheme under reasonable hypotheses (see [3] for the proof). The proof assumes the more usual form of the mixed method in which

$$(D^{-1}Z^n, v) - (C^n, \nabla \cdot v) = 0, \quad v \in V_h, \quad (12)$$

$$\tilde{C}^{n-1} = \mathcal{P}(C^{n-1}, Z^{n-1}), \quad (13)$$

replaces (10b)–(10d), and also that $\mathcal{P} : W \times V \rightarrow \tilde{W}_h$, with

$$(D\nabla \tilde{\omega} + v, \nabla \tilde{w})_R = 0, \quad \tilde{w} \in \tilde{W}_h \quad (14)$$

replacing (11b).

Theorem. If (12)–(13) replaces (10b)–(10d) and (14) replaces (11b), then for h and Δt sufficiently small,

$$\max_n \|\tilde{C}^n - c^n\| \leq C\{h^{3/2} + \Delta t\}, \quad (15a)$$

$$\left\{ \sum_{n=1}^N \|D^{1/2}(Z^n - z^n)\|^2 \Delta t \right\}^{1/2} \leq C\{h + \Delta t\}, \quad (15b)$$

where $\|\psi\| = (\psi, \psi)^{1/2}$ is the $L^2(\Omega)$ -norm.

Preliminary results by the authors indicate that the proof extends to the formulation (10a)–(10d), (11b), with (15b) replaced by

$$\left\{ \sum_{n=1}^N \|D^{1/2}(\tilde{Z}^n - \tilde{z}^n)\|^2 \Delta t \right\}^{1/2} \leq C\{h + \Delta t\}. \quad (16)$$

We remark that under special circumstances and if \tilde{W}_h is replaced by the discontinuous, piecewise quadratic functions, then $h^{3/2}$ can be replaced by $h^{7/4}$ in the theorem.

4. PARALLEL IMPLEMENTATION

In our numerical formulation for modeling (1)–(4), we first approximate u by U by applying to (4) our mixed finite element procedure with the lowest order Raviart-Thomas space (5) as described in the last section. In (5a) we employ the following quadrature rule for the i th component: the trapezoidal rule in the i th direction and midpoint rule in the other two directions. The resulting algorithm is equivalent to the cell-centered finite difference method [28,33]. For a diagonal tensor K one obtains a finite stencil for pressure, five points if the dimension $d = 2$ and seven if $d = 3$.

A nonoverlapping parallel domain decomposition algorithm has been applied to solving the discrete system. The basic idea is to decompose the domain Ω into a number of subdomains Ω_j , one associated with each processor. We then have a series of boundary value problems similar to (4) in each Ω_j . We obtain a guess for the boundary data on the internal interfaces $\partial\Omega_j$, and solve the local problems in the subdomains. If the solutions and their normal derivatives match across subdomain boundaries, then the problem in Ω is solved. If not, then interface boundary data are updated and we iterate. In other words, in domain decomposition the solution process of the large global problem is decomposed into the repeated solution of numerous smaller, *independent* problems.

In such a domain decomposition algorithm, we must describe how we choose the guess for the internal interfaces boundary data. We use Method 2 of Glowinski and Wheeler [21], which uses Dirichlet interface boundary data. From any convenient initial guess, the succeeding guesses are given as the solution of a positive definite, symmetric problem posed on the interfaces. There have been several interface problem solution techniques proposed [10,11]; however, the one used for the calculations reported in §5 is Balancing. This procedure was defined and analyzed by Cowsar, Mandel, and one of the authors [10] and implemented by Cowsar. There are three components to multi-domain balancing. The first involves the solution of the subdomain problems with Dirichlet data provided on internal interfaces. The second involves the solution of subdomain problems with Neumann data. The third involves a global coarse grid problem with subdomains treated as “elements” to insure the well-posedness of the Neumann solves and to provide a mechanism of global exchange of information.

The number of iterations of the Balancing procedure is of the order $1 + \log(H/h)$, where the diameter of the global domain is $O(1)$, the diameter of the subdomain is $O(H)$, and the diameter of the cell is $O(h)$. Balancing scales almost linearly provided that care is taken treating the coarse grid problem. For massively parallel machines the coarse grid problem can be a costly bottleneck and a domain decomposition procedure needs to be applied to the coarse grid.

Since the approximate velocity U is discontinuous, there are certain numerical difficulties in obtaining good approximations to the characteristics (8). Therefore, we postprocess it into a continuous velocity \tilde{U} in the space of piecewise discontinuous trilinear functions. This velocity field is actually more accurate than U because it exploits superconvergence [33].

Given the velocity approximation \tilde{U} , the advection-diffusion-reaction system involving donor, acceptor and biological mass equations are approximated using a time splitting scheme. One global time step involves the following three sequential steps:

- (i) Pure transport. For each electron donor or acceptor, characteristics are traced backwards in time to locate their origin at the previous time level. This may be done by taking small micro time steps. The trace-back points are joined to form a "twisted" grid. The time-step size is controlled so that this twisting is not excessive, and every grid cell is mapped to a distinct twisted grid cell. For each given cell, we average the postprocessed concentration from the previous time step over the corresponding "twisted" cell (i.e. we integrate and divide by the volume). This average is the transported concentration in the absence of reactions and diffusion/dispersion.
- (ii) Reactions. The coupled system of reaction equations (i.e. (1)–(3) without the two divergence terms and without the g_i source terms) are approximated using a fourth order Runge-Kutta procedure. Initial conditions are the "twisted" cell averages from (i) for acceptors and donors, and the previous time step concentrations for the microbes. Many small time steps may be taken to improve the accuracy.
- (iii) Diffusion/dispersion. The diffusion/dispersion step involves approximating a parabolic system for each donor or acceptor using initial data from (ii) and applying the mixed finite element method (10a)–(10d), with $C = S_i$ or $C = N_i$. In (10b) the same quadrature is used as described above for the flow. A tensor product trapezoidal rule is used in (10c). As in the case of the flow, a finite stencil is obtained for each component, nine points in two dimensions and nineteen in three. As in previous MMOC-Galerkin calculations [19,34], the discrete system is solved using a Jacobi preconditioned conjugate gradient algorithm. Respective concentrations and their spatial gradients \tilde{Z} are thereby obtained. The latter are used to construct a higher order approximation to the concentrations in each grid cell as in (10d)–(11). Finally, a slope-limiting scheme is used to prevent overshoot and undershoot.

Using the previous time step as initial data, the global time step is repeated to some final time T .

The implementation of this time splitting reactive transport scheme in parallel was done by one of the authors, Ashokumar Chilakapati, and Doug Moore.

5. SOME BIOREMEDIATION RESULTS

The Hanford Site in Washington State in the United States occupies approximately 560 square miles of semiarid terrain and was selected in 1943 for producing materials (primarily plutonium) in support of the United States' World War II efforts. Chemical processes employed to recover and purify plutonium produced a waste stream containing actinide compounds as well as the typical aqueous and organic liquid industrial wastes. The primary organic contaminant carbon tetrachloride (CCl_4) totaled 637 to 1200 tons discharged. Today, plutonium production has ceased, and the primary mission has shifted to environmental restoration of the Hanford Site [22,25].

Rice University and Pacific Northwest Laboratory (PNL) began a collaborative research effort in 1992 that involves laboratory, field, and simulation work directed toward validating remediation strategies, and includes both natural and *in situ* bioremediation. We discuss below some preliminary computational results based on some recent microbial CCl_4 destructive kinetics developed by Skeen and Chan of PNL [30].

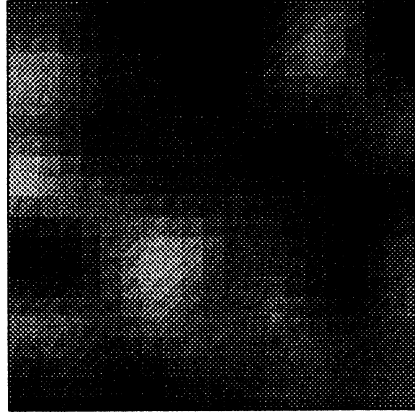
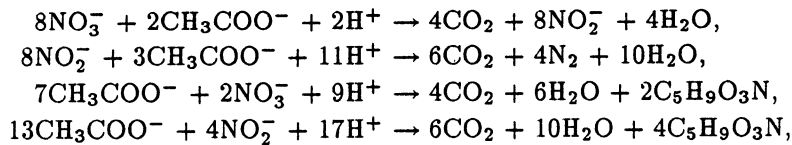


Fig. 1. Horizontal cross-section of permeability field K .

We assume that the domain is a $20\text{ m} \times 20\text{ m} \times 5\text{ m}$ aquifer and that the grid is $20 \times 20 \times 5$. The permeability is taken to be a scalar; a horizontal cross-section is shown in Figure 1. (In all the figures, horizontal cross-sections are taken at $z = 2.5\text{ m}$, and white is the highest value, black the lowest.) The model has six components: electron acceptors nitrate NO_3^- , nitrite NO_2^- , and acetate CH_3COO^- , donor CCl_4 , microbes $\text{C}_5\text{H}_9\text{O}_3\text{N}$, and a nonreactive tracer. We also assume that the retardation factor R for acetate is 1.8. The chemical reactions for this system are:



and bioremediation is described by

$$\frac{d(\text{CCl}_4)}{dt} = \frac{-\mu(\text{CCl}_4)(\text{microbes})}{1 + k_i((\text{NO}_3^-) + (\text{NO}_2^-))}.$$

The problem is a linear flow from the left to the right face of the aquifer with pressure specified on the left and right faces and no flow or zero Neumann conditions specified on the remaining faces. The nutrient electron acceptors nitrate and acetate are introduced into the system on the left face for 20 days, with the goal of increasing the microbial population. We assume that the substrate CCl_4 is flowing through the system (i.e. it is continuously injected at its original concentration on the left face) so that any concentration reduction observed is due not to CCl_4 flowing out of the system, but rather to microbial degradation.

In Figure 2, horizontal cross-sections of a nonreactive tracer are shown at 2.5 days and at 5 days, respectively, and in Figure 3 a contour of the .5 concentration of the nonreactive tracer at 5 days. From Figures 1 and 2, we clearly observe the effect of the permeability; that is, the tracer moves into the high permeability zones. Figures 4–7 are horizontal cross-sections of carbon tetrachloride, microbial mass, acetate, and nitrate at 2.5 and 5 days respectively. One can observe the growth of the microbial mass when nitrate and acetate are both available, and the successful degradation of CCl_4 .

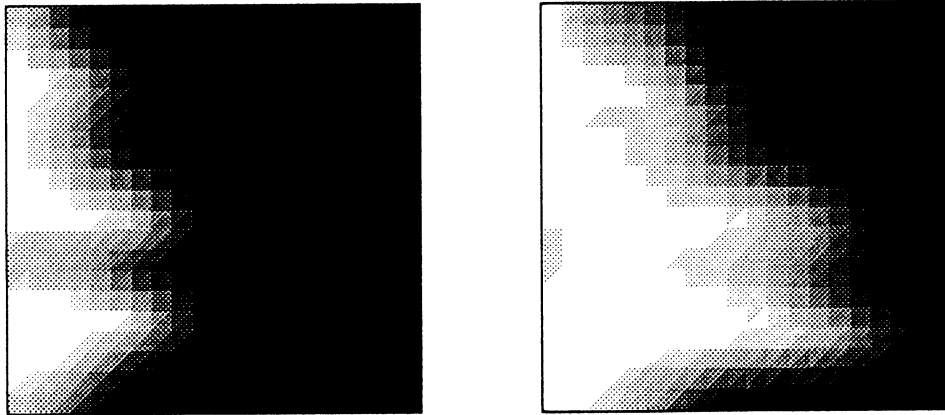


Fig. 2. Horizontal cross-section of nonreactive tracer at 2.5 and 5 days.

The effects of retardation on acetate are clear from the figures by noting that acetate has not moved as fast as the nitrate or the tracer. Since all the assumed chemical reactions require acetate, this example illustrates the danger of a poor application of the technology: Some nitrate outruns the acetate and pollutes the aquifer (though nitrate is preferable to CCl_4 !). A series of simulation studies could be used to identify the proper rates of nutrient injection.

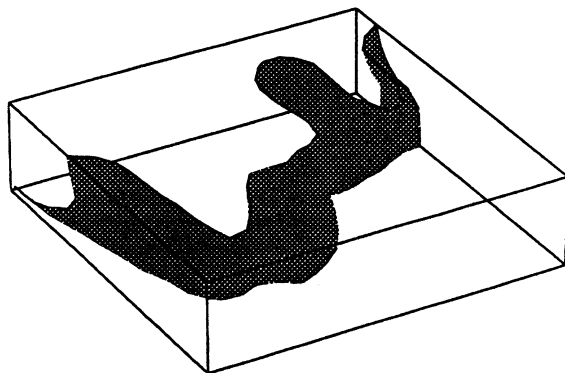


Fig. 3. Contour of nonreactive tracer concentration .5 at 5 days.

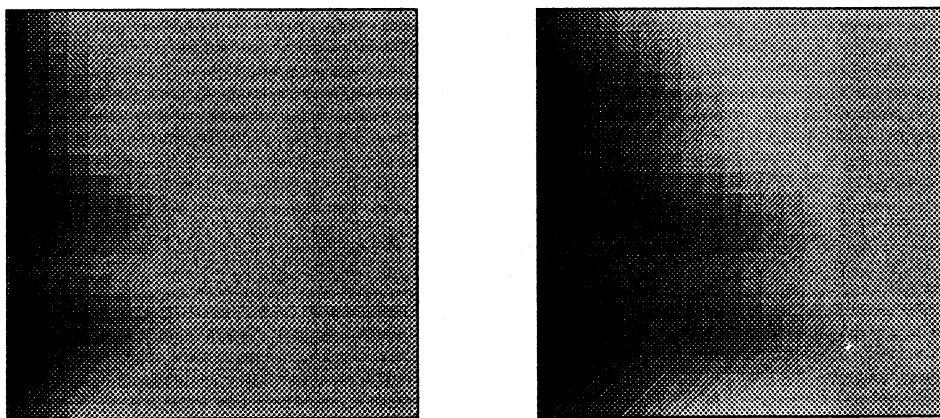


Fig. 4. Horizontal cross-section of CCl_4 at 2.5 and 5 days.

Finally in Figure 8, we observe the performance of the Rice 3D Parallel Groundwater Reactive Flow and Transport Code (RPGW). Here, speed-up is plotted as a function of the number of processors, normalized to the time taken on two processors. The dotted line indicates the theoretical linear speed-up. Since the INTEL iPSC/860 and the INTEL DELTA have roughly the same speed, some of the experiments were run on only one machine; in particular the longer runs using two and four processors on the i860 were not repeated on the DELTA.

The reader should note that the subdomain grids are only $4 \times 4 \times 5$ when run on 25 processors, so then the surface to volume ratio is 80:80 (since the z -direction is not subdivided). This ratio is quite high, and it is proportional to the amount of



Fig. 5. Horizontal cross-section of microbial mass at 2.5 and 5 days.

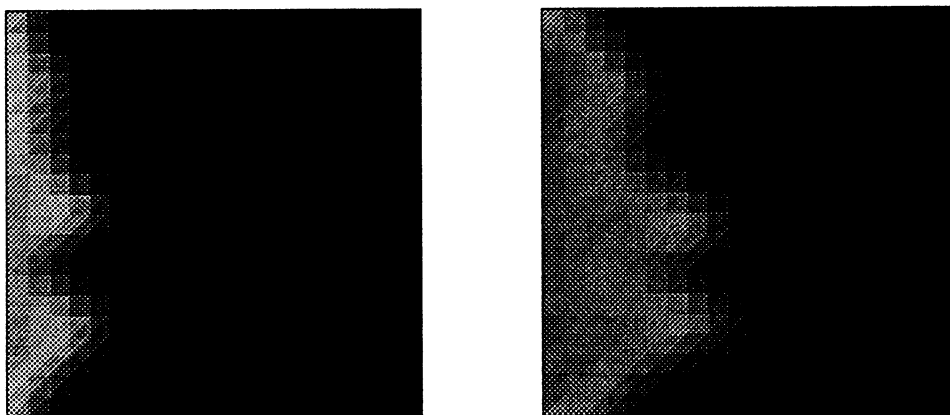


Fig. 6. Horizontal cross-section of acetate at 2.5 and 5 days.

interprocessor communication needed to solve the problem. The observed speedup is almost linear even up to this high level of surface to volume ratio.

6. CONCLUSIONS AND FUTURE DIRECTIONS

Rice 3D Parallel Groundwater Reactive Flow and Transport is a parallel code under development entirely at Rice University. Its purpose is to simulate the flow and transport of reacting chemical species in the groundwater. This code is based on

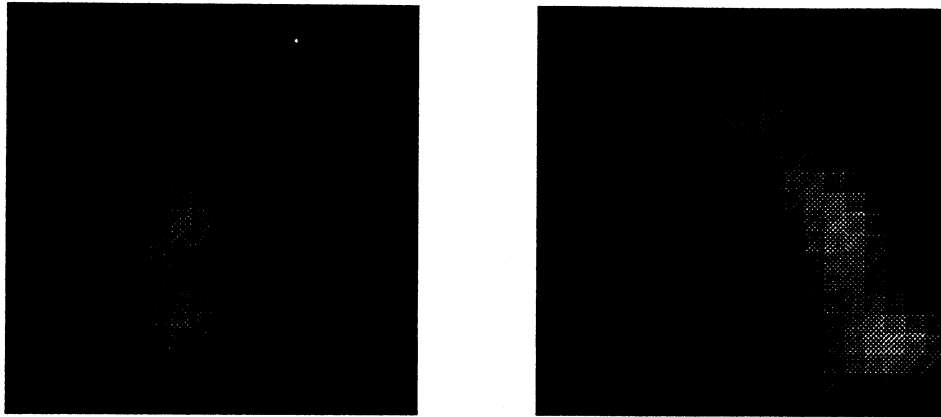


Fig. 7. Horizontal cross-section of nitrate at 2.5 and 5 days.

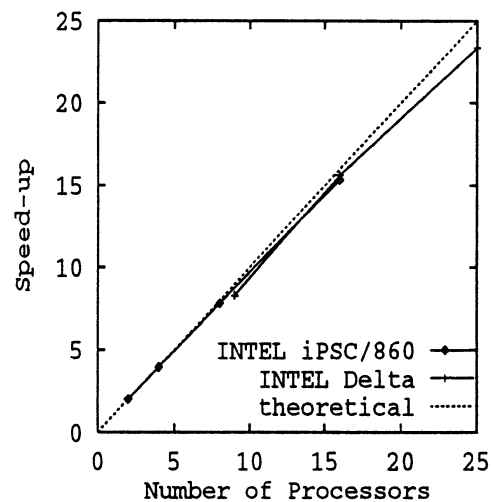


Fig. 8. Speed-up for RPGW.

combining locally conservative schemes: a mixed finite element method for flow with a characteristics-mixed finite element method for transport. Computational experiments indicate that this approach is useful in solving grand challenge problems such as bioremediation and that the code scales almost linearly even on small problems.

We are presently adding general wells and boundary conditions to the transport code as well as coupling this code to a three phase (gas, non-aqueous phase liquid, and aqueous) flow code. Future plans include the incorporation of meshes defined by fairly general geometry. In addition we plan to add more chemistry and microbiology

as well as the capability of simulating fractured media. Since most environmental companies do not have access to large parallel machines, we plan to replace the present communications package PICL with PVM so that a collection of workstations can also be used.

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