ACCURATE NUMERICAL SIMULATION OF BIOBARRIER FORMATION IN POROUS MEDIA

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ABSTRACT

Biofilm-forming microbes have complex effects on the flow properties of natural porous media. Subsurface biofilms have the potential for biotransformation of organic contaminants to less harmful forms, and also to form biobarriers to inhibit contaminant migration in groundwater.

To describe the population distribution and movement of bacteria in porous media, we consider the convection-dispersion equation with nonlinear reactions. The reactive solute transport equation is one for which numerical solution procedures continue to exhibit significant limitations. Accurate numerical simulations are crucial to the development of contaminant remediation strategies.

A new "exact" numerical method is developed for simulation of reactive bacterial transport in porous media that leads to solutions free from numerical instabilities. Applications to different biofilm models are examined and numerical results are presented to demonstrate the performance of the proposed non-standard numerical approach.

Key words: *bioremediation, biobarrier, "exact" methods*

INTRODUCTION

In situ biorestoration techniques are a promising approach for the successful cleanup of contaminated aquifers. One such technology is the creation of biobarriers for containment and remediation of soil and groundwater contaminated with organics and heavy metals. Biobarriers are *in situ* barriers that are formed by stimulating growth of biofilm-forming microbes introduced into the subsurface (James et al., 1995). Microbial biomass plugs the free-pore-space flow paths through porous media, thereby reducing the hydraulic conductivity and mass transport properties. Selective plugging of permeable strata may be used for preventing migration of groundwater contaminants from hazardous waste sites. In addition, biobarriers may be capable of simultaneously degrading and containing a contaminant plume. Simple nutritional differences may be used to deliver bacteria to any location in the subsurface environment.

The objectives of our research work are to develop mathematical models for flow, transport, and biofilm accumulation in porous media; to develop reliable, accurate, and efficient numerical methods for the given models; and to apply the methods to subsurface biobarrier formation. The outline of the paper is as follows. The governing system of partial differential equations is formulated for a two-phase, four-species mixture. In the next section, standard numerical techniques are presented for solving the equations governing the fluid flow and solute transport in porous media. The new "exact" numerical method for simulation of reactive bacterial transport in porous media is developed in Section 4. To demonstrate the performance of the proposed new method and the effectiveness of microbial biobarriers for reducing the hydraulic conductivity, numerical results are

presented in Section 5. In the last section, summary of results and future research directions are outlined.

GOVERNING SYSTEM OF EQUATIONS

In many practical cases of flow of liquids, the variation in density of the liquid may be ignored. In such cases the liquid is said to be incompressible (Currie, 1993), which means that as a given mass of liquid is followed, its density remains constant. For the case of homogeneous, incompressible liquids, the equation governing transient fluid flows in saturated porous media can be written in the form (Allen, 1988):

$$S_s \frac{\partial h}{\partial t} - \frac{\partial}{\partial x}\left(K(c_M, c_N) \frac{\partial h}{\partial x} \right) = f. \quad \text{(fluid flow)} \tag{1}$$

Here, $h(x,t)$ denotes the hydraulic head; S_s is the specific storage; K is the saturated hydraulic conductivity; and $f(x,t)$ represent sources or sinks.

The transport of microbes and nutrients is governed by the partial differential equations:

$$\begin{aligned} &\frac{\partial}{\partial t}(\hat{R}_M \phi c_M) + \frac{\partial}{\partial x}(v c_M) - \frac{\partial}{\partial x}\left(D_M \frac{\partial c_M}{\partial x} \right) = R_M(c_M, c_N), \quad \text{(microbes)} \\ &\frac{\partial}{\partial t}(\hat{R}_N \phi c_N) + \frac{\partial}{\partial x}(v c_N) - \frac{\partial}{\partial x}\left(D_N \frac{\partial c_M}{\partial x} \right) = R_N(c_M, c_N), \quad \text{(nurtients)} \end{aligned} \tag{2}$$

respectively. Here c_i, $i=M, N$, represents the mass concentration of species i per unit volume of the liquid phase. For single-fluid flow, the quantity ϕ is usually identified as the porosity of the rock matrix, $D_i(x,t)$; $i = M, N$ is the hydrodynamic dispersion coefficient; and $\hat{R}_i$, $i = M, N$ is the retardation factor accounting for linear equilibrium sorption. The pore water velocity $v(x,t)$, called superficial or Darcy velocity, represents the speed of the moving front.

We assume that the solid rock matrix is stationary and that the diffusion of microbial and nutrient species in the solid phase is negligible. The rate of biofilm growth is given by the Monod kinetics reactions:

$$\mu(c_N) = \frac{\mu_{\max} c_N}{K_s + c_N}, \tag{3}$$

where $\mu_{\max}$ is the maximum specific growth rate, and K_s is that value of the concentration of nutrients c_N where the specific growth rate $\mu(c_N)$ has half its maximum value (Bailey and Ollis, 1986). Also, the microbial death rate is assumed to be proportional to the size of the biofilm population.

Invoking all simplifying assumptions to equations (2) gives the final form of the governing system of differential equations

$$S_s \frac{\partial h}{\partial t} - \frac{\partial}{\partial x}\left(K(c_M, c_N) \frac{\partial h}{\partial x} \right) = f,$$

$$\frac{\partial}{\partial t}(\hat{R}_M \phi c_M) + \frac{\partial}{\partial x}(v c_M) - \frac{\partial}{\partial x}\left(D_M \frac{\partial c_M}{\partial x} \right) = \frac{\mu_{\max} c_N}{K_s + c_N} c_M - k_r c_M, \tag{4}$$

$$\frac{\partial}{\partial t}(\hat{R}_N \phi c_N) + \frac{\partial}{\partial x}(v c_N) - \frac{\partial}{\partial x}\left(D_N \frac{\partial c_N}{\partial x} \right) = -\frac{1}{Y} \frac{\mu_{\max} c_N}{K_s + c_N} c_M,$$

where k_r is the first-order endogenous decay rate.

NUMERICAL SOLUTION STRATEGY

Equations (4) represent a coupled system of nonlinear, time-dependent partial differential equations that is very difficult to solve numerically. A key objective of the numerical simulation is to develop time-stepping procedures that are reliable, accurate, and computationally stable. One possible time-stepping approach is the sequential solution technique (Russell and Wheeler, 1983). The nonlinear partial differential system is decoupled at each time step using a linearization technique and each equation is solved implicitly at the current time step (Ewing and Russell, 1982). This allows multiple concentration time steps for each head time step.

Mixed Finite-Element Methods for the Flow Equation

Classical techniques for solving the fluid flow equation (1)

$$S_s \frac{\partial h}{\partial t} - \frac{\partial}{\partial x}\left(K \frac{\partial h}{\partial x} \right) = f, \quad x \in \Omega \tag{5}$$

include the standard finite difference and Galerkin finite-element methods, applied on uniform spatial grids. The resulting linear algebraic systems are symmetric and positive definite, so one can solve for the approximate hydreaulic head $\hat{h}$ using a variety of iterative numerical schemes. Having computed $\hat{h}$, one can differentiate numerically to obtain the velocity

$$\hat{v} = -K(x,t) \frac{\partial \hat{h}}{\partial x}. \tag{6}$$

A major problem with those approaches is that the approximate velocity $\hat{v}$ is one order lower in spatial accuracy than the approximate hydraulic head. In groundwater contaminant hydrology, inaccurate velocities are of serious concern, since the hydraulic head appears in the species concentration equations (2) only through its velocity field.

To overcome these difficulties, it is more appropriate to choose a numerical method that approximates the velocity field v directly, such as the mixed finite-element method or cell-centered finite differences in space (Allen and Wang, 1994). Mixed finite-element methods use a different discretization approach than the classical numerical methods.

The single fluid-flow equation (1) arises from the mass balance law

$$S_s \frac{\partial h}{\partial t} + \frac{\partial v}{\partial x} = f, \tag{5}$$

we substitute for the groundwater velocity v using the Darcy's law

$$v = -K \frac{\partial h}{\partial x}.$$

Here, one solves simultaneously the mass balance and Darcy's laws. The corresponding mixed finite-element method for solving the first-order system (5)-(6) is as follows: Find a pair $(\hat{v}, \hat{h}) \in \hat{\mathrm{U}} \times \hat{\mathrm{Q}}$ such that

$$\begin{aligned} &\int_\Omega K^{-1} \hat{v} u - \int_\Omega \hat{h} \frac{\partial u}{\partial x} = 0 \qquad \forall u \in \hat{\mathrm{U}}, \\ &\int_\Omega q S_s \frac{\partial \hat{h}}{\partial t} + \int_\Omega q \frac{\partial \hat{v}}{\partial x} = \int_\Omega q f \qquad \forall q \in \hat{\mathrm{Q}}, \end{aligned} \tag{7}$$

$\hat{\mathrm{U}}$ and $\hat{\mathrm{Q}}$ are finite-dimensional subspaces of given Hilbert spaces U and Q, respectively (Allen et al., 1992).

Among the simplest choices for subspaces are the lowest-order Raviart-Thomas spaces (Raviart and Thomas, 1977) on uniform grids, where the "hydraulic head" space $\hat{\mathrm{Q}}$ consists of piecewise-constant functions and the "velocity space" $\hat{\mathrm{U}}$ is the space of functions that are piecewise-linear with respect to the uniform grid on Ω. The scheme exhibits good convergence properties in the presence of fine spatial grids and effectively handles variable coefficients K (Allen et al., 1992).

Standard Methods for Transport Equations

Consider the equations governing transient species transport in porous media (2) in the following non-dimensional form:

$$\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} - \frac{\partial}{\partial x}\left(D \frac{\partial c}{\partial x} \right) = R(c). \tag{8}$$

Here, c is the species concentration; v is the barycentric velocity of the mixture; D is the hydrodynamic dispersion tensor; and $R(c)$ is the total production rate via reactions and sources.

While classical techniques, such as standard finite-differences or Galerkin finite-elements, work well for problems of species transport that are dominated by dispersive movement, they suffer from severe nonphysical oscillations and excessive numerical dispersion when convection, associated with the velocity field v, dominates the dispersive effects. Equation (8) is a parabolic-type partial differential equation which changes to hyperbolic if the hydrodynamic dispersion coefficient D is set to zero. Therefore, it is logical to design numerical procedures that recognize the hyperbolic nature of the convection-dominated solute transport problems. Many such schemes have been developed that incorporate ideas from the modified method of characteristics (*MMOC*) (Douglas and Russell, 1982) and the Eulerian-Lagrangian localized adjoint method (*ELLAM*) (Celia et al., 1990). In ELLAM, it can be difficult to evaluate the resulting integrals, in contrast with the MMOC which is relatively easy to implement but does not hold local mass balance of the system. In recent years, several MMOC-based local mass conservative schemes have been developed but still little has been done to improve the numerical solutions of problems in which nonlinear reactions are present.

NON-STANDARD METHODS FOR TRANSPORT EQUATIONS

Nonlinear reaction terms play a significant role in applications involving bacterial growth and contaminant biodegradation in subsurface regions.

We propose a new Eulerian-Lagrangian numerical method for solving the reactive solute transport equation (8):

$$\frac{\partial c}{\partial t} + v\frac{\partial c}{\partial x} - \frac{\partial}{\partial x}\left(D\frac{\partial c}{\partial x}\right) = R(c). \tag{9}$$

numerical solution of the convection-reaction part of Equation (9) is defined using an "exact" time-stepping scheme. This enables us to follow the transport and track sharp fronts much more accurately than with the standard numerical schemes. Having dealt with the most difficult part of the transport problem, only the smoothing property of the dispersion term remains. Then, standard finite differences or finite elements are well suited for solving the dispersion part.

"Exact" Time-Stepping Scheme

Our goal in this section is to construct such an "exact" time-stepping scheme for the convection-reaction part of Equation (9):

$$\frac{\partial c}{\partial t} + v\frac{\partial c}{\partial x} = R(c), \tag{10}$$

subject to the initial condition $c(x,0) = f(x)$, where f is a given function.

To introduce the concept of "exact" time-stepping schemes, let us consider the following numerical scheme:

$$C^m(x) = \mathrm{F}\left(C^{m-1}(x), \Delta t, m\right),$$

where Δt is the time-step size and $C^m(x)$ is the numerical solution at time $m\Delta t$. Assume that it has a solution

$$C^m(x) = \mathrm{G}(C^0(x), \Delta t, m) = \mathrm{G}(f(x), \Delta t, m).$$

The numerical scheme is said to be an "exact" time-stepping scheme if the relationship $C^m(x) = c(x, m\Delta t)$ holds for arbitrary time-step size Δt and at every spatial location x (Mitchell and Griffiths, 1980).

As a first case, consider the dimensionless logistic growth equation (Murray, 1993)

$$\frac{\partial c}{\partial t} + v\frac{\partial c}{\partial x} = \lambda c(1-c). \tag{11}$$

Here, the parameter λ is a positive constant, and the species concentration $c(x,t)$ ranges in the interval [0,1].

The nonlinear partial differential equation (11) can be easily solved using the *method of characteristics* (John, 1991). The general solution assumes the form

$$c(x,t) = \frac{f(s)}{e^{-\lambda t} + (1-e^{-\lambda t})f(s)}, \tag{12}$$

where s is the initial condition for the following ordinary differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t}x(t) = v(x,t). \tag{13}$$

Using linear in space, time-dependent velocity fields $v(x,t) = (ax+b)P_{n-1}(t)$, the solution of Equation (13) is given by the expression

$$x(t) = e^{aP_n(t)}(s + b/a) - b/a.$$

Here, $P_{n-1}(t)$ is a polynomial of (n-1) degree and $P_n(t) = \int_0^t P_{n-1}(\tau)\mathrm{d}\tau$. Substitution of $s = e^{-aP_n(t)}(x + b/a) - b/a$ into (12) yields

$$c(x,t) = \frac{f(e^{-aP_n(t)}(x+b/a) - b/a)}{e^{-\lambda t} + (1-e^{-\lambda t})f(e^{-aP_n(t)}(x+b/a) - b/a)}. \tag{14}$$

Based on comparison of the analytical solution (14) at time t with the analytical solution at time $t + \Delta t$, we construct the "exact" time-stepping scheme (Kojouharov and Chen, 1998) for solving Equation (11):

$$\frac{C^{m+1}(x) - C^m(\bar{x}^m)}{\frac{e^{\lambda\Delta t} - 1}{\lambda}} = \lambda C^m(\bar{x}^m)(1 - C^{m+1}(x)), \tag{15}$$

where the backtrack point $\bar{x}^m$ has the following expression

$$\bar{x}^m = e^{-a[P_n((m+1)\Delta t) - P_n(m\Delta t)]}(x + b/a) - b/a. \tag{16}$$

The left-hand side of the numerical scheme (15) can be viewed as a non-standard backward difference approximation of the characteristic derivative

$$\frac{Dc}{Dt} = \frac{\partial c}{\partial t} + v(x,t)\frac{\partial c}{\partial x},$$

while the right-hand side represents a nonlocal modeling of the nonlinear reaction term $R(c) = \lambda c(1-c)$. Another distinctive feature of the "exact" time-stepping scheme (15) is the more complicated denominator function

$$\delta(\Delta t) = \frac{e^{\lambda\Delta t} - 1}{\lambda}.$$

As a second case, consider the dispersion-free system of dimensionless differential equations governing the transport of microbes and nutrients in an incompressible porous media (Huyakorn and Pinder, 1983):

$$\begin{aligned} &\frac{\partial c_M}{\partial t} + v\frac{\partial c_M}{\partial x} = \frac{\mu_{\max} c_N}{K_s + c_N} c_M - k_r c_M, \qquad \text{(microbes)} \\ &\frac{\partial c_N}{\partial t} + v\frac{\partial c_N}{\partial x} = -\frac{1}{Y}\frac{\mu_{\max} c_N}{K_s + c_N} c_M. \qquad \text{(nutrients)} \end{aligned} \tag{17}$$

Similar to the case of logistic growth reaction terms, we can construct the new "exact" time-stepping scheme for the microbial transport equation (17)

$$\frac{C_M^{m+1}(x) - C_M^m(\bar{x}^m)}{\frac{e^{\lambda^m\Delta t} - 1}{\lambda^m}} = \lambda^m C_M^m(\bar{x}^m), \tag{18}$$

where

$$\lambda^m = \frac{\mu_{\max} C_N^m(x)}{(K_s + C_N^m(x))} - k_r,$$

and the backtrack point $\bar{x}^m$ has the expression (16).

The "exact" time-stepping scheme for solving the nutrients transport equation:

$$\frac{\partial c_N}{\partial t} + v\frac{\partial c_N}{\partial x} = -\frac{1}{Y}\frac{\mu_{\max} c_N}{K_s + c_N} c_M ,$$

is given by the expression

$$\frac{C_N^{m+1}(x) - C_N^m(\bar{x}^m)}{\Delta t} = \lambda^m - \frac{K_s}{\Delta t}\ln\left(\frac{C_N^{m+1}(x)}{C_N^m(\bar{x}^m)}\right), \tag{19}$$

where

$$\lambda^m = -\frac{\mu_{\max} C_M^{m+1}(x)}{Y} .$$

More details on the derivation of "exact" time-stepping schemes for species transport equations with first-order reactions and a variety of nonlinear reaction terms are given in Kojouharov and Chen (1998).

Dispersive Solute Transport Equations

Without loss of generality, we confine our discussion to the development of the non-standard method for solving the dimensionless differential equation governing the transport of microbes in an incompressible porous medium

$$\frac{\partial c_M}{\partial t} + v\frac{\partial c_M}{\partial x} - \frac{\partial}{\partial x}\left(D_M \frac{\partial c_M}{\partial x}\right) = \frac{\mu_{\max} c_N}{K_s + c_N} c_M - k_r c_M . \tag{20}$$

Applying the "exact" time-stepping scheme (18) to Equation (20) yields the following implicit-in-nature, semi-discrete procedure

$$\frac{C_M^{m+1}(x) - C_M^m(\bar{x}^m)}{\dfrac{e^{\lambda^m \Delta t} - 1}{\lambda^m}} - \frac{\partial}{\partial x}\left(D_M^{m+1}\frac{\partial C_M^{m+1}(x)}{\partial x}\right) = \lambda^m C_M^m(\bar{x}^m). \tag{21}$$

To complete the construction of the new non-standard method, we need to introduce an approximation technique for discretizing the spatial derivatives involved in (21).

Let us consider the centered, weighted second difference approximation of the dispersion term (Huyakorn and Pinder, 1983):

$$\frac{\partial}{\partial x}\left(D_M^{m+1}\frac{\partial C_M^{m+1}(x)}{\partial x}\right) \approx \frac{D_{M_{i+\frac{1}{2}}}^{m+1}\left(C_{M_{i+1}}^{m+1} - C_{M_i}^{m+1}\right) - D_{M_{i-\frac{1}{2}}}^{m+1}\left(C_{M_i}^{m+1} - C_{M_{i-1}}^{m+1}\right)}{\Delta x^2}, \tag{22}$$

where $D_{M_{i+\frac{1}{2}}}^{m+1}$ is the hydrodynamic dispersion coefficient located at the center of a space increment and Δx is the spatial grid size. The finite element method can be used as successfully as the finite

difference method; however, we shall not present it here since the general idea of constructing the non-standard method is the same.

Combining the semi-discrete procedure (21) with the above spatial approximation of the dispersion term yields the new non-standard method for solving the microbial transport equation (20)

$$\frac{C_{M_I}^{m+1} - C_M^m(\bar{x}_i^m)}{\dfrac{e^{\lambda_i^m \Delta t} - 1}{\lambda_i^m}} - \delta_{\bar{x}}\left(D_M^{m+1}\delta_x C_M^{m+1}\right)_i = \lambda_i^m C_M^m(\bar{x}_i^m), \tag{23}$$

where

$$\lambda_i^m = \frac{\mu_{\max} C_{N_i}^m}{(K_s + C_{N_i}^m)} - k_r, \text{ and } \delta_{\bar{x}}\left(D_M^{m+1}\delta_x C_M^{m+1}\right)_i$$

denotes the finite difference approximation (22). Here, $C_{M_i}^{m+1}$ is the approximate value of the microbial concentration $c_M(x,t)$ at the grid point xi at the advanced time level $(m+1)$, and the backtrack point $\bar{x}_i^m$ has the expression

$$\bar{x}_i^m = e^{-a[P_n((m+1)\Delta t) - P_n(m\Delta t)]}(x_i + b/a) - b/a.$$

Similarly, the non-standard method for solving the differential equation governing the transport of nutrients in an incompressible porous media:

$$\frac{\partial c_N}{\partial t} + v\frac{\partial c_N}{\partial x} - \frac{\partial}{\partial x}\left(D_N \frac{\partial c_N}{\partial x}\right) = -\frac{1}{Y}\frac{\mu_{\max} c_N}{K_s + c_N} c_M, \tag{24}$$

is given by the expression

$$\frac{C_{N_i}^{m+1} - C_N^m(\bar{x}_i^m)}{\Delta t} - \delta_{\bar{x}}\left(D_N^{m+1}\delta_x C_N^{m+1}\right)_i = \lambda_i^m - \frac{K_s}{\Delta t}\ln\left(\frac{C_{N_i}^{m+1}}{C_N^m(\bar{x}_i^m)}\right),$$

where

$$\lambda_i^m = -\frac{\mu_{\max} C_{M_i}^{m+1}}{Y}.$$

NUMERICAL RESULTS

We now turn to a set of numerical experiments to demonstrate the performance of the proposed new method and the effectiveness of microbial barriers for reducing the hydraulic conductivity.

The governing system of equations (4) examined here has the following form:

$$-\frac{\partial}{\partial x}\left(K\frac{\partial h}{\partial x}\right)=f, \qquad \text{(fliud flow)}$$

$$\frac{\partial c_M}{\partial t}-\frac{\partial}{\partial x}\left(D_M\frac{\partial c_M}{\partial x}\right)=\frac{\mu_{\max}c_N}{K_s+c_N}c_M-k_r c_M, \qquad \text{(microbes)} \tag{25}$$

$$\frac{\partial c_N}{\partial t}+v\frac{\partial c_N}{\partial x}-\frac{\partial}{\partial x}\left(D_N\frac{\partial c_N}{\partial x}\right)=-\frac{1}{Y}\frac{\mu_{\max}c_N}{K_s+c_N}c_M, \qquad \text{(nutrients)}$$

where h is the hydraulic head; c_M is the biofilm density; and c_N is the nutrients concentration. Assumptions made in the above mathematical model (25) are that all bacteria are attached to the rock surface, as a part of the biofilm structure, and that the concentration of nutrients present in the solid phase is negligible.

Two numerical simulations are carried out with the non-standard "exact" method. Dimensionless model parameters of the correct magnitude are chosen as mesh size $\Delta x = 0.01$, time-step size $\Delta t = 0.02$, dispersion coefficients D_M= 0.0002 and D_N= 0.003, source term f=0.01, and initial hydraulic conductivity K = 0.015. We consider a spatial domain Ω = [0, 1], and assume that h=50 at x=0, and h=0 at x=1. No endogenous respiration is used and the Monod kinetics coefficients are taken as $\mu_{\max} = 0.05$, K_s = 0.32, and Y = 0.16. The initial biofilm distribution is represented by the "cutoff" *Gaussian hill* centered at x_0

$$c_M(x,0)=\begin{cases}0.7\exp\{-\sigma(x-x_0)^2\}, & |x-x_0|\le 1/16\\ 0, & \text{otherwise}\end{cases} \tag{26}$$

where x_0= 0.2 and s= 800.

In the first numerical experiment, the initial nutrients distribution

$$c_N(x,0)=\begin{cases}0.5, & 0\le x\le 0.1\\ 0.4, & 0.1< x\le 1\end{cases}$$

corresponds to a nutrients saturation of c_N = 0.4 that is subsequently increased to c_N = 0.5 at the left end of the porous media domain Ω. Results for this problem, after 800 time-step iterations, are shown in Figure 1. The initial conditions are given in dotted lines (...), and the numerical solutions in dashed (_ _) and solid (___) lines. Figure 1 demonstrates the ability of the non-standard method to model convection-dominated nutrients transport without distorting sharp concentration fronts (Kojouharov and Chen, 1998).

The potential of microbial biobarriers for reducing the hydraulic conductivity is demonstrated in Figure 2. A relative increase of 23% in the biofilm density, after 500 time-step iterations, results in a

corresponding decrease in the hydraulic conductivity of about 40 %.

In the second numerical experiment, we consider the "step-function" type initial nutrients distribution:

$$c_N(x,0) = \begin{cases} 0.8, & 0 \le x \le 0.1 \\ 0.4, & 0.1 < x \le 1 \end{cases},$$

which corresponds to a subsequent increase of the initial nutrients saturation from $c_N = 0.4$ to $c_N = 0.8$ (Figure 3). The 60 % increase in the nutrients concentration, with respect to the first numerical experiment, results in a much bigger growth rate of the biofilm-forming microbes. Figure 4 shows the 50% reduction in the hydraulic conductivity, after 500 time-step iterations, due to the 33% decrease in the biofilm density.

CONCLUSIONS AND FUTURE RESEARCH DIRECTIONS

Non-standard numerical methods have been developed for solving one-dimensional, transient convective-dispersive transport equations with nonlinear reactions. Large time steps can be taken without affecting the accuracy of the numerical solution. The appropriate time-step size for a particular model problem can be determined by physical considerations, rather than stability, convergence, or consistency reasons.

The proposed new methods have been successfully applied to biobarrier formation models incorporating Monod kinetics reactions. Numerical results confirmed the theoretical and experimental predictions that microbial barriers are effective for manipulating the porous media properties in general, and for reducing the hydraulic conductivity and mass transport in particular.

There are currently two research directions that we are pursuing. Our main effort is to extend the ideas of the "exact" time-stepping scheme to multi-dimensional reactive solute transport problems. The second research direction is toward an improved treatment of spatial derivatives in the dispersion term. Comparison with experimental results obtained from the Montana State's Center for Biofilm Engineering for validation and calibration of the developed mathematical models is in progress.

ACKNOWLEDGMENTS

The Department of Mathematics, University of Wyoming and the Great Plains/Rocky Mountain Hazardous Substance Research Center are acknowledged for financial support.

Although this article has been funded in part by the U.S. Environmental Protection Agency under assistance agreement R-819653, through the Great Plains/Rocky Mountain Hazardous Substance Research Center, it has not been subjected to the agency's peer and administrative review and, therefore, may not necessarily reflect the views of the agency. No official endorsement should be inferred.

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Figure 1. Numerical solutions generated by the non-standard method for the biofilm density (___) and the nutrients concentration (_ _) after 800 time-step iterations. The dotted lines (...) are the initial biofilm and nutrients distributions.

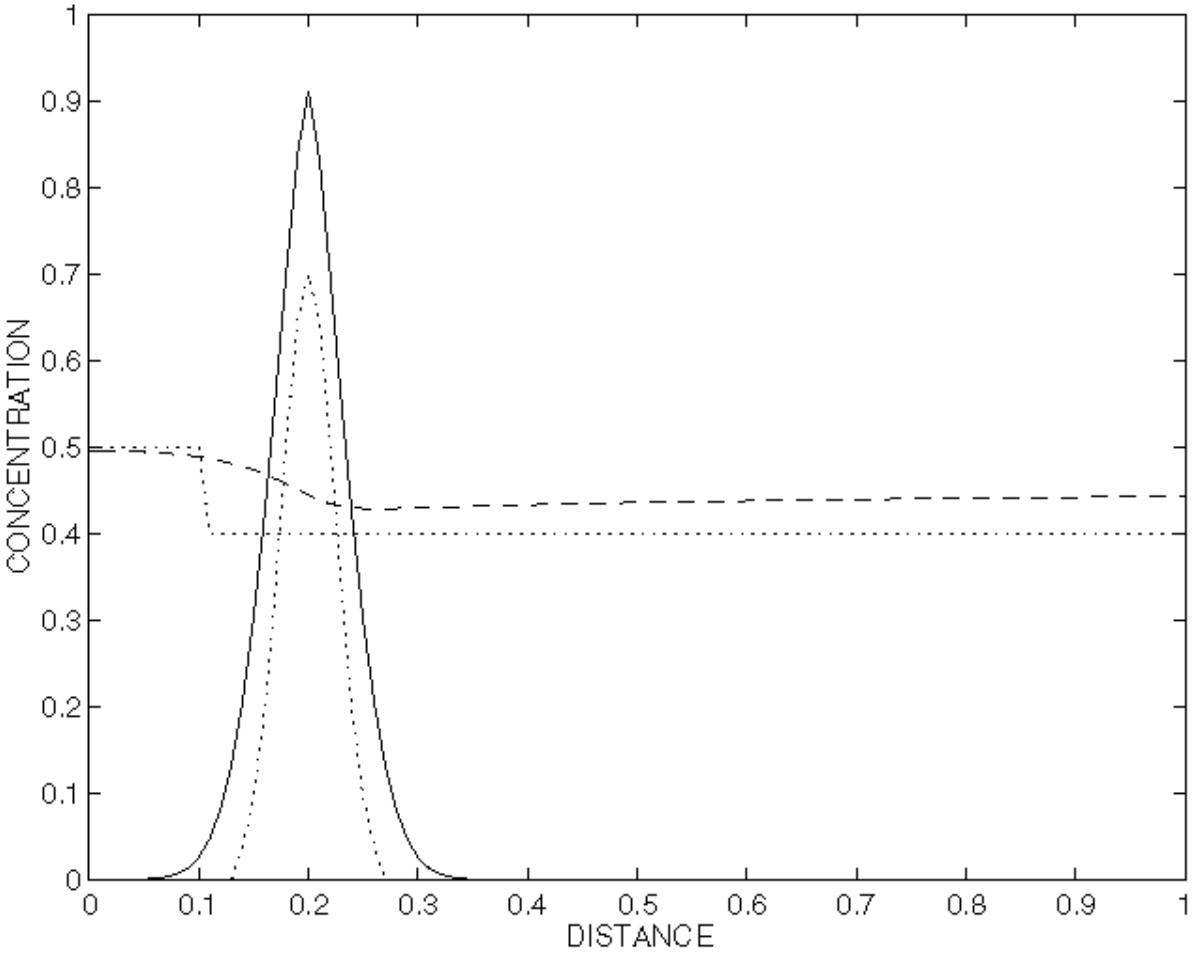

Figure 2. Effectiveness of the microbial barriers for reducing the hydraulic conductivity.

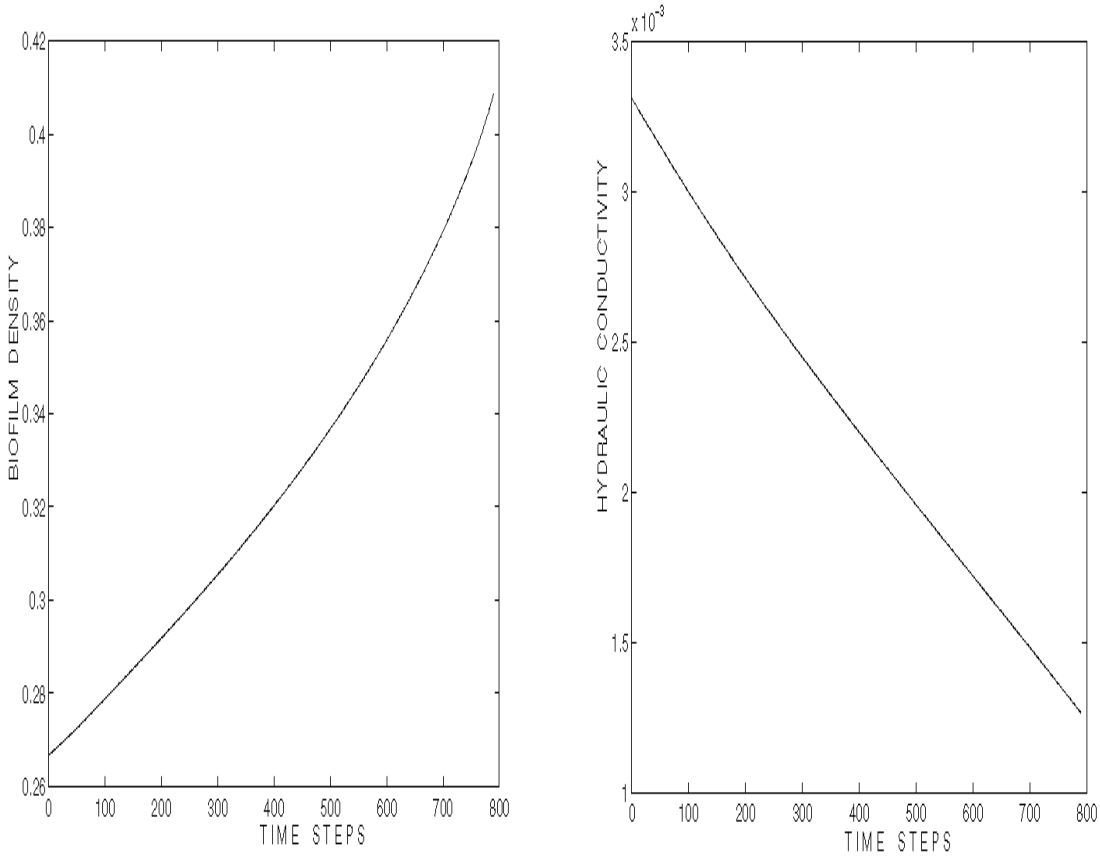

Figure 3. Numerical solutions generated by the non-standard method for the biofilm density (___) and the nutrients concentration (_ _) after 550 time-step iterations. The dotted lines (...) are the initial biofilm and nutrients distributions.

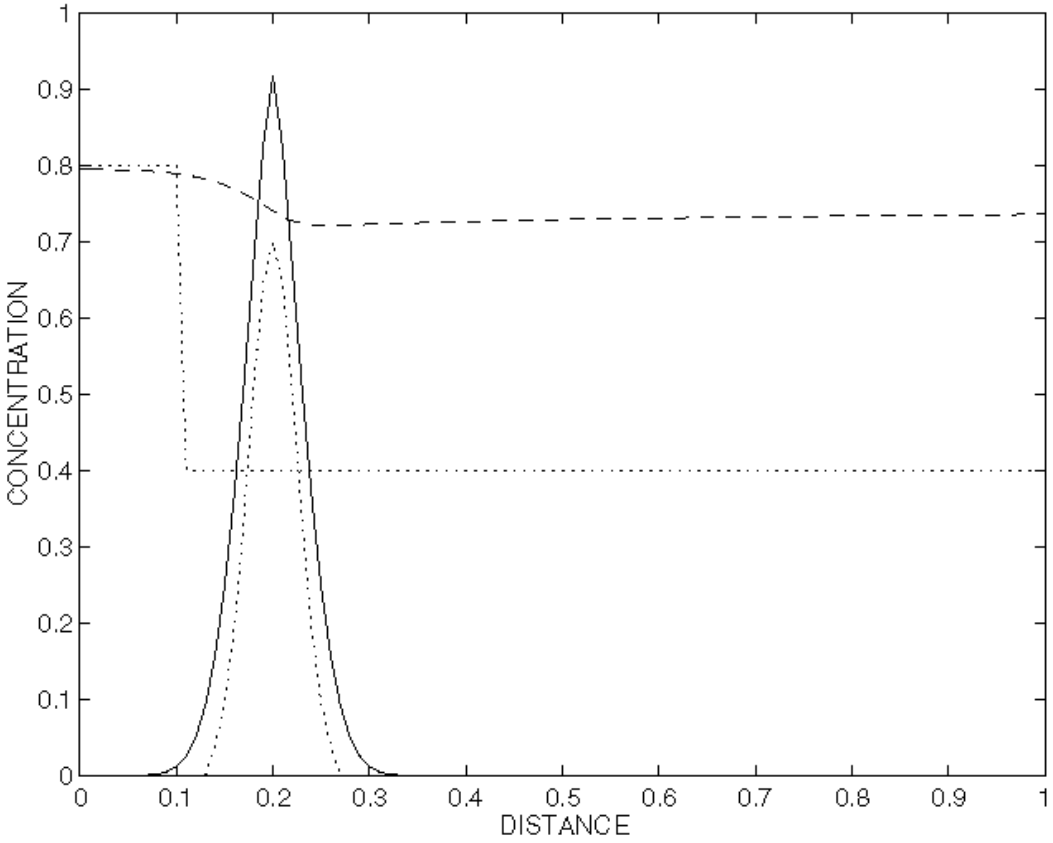

Figure 4. Effectiveness of the microbial barriers for reducing the hydraulic conductivity.