

MODELING OF SUBSURFACE BIOBARRIER FORMATION

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ABSTRACT

Biofilm-forming microbes can form biobarriers to inhibit contaminant migration in groundwater. Also subsurface biofilms have the potential for biotransformation of organic contaminants to less harmful forms, thereby providing an *in situ* method for treatment of contaminated groundwater supplies. We present a mathematical and numerical model to describe the population distribution and growth of bacteria in porous media. The model is based on the convection-dispersion equation with nonlinear reaction terms. Accurate numerical simulations are crucial to the development of contaminant remediation strategies. We use the nonstandard numerical approach that is based on nonlocal treatment of nonlinear reactions and modified characteristic derivatives. It leads to significant, qualitative improvements in the behavior of the numerical solution. Numerical results for a simple biobarrier formation model are presented to demonstrate the performance of the proposed new method. We show comparisons with experimental results obtained from Montana State's Center for Biofilm Engineering.

Key words: *biobarriers, models, biofilms, simulations*

INTRODUCTION

Controlling pollution in underground water is a very important and difficult problem. There are bacteria that will destroy many organic contaminants in subsurface regions. But for most pollutants, including heavy metals, a more promising concept is the creation of biobarriers for containment and remediation of contaminated soil and groundwater. Biobarriers are *in situ* barriers that are formed by stimulating the growth of biofilm-forming microbes that are already present or are introduced into the aquifer. As the microbial biomass increases it plugs the free pore space flow paths through porous media, thereby reducing the hydraulic conductivity and mass transport properties (Cunningham et al., 1991). By adequately choosing where to plug the porous medium, it is possible to prevent the migration of groundwa-

ter contaminants from hazardous waste sites.

An even better scenario is to have biobarriers that will not only contain the contaminant plume but will also degrade it.

Mathematical models are needed to complement experimental work into the use of biofilms to form biobarriers. Mathematical models help to explain the mechanisms for flow, solute transport, biological and chemical reactions, biofilm accumulation, and natural biodegradation in porous media. These generally lead to strongly coupled systems of nonlinear partial differential equations that are difficult to solve. Analytical solutions for the full, coupled problems are nonexistent, and numerical methods have problems such as instabilities and artificial diffusion. Here we use new methods that are reliable, accurate, and efficient for the given models. We apply the methods to subsurface

biobarrier formation. Without these methods, results of numerical simulations are of doubtful value.

In this article, we use a new Eulerian-Lagrangian numerical scheme that efficiently handles the numerically difficult convection-dominated transport problems with nonlinear reaction terms. The convection-reaction part of a transport equation is approximated using an “exact” time-stepping scheme. Some of the important features of the scheme are the nonlocal modeling of nonlinear reactions and the more sophisticated discretization of time derivatives. It enables us to track sharp concentration fronts much more accurately than with standard numerical schemes. Having dealt with the most difficult part of the problem, standard finite differences are well suited for solving the remaining dispersion term. This method was presented by Kojouharov and Chen (1999).

We compare the results obtained from using our numerical simulator with some of the experimental results for short cores done by Cunningham et al. (1991). The results compare very well, which is a very good validation of the model. The simulator can now be used as a predictive tool to determine values of parameters which are difficult or impossible to measure, and to help design experiments, field studies, and actual biobarriers.

The outline of the paper is as follows. In the next section, the governing system of partial differential equations is formulated for a two-phase, two-species mixture. In section three, the non-standard numerical method for solving the reactive solute transport problem in porous

media is given. To demonstrate the performance of the proposed method of solution for the model and the effectiveness of biobarriers for reducing the hydraulic conductivity, numerical results and comparisons with experiments are presented in section four. In the last section, a summary of results is presented.

GOVERNING SYSTEM OF EQUATIONS

Consider a three-phase mixture consisting of a liquid phase, a solid rock phase, and a biofilm phase. Even though the biofilm can be considered to be part of the solid phase, it is simpler to take it as a separate phase. The four molecular species present in the porous medium are the biofilm-forming microbes, labeled M ; the soluble contaminants or nutrients, labeled N ; and the water and rock species. We assume that interactions in the system occur only between the microbial and nutrients species. Furthermore, we assume that the microbes are immobile; i.e., they are attached to the rock as biofilm.

The fundamental equation for transient groundwater flow of constant density can be written in the following form (Allen, 1988):

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

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

$$S_s \frac{\partial h}{\partial t} + \frac{\partial v}{\partial x} = f, \quad (2)$$

when we substitute for the specific discharge vector v using the Darcy's law

$$v = -K \frac{\partial h}{\partial x}. \quad (3)$$

$h(x,t)$ 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 specific discharge vector $v(x,t)$, called Darcy velocity, represents the speed of the water.

The transport and reaction of nutrients and the growth of microbes are governed by a system of partial differential equations. Since the rock phase doesn't change, we assume that the solid rock matrix is stationary and that the diffusion of microbial and nutrient species in the solid phase is negligible. Therefore we can work only with the liquid and biofilm phases as follows:

$$\frac{\partial}{\partial t}(\phi_M \rho_M) = r_M(\rho_M, \rho_N) \quad (\text{microbes})$$

$$\frac{\partial}{\partial t}(\phi_N \rho_N) + \frac{\partial}{\partial x}(v \rho_N) - \frac{\partial}{\partial x}\left(D_N \frac{\partial \rho_N}{\partial x}\right) = r_N(\rho_M, \rho_N). \quad (\text{nutrients}) \quad (4)$$

Here $\rho_i, i=M,N$, represents the intrinsic mass density of microbes and nutrients, respectively. For a single-fluid flow, the quantity f_N is the volume fraction occupied by the liquid divided by the volume of the liquid plus the volume of the biofilm; f_M is the volume of the biofilm again divided by the volume of the liquid and biofilm; $D_N(x,t)$ is the hydrodynamic dispersion coefficient for the nutrients; and r_i represents the total rate at which species i is produced via reactions and sources.

The growth rates are usually written in terms of concentrations and we will do that too. The microbial death rate is assumed to be proportional to the size of the biofilm population. The rate of biofilm growth is given by the

following Monod kinetics reactions:

$$\mu(S) = \frac{\mu_{MAX} S}{K_s + S}, \quad (5)$$

where μ_{MAX} is the maximum specific growth rate; and K_s is that value of the concentration of nutrients S (mass of nutrients per unit of liquid volume) where the specific growth rate $\mu(S)$ has half its maximum value (Bailey and Ollis, 1986). We assume that only the growth and accumulation of biofilm in the pore spaces cause changes in the porous media properties. Let X_f be the current biofilm concentration; then

$$\tilde{X}_f = \frac{X_f}{\rho_M}$$

is the normalized biofilm concentration. It follows that the change in porosity, for small initial biofilm concentrations, is given by

$$\phi = \phi_0 (1 - \tilde{X}_f),$$

where ϕ_0 is the clean surface porosity. For the saturated hydraulic conductivity K we assume the following form:

$$K = K_0 (1 - \tilde{X}_f)^{n_k} \quad (6)$$

where K_0 is the initial hydraulic conductivity, and n_k is an experimentally determined parameter which takes values around 3 (Clement et al., 1996). For simplicity, from now on we will drop the tilde from the normalized biofilm concentration. We assume there are no sources and sinks for the fluid; therefore, $f=0$. Also we are modeling very short cores with uniform biofilm distribution so we can take the velocity to be independent of x .

Invoking all simplifying assumptions to equations (4) and using concentrations as the

unknowns gives the following final form of the governing system of differential equations:

$$\begin{aligned} -\frac{\partial}{\partial x} \left(K(X_f) \frac{\partial h}{\partial x} \right) &= 0, \\ \frac{\partial}{\partial t} (X_f) &= \frac{\mu_{\max} S}{K_s + S_N} X_f - k_r X_f, \\ \frac{\partial}{\partial t} (S) + \frac{\partial}{\partial x} (vS) - \frac{\partial}{\partial x} \left(D_N \frac{\partial S}{\partial x} \right) &= -\frac{1}{Y} \frac{\mu_{\max} S}{K_s + S} X_f, \end{aligned} \quad (7)$$

where k_r is the first-order endogenous decay rate, and Y is the yield rate coefficient.

NUMERICAL METHODS FOR BIOFILM GROWTH

Equation (7) represents 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 accurate and computationally stable. Different time-stepping ideas can be applied to solve the governing system of equations (Russell and Wheeler, 1983). One possible time-stepping approach is the sequential solution technique. The sequential method first solves implicitly for the Darcy velocity v at the current time level by solving the fluid flow equation (1). Then the species transport system (4) is solved implicitly for the concentrations S and X_f in a decoupled fashion (Ewing and Russell, 1982). New values of porosity and permeability are then calculated and the cycle is repeated by calculating the new velocities. For the solution of the ordinary differential equation modeling the flow, we use a standard finite-difference method to calculate h . Then we numerically differentiate using

$$v = -K \frac{\partial h}{\partial x}, \quad (8)$$

to get the velocity field.

Consider the following reaction-diffusion-advection equation governing reactive species transport in porous media:

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

Here, c is the species concentration; v is the velocity; and D is the hydrodynamic dispersion tensor. Since v is independent of x , the nonlinear reaction term $R(c)$ has the expression

$$R(c) = r(c), \quad (10)$$

where $r(c)$ represents the total rate at which the species is produced via reactions and sources.

Unfortunately, there are only few cases for which analytic solutions to the solute transport equation (9) exist. The form of equation (9) ranges from parabolic to almost hyperbolic, depending on the ratio of convection to dispersion. While classical numerical techniques, such as the standard finite-differences or Galerkin finite-elements, work well for problems of solute transport that are dominated by dispersive movement, they suffer from severe nonphysical oscillations and excessive numerical dispersion when convection dominates the dispersive effects. Solutions of hyperbolic-type equations can be represented from the initial data propagating over characteristic paths in the surface and can be viewed as dispersing away from these paths, along which the concentration c is a smooth function (Douglas and Russell, 1982). Therefore, it is logical to design numerical

procedures that recognize the hyperbolic nature of the convection-dominated solute transport problems, such as the Eulerian-Lagrangian methods. In recent years, many such schemes have been developed but still little has been done to improve the numerical solutions of problems in which nonlinear reactions are present. Nonlinear reaction terms play a significant role in applications involving bacterial growth and contaminant biodegradation in subsurface regions.

Referring to Kojouharov and Chen (1999), we proposed a new Eulerian-Lagrangian numerical method for solving the reactive solute transport equation (9). The numerical solution of the convection-reaction part 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 (9), only the smoothing property of the dispersion term remains. Then, standard finite differences or finite elements are well suited for solving the dispersion part.

We now apply the new method to the following dispersion-free system of differential equations:

$$\begin{aligned} \frac{\partial X_f}{\partial t} &= \frac{\mu_{\max} S}{K_s + S} X_f - k_r X_f, \quad (\text{microbes}) \\ \frac{\partial S}{\partial t} + v \frac{\partial S}{\partial x} &= -\frac{1}{Y} \frac{\mu_{\max} S}{K_s + S} X_f. \quad (\text{nutrients}) \end{aligned} \quad (11)$$

The microbes equation is a linear first order ordinary differential equation whose “exact solution” is given by

$$\frac{X_f^{m+1}(x) - X_f^m(x^m)}{e^{\lambda^m \Delta t} - 1} = \lambda^m X_f^m(x^m), \quad (12)$$

$$\text{where } \lambda^m = \frac{\mu_{\max} S^m(x)}{(K_s + S^m(x))} - k_r.$$

The “exact” time-stepping scheme for solving the nutrients transport equation from system (11) is given by the expression

$$\frac{S^{m+1} - S^m(\bar{x}^m)}{\Delta t} = \lambda^m - \frac{K_s}{\Delta t} \ln \left(\frac{S^{m+1}(x)}{S^m(\bar{x}^m)} \right), \quad (13)$$

$$\text{where } \lambda^m = -\frac{\mu_{\max} X_f^{m+1}(x)}{Y}, \text{ and the back-}$$

track point \bar{x}^m has the expression

$$\bar{x}^m = x - \left[P_n((m+1)\Delta t) - P_n(m\Delta t) \right],$$

for constant in space, time-dependent velocity fields: $v(t) = P_{n-1}(t)$.

We now add a diffusion term to the transport equation for the following nutrients:

$$\frac{\partial S}{\partial t} + v \frac{\partial S}{\partial x} - \frac{\partial}{\partial x} \left(D_M \frac{\partial S}{\partial x} \right) = -\frac{1}{Y} \frac{\mu_{\max} S}{K_s + S} X_f. \quad (14)$$

Applying the “exact” time-stepping scheme (13) to equation (14) yields the following implicit in nature, semi-discrete procedure:

$$\begin{aligned} \frac{S^{m+1}(x) - S^m(\bar{x}^m)}{\Delta t} - \frac{\partial}{\partial x} \left(D_M^{m+1} \frac{\partial S^{m+1}(x)}{\partial x} \right) = \\ \lambda^m - \frac{K_s}{\Delta t} \ln \left(\frac{S^{m+1}(x)}{S^m(\bar{x}^m)} \right). \end{aligned} \quad (15)$$

To complete the construction of the new Eulerian-Lagrangian method for solving equation (14), we need to introduce an approximation

technique for discretizing the spatial derivatives involved in the dispersion term. Let us consider the following centered, weighted second difference approximation (Huyakorn and Pinder, 1983):

$$\frac{\partial}{\partial x} \left(D_M^{m+1} \frac{\partial S^{m+1}(x)}{\partial x} \right)_i \approx \delta_{\bar{x}} \left(D_N^{m+1} \delta_x S^{m+1} \right) = \frac{D_{M_{i+\frac{1}{2}}}^{m+1} (S_{i+1}^{m+1} - S_i^{m+1}) - D_{M_{i-\frac{1}{2}}}^{m+1} (S_i^{m+1} - S_{i-1}^{m+1})}{\Delta x^2}, \quad (16)$$

where

$$D_{M_{i+\frac{1}{2}}}^{m+1} = D_M \left(\left(\frac{x_i + x_{i+1}}{2} \right), (m+1)\Delta t \right) \quad (17)$$

is the hydrodynamic dispersion coefficient located at the center of a space increment, and Δx is the spatial grid size.

Combining the semi-discrete procedure (15) with the above spatial approximation of the dispersion term yields the non-standard difference method for solving equation (14):

$$\frac{S_i^{m+1} - S^m(\bar{x}_i^m)}{\Delta t} - \delta_{\bar{x}} \left(D_N^{m+1} \delta_x S^{m+1} \right)_i = \lambda_i^m - \frac{K_s}{\Delta t} \ln \left(\frac{S_i^{m+1}}{S^m(\bar{x}_i^m)} \right), \quad (18)$$

where

$$\lambda_i^m = -\frac{\mu_{\max} X_{f_i}^{m+1}}{Y}$$

and the backtrack point \bar{x}_i^m has the expression

$$\bar{x}_i^m = x_i - \left[P_n \left((m+1)\Delta t \right) - P_n \left(m\Delta t \right) \right].$$

Remark. - In general, the “backtrack” point \bar{x}_i^m does not lie at a grid point. If the approximate solution S is being determined by a finite-difference procedure, the convective concentra-

tion $S^m(\bar{x}_i^m)$ must be evaluated by an interpolation of the approximate solution values $\{S_i^m\}$ at the grid points x_i .

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 property of porous media. The governing system of equations examined here has the following form:

$$-\frac{\partial}{\partial x} \left(K \frac{\partial h}{\partial x} \right) = 0, v = -K \frac{\partial h}{\partial x} \quad (\text{fluid flow})$$

$$\frac{\partial X_f}{\partial t} = \frac{\mu_{\max} S}{K_s + S} G(X_f) X_f - k_r X_f, \quad (\text{microbes})$$

$$\frac{\partial S}{\partial t} + v \frac{\partial S}{\partial x} - D_N \frac{\partial^2 S}{\partial x^2} =$$

$$-\frac{1}{Y} \frac{\mu_{\max} S}{K_s + S} G(X_f) X_f, \quad (19)$$

where

$$G(X_f) = \frac{1 - X_f}{1 - X_f + \gamma},$$

with γ typically small, is introduced to restrict the growth of the microbes as the pores are being plugged. h is the hydraulic head; X_f is the normalized biofilm concentration; and S is the nutrients concentration. The non-dimensional spatial domain considered here is $\Omega = [0, 1]$.

Assumptions made in the above mathematical model (20) are that all bacteria are attached to the solid rock surface as a part of the biofilm structure and that the concentration of nutrients present in the solid phase is negligible. Changes in the hydraulic conductivity K

are caused by the accumulation of solid-phase biomass in the pore spaces. We assume a piecewise steady-state fluid flow, due to the relatively slow changes in the porous media properties (Cunningham et al., 1991). The biofilm concentration-porosity relation used is

$$\phi = \phi_0 (1 - X_f). \quad (20)$$

This formula is valid for small initial biofilm concentrations which is the case in the examples that we do. The conductivity-reduction relationship examined here is given by the following expression:

$$K = K_0 (1 - X_f)^3. \quad (21)$$

We simulate two of the experiments done by Cunningham et al. (1991): the ones for .70 mm and .54mm sands. The experimental values are as follows:

- For .70mm sand: permeability $k = 3.19 \times 10^{-6} \text{ cm}^2$, i.e., hydraulic conductivity $K = .2404 \text{ cm/s}$ for water at 15°C .
- For .54mm sand: $k = 2.17 \times 10^{-6} \text{ cm}^2$, i.e., $K = .1635 \text{ cm/s}$.

For both sands, the initial porosity is $\phi_0 = 0.35$ and the reactor's length is 5 cm, which was scaled to 1 for the calculations. The boundary and initial conditions considered in the model in agreement with Cunningham et al. (1991) are as follows:

$$\begin{aligned} S(0,t) &= S^0 = 25 \text{ mg/L (the numerical results were scaled by a factor of 50, s.t. } S^0 = 0.5 \text{ for calculation and graphing purposes),} \\ h(0,t) &= 0.5 \text{ cm, } h(1,t) = 0 \text{ cm, i.e., head gradient} = 0.5 \text{ cm/cm,} \\ S(x,0) &= 0.5, \text{ and } X_f(x,0) = 0.02. \end{aligned}$$

The following reaction parameters are taken from Taylor and Jaffe (1990):

$$\mu_{\max} = 0.0001041/\text{s},$$

$$K_s = 0.799 \text{ mg/L and}$$

$$Y = 0.0975.$$

Other parameters used are as follows:

$k_r = 0.00007161/\text{s}$, which was obtained from calibrating the model, and

$D_N = 0.0005 \text{ cm}^2/\text{s}$ (The model has a very low sensitivity to this parameter.).

The figures present the results of our calculation, together with some of the experimental values shown in Figures 5 and 8 from Cunningham et al. (1991). We use concentrations instead of biofilm thickness since we cannot calculate the thickness without making assumptions on the distribution of microbes. But, it is reasonable to assume that there is a linear relation between biofilm thickness and microbial concentration.

Figure 1 shows the variation of the normalized porosity with the normalized biofilm concentration. $X_{f\max}$ is the maximum value of the microbial concentration, and the Δ and * symbols represent some experimental results.

Figure 2 is a plot of the permeability decrease and the increase in the microbial concentration with time. In our results, the normalized biomass goes to 1 in about 2 days, the same time it takes the normalized permeability to decrease to about 0.1. In Figure 5 (Cunningham et al., 1991), the permeability also decays to 0.1 in about 2 days, but the normalized biofilm thickness takes about 6 days to tend to 1. The difference is due to the averag-

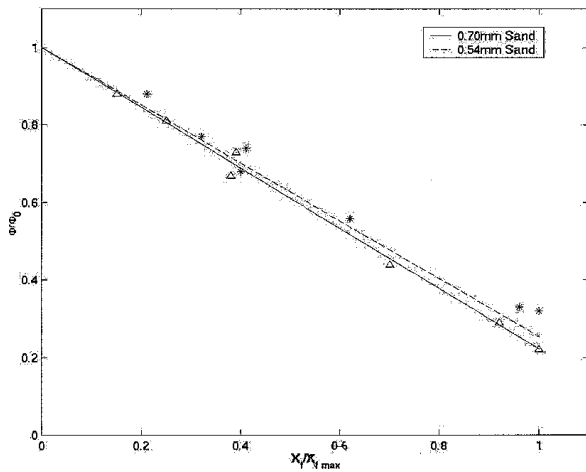


Figure 1. Variation in simulated normalized media porosity with normalized biofilm concentration. The triangles and the stars represent the experimental values for .70 mm and .54 mm sands, respectively, from Cunningham et al., 1991.

ing of the biofilm thickness done by Cunningham et al. (1991), where the dominant component is for 1mm glass spheres (which we are not modeling).

Figure 3 shows the growth of biomass together with the decrease in nutrients. The amount of biomass reaches a maximum steady state at about 2 days, which coincides with the time it takes for the nutrients to reach their minimum.

CONCLUSIONS

A new class of numerical methods has 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, conver-

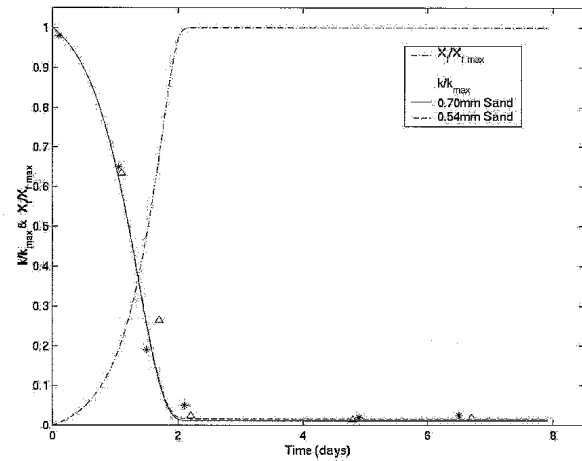


Figure 2. Normalized porous media permeability decrease corresponding to increased normalized microbial concentration versus time. The microbial concentration curve is the average for both types of sand. The triangles and the stars represent experimental permeability values for .70mm sands and .54mm sands, respectively, from Cunningham et al., 1991.

gence, 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 in particular. The agreement is very good and shows that the model can reproduce experimental results and in the future be used as a predictive tool. However, the curves in Figure 1 are closer together than the corresponding experimental ones. One reason is that we are plotting biomass concentrations instead of biofilm thickness. Another possible reason is that we took all the bacteria to be in biofilm form with no significant detachment, so all the biomass reduces the porosity and perme-

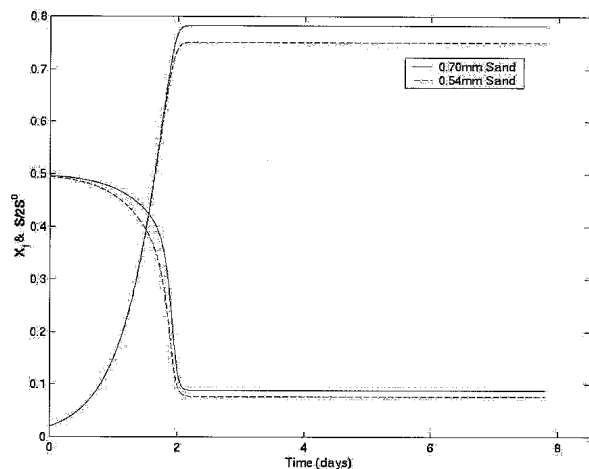


Figure 3. Increase in microbial concentration and decrease of normalized nutrient concentration with time.

ability. In practice there is detachment and the free-floating microbes will not change the physical properties of the medium. Also, for the .54 mm sand, the pore channels are smaller and the velocities higher, which would increase the detachment in this case and add to the separation of the curves.

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