Design of a Passive Biobarrier System for Chromium Containment in Confined Aquifers

T. Shashidhar[1]; Nisha Nandanan[2]; Ligy Philip[3]; and S. Murty Bhallamudi[4]

Abstract: Trench-type biobarrier is one of the commonly used in situ systems for bioremediation of contaminated aquifers. Design variables for such a system are the length of the biobarrier, L, initial microbial concentration, M_0, and inlet substrate concentration, S_0. In this work, a procedure, based on a simple mathematical model, was developed for obtaining the interrelationship between these design variables for containing Cr(VI) in contaminated confined aquifers. The microbial characteristics used in this study were obtained by batch and bench scale column studies. A simulation-optimization model is presented for obtaining the screening level optimal solutions, corresponding to a minimal cost. Variation of values of design variables are presented as a function of a nondimensional parameter π_1, which represents the relative magnitude of microbial growth rate and aquifer flow conditions. As π_1 increases, the optimal length of the biobarrier and, hence, the cost of the treatment system is reduced. The screening level design procedure presented here can be the starting point for design using more sophisticated mathematical models.

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Introduction

Groundwater resources in many places have been contaminated by hydrocarbons, heavy metals, nutrients, microorganisms, etc. (Chen et al. 1992; Riley et al. 1992). Several of these aquifers have been contaminated by hexavalent chromium from wastes generated by leather tanning, wood preservative, and electroplating industries (Fetter 1993). Cr(VI) is highly toxic, highly soluble in water, does not get adsorbed easily, and therefore, it is highly mobile. A maximum acceptable concentration of 0.05 mg/L for chromium in drinking water has been established on the basis of health considerations (EPA 1990). Therefore, aquifers contaminated with chromium require treatment.

Physical, chemical, and biological methods can be used for treating the Cr(VI) contaminated groundwater. Among these, biological methods are more environmentally friendly and economical as they do not involve use of large quantities of chemicals. It has been reported that many microorganisms, under various environmental conditions, can reduce highly toxic Cr(VI) to less toxic and less mobile Cr(III) (Chen and Hao 1998; Rama Krishna and Philip 2005). The biological treatment of groundwater can be carried out either ex situ, using pump and treat technology, or in situ, using biotransformation. The biotransformation process can be aerobic/ anaerobic/ anoxic or a combination of the three. It can be achieved either through biostimulation or bioaugmentation (Eguchi et al. 2000, 2001; Lendvay et al. 2003; Evans et al. 2003; Trindade et al. 2005; Fantroussi and Agathos 2005). Bioaugmentation involves introduction of specific, pregrown microbial cultures to perform a specific remediation task in a given contaminated environment, with the help of biobarriers (Hwang and Cutright 2002; Jianlong et al. 2002; Quan et al. 2004).

Several of the recent research studies have focused on the engineered passive bioreactive barrier technology as it is becoming popular at commercial scale to manage contaminated soil and groundwater risks (Kalin 2004). Borden et al. (1997) reported a field study for control of BTEX migration using a biologically enhanced permeable barrier. Warith et al. (1999) conducted laboratory experiments for the development of an in situ microbial filter for the remediation of groundwater contaminated with naphthalene. Puls et al. (1999) conducted a small-scale field test to evaluate the in situ remediation of groundwater contaminated with chromate using permeable reactive barrier of a mixture of Fe^0, sand, and aquifer sediment. Kao et al. (2001) conducted laboratory experiments for development of a biobarrier for the remediation of PCE-contaminated aquifer. The proposed biobarrier system included a peat layer to enhance the anaerobic reductive dechlorination of PCE in situ. Vogan et al. (1999), Devlin et al. (2004), and Birke et al. (2003) conducted experiments and obtained optimal parameters for the design and performance evaluation of permeable reactive barriers for different volatile organic compounds , under various conditions. Wilkin et al. (2005) studied geochemical and microbiological factors that control long-term performance of subsurface reactive barriers.

Construction and operation of the biobarriers is costly, involving large volume of earth work, mixing of the soil with appropriate microbes, backfilling of the trench, and continuous feeding of aquifer with the substrate required for the microbial growth. In any bioaugmentation problem, the design variables that need to

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be determined are length of the biobarrier (L), initial microbial concentration (M_0), and the substrate to be provided for the microbial growth (S_0). A good understanding of the subsurface transport (advection and dispersion) processes along with chemical (adsorption, ion exchange, precipitation, etc.) and biochemical reactions is essential for optimal design of the biobarriers.

Optimal design of ground water remediation systems has become an active area of research in the last several years (Yoon and Shoemaker 1999; Zheng and Wang 1999; Shieh and Peralta 2005). A variety of optimization methods have been used for this purpose. Computational performances of eight such optimization algorithms were compared by Yoon and Shoemaker (1999). Results showed that no one algorithm is consistently the most accurate on all the problems. Maskey et al. (2002) have developed a ground water remediation strategy using global optimization algorithms, for pump and treat systems. Hu et al. (2006) have developed a dynamic predictive control system for in situ bioremediation process. This control system includes an optimization tool that consists of a simulation model and an optimization function. Shieh and Peralta (2005) developed a model combining genetic algorithms and simulated annealing with BIOPLUME II for the optimal design of bioremediation systems. Liu and Minsker (2004) developed a full multiscale approach to exploit interaction between partial differential equation discretization and optimization, and achieved significant computational saving.

Literature review revealed that although many generic simulation-optimization packages are available for optimal design of aquifer remediation strategies, most of them have been applied to the case of pump and treat method. Very few attempts are made on the optimal design of trench-type biobarrier, especially for the containment of Cr(VI) in contaminated confined aquifers. The objective of this work is to develop a methodology for the optimal design of a trench-type biobarrier, for given hydrogeologic conditions and microbial characteristics.

Simulation Model

In the present study, the design problem was solved as a simulation-optimization problem, wherein the optimization model made several function calls to the simulation model. The simulation model was used to determine the Cr(VI) concentration at the control point, given the values of the decision variables (M_0, S_0, and L), the hydrogeological conditions of the aquifer (pore velocity, soil characteristics), the biokinetic parameters, and the initial Cr(VI) concentration. In the simulation model, the governing advection-dispersion-reaction equations for one-dimensional transport of hexavalent chromium, substrate, and the microbial growth equation were numerically solved. These equations (Guha 2004; Shashidhar et al. 2007) are given in the following:

$$R_c\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}=D\frac{\partial^2 C}{\partial x^2}-R_{\text{sink}C} \tag{1}$$

$$R_s\frac{\partial S}{\partial t}+u\frac{\partial S}{\partial x}=D\frac{\partial^2 S}{\partial x^2}-R_{\text{sink}S} \tag{2}$$

$$\frac{1}{M}\left(\frac{dM}{dt}\right)=\lambda(\mu-k_d) \tag{3}$$

$$R_{\text{sink}S}=\frac{dS}{dt} \tag{4}$$

$$\frac{dS}{dt}=\frac{\lambda\mu M}{Y} \tag{5}$$

$$\mu=\left(\frac{\mu_{\max}Su}{K_s+Su}\right)\left(\frac{K_i}{K_i+C}\right),\quad =0 \;\; if \;\; Su<0 \tag{6}$$

$$S_u=S-0.63S_T \tag{7}$$

$$R_{\text{sink }kC}=\frac{M\lambda\eta\mu}{Y} \tag{8}$$

in which C=hexavalent chromium concentration in the liquid medium (mg/L); S=molasses concentration in the liquid medium (mg/L); M=bacterial concentration expressed as mg/L of liquid in the column; S_u=utilizable concentration of molasses (mg/L); S_T=total inlet molasses concentration (mg/L); u=pore water velocity (cm/h); D=coefficient of dispersion (cm^2/h); R_c=retardation coefficient for hexavalent chromium; R_s=retardation coefficient for substrate, $R_{\text{sink}C}$=sink term for hexavalent chromium due to biotransformation, $R_{\text{sink}S}$=sink term for substrate due to microbial utilization; μ=specific growth rate (1/h), $\mu_{\max}$=maximum specific growth rate (1/h); k_d=decay constant (1/h); Y=observed yield coefficient; η=efficiency factor for chromium reduction with respect to substrate utilization; and λ=proportionality constant, which takes care of the differences between the microbial growth in suspended batch and attached continuous systems. It also implicitly accounts for metabolic retardation due to starving in the stabilization and acclimatization periods. The coefficient of dispersion, $D=u\alpha_L$ (α_L=dispersivity, cm). Computation of the retardation coefficients for hexavalent chromium and substrate is based on the equilibrium adsorption studies. In this study, Freundlich isotherm model was used. The basic assumptions made in deriving the model can be summarized as follows.

1. The flow in the aquifer is one dimensional. It is emphasized here that the present work dealt with only a screening level design. Therefore, although the subsurface transport of contaminants in nature is three dimensional, it was approximated to one dimensional flow along the movement of the plume.
2. The porous medium is homogeneous, and the porosity remains constant throughout the study period. It has been reported that there is some reduction in the porosity due to microbial growth and contaminant precipitation/adsorption. Also, the writers' earlier studies (Shashidhar et al. 2006) have shown that there was some change in the hydrogeological conditions in the biobarrier due to microbial activity and the associated gas release. These effects are not considered in this screening level design model.
3. Adsorption occurs under equilibrium conditions.
4. The model is based on the "macroscopic modeling," in which it is assumed that all the microorganisms present in a given control volume are equally exposed to the substrate concentration prevailing in the bulk liquid volume (Baveye and Valocchi 1989).
5. The microbes are immobile.
6. The Monod's equation with inhibition describes the microbial growth.

7. Only a fraction of substrate is available for Cr(VI) reduction (Ribesa 2004).
8. Cr(III) generated due to biotransformation is either adsorbed or precipitated and retained on the soil matrix. Therefore, concentration of Cr(III) in liquid phase is assumed to be zero.
9. The temperature is constant, and biokinetic parameters remain invariant.

Numerical Method

A sequential iterative technique is used to solve the nonlinear partial differential equations (Herzer and Kinzelbach 1989; Yeh and Tripathi 1991; Steefel and MacQuarrie 1996). In these equations, the advection part was discretized based on the Monotone Upwind Scheme for Conservation Laws (Van Leer 1977), which is globally second-order accurate and nonoscillatory. The spatial discretization for advection term is based on an essentially nonoscillating scheme in which MINMOD limiter is employed for suppressing numerical oscillations. A central difference scheme is used for spatial discretization of the dispersive term. The mathematical model was calibrated and validated using bench-scale column studies (Shashidhar et al. 2006, 2007)

Development of Design Charts

Construction and operation of biobarriers involve cost of trenching, mixing the soil with appropriate microbes, refilling, and continuous feeding of aquifer with the substrate required for microbial growth. So it is useful to develop charts showing the interrelationship between the length of the biobarrier (L), initial microbial concentration (M_0), and the substrate to be provided for the microbial growth (S_0). The initial microbial concentration to be introduced into the biobarrier depends upon time available for remediation and the permissible limit of the contaminant. If the initial concentration of microbes is very high, the time required for cleaning up the aquifer is less. The main management constraint to be satisfied is that the concentration of Cr(VI) at the outlet of the biobarrier should be within the specified limit at all times t greater than or equal to the time specified. For specified microbial and hydrogeological characteristics of the aquifer, the mathematical model described in the previous section was run for different initial microbial concentrations, M_0 (M_0=10, 20, 30, 40, 50, 100, and 500 mg/L of liquid pore volume) and inlet substrate concentrations, S_0 (S_0=500, 1,000, 2,000, 3,000, and 5,000 mg/L as COD). From these simulation runs, Cr(VI) concentration with respect to distance from upstream end of the biobarrier, at different times from the start of simulation, T, was determined. Minimum length required for remediation was determined from the above-mentioned plots. It is the distance from the upstream at which Cr(VI) concentration is just below 0.05 mg/L, as per the EPA drinking water standards. The design chart was then developed between initial microbial concentration and minimum biobarrier length, for different inlet substrate concentrations, and for different times available for remediation.

Optimization Model Formulation

In any bioaugmentation system that uses a trench-type passive biobarrier, the design variables are length (along the flow direction), L, width (across the flow direction), W, and depth, D of the barrier, initial microbial concentration, M_0 in the barrier, and the substrate (electron donor/electron acceptor), S_0, to be provided for the microbial growth. For a one-dimensional system such as that considered in this study, barrier is assumed to extend for the entire width, and depth of the plume. Hence, only L, M_0, and S_0 are considered as decision variables in the optimization model. These variables are determined such that the total cost, including the capital cost of trenching, cost of providing the initial microbial population in the barrier, and the operational cost of injecting the substrate throughout the period of remediation, is a minimum.

When designing the biobarrier, it should be ensured that the length of the barrier is not less than a minimum value, and not greater than a maximum value because of construction and space requirements. Also, the initial microbial concentration is not allowed to exceed a maximum value in order to prevent the clogging of the barrier during the remediation period. The remediation period is taken as that time after which the Cr(VI) concentration on the downstream side of the barrier is less than the allowable limit of 0.05 mg/L. Lower and higher limits can also be put on the inlet substrate concentration, if required. Besides these, the main management constraint to be satisfied is that the concentration of Cr(VI) at the control point, on the downstream side of the biobarrier, should be within the specified limit at all time "t" greater than or equal to a specified time. This time is equal to the time of travel for Cr(VI) plume to the control point, in the case of a slug discharge and if there is no remediation. In case of contamination due to a continuous source, the above-mentioned time is specified by the user, depending upon the source characteristics, and/or the longevity of the biobarrier. The optimization problem can be stated as follows:

Objective function

$$\text{Min } Z_1 = C_1AL + \frac{C_2M_0AL\phi 1{,}000}{10^6} + \frac{C_3S_0QT1{,}000}{10^6} \tag{9}$$

where Z_1=total cost of biobarrier; C_1=cost of trenching per m^3 of soil; A=cross-sectional area in m^2; L=length of the biobarrier in m; C_2=cost of microbes per kg; M_0=initial microbial concentration in mg/L; ϕ=porosity; C_3=cost of substrate per kg; S_0=inlet concentration of substrate in mg/L; Q=flow rate in m^3/h; and T=time for which the substrate is applied for remediation in hours.

Constraints

The following constraints have to be satisfied when minimizing the objective function:

1. $[C]_{\text{outlet}} \leq 0.05$ mg/L $\quad \forall t \leq t_{\text{specified}}$;
2. $L_{\min} < L < L_{\max}$;
3. $M_{0\,\min} < M_0 < M_{0\,\max}$;
4. $S_{\min} < S < S_{\max}$; and
5. $[C]_{\text{outlet}} = f$ (M_0, S_0, L, hydrogeologic conditions, biokinetic parameters). This relationship is represented by the Cr(VI) transport and transformation equations [Eqs. (1)–(8)].

Genetic Algorithms

A simple genetic algorithm was used for solving the optimization problem. Genetic algorithms (GA) (Goldberg 1989; Deb 1995) are nondeterministic search/optimization methods that utilize the theories of evolution and natural selection to solve an optimization problem within a complex solution space. They are not likely to get stuck in a local minimum, which may be the case with traditional methods. Description of the GA is given in detail by Goldberg (1989) and Deb (1995). The particular version used in this study is taken from MATLAB, and is presented in the form of

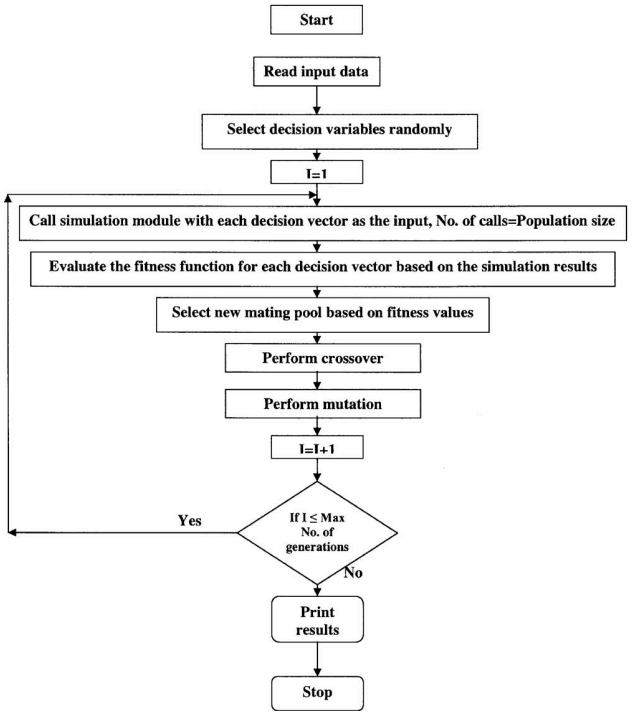

Fig. 1. Flow chart for the simulation-optimization model

a flow chart in Fig. 1. The important parameters of a GA are the population size, the number of generations, and the probabilities of crossover and mutation. All these have to be given as an input by the user and vary depending on the problem. It has been established in literature (Deb 1995) that the population size should be approximately equal to ten times the number of decision variables. The string length for each variable is taken based on the accuracy required. Accuracy$=1/(2^{SL}-1)$ where SL=string length. In the present study, SL is equal for all the decision variables. The probability of crossover generally varies from 0.6 to 1.0. The probability of mutation is typically equal to 1/L (Deb 1995). In this work, the Genetic Algorithm module given in the MATLAB toolbox was used. Probability of crossover and mutation were taken equal to their default values in this toolbox. The number of generations to be considered depends strongly on the number of decision variables. Practically, the computational overburden also dictates the selection of the number of generations. In this study, the number of generations was equal to 100.

Penalty Function Approach

The classical GA presented in the earlier section is designed for application to an unconstrained optimization problem. However, its application to a constrained optimization problem requires modifications. In the constrained optimization problem, the constraints pertaining to lower and upper bounds on the decision variables L, M_0, and S_0 are easily implemented through the specification of maximum and minimum values of the decision variables, which in any case are needed for decoding of the strings representing the variable. However, there is an inequality constraint on the concentration of Cr(VI) at the end of the biobarrier. This constraint is implemented using the penalty function approach. In this approach, a constrained optimization problem is transformed to an unconstrained problem by associating a penalty with all constraint violations, and changing the value of objective function accordingly. For this purpose, the objective function is written as follows:

Minimize

$$\mathrm{OF} = Z_1 + B \tag{10}$$

where Z_1=total cost involved and B=penalty factor. In Eq. (10), B is assigned a nonzero constant value if the inequality constraint on the concentration of Cr(VI) at the end of the biobarrier is violated. Increase in the objective function value corresponding to a particular decision vector reduces the chance of survival of that decision vector in the next generation. This ensures that only those decision vectors that nearly satisfy the constraints remain in the population at the end of the run. A very high value of 10^{10} was used for B in the present study so that a heavy penalty was levied when this constraint was violated.

Nondimensionalization of Optimal Design Parameters

It is convenient if charts, which show the interrelationship between design variables (L, M_0, and S_0) and nondimensional system characteristics, are available to aid the design. The idea of nondimensionalization of governing equations is to combine all the variables involved in the present problem into a few nondimensional parameters, and to study the interrelationship between them. In this study, variations of optimal cost (Z_1), length of the biobarrier (L), microbial concentration (M_0), and concentration of substrate at inlet (S_0) corresponding to the optimal design were studied with respect to these nondimensional parameters. In the present study, only one type of microbe was used. Hence, biokinetic parameters were taken as constant. The nondimensional governing equations are

$$R_c\frac{\partial C^*}{\partial t^*} + \frac{\partial C^*}{\partial x^*} = \frac{\partial^2 C^*}{\partial x^{*2}} - R^*_{\mathrm{sink}Cr6} \tag{11}$$

$$R^*_{\mathrm{sink}Cr6} = \pi_5 \lambda M^* \left[\frac{S^*}{\pi_2 + S^*}\right]\left[\frac{\pi_3}{\pi_3 + C^*}\right] \tag{12}$$

$$R_s\frac{\partial S^*}{\partial t^*} + \frac{\partial S^*}{\partial x^*} = \frac{\partial^2 S^*}{\partial x^{*2}} - R^*_{\mathrm{sink}S} \tag{13}$$

$$R^*_{\mathrm{sink}S} = \pi_4 \lambda M^* \left[\frac{S^*}{\pi_2 + S^*}\right]\left[\frac{\pi_3}{\pi_3 + C^*}\right] \tag{14}$$

$$\frac{1}{M^*}\frac{dM^*}{dt^*} = \pi_1 \lambda \left[\frac{S^*}{\pi_2 + S^*}\right]\left[\frac{\pi_3}{\pi_3 + C^*}\right] \tag{15}$$

where

$$C^* = \frac{C}{C_0}, \quad x^* = \frac{x}{\alpha_L}, \quad t^* = \frac{t}{\alpha_L}u, \quad S^* = \frac{S - 0.63S_T}{C_0}, \quad M^* = \frac{M}{C_0} \tag{16}$$

$$\pi_1 = \frac{\mu_{\max}\alpha_L}{u} \tag{17}$$

$$\pi_2 = \frac{K_s}{C_0} \tag{18}$$

Table 1. Input Values for Mathematical Simulations

Serial No.	Parameter	Value
1	μ_{max} (1/h)	0.3
2	Y	0.263
3	η	0.3
5	λ	0.1
6	K_s (mg/L)	40.0
7	K_i (mg/L)	3.049
8	K_d (1/h)	0.0
9	Dispersivity (α_L) (cm)	1
10	Darcy velocity (m/day)	0.1
11	Porosity	0.35
12	Time for remediation (days)	14.5 and 21
13	Maximum length (cm)	100
14	Bulkdensity (g/cc)	1.8
15	Freundlich constants for Cr(VI)	K_f=0.012; n=1.9
16	Freundlich constants for molasess	K_f=0.055; n=0.764
17	Upstream Cr(VI) concentration (mg/L)	25
18	Maximum microbial concentration (mg/L)	530

$$\pi_3 = \frac{K_i}{C_0} \tag{19}$$

$$\pi_4 = \pi_1\left(\frac{1}{Y}\right) \tag{20}$$

$$\pi_5 = \pi_4\eta \tag{21}$$

The transport and biotransformation of Cr(VI) depends upon the flow characteristics and biokinetics of the microbes used. Flow characteristics are determined by pore velocity and longitudinal dispersivity. The biokinetic parameters of the system are represented by the maximum specific growth rate, μ_{max}, half saturation constant, K_s, yield coefficient, Y, and inhibition constant, K_i. For a given type of microbes, these parameters are constant. Similarly, η and λ are also constants for a given system. Therefore, the nondimensional parameters π_2 and π_3 are constant for given conditions. The nondimensional parameter π_1 incorporates the relative effects of microbial growth and transport on pollutant containment. Therefore, in this study, optimal design values of L, M_0, and S_0 were determined as a function of this parameter π_1, for given microbial and soil system. The plots between the design variables and π_1 indicate how the design changes depending upon the transport conditions.

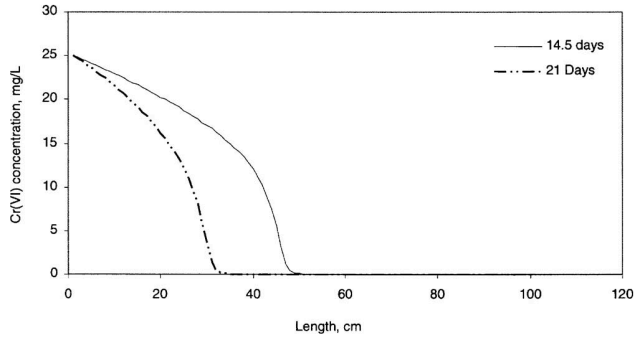

Fig. 2. Cr(VI) concentration with respect to distance at 14.5 and 21 days

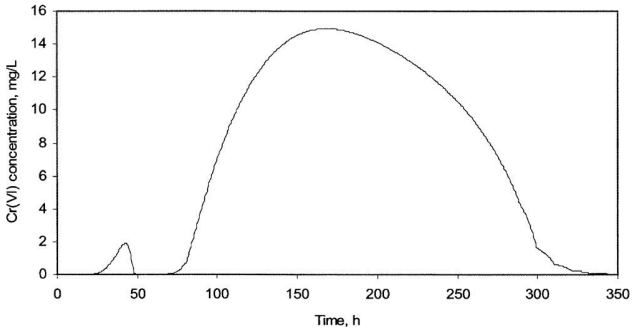

Fig. 3. Cr(VI) breakthrough at 50 cm for the initial bacterial concentration of 30 mg/L and substrate concentration of 1,000 mg/L as COD

Results and Discussion

Design Charts for the Remediation of a Cr(VI) Contaminated Aquifer

The procedure given for preparing the design charts for the remediation of a Cr(VI) contaminated site is illustrated in this section using the input parameters given in Table 1.

The mathematical model was used to simulate the transport and biotransformation within the biobarrier for different combinations of microbial and substrate concentrations. From these simulation runs, variation of Cr(VI) concentration with respect to distance, at the end of 14.5 and 21 days, was obtained. Fig. 2 shows a typical graph for spatial variation of Cr(VI) concentration for the combination of 30 mg/L of initial microbial concentration and 1,000 mg/L of inlet substrate concentration. Fig. 3 shows the Cr(VI) concentration at 50 cm distance from the upstream end of the biobarrier in time domain. For the above-presented combination of M_0 and S_0, the minimum length required for remediation is the length of the barrier from the upstream end at which Cr(VI) concentration is just below the EPA drinking water standards. The minimum length corresponding to various combinations of M_0 and S_0 were determined using numerical experiments. The screening level design chart was then

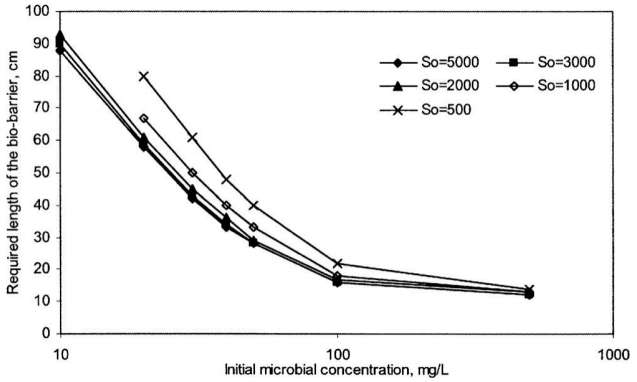

Fig. 4. Design chart for 14.5 days of remediation period

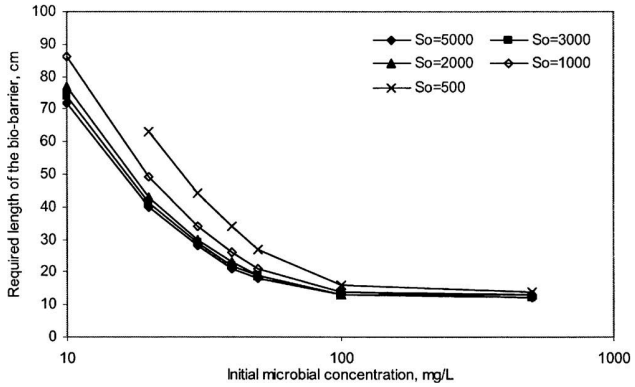

Fig. 5. Design chart for 21 days of remediation period

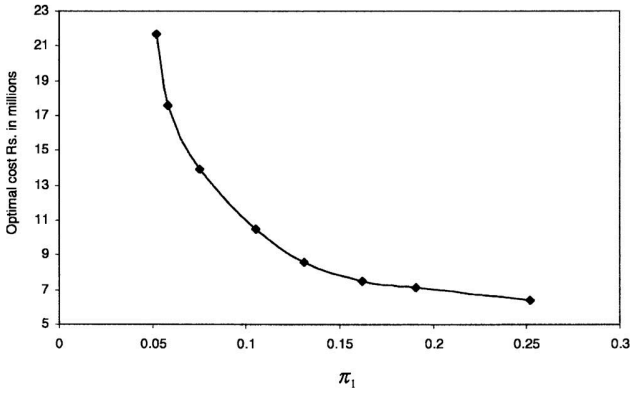

Fig. 6. Variation of optimal cost with π_1, Set A

drawn between the initial microbial concentration, M_0, and the minimum biobarrier length, L, for different inlet substrate concentrations, S_0, for different remediation periods. Figs. 4 and 5 show the minimum length of the barrier required for various substrate concentrations for 14.5 and 21 days of remediation periods, respectively.

From Figs. 4 and 5, it is clear that the minimum biobarrier length required depends on both substrate and initial bacterial concentrations. It is also observed that minimum barrier length required remains almost the same if the initial microbial concentration is above a particular level (100 mg/L for the conditions chosen here). Microbial concentration of 100 mg/L and substrate concentration of 1,000 mg/L combination can contain Cr(VI) concentration of 25 mg/L with a minimum barrier length of 15 cm. For further improvement of design procedure, optimization techniques can be used wherein the cost of the biobarrier is minimized, as discussed in the following section.

Table 2. Input Values for the Optimization Model

Serial No.	Variable	Set A	Set B	Set C
1	L_{min} (cm)	10	10	10
2	L_{max} (cm)	100	100	100
3	$M_{0\,min}$ (mg/L)	0	0	0
4	$M_{0\,max}$ (mg/L)	300	300	300
5	$S_{0\,min}$ (mg/L)	50	1,000	50
6	$S_{0\,max}$ (mg/L)	1,000	2,000	1,000
7	C_1 (Rupees)	200	200	200
8	C_2 (Rupees)	1,000	1,000	500
9	C_3 (Rupees)	14	14	14
10	T (days)	14.5	14.5	14.5

Optimal Design of a Biobarrier

The cost of construction of biobarriers and time taken for remediation depend upon the design variables. Hence, it is necessary to determine the optimal solutions of the decisions to be made for the proper design and management of a bioremediation system for given specific site conditions. As mentioned earlier, the main objective is to determine the decision variables in such a way that the cost involved in the implementation of these decisions is a minimum.

In the present problem, the one-dimensional simulation optimization model was run for different pore velocities, varying from 1 to 6 cm/h. The system parameters used in these optimization runs were the same as those presented in Table 1. In all these runs, $\Delta x=1$ cm and Courant number=0.65 were used. The biobarrier size was 10 km wide normal to the contaminant plume and 10 m deep. Other input values required for the optimization model, for different runs, are presented in Table 2. The obtained optimal decision for each case was cross checked with the simulator in order to determine whether the constraints were satisfied. Design charts were prepared based on these optimal solutions and are discussed in the following.

Optimal solutions obtained for Set A, for different groundwater velocities, are presented in Table 3, and in Figs. 6–9. In this set of runs, the Darcy velocity varied from 0.417 to 2.0 cm/h, which corresponds to a variation of 0.0525 to 0.252 in the π_1 value. It was observed that, as π_1 increased, the length of the biobarrier decreased, and consequently, the cost of the biobarrier decreased. A high value of π_1 implies that microbial activity and dispersion

Table 3. Optimal Solution for Different Groundwater Velocities for Set A

Darcy velocity (cm/h)	Pore velocity (cm/h)	π_1	L (cm)	M_0 (mg/L)	S_0 (mg/L)	Cost (Rupees)
2.0	5.71	0.0525	69.5	150.5	420.3	2.17E007
1.8	5.14	0.0584	48.5	208.5	500.8	1.76E007
1.4	4.0	0.075	39.5	215.2	450.5	1.39E007
1.0	2.86	0.1049	30.4	190.3	492.5	1.05E007
0.8	2.29	0.131	25.7	220.3	378.0	0.86E007
0.65	1.86	0.162	24.5	163.3	384.1	0.75E007
0.55	1.57	0.191	23.2	128.9	507.4	0.71E007
0.417	1.19	0.252	21.5	93.2	671.6	0.64E007

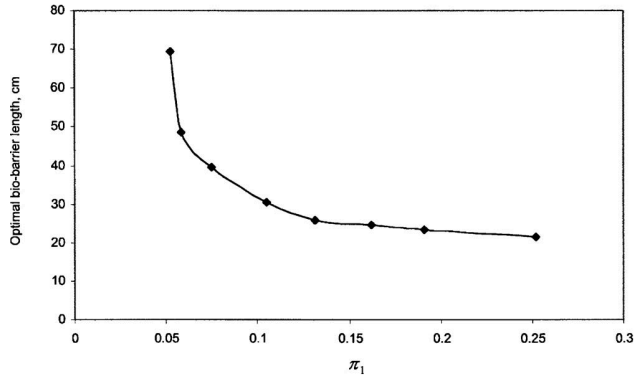

Fig. 7. Variation of optimal length with π_1, Set A

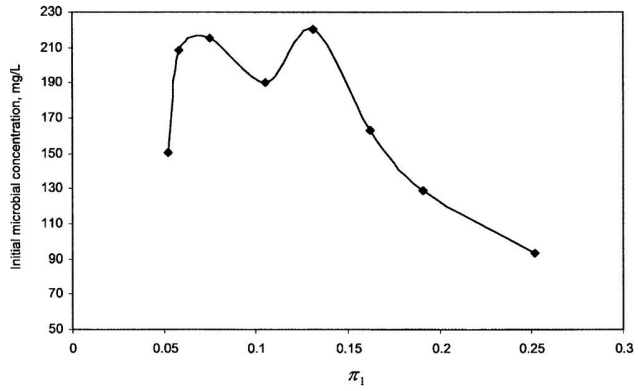

Fig. 8. Variation of optimal initial microbial concentration with π_1, Set A

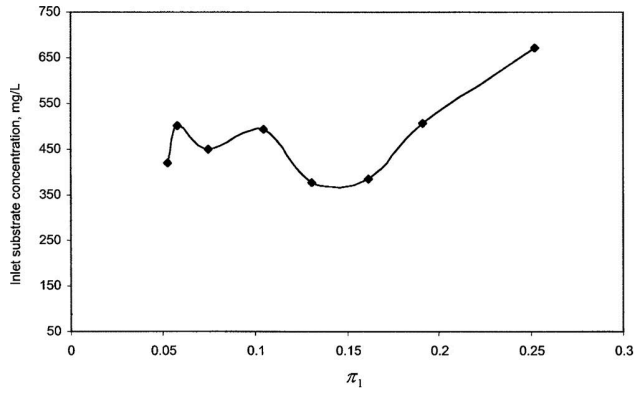

Fig. 9. Variation of optimal inlet substrate concentration with π_1, Set A

effects are more significant compared to the advection effect. Therefore, the residence time of the pollutant inside the barrier is higher. Moreover, because of high dispersion, the concentration of the pollutant coming in contact with the microbes at the plume front is lower compared to that in the case of high advection. This reduces the inhibition effect.

As the π_1 value increased, required initial biomass concentration also decreased in general. This was compensated for by a general increase in the inlet substrate concentration. Microbial concentration at any instant depends on both the initial microbial concentration and the specific growth rate. The specific growth rate can be increased by taking a higher substrate concentration. For lower values of π_1, there was a trade-off between the M_0 and S_0 values, and the actual values chosen depended upon the unit costs of M_0 and S_0.

Optimal solutions obtained for Set B, for different groundwater velocities, are presented in Table 4. The difference between Sets A and B was only in terms of range for the S_0 value. In Set B, higher substrate concentrations were considered. Results for the optimal cost and the optimal biobarrier length followed a similar trend as before. However, the optimal substrate concentration, S_0, was mostly taken near the lower end of the range. This might be due to the fact that the specific growth rate cannot be greater than μ_{max} value whatever the substrate concentration may be.

Optimal solutions obtained for Set C, for different groundwater velocities, are presented in Table 5. The difference between Sets A and C was only in terms of the unit cost for microbes. Unit cost for the microbes in Set C was only half of that in the case of Set A. These runs were made to demonstrate how the optimal solution depends on the relative costs of trenching, microbes, and the substrate. Results for the optimal cost and the optimal biobarrier length followed a similar trend as before. However, there was a trade-off between the initial microbial concentration, M_0, and the inlet substrate concentration, S_0. If there was an increase in the M_0 value with π_1, there was a corresponding decrease in the S_0 value, and vice versa. There was no definitive trend in the variations of M_0 and S_0 with π_1.

It should be noted that the results presented here indicate only a general trend in the optimal design parameters. Optimal solution depends on system characteristics, bounds on the decision variables, and unit costs. Nonlinearities are involved in the objective function as well as the constraints in the optimization problem. This underscores why the design parameters should be determined using formal optimization techniques. It should also be noted that the optimal design is limited by the limitations of the simulator. The simulator was developed based on a simple model for the microbial growth. The stationary phase was simulated by limiting the microbial concentration to a prefixed maximum value

Table 4. Optimal Solution for Different Groundwater Velocities for Set B

Darcy velocity (cm/h)	Pore velocity (cm/h)	π_1	L (cm)	M_0 (mg/L)	S_0 (mg/L)	Cost (Rupees)
2.0	5.714	0.0525	53.8	147.9	1,033.7	2.36E007
1.8	5.1429	0.0583	45.7	165.4	1,010.7	2.06E007
1.4	4.0	0.075	40.3	142.4	1,020.4	1.70E007
1.0	2.857	0.105	30.6	133.0	1,030.3	1.26E007
0.8	2.286	0.131	29.9	108.3	1,010.7	1.11E007
0.65	1.857	0.162	22.9	121.5	1,050.2	0.89E007
0.55	1.5714	0.191	22.9	98.8	1,244.8	0.87E007
0.417	1.1914	0.252	22.9	75.2	1,253.3	0.77E007

Table 5. Optimal Solution for Different Groundwater Velocities for Set C

Darcy velocity (cm/h)	Pore velocity (cm/h)	π_1	L (cm)	M_0 (mg/L)	S_0 (mg/L)	Cost (Rupees)
2.0	5.71	0.0525	67.7	151.6	440.6	1.96E007
1.8	5.14	0.0584	55.5	132.9	796.4	1.94E007
1.4	4.0	0.075	44.8	175.8	415.3	1.32E007
1.0	2.86	0.1049	33.6	196.9	349.5	0.96E007
0.8	2.29	0.131	30.6	131.2	508.2	0.88E007
0.65	1.86	0.162	21.9	193.9	413.7	0.64E007
0.55	1.57	0.191	20.3	205.4	360.3	0.58E007
0.417	1.19	0.252	20.1	130.8	414.1	0.53E007

(in this work, found from the writers' batch experiments). This may not truly represent the field scenario. Also, the simulator did not incorporate the change in hydrogeology due to bacterial growth and associated activities. The simulator used in this study is applicable for homogeneous and isotropic aquifers. This is far from the real situation, wherein the nonhomogeneities play a significant role in the plume migration. Therefore, the present simulation-optimization model should be used only for screening level designs. Sophisticated optimal design tools, particularly those using evolutionary techniques such as GA for finding optimal solution, would require the range over which the search for optimal solution should be made. This is required not only to cut down the computational cost, but also to determine the feasible solution space. The present screening level model will be very helpful for this purpose. Also, many times, particularly at planning stage, screening level solutions are sufficient. It may be noted that nonhomogeneities introduce local scale dispersion, which is equivalent to having a higher value of α_L in the present simple model. This increases the π_1 value. As a result, thinner biobarriers would be able to contain the contaminant plume.

Conclusions

In this study, a methodology has been proposed for the screening level design of trench-type biobarrier system for remediation of chromium-contaminated confined aquifers. The developed charts show the interrelationship between the length of the biobarrier (L), initial microbial concentration (M_0), and the substrate to be provided for the microbial growth (S), for a specific aquifer and microbial system. These charts can be developed for different remediation periods. These design charts will be useful in selecting the best combinations of initial microbial concentration in the biobarrier, length of biobarrier, and the substrate concentration for cost effectiveness, minimization of residual contamination in the aquifer, and the bioremediation time. An optimization model, using the simulation-optimization framework, has been developed for this purpose. Nondimensionalization of the governing equations showed that the optimal values of the length of the biobarrier, the initial microbial concentration, and the inlet substrate concentration depend on nondimensional parameter π_1, which indicates the relative significance of maximum specific growth rate and dispersivity with respect to pore velocity. The optimal length and the cost of the biobarrier reduce with an increase in π_1 value.

Notation

The following symbols are used in this paper:

A = cross-sectional area in m^2;
B = penalty factor;
C = hexavalent chromium concentration in the liquid medium (mg/L);
C_1 = cost of trenching per m^3 of soil;
C_2 = cost of microbes per kg;
C_3 = cost of substrate per kg;
D = coefficient of dispersion (cm^2/h);
K_i = inhibition concentration;
K_s = half saturation constant;
k_d = decay constant (1/h);
L = length of the biobarrier in m;
M = bacterial concentration expressed as mg/L of liquid in the column;
M_0 = initial microbial concentration in mg/L;
Q = flow rate in m^3/h;
R_c = retardation coefficient for hexavalent chromium;
R_s = retardation coefficient for substrate;
R_{sinkC} = sink term for hexavalent chromium due to biotransformation;
R_{sinkS} = sink term for substrate due to microbial utilization;
S = molasses concentration in the liquid medium (mg/L);
S_T = total inlet molasses concentration (mg/L);
S_u = utilizable concentration of molasses (mg/L);
S_0 = inlet molasses concentration in the liquid medium (mg/L);
T = time for which the substrate is applied for remediation in hours;
u = pore water velocity (cm/h);
Y = observed yield coefficient;
Z_1 = total cost of biobarrier;
α_L = dispersivity;
η = efficiency factor for chromium reduction with respect to substrate utilization;
λ = proportionality constant which takes care of the differences in the microbial growth in a suspended batch system and attached continuous system;
μ = specific growth rate (1/h);
μ_{max} = maximum specific growth rate (1/h);

π_1, π_2, π_3 = Nondimensional parameters that incorporate the relative effects of microbial growth and transport on pollutant containment; and

ϕ = porosity.

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