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TRANSPORT AND RETENTION OF MICROORGANISMS IN POROUS MEDIA: COMPARISON OF NUMERICAL TECHNIQUES AND PARAMETER ESTIMATION*

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ABSTRACT

Governing equations for the transport and retention of microorganisms in porous medium are reviewed and modified to describe various experimental conditions. Analytical solution and a numerical solution by Galerkin finite element method (GFEM) are available for a simplified case of transport of microorganisms in one dimensional flow through saturated porous medium. This article investigates a different numerical method, orthogonal collocation method (OCM), which is known to be more efficient and effective computationally, for solving the transport equations. The solutions obtained by these two numerical methods are compared with the analytical solution for the simplified case. The agreement between the numerical prediction by OCM and the analytical solution was observed to be better than that between the analytical solution and GFEM solution. The governing equations and the boundary conditions were further modified for unsaturated soil condition and solved by the OCM to verify the model using the experimental data available in the literature. As the values of the constants in the model for transport of microbes through porous media have never been established, a sensitivity analysis was performed to find the coefficients for effective dispersion, clogging and declogging of microbes in soil medium.

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INTRODUCTION

The transport of bacteria in porous media has long been a subject of great importance in many areas of study, particularly ground water pollution. The use of soils for applying waste materials has also resulted in a growing concern for the potential movement of microorganisms through soil layers, as the pathogenic bacteria present in the waste materials may contaminate ground water. Septic tanks, cesspools, and the direct injection and percolation of domestic waste water from land application for ground water recharge, crop irrigation and leachate from sanitary and hazardous landfills are some of the sources for ground water contamination. These wastes contain bacteria, viruses and protozoa which are pathogenic to human beings resulting in the potential to cause large outbreaks of water borne diseases due to contamination of ground water.

The recent trend in treating the landfill sites and contaminated soils has been to use the naturally occurring or commercially available microorganisms to degrade the hazardous chemical compounds. This process is known as in-situ biodegradation or in-situ bioremediation. The in-situ bioremediation is achieved by using indigenous populations or by introducing adapted microorganisms acclimatized in the laboratory into the subsurface with necessary nutrients. In either case the retention and movement of these microorganisms in the subsurface has to be studied to quantify the effectiveness of this process.

The fate of microorganisms in the subsurface is determined by their survival and retention by soil particles. The survival and transport of these microorganisms depend on many factors, including soil type, moisture, pH, sunlight, temperature, organic matter, type of microorganisms, and their interaction with other microorganisms [1]. A number of research studies have reported experimental results on transport and fate of bacteria in porous media without any mathematical model development [2-4]. On the other hand, Corapcioglu and Haridas [5, 6] formulated a mathematical model for the transport of microorganisms in porous media and developed a numerical solution for the same. This model was not verified using suitable experimental data and, therefore, the validity of the model remains to be established. A recent research work predicted the position of the retarded bacterial concentration fronts using an analytical model and verified the same with experimental data [7]. Fortunately, because of the availability of this data, it is now possible to calibrate and verify mathematical models for transport of microorganisms through porous media.

The purpose of this article is to:

1. Review and propose a general model for transport of microorganisms through porous media;
2. Establish an appropriate numerical solution technique for the proposed model;
3. Verify the model by making necessary modifications of the model to suit the available experimental data; and

4. Obtain representative values for dispersion coefficients, clogging and declogging coefficients for microorganisms necessary for the solution of the transport equations.

THEORY

The governing equations for the transport and retention of microorganisms can be obtained from the macroscopic conservation of mass for microbial particles in porous media.

The capture of microbial particles from water passing through soil is the result of simultaneous action of shearing and viscous forces along with other forces that act between the particles and the collector [8]. The removal mechanisms for bacteria in the porous media can be conceptualized as similar in nature to those observed for the filtration mechanisms. A review of the filtration theory [9-11] suggests that the rate of deposition of bacteria can be expressed by a kinetic equation:

$$R_a = k_c (\theta C) - k_d (\rho \sigma^h), \tag{1}$$

where,

R_a = rate of deposition of microbial particles per unit volume of soil (M/L^3T),
k_c = clogging rate constant takes into account screening and adsorption phenomena (1/T),
θ = effective porosity, i.e., volume occupied by the flowing suspension per unit of the total volume (L^3/L^3),
C = concentration of suspended microbial particles per unit volume of flowing suspension (M/L^3),
k_d = declogging rate constant (1/T),
ρ = density of the microbial particles (M/L^3),
σ = volume of deposited bacteria per unit volume of bulk soil (L^3/L^3), and
h = constant which has to be found experimentally ($h = 1$ was proposed by Mints [12], and is used here).

The first term on the right hand side of the equation is the accumulation or clogging of bacteria and is considered to be primarily due to adsorption, straining, sedimentation, and interception. Other mechanisms which may influence the removal of microbes in the porous media are explained later. The second term is the detachment or declogging which is due to the breaking of bacterial clusters. It is apparent from this equation that the rate of clogging is a function of the concentration of the bacterial suspension and effective porosity of the bed, whereas the declogging rate is a function of deposited bacterial volume. The kinetic equation assumes that these two processes are simultaneous, which may not be true in the early stage of the process.

A significant volume of research has been done on adsorption of viruses to soil surfaces, but there are only a few studies on the adsorption of bacteria. The adsorption of bacteria like viruses was found to follow a Freundlich isotherm when straining is absent (e.g., sands) and the constants are different for different types of sands [7]. But the validity of this expression for cases where straining is present (e.g., clays), is not known. In the case of soils containing clay, adsorption could be an important removal mechanism [13].

A particle will be strained if the particle size is larger than the pore opening. Straining results in the accumulation of particles on the soil grains thereby decreasing the pore space and hence, increasing the straining effect. The deposited bacterial volume can be estimated based on purely geometric considerations. Herzig demonstrated that for bacteria the effect of straining is considerable and needs to be included in the formulation [14]. Microbial removal by straining may not play a significant role if the mean diameter of microbes is much less than the mean diameter of the soil grains. The effect of straining may not be significant for sand medium because of the larger pores [7].

The removal of suspended particles by interception is due to the inability of particles to follow the tortuous streamlines of the fluid even though they may have the same density as the fluid. However, because of their very small size it is not an important mechanism for microbes.

The net rate of change of deposited microbial mass should also include the growth and death of microorganisms. If R_{dd} and R_{gd} are decay and growth terms of the deposited microbes, respectively, then the equation for deposited particles can be written as

$$\frac{\partial (\rho \sigma)}{\partial t} = R_a - R_{dd} + R_{gd} \tag{2}$$

Substituting for R_a from Equation (1) in Equation (2), we will get the first governing equation for the transport process:

$$\frac{\partial (\rho \sigma)}{\partial t} = k_c (\theta C) - k_d (\rho \sigma) - R_{dd} + R_{gd} . \tag{3}$$

A mass balance for suspended microbial population is the control volume at the macroscopic level can be written as:

$$\frac{\partial (\theta C)}{\partial t} = -\nabla \cdot J - R_a - R_{ds} + R_{gs} , \tag{4}$$

where,

R_{ds} = rate of decay of suspended microbial particles (M/L^3T);
R_{gs} = rate of growth of suspended microbial particles (M/L^3T); and
J = specific mass discharge of flowing suspension (M/L^2T).

The specific mass discharge (J) is composed of advection and mechanical dispersion, Brownian diffusion, chemotaxis and tumbling and movement due to sedimentation. The detailed explanation of these mechanisms is given elsewhere [5]. Hence,

$$J = J_A + J_B + J_{CT} + J_{vg}, \tag{5}$$

where,

J_A = flux due to advection and mechanical dispersion (M/L^2T);
J_B = flux due to Brownian diffusion (M/L^2T);
J_{CT} = flux due to chemotaxis and tumbling (M/L^2T); and
J_{vg} = flux due to sedimentation (M/L^2T).

Advection and mechanical dispersion flux is the component of movement attributed to transport by the flowing suspension. The flux term J_A would contain

$$J_A = -D_a \theta \nabla C + v_f(\theta C), \tag{6}$$

where,

D_a = coefficient of mechanical dispersion (L^2/T); and
v_f = superficial longitudinal velocity of flow (L/T).

Because of their small size, bacteria rely partially on Brownian diffusion for their movement. Even though the path of the individual particles appears to be quite erratic, the average particle flux is proportional to the concentration gradient. The flux due to Brownian motion is given by [5]:

$$J_B = -D_B \theta \nabla C, \tag{7}$$

where, D_B is diffusion coefficient of bacteria (L^2T). D_B can be estimated by the Stokes-Einstein equation:

$$D_B = k_b T / 3\pi\mu_w d, \tag{8}$$

where,

k_b = Boltzmann constant (energy per degree, ML^2/T^2);
T = absolute temperature (°K);
μ_w = viscosity of the flowing fluid (M/LT); and
d = diameter of the suspended particle (L).

Chemotaxis or systematic movement of bacteria is the directed movement of bacteria toward higher concentrations of substrate. The chemotactic phenomena is a function of the substrate concentration gradient. Flux due to chemotaxis (J_C) can be expressed as:

$$J_C = \theta(v_m C), \tag{9}$$

where, v_m = the migration velocity (L/T).

The migration velocity is a function of relative concentration gradient and it can be formulated as a log function of the concentration gradient [15]:

$$v_m = k_m \nabla \ln C_F = \frac{k_m}{C_F} \nabla C_F , \tag{10}$$

where,

k_m = migration rate constant or chemotactic coefficient (1/T); and
C_F = substrate concentration in the porous space (M/L^3).

However, the chemotactic motion of bacteria is frequently accompanied by another phenomenon known as tumbling which is due to chaotic motion of bacteria. The flux due to tumbling can be formulated in the same manner as is done for Brownian diffusion. However, the diffusion coefficient D_T in this case is known as motility coefficient or effective diffusivity and is always positive and the flux due to tumbling can be superimposed on the systematic movement, therefore the flux due to chemotaxis and tumbling is given by:

$$J_{CT} = \theta (v_m C - D_T \nabla C) . \tag{11}$$

Sedimentation occurs if the density of the suspended particles is greater than that of the fluid. Since the bacteria and viruses have densities very close to that of water, they do not tend to settle. But for some bacteria, sedimentation could be a removal mechanism [13]. Settling velocity (v_g) can be used to quantify the significance of sedimentation and it is expressed as [11].

$$v_g = \left(1 - \frac{\rho_w}{\rho}\right) \frac{m_d g}{3\pi \mu_w d} , \tag{12}$$

where,

ρ = density of microbial particles (M/L^3);
d = diameter of microbial particles (L);
g = gravitational acceleration (L/T^2);
m_d = mass of microbial particle (M);
ρ_w = density of water (M/L^3); and
μ_w = viscosity of water (M/LT).

Therefore, flux due to settling can be expressed as:

$$J_{vg} = \theta v_g C . \tag{13}$$

Substituting for all the flux components from Equations (6-7) and Equations (11-13) in Equation (5), J will become:

$$J = -\theta D \nabla C + \theta C(v_f + v_g + v_m), \tag{14}$$

where D, the coefficient of hydrodynamic dispersion (L^2/T), is the sum of the Brownian diffusion coefficient, coefficient of mechanical dispersion and effective diffusivity coefficient due to tumbling of bacteria, i.e., $D = D_a + D_B + D_T$.

A mass balance for the microorganisms both in the deposited and suspended forms results in the second governing equation. This can be formulated by combining Equations (3) and (4).

$$\frac{\partial(\theta C)}{\partial t} + \frac{\partial(\rho\sigma)}{\partial t} = -\nabla \cdot J - R_a - R_{ds} + R_{gs} + R_a - R_{dd} + R_{gd}. \tag{15}$$

Substituting for J, from Equation (14), and canceling R_a, the modified form of the second governing equation is:

$$\frac{\partial(\rho\sigma)}{\partial t} + \frac{\partial(\theta C)}{\partial t} = -\nabla \cdot \left[-\theta D \nabla C + \theta C (v_f + v_g + v_m) \right] + R_{gs} + R_{gd} - R_{ds} - R_{dd}. \tag{16}$$

The decay and growth of bacteria may play significant roles in case of long retention times for microbes in the porous media. Gerba reviewed the factors that affect the survival of enteric bacteria [13]. The decay of microorganisms is considered as a first order irreversible reaction. Assuming the decay rate to be the same in both the adsorbed and free states, the decay term becomes:

$$R_d = R_{dd} + R_{ds} = b(\theta C + \rho\sigma), \tag{17}$$

where,

R_d = decay of particles in both the phases (M/L^3T); and
b = the specific decay rate (1/T).

The specific decay rate (b) is typically a constant value for a particular type of bacteria and environment. Matthess and Pekdeger assumed that the decay in the adsorbed state is negligible [16].

The growth of bacteria can be assumed to follow Monod's equation, which describes the relationship between the concentration of a limiting substrate and the growth rate of microbes. The specific growth rate, μ (1/T), is given by:

$$\mu = \frac{\mu_{max} C_F}{K_s + C_F}, \tag{18}$$

where,

μ_{max} = maximum specific growth rate (1/T);
K_S = half saturation constant (M/L^3); and
C_F = concentration of substrate (M/L^3).

For real world situations where most of the organic matter is attached to the soil grains, the growth rate of microorganisms in the adsorbed phase may be different from that of the free phase. However, for most laboratory experiments where there is little or no organic matter available for the growth of microorganisms, the specific growth rate is likely to be very small. In such cases, the specific growth rate of both phases can be assumed to be the same. With that assumption, the growth rate of microbial mass in the control volume is given by:

$$R_g = R_{gd} + R_{gs} = \mu\,(\theta\, C + \rho\, \sigma)\,, \tag{19}$$

where R_g is the growth of microbial particles in both the phases (M/L^3T).

Substituting the decay and growth terms of Equations (18) and (19) into Equation (17), the final form of the second governing equation will become:

$$\frac{\partial\,(\rho\,\sigma)}{\partial t} + \frac{\partial\,(\theta\, C)}{\partial t} = -\nabla \cdot \left[-\theta D \nabla\, C + \theta C(v_f + v_g + v_m)\right] + \left[\theta\, C + \rho\, \sigma\right](\mu - b)\,. \tag{20}$$

The third governing equation is obtained from the mass conservation equation for the organic matter which acts as substrate for the microorganisms in the control volume, by following the similar procedure:

$$\frac{\partial\,(\rho_s\, S_F)}{\partial t} + \frac{\partial\,(\theta\, C_F)}{\partial t} = -\nabla \cdot \left[-D_e\, \theta\, \nabla C_F + \theta v_f C_F\right] - \frac{\mu}{Y}\,(\theta\, C + \rho\, \sigma)\,, \tag{21}$$

where,

ρ_s = bulk mass density of dry soil (M/L^3);
S_F = mass of adsorbed substrate per unit mass of soil particles;
C_F = the mass of substrate per unit volume (M/L^3);
$D_e = D_{dl} + D_m$, effective diffusivity coefficient (L^2/T);
D_{dl} = coefficient of mechanical dispersion of substrate (L^2/T);
D_m = coefficient of molecular diffusion (L^2/T); and
Y = true yield coefficient.

Equations (3), (20), and (21) are the governing equations for the bacterial transport in porous medium. These three equations are to be solved to describe bacterial transport in a porous medium.

Selection of Numerical Methods

As can be seen, the governing equations are complex with a high degree of non-linearity and coupling. It is very difficult to obtain a closed form solution for the unknowns even for a one-dimensional space. Numerical techniques are needed for a solution of these equations. The above governing equations can be modified to accommodate different experimental conditions. Because of the paucity of

experimental data, numerical solution techniques were performed on a simplified one-dimensional transport equation. In case of saturated soils, the volumetric water content θ is equal to the effective porosity, $(n - \sigma)$, and the velocity of flow will be a constant. If the flow is considered to be one-dimensional, then the divergence term in those above equations will become partial derivative with respect to the direction of flow. To analyze experimental conditions with no substrate present for the biological growth, the third equation need not be considered. Furthermore, in the absence of substrate, chemotactic phenomena is absent. By incorporating all these facts and setting $C^* = \theta C$, $\sigma^* = \rho\sigma$, $k = \mu - b$, in the governing Equations (3) and (20) and rearranging

$$\frac{\partial \sigma^*}{\partial t} = k_c C^* - k_d \sigma^* + k \sigma^* \tag{22}$$

$$\frac{\partial C^*}{\partial t} = D\frac{\partial^2 C^*}{\partial X^2} - \mu \frac{\partial C^*}{\partial X} - k_c C^* + k_d \sigma^* + kC^* \tag{23}$$

where $u = v_f + v_m + V_g$, sum of the velocities of flow, migration, and sedimentation. However, v_m is zero for this particular case.

The boundary and initial conditions for this problem are:

$C^* = C^*_0$ at $X = 0$;
$C^* = 0$ at $X = \infty$;
$C^* = 0$ at $t = 0$; and
$\sigma^* = 0$ at $t = 0$.

These equations are the same as those presented by Corapcioglu and Haridas for similar conditions [6]. They obtained the analytical solution and also solved these equations numerically using Galerkin finite element method (GFEM). In this article another well-known numerical technique, orthogonal collocation method (OCM), is used for solving the governing equations. OCM is a combination of the collocation method and finite difference method [17]. It uses the orthogonal polynomial expansions. The trial function is assumed as a series of orthogonal polynomials $F_N(x)$ defined as:

$$F_N(X) = \sum_{j=1}^{N} C_j X^j . \tag{24}$$

The coefficients (C_j) in Equation (24) are defined by requiring that F_1 be orthogonal to F_0, F_2 be orthogonal to both F_1 and F_0, and F_N be orthogonal to each F_k, where $k \leq (N-1)$. The orthogonal condition can include a weighing function $w(X) \geq 0$. Thus,

$$\int_a^b w(X)F_k(X)F_N(X)dX = 0, \quad k = 0, 1, 2, \ldots, N-1, \tag{25}$$

where a and b are the limits of integration. The polynomials satisfying Equation (25) with w = 1 are called shifted Legendre polynomials, and the roots for these polynomials are readily available in tabular form [17].

The collocation points are taken as the N roots to $F_N(X) = 0$, where the roots are between zero and one. The collocation points are then $X_1 = 0.0$, $X_{N+2} = 1.0$, and $X_2, \ldots, X_{N+1}$ are the interior roots. The solution for the trial function at the collocation points $C^*(X_j)$, can be written as:

$$C*(X_j) = \sum_{i=1}^{N+2} d_i X^{i-1}. \tag{26}$$

The first and second derivatives at the N + 2 collocation points are:

$$\frac{dC*(X_j)}{dX} = \sum_{i=1}^{N+2} d_i(i-1)X_j^{i-2} \tag{27}$$

$$\frac{d^2C*(X_j)}{dx^2} = \sum_{i=1}^{N+2} d_i(i-1)(i-2)x_j^{i-3}. \tag{28}$$

These equations can be written in matrix notation:

$$\begin{aligned} C* &= Qd, \\ \frac{dC*}{dX} &= Ed, \text{ and} \\ \frac{d^2C*}{dX^2} &= Dd, \end{aligned} \tag{29}$$

where Q, E, and D are (N + 2)*(N + 2) matrices.

The first and second derivatives can be obtained by eliminating d from Equation (29):

$$\frac{dC*}{dX} = EQ^{-1}C* = AC* \tag{30}$$

$$\frac{d^2C*}{dX^2} = DQ^{-1}C* = BC*. \tag{31}$$

When orthogonal collocation method is applied to solve Equations (22) and (23), the spatial derivatives are replaced by the following matrices:

$$\frac{\partial C^*}{\partial X} x_i = \sum_{j=1}^{N+2} A_{ij} C^*_j, \quad \frac{\partial_2 C^*}{\partial X^2} x_i = \sum_{j=1}^{N+2} B_{ij} C^*_j . \tag{32}$$

Then, by substituting these, Equations (22) and (23) become:

$$\frac{d\,\sigma^*_i}{dt} = k_c C^*_i + (k - k_d)\sigma^*_i \tag{33}$$

$$\frac{dC^*_i}{dt} = D\sum_{j=1}^{N+2} B_{ij} C^*_j - u \sum_{j=1}^{N+2} A_{ij} C^*_j + (k - k_c)\, C^*_i = k_d \sigma^*_i . \tag{34}$$

Runge-Kutta method was employed to integrate the above equations numerically. However, it should be noted that the above equations can also be converted to linear algebraic equations by using the Laplace transform. The solution of the orthogonal collocation method is plotted in Figure 1, with relative concentration of bacteria in suspension on the Y axis and distance along the X axis. The analytical solution and the Galerkin finite element method solution obtained by Corapcioglu and Haridas are also plotted on the same figure for comparison [6].

To compare the solutions of orthogonal collocation method and Galerkin finite element method with the analytical solution, the values of the constants and parameters used were the same as those reported by Corapcioglu and Haridas [6]

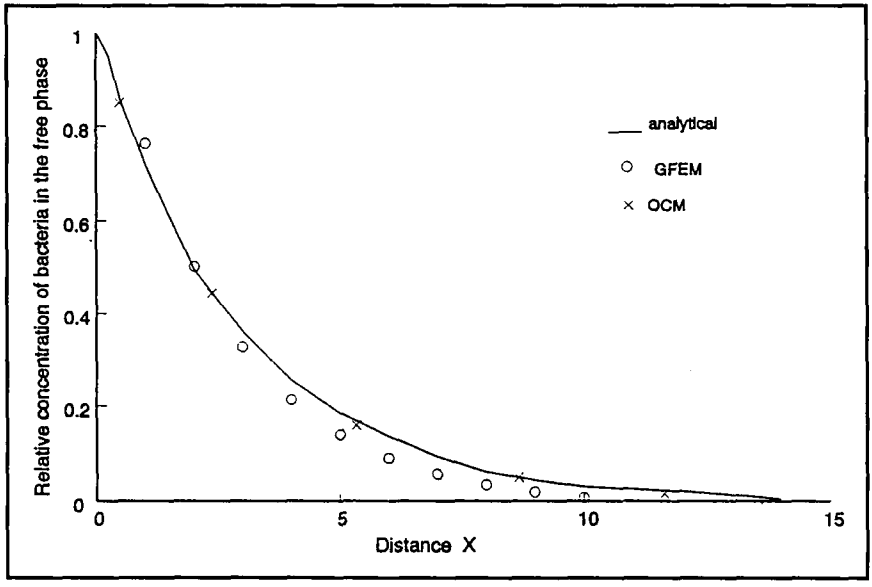

Figure 1. Comparison of the solutions of OCM and GFEM with the analytical solution.

Table 1. Values of the Parameters Used in the Literature [6]

Parameter	Value Used in the Literature
Dispersion coefficient (D)	0.04 cm^2/sec
Clogging rate constant (k_c)	6.5×10^{-3}/sec
Declogging rate constant (k_d)	4.35×10^{-4}/sec
Velocity (μ)	3.0×10^{-2} cm/sec

and are presented in Table 1. The other constants used are specific decay coefficient 10^{-3}/sec, maximum specific growth 4.2×10^{-5}/sec and Monod half saturation constant 2×10^{-3}mg/l and yield coefficient 0.04. As can be seen from this plot, the solution of the orthogonal collocation method (N = 6) fits the analytical solution better than that of the Galerkin finite element method. Moreover, the OCM has the following advantages over the GFEM. It uses one high degree polynomial over the entire domain where as for GFEM linear polynomials are used on each element [18] and the higher order methods converge rapidly and give more accuracy than lower order method. If the solution is symmetric, this fact can be incorporated in the trial functions and computations can be reduced by half in the OCM. Moreover, for one-dimensional partial differential equations it is easy and convenient to use OCM rather than GFEM and also, by increasing the number of collocation points, the error can be decreased appreciably. Hence, the orthogonal collocation method is recommended for solving bacterial transport equations through porous media.

Bacterial Transport through Unsaturated Porous Media

Experimental data for one of the special cases of an unsaturated soil water flow problem have been reported in the literature [7]. The governing equations for the experimental data are obtained by modifying Equations (3), (20), and (21) to reflect the following experimental conditions:

1. The flow is unsaturated and one-dimensional;
2. No substrate is present;
3. Effects of straining and sedimentation are negligible for the medium used; and
4. The growth and decay of bacteria are neglected during the short time periods of the experiment.

Therefore, the first governing equation (Equation (3)), becomes:

$$\frac{\partial(\rho\,\sigma)}{\partial t} = k_c \theta C - k_d\,\rho\,\sigma\,. \tag{35}$$

Table 2. Variation of Volumetric Water Content with Similarity Variable (λ)

Similarity Variable	Volumetric Water Content	Similarity Variable	Volumetric Water Content
0.0	0.370	4.5	0.242
0.5	0.340	5.0	0.233
1.0	0.311	5.5	0.228
1.5	0.292	6.0	0.218
2.0	0.278	6.5	0.208
2.5	0.265	7.0	0.190
3.0	0.255	7.5	0.120
3.5	0.250	8.0	0.015
4.0	0.246	10.0	0.000

In the absence of organic matter, chemotaxis is absent ($v_m = 0$). The effect of sedimentation is neglected because of the low settling velocity of microorganisms. Then, the second governing equation becomes:

$$\frac{\partial(\rho\,\sigma)}{\partial t} + \frac{\partial(\theta\,C)}{\partial t} = -\,\nabla\cdot\left[-\theta\,D\nabla C + \theta\,C(v_f)\right] + \left[\theta\,C + \rho\,\sigma\right](\mu - b)\,. \tag{36}$$

Considering the flow as one-dimensional, the divergence will become the partial derivative with respect to the direction of flow, so the above equation reduces to:

$$\frac{\partial(\theta C)}{\partial t} = \frac{\partial}{\partial X}\left[\partial D\,\frac{\partial C}{\partial X}\right] - \frac{\partial v_f\,\theta C}{\partial X} - k_c\theta C + k_d\,\rho\,\sigma\,. \tag{37}$$

As there is no substrate available, the third governing equation need not be considered. Since there are two equations (Equations (35) and (37)) and three unknowns (σ, θ, and C), we need additional information about the soil water content. The variation of θ for this experiment is available [7]. Table 2 shows the variation of volumetric water content with Boltzmann's similarity variable λ which is defined as $X/\sqrt{t}$ for a diffusion type equation [19]. The similarity variable (λ) is used to eliminate the X and t from the one-dimensional transport equation.

The above governing equations (35) and (37) can be reduced to ordinary differential equations by taking N collocation points along the direction of flow. The reduced equations are:

$$\frac{d(\rho\,\sigma_j)}{dt} = k_c\,\theta_j\,C_j - k_d\,\rho\,\sigma_j \tag{38}$$

$$\frac{d(\theta C)}{dt} = \sum_{i=1}^{N+2} A_{ji} D(\theta_i C_i) \sum_{i=1}^{N+2} A_{i1}\, \theta_1 C_1 - v_f \sum_{i=1}^{N+2} A_{ji}\, \theta_i C_i - k_c\, \theta_j C_j + k_d\, \rho\, \sigma_j . \tag{39}$$

Initial and boundary conditions are:

1. When $t = 0$, $X > 0$, $C_i = 0$, $\sigma_i = 0$, $\theta_i = 0$;
2. When $X = \infty$, $C = 0$, $\sigma = 0$, $\theta = 0$; and
3. When $X = 0$, $C_1 = C \mid_{x=0} = C_0 = 1.0$ (relative concentration is used), and $\theta \mid_{x=0} = \theta_0 = 0.37$.

When $j = 1$ ($X = 0$), Equation (38) reduces to:

$$\frac{d(\rho\, \sigma_1)}{dt} = 0.37 k_c - k_d \rho\, \sigma_1 . \tag{40}$$

Now, taking the Laplace transform on both sides of Equation (40):

$$S\, \rho\, \sigma_1(s) = 0.37 \frac{k_c}{S} - k_d\, \rho\, \sigma_1\, (s) \rightarrow \rho\, \sigma_1\, (s)\, (S + k_d) = 0.37\, \frac{k_c}{S} . \tag{41}$$

The solution is obtained by taking the inverse Laplace transform:

$$\rho\, \sigma_1(t) = 0.37\, \frac{k_c}{k_d} (1 - e^{k_d t}) . \tag{42}$$

Equation (42) is a boundary condition for σ at $X = 0$ and is a function of time. Equations (38) and (39) are non-linear ordinary differential equations. There are several techniques to solve these equations. The Runge-Kutta method is adopted here.

Equations (38) and (39) cover three sets of variables (θ_i, σ_i, C_i). One can set $C^* = \theta\, C$ and $\sigma^* = \rho\, \sigma$, then Equations (38) and (39) reduces to

$$\frac{d\, \sigma^*_j}{dt} = k_c C^*_j - k_d\, \sigma^*_j \tag{43}$$

$$\frac{dC^*_{30j}}{dt} = \sum_{i=1}^{N+2} A_{ji}\, DC^*_i \sum_{1=i}^{N+2} A_{i1}\, C^*_1 - v_f \sum_{i=1}^{N+2} A_{ji}\, C^*_i - k_c C^*_j + k_d\, \sigma^*_j . \tag{44}$$

Equations (43) and (44) can be solved simultaneously for C^*_j and σ^*_j. Knowing the values of θ_j from Table 2, $C_j = C^*_j/\theta_j$ and $\sigma_j = \sigma^*_j/\rho$ can be calculated. The total concentration of bacteria (C_t) can be obtained by summing C_j and σ_j .

Parameter Estimation and Model Verification

The above equations can be solved, if the values of the parameters D, k_c, and k_d are known. These parameters for the transport of microorganisms are not available

in the literature. For the numerical solution of the governing equations, Corapcioglu and Haridas [6] used the values of the parameters from studies on the leachate movement and filtration [20-22]. It should be noted that the leachate movement and filtration is somewhat different from that of transport of organisms through porous media.

Our approach in this research is to establish the values of the parameters D, the dispersion coefficient, k_c, the clogging coefficient and k_d, the declogging coefficient, which would fit the experimental data available in the literature [7]. For this experiment, the flow is unsaturated and velocity of flow through the column is not stated. However, one can use the known range of values for the hydraulic conductivity of sand (10^{-4} to 10^{-1} cm/sec) [23], which is the medium used for the experiment and the reported experimental head of water (12 mm), to calculate the range of values for flow velocity by Darcy's Law. A sensitivity analysis was performed to obtain the best value of flow velocity, which minimizes sum of squared residual between the model prediction and the experimental values. The model predictions and the experimental data are presented in Figure 2. It should be noted that the total concentration of bacteria (bacteria in both the adsorbed and free phases) is plotted as a function of a parameter defined earlier as the similarity variable (λ). The initial trial values of the parameters D, k_c, and k_d are presented in Table 1. The other parameters used for the sensitivity analysis are density of bacteria (1 gm/cc) and the porosity of bed (0.37). It is apparent from Figure 2 that the solution is not sensitive to flow velocity for the range of velocities used. A

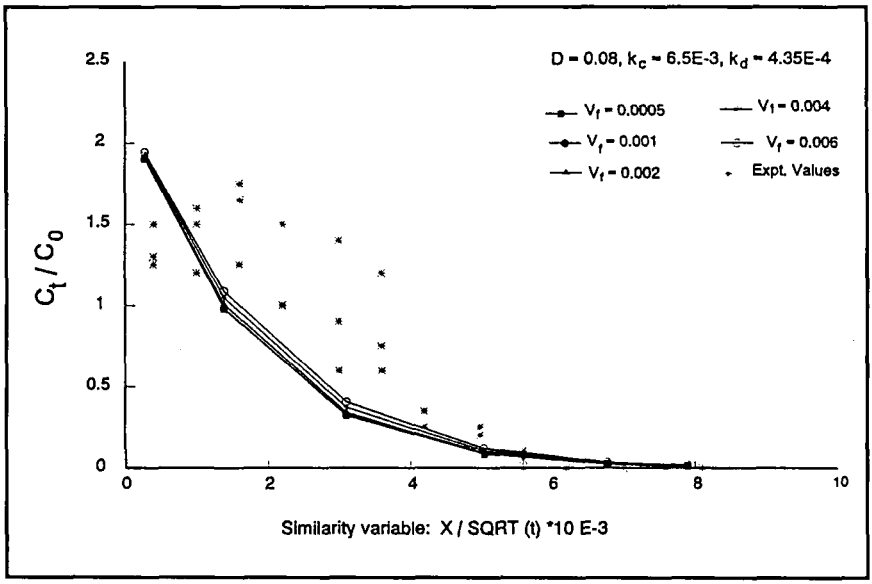

Figure 2. Effect of varying the flow velocity on the model prediction.

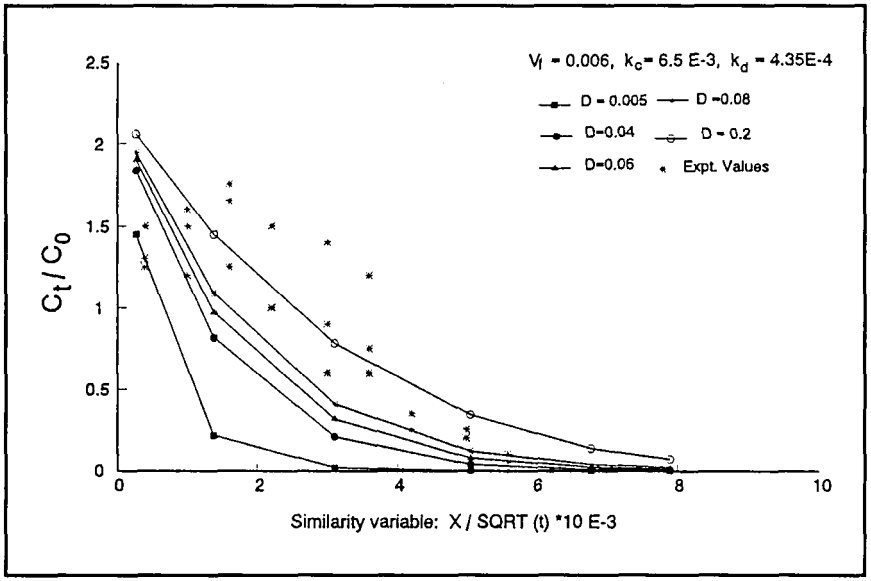

Figure 3. Effect of varying the dispersion coefficient on the model prediction.

velocity of 6.0×10^{-3} cm/sec produced the minimum sum of the squared residual and hence is used here.

Dispersion coefficient, D, clogging coefficient, k_c, and declogging coefficient k_d are the three important parameters for the prediction of the microbial transport in porous media. The effect of variation of these parameters on the model prediction was analyzed by the sensitivity analysis in a manner similar to the one described above for the velocity. The effect of the variation of D on the model prediction (Figure 3) suggests that the solution is sensitive to D for the range of values used. The values of D, less than the order of 10^{-2} are under predicting and the values more than the order of 10^{-1} are over predicting the relative concentration of bacteria for all λ values. Hence, the value of D is likely to be of the order of 10^{-2}. The least square analysis confirmed this, a D value of 8.0×10^{-2} produced the minimum sum of the squared residual and is used for further computations. It should be noted that the value of D obtained in this study is approximately twice the D value used by Corapcioglu and Haridas [6]. Figure 4 shows the effect of the variation of k_c, the clogging coefficient on the model prediction. As can be seen from this figure, the model solution is sensitive to clogging coefficient. For all k_c values, the trend of prediction changes direction at a n value of 1.6×10^{-3}. The iterative search method employed to estimate the clogging coefficient yielded a k_c value of 3.9×10^{-3}/sec. This value is about two-thirds of that used by Corapcioglu and Haridas [6]. Sensitivity analysis on the model prediction performed by varying the declogging coefficient is shown in Figure 5. It appears that the model

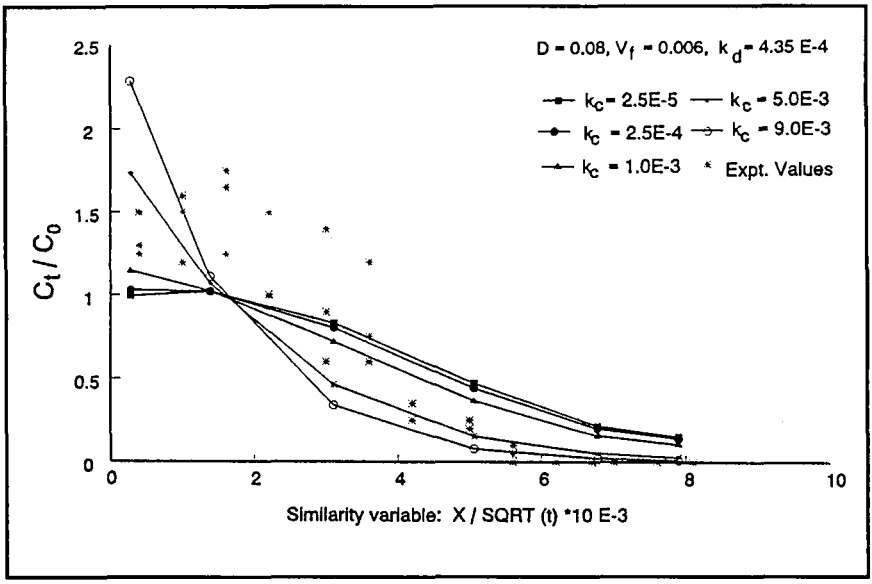

Figure 4. Effect of varying the clogging coefficient on the model prediction.

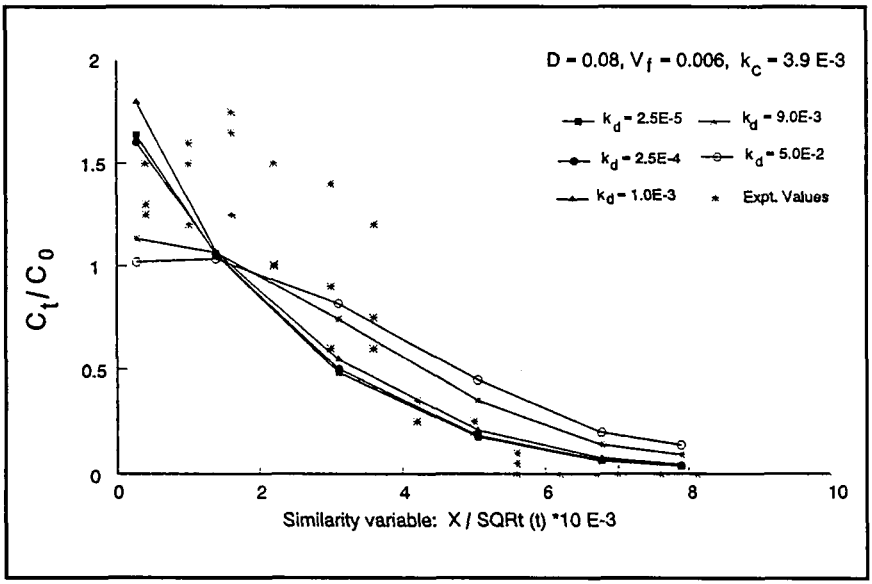

Figure 5. Effect of varying the declogging coefficient on the model prediction.

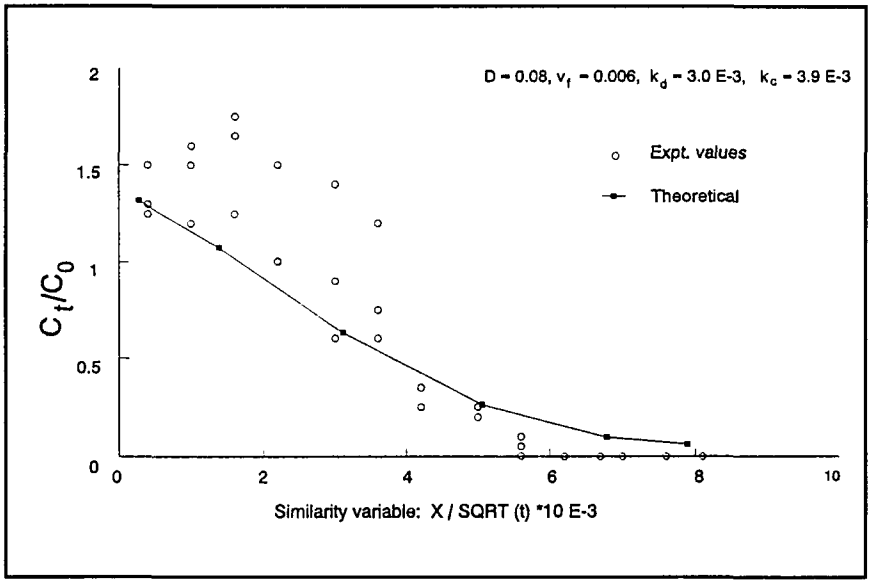

Figure 6. The predicted values of the relative concentration of bacteria along with the experimental values.

Table 3. Values of the Parameters Obtained in This Study

Parameter	Value Obtained in This Study
Dispersion coefficient (D)	0.08 cm^2/sec
Clogging rate constant (k_c)	3.9×10^{-3}/sec
Declogging rate constant (k_d)	3.0×10^{-3}/sec
Velocity (u)	6.0×10^{-3} cm/sec

solution is sensitive to declogging coefficient and for all k_d values the trend of prediction changes direction at a 1 value of 1.4×10^{-3}. Once again the search method of minimizing the sum of squared residuals resulted in a k_d value of 3.0×10^{-3}/sec. The k_d value of this study is almost seven times of that used by Corapcioglu and Haridas [6]. The values of the parameters obtained in this study are summarized in Table 3.

Using the parameters from Table 3, the model is solved for C^* and σ^* by the orthogonal collocation method together with the Runge-Kutta method. The results of the numerical solution using the parameters obtained in this study and the experimental data from Tan et al. [7] are presented in Figure 6. The plot shows that

the model under predicts the relative concentration of bacteria when $\lambda < 3.6 \times 10^{-3}$ and over predicts the relative concentration of bacteria when $\lambda > 3.6 \times 10^{-3}$.

CONCLUSIONS

The general governing equations for the transport of microorganisms in porous media are reviewed and modified to describe various experimental conditions. Two different numerical techniques were compared for effectiveness in solving the governing equations. Based on the results of this study, the following conclusions can be drawn:

1. The orthogonal collocation method is found to fit the analytical solution better than the Galerkin finite element method.
2. Fewer steps, simplicity for one-dimensional problems, and accuracy are the advantages of the orthogonal collocation method when compared with the Galerkin finite element method, particularly for experiments which extend over long time periods.
3. The model under-predicts the relative concentration of bacteria when $\lambda < 3.6 \times 10^{-3}$ and over-predicts the relative concentration of bacteria when $\lambda > 3.6 \times 10^{-3}$.
4. Sensitivity analysis was useful in obtaining estimates for the parameters necessary for solving bacterial transport model for porous media. However, simultaneous optimization of all of the parameters concurrently may have led to even better estimates of these parameters.

LIST OF SYMBOLS

b = the specific decay rate (1/T)
C = concentration of suspended microbial particles per unit volume of flowing suspension (M/L^3)
C_F = substrate concentration in the porous space (M/L^3)
D = coefficient of hydrodynamic dispersion (L^2/T) = $D_a + D_B + D_T$
D_a = coefficient of mechanical dispersion (L^2/T)
D_B = diffusion coefficient of bacteria (L^2/T)
D_e = $D_{dl} + D_m$, effective diffusivity coefficient (L^2/T)
D_{dl} = coefficient of mechanical dispersion of substrate (L^2/T)
D_m = coefficient of molecular diffusion (L^2/T)
D_T = motility coefficient or effective diffusivity coefficient (L^2/T)
d = diameter of microbial particles (L)
g = gravitational acceleration (L/T^2)
h = constant which has to be found experimentally
J = specific mass discharge of flowing suspension (M/L^2T)
J_A = flux due to advection and mechanical dispersion (M/L^2T)

J_B = flux due to Brownian diffusion (M/L^2T)
J_{CT} = flux due to chemotaxis and tumbling (M/L^2T)
J_{vg} = flux due to sedimentation (M/L^2T)
k = net specific growth rate ($1/T$)
k_b = Boltzmann constant (energy per degree, ML^2/T^2)
k_e = clogging rate constant takes into account screening and adsorption phenomena ($1/T$)
k_d = declogging rate constant ($1/T$)
k_m = migration rate constant or chemotactic coefficient ($1/T$)
K_s = half saturation constant (M/L^3)
λ = similarity variable (distance over square root of time, $LT^{-1/2}$)
m_d = mass of microbial particle (M)
R_a = rate of deposition of microbial particles per unit volume of soil (M/L^3T)
R_d = decay of particles in both the phases (M/L^3T)
R_{dd} = growth term of the deposited microbes (M/L^3T)
R_{ds} = rate of decay of suspended microbial particles (M/L^3T)
R_g = growth of particles in both the phases (M/L^3T)
R_{gs} = rate of growth of suspended microbial particles (M/L^3T)
R_{gd} = decay term of the deposited microbes (M/L^3T)
ρ = density of the microbial particles (M/L^3)
ρ_s = bulk mass density of dry soil (M/L^3)
ρ_w = density of water (M/L^3
θ = effective porosity, i.e., volume occupied by the flowing suspension per unit of the total volume (L^3/L^3)
S_F = mass of adsorbed substrate per unit mass of soil particles (M/L^3)
σ = volume of deposited bacteria per unit volume of bulk soil (L^3/L^3)
t = time
T = absolute temperature (°K)
μ = specific growth rate ($1/T$)
μ_{max} = maximum specific growth rate ($1/T$)
μ_w = viscosity of the flowing fluid (L/T)
v_f = superficial longitudinal velocity of flow (L/T)
v_g = settling velocity
v_m = the migration velocity (L/T)
X = distance
Y = true yield coefficient

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