

Microbial transport in soils and groundwater: A numerical model

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To serve as a tool in the long term evaluation of the risk of accumulation of microbial contaminants (bacteria and viruses) entering soil and groundwater, a mathematical model is developed to predict the spatial and temporal distribution of pollutant concentration. The governing equation for bacterial transport is coupled with a transport equation for the bacterial nutrient present in the seeping wastewater. The deposition and declogging mechanisms are incorporated into the model as a rate process for bacteria and as an equilibrium partitioning for viruses. While the decay is assumed to be a first order reaction and the growth of bacteria is assumed to follow the Monod equation, the model equations exhibit nonlinearity and coupling. A simplified set of equations is solved analytically to test the numerical results. Coupled numerical solutions in one and two dimensions are obtained by the Galerkin method at spatial and temporal locations of interest. Cases studied included a soil column and a horizontal two-dimensional field coupled with the one dimensional solution. For these examples, the bacteria are removed almost totally within the top 7 cm of soil with minimal risk of clogging.

INTRODUCTION

Recently, microbial contamination of groundwater by bacteria and viruses as a result of numerous wastewater disposal activities has gained considerable attention because of public health concerns. The application of wastewater onto land poses the possible risk of microbial contamination of groundwater. In addition to the land application of wastewater, the septic system is an acceptable method of sewage disposal in unsewered areas, but its use frequently results in the contamination of soil and groundwater, thus constituting a public health hazard. Rain infiltrating through sanitary landfills and artificial recharge of groundwater aquifers by treated sewage water are additional sources for biological contamination of groundwater. Once in the ground the wastes move through the soil until they enter the groundwater system that may be in use as a source of water supply. While natural processes can in some cases help to reduce the pollution, most biological contaminants can travel through the earth until they either enter someone's water well or are discharged into a stream.

A literature survey presented by Corapcioglu and Haridas¹ shows evidence that microbial contamination of groundwater does occur when human wastes enter into the soil and that microbes can travel long distances in groundwater under proper conditions. Romero² reviewed various case studies of microbial groundwater pollution until 1970. Butler *et al.*³ and Hagedorn⁴ studied the underground movement of bacteria in field and pilot scale studies. They conclude that bacteria may travel little more than 5 feet in moist or dry fine soil, but will travel much further through such means as root channels and rodent holes.

Although some studies find the microbial mass transport negligible for granular filters and soil-microbial mass systems (e.g.^{5,6}), many others consider the transport of microorganisms significant and have used bacteria and viruses to trace groundwater movement in much the same manner as chemical tracers are used. A review presented by Keswick *et al.*⁷ finds that bacterial viruses appear to be the microorganisms most suited as a microbial tracer because of their size, ease of assay and lack of pathogenicity.

In addition to the traditional practice of the septic tank disposal system, land application of waste water brings a new dimension to environmental problems. Sewage contains many pathogenic microbial organisms with bacteria and virus probably being the most prevalent. The results of a groundwater study in the Milwaukee, Wisconsin area show that bacterial contamination is, in part, the result of leakage from sewer lines⁸. Hain and O'Brien⁹ documented movement of indigenous enteric viruses into shallow groundwater. These few samples are among many other cases reported in the literature. The most important pathogenic bacteria and viruses which might be transported through groundwater are salmonella sp., shigella sp., *Escherichia coli*, vibrio sp., and viruses, hepatitis, echovirus, poliovirus, and coxsachievirus^{10,11}. These pathogens have been associated with a wide variety of diseases, including typhoid, gastroenteritis, diarrhea, hepatitis, gastrointestinal illness, etc. Wilson *et al.*¹² reported that of all waterborne diseases outbreaks between 1971 and 1979 in the United States, 42% were attributed to contaminated groundwater.

A number of environmental factors affect the transport and survival of bacteria and viruses in soils. The factors determining the survival of bacteria include bacteria type, rainfall, soil moisture, temperature, soil composition, pH,

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presence of oxygen and nutrients, and availability of organic matter. Viruses are more resistant to environmental changes and have a larger life span in the subsurface than bacteria. Keswick and Gerba¹⁰ discuss the factors affecting survival of viruses in soils and conclude that, like bacteria, low pH and high ionic strength water favour their removal. Smith *et al.*¹³ measured the effects of soil type, flow rate, soil moisture and other factors on transport of *E. coli* through soils on disturbed and intact soil columns and showed that suspended bacteria can move rapidly through 25–30 cm deep soil profiles.

As is apparent from this short review, bacteria and viruses in groundwater pose a proven hazard to health as evidenced by outbreaks of waterborne diseases caused by contaminated groundwater. A critical issue in groundwater quality management associated with this problem is to predict survival and transport of microbial pollutants in the subsurface environment. Although the problem has a great practical importance, the mathematical statement of the phenomenon has been attempted only in a few recently published studies. The first conceptual model for the bacterial movement in soils was presented by Matthess and Pekdeger¹⁴. Later, Sykes *et al.*⁵ presented a model to predict the concentrations of leachate organics, measured as chemical oxygen demand in groundwaters below sanitary landfills. Simultaneous substrate utilization and microbial mass production equations, with convection and dispersion included for the former, are used for modeling biodegradation. The only processes considered for the latter are the microbial growth and decay. Chetboun and Bachmat¹⁵ have presented a generalized model which considers biological and mass transfer processes by taking the total mineral nitrogen as the substrate. A one-dimensional, steady state solution is mentioned in their publication. None of these modeling studies present a complete picture of the phenomenon, that is, complete coupling of microbial and substrate mass conservation equations, transient conditions, convective transport of microbial population, etc. Therefore, the purpose of this study is to present a coupled mathematical model for the transport and fate of bacteria and viruses in soils and groundwater. The model is designed to predict how long a given population of microorganisms can live in soils and how far they can spread while they are alive.

MATHEMATICAL FORMULATION

Corapcioglu and Haridas¹ have developed the governing equations for the transport and fate of microbial contaminants in the presence of a substrate. The details of the derivation can be found in Corapcioglu and Haridas¹. Here, we will give the basic steps of the derivation.

The starting point is the macroscopic mass conservation equation for species in a porous medium in a three dimensional space,

$$R_a + \frac{\partial(\theta C)}{\partial t} = -\nabla \cdot J + R_d + R_g \quad (1)$$

where C is the concentration of suspended particles (bacteria and/or viruses), R_a is the rate of deposition of particles on grains, R_d and R_g are the decay and growth terms of the suspended particles, respectively, and θ denotes the volume occupied by the flowing suspension

per unit total volume. Some of the removal mechanisms of bacteria and the transport processes are summed up in the term denoted by J which is the specific mass discharge of suspended particles.

The capture of suspended particles from water passing through soil is characterized by the simultaneous action of forces of fluid-mechanical origin along with the forces of other origin that act between the particle and collector¹⁶. The removal of bacteria is attributed to straining in the contact zones of adjacent pores, sedimentation in the pores, and adsorption. Adsorption is the primary removal mechanism for viruses due to their very small size. A detailed discussion of removal mechanisms is given in Corapcioglu and Haridas¹.

Straining

Particles cannot pass through pores smaller than a particular size. Theoretically, a particle of any diameter may wedge in a void between two tangent soil grains; this interpretation is no longer relevant if the ratio of suspended particle diameter to soil grain diameter is small (≤ 0.05) because the predominating mechanism for attachment to surface sites will then be surface forces. This process is reported to be one of the limitations for bacteria travelling through soils^{17,18}. For viruses this effect can easily be neglected.

Adsorption

Adsorption of microbial particles heavily relies on various factors: (a) the physical and chemical nature of absorbate (viruses) and absorbent (soil), (b) the pH of the solution, (c) the characteristics of the flow, and (d) the degree of saturation. Soil type, ionic strength of soil solution, amount of organic matter and humic substances are all considered in the first category. High salt content in groundwater would increase the adsorption due to double layer compression. Also, it is usually agreed that fine-textured soils like clay retain more viruses^{18,19,20} and bacteria⁴ than do sandy soils. Increasing adsorption occurs with the reduction of pH below 8.0 and with the addition of cations, especially the divalent species²¹. It was also concluded that retention mechanisms by soil was due to an adsorption mechanism which increased with decreasing soil moisture. Bitton *et al.*¹⁹ critically examined the various methods frequently used to assess soils' potential to retain viruses.

Various studies^{20,22,23} have shown that adsorption data of viruses to soils were found to fit a Freundlich isotherm and were not describable by a Langmuir isotherm.

Sedimentation

Gravitational deposition on grains can occur if the particles have a density different from that of the liquid. Usually, viruses and some bacteria are neutrally buoyant and tend not to settle. But, Gerba *et al.*¹⁸ reported that sedimentation could be a mechanism of removal for some bacteria. Yao *et al.*²⁴ noted that gravitational settlings play a significant part only in the capture of relatively large particles ($> 5 \mu$); for these particles the removal efficiency is proportional to the square of the particle diameter.

Formulation of the deposition of particles on grain surfaces

The accumulation of bacteria on grain surfaces forms clusters called dendrites. The straining effects increase

with dendritic growth, resulting in further growth, until the clusters become unstably large and break off. The process is repeated at sites below, resulting in the movement of a 'saturated front' of clusters. The rate of removal depends on the flow rate and the size and density of the bacterial clusters¹⁷. If the deposition (clogging) of the bacteria by various mechanisms (straining, sedimentation, adsorption) and sloughing off of clusters (declogging) are simultaneous, the conservation equation for the deposited material may be written as

$$\frac{\partial \rho \sigma}{\partial t} = R_a + R_d + R_g, \quad (2)$$

where R_g and R_d are the growth and decay terms respectively in the deposited state, ρ is the density of bacteria and σ is the volume of deposited bacteria per unit volume of bulk soil. The term R_a can be expressed by a kinetic equation

$$R_a = k_c(n - \sigma)C - k_y \rho \sigma^h \quad (3)$$

where k_c and k_y are the clogging and declogging rate constants respectively, and h is a constant. When $h=1$, equation (3) reduces to the kinetic equation proposed by several researchers (e.g., Mints²⁵, see Sakthivadival and Irmay²⁶, for a review). The exponent h , which has to be determined experimentally, scales the importance of C on σ . For values of h greater than 1, the concentration has a decreasing effect on the amount of deposited material.

In the case of viruses, since adsorption is the major removal mechanism (2) should be replaced by

$$\frac{\partial \rho S}{\partial t} = R_a + R_d, \quad (4)$$

where S is the mass of adsorbed phase per unit mass of the solid part of the porous medium and it is related to C by an equilibrium isotherm. Note that $R_g=0$ for viruses, since viruses reproduce only inside an appropriate host cell.

In summary, R_a is a rate controlled reaction for bacteria, and an equilibrium controlled reaction due to surface and electrokinetic forces for viruses.

Diffusion by Brownian motion

Like other colloids, bacteria and viruses are subject to Brownian motion by which the path of the individual particle appears quite erratic, while the average particle flux is proportional to the concentration gradient. Then, the mass discharge of bacteria or viruses by Brownian motion is expressed by

$$J_B = -D_B \theta \nabla C \quad (5)$$

where D_B is the diffusion coefficient of the suspended particles (bacteria or viruses), which could be estimated by the Stokes-Einstein's equation.

Chemotaxis and tumbling of bacteria

In natural water systems there exist concentration gradients of various solutes, some of which stimulate response from microbes. Some microbes move systematically toward a richer food supply, and this motion, induced by presence of a solute gradient, is termed chemotaxis. In chemotaxis the motion of a cell is

influenced by the molecules of the substrate through a chemical interaction rather than by the direct impact characteristic of Brownian motion.

The chaotic, random movement of motile bacteria which was referred to as 'tumbling'²⁷ above gives rise to an effective diffusivity or motility coefficient D_T . This random movement may be assumed to be superimposed upon any systematic migration induced by substrate, so the two effects (random and systematic) may be considered to be additive. Note that although the random motion is a sign of vitality, the Brownian motion is exhibited by any particle. Keller and Segel²⁷ note that the additive property of Brownian and chemotactic particle migration by saying that 'the chemotactic response of unicellular microscopic organisms is viewed as analogous to Brownian motion. Local assessments of chemical concentrations made by individual cells give rise to fluctuations in path. When averaged over many cells, on a long time interval, a macroscopic flux is derived which is proportional to the chemical gradient.' The detailed discussion of the subject is given by Corapcioglu and Haridas¹. The total flux J_{CT} , due to chemotactic movement and tumbling can be expressed by²⁸

$$J_{CT} = \theta (C k_m \nabla \ln C_F - D_T \cdot \nabla C) \quad (6)$$

where k_m is the migration rate constant, C_F is the substrate concentration, and D_T is the motility coefficient. The anatomy of viruses is very much different than that of bacteria. Viruses reproduce only inside an appropriate host cell; therefore, chemotaxis is irrelevant for viruses.

Decay and growth

Gerba *et al.*¹⁸ concluded that in most cases, 2 to 3 months is sufficient for reduction of pathogenic bacteria to negligible numbers once they have been applied to the soil. The decay mechanism of viruses is similar to that of bacteria, but certain types which are more resistant to environmental changes might survive longer (1 to 6 months) than their bacterial counterpart. Gerba *et al.*¹⁸ concluded that the survival of the enteroviruses in soil is dependent on the nature of the soil, temperature, pH and moisture.

The death of microorganisms is expressed as an irreversible first order reaction, for bacteria

$$R_{d_j} = -k_d \theta C; \quad R_{d_s} = -k_d \rho \sigma \quad (7)$$

and similarly for viruses

$$R_d = -k_d (\theta C + \rho S) \quad (8)$$

where k_d is the specific decay rate, R_d is the decay term in free state in water, and R_{d_s} is the decay rate in adsorbed state. We assume that k_d is the same in free and adsorbed states.

Bacterial growth occurs with the utilization of the substrate. The growth of bacteria is assumed to follow the Monod equation. This equation describes a relationship between the concentration of a limiting nutrient and the growth rate of microorganisms. As stated earlier, nutrients needed for proper biological growth can be present in a sewage water. Bacterial growth in a subsurface environment is slow and the Monod equation may be safely used. Similar to the decay process, we assume that bacteria can grow in the deposited state as

well as in the suspension at the same rate. Then, a generalized Monod equation can be written as

$$R_{g_f} = \mu \theta C \quad R_{g_s} = \mu \rho \sigma \quad (9)$$

where μ is the specific growth rate and R_{g_f} and R_{g_s} denote the growth terms in free and adsorbed states respectively. The functional relationship between μ and an essential nutrient's concentration C_F was proposed by Monod²⁹,

$$\mu = \frac{\mu_m C_F}{K_s + C_F} \quad (10)$$

Here μ_m is the maximum growth rate achievable when $C_F \gg K_s$ and the concentration of all other essential nutrients is unchanged. K_s is that value of the concentration of the substrate where the specific growth rate has half its maximum value; roughly speaking, it is the division between the lower concentration range where μ is linearly dependent on C_F , and the higher range, where μ becomes independent of C_F .

COMPLETE SET OF MODEL EQUATIONS

After substitution of (7) and (9) into the macroscopic mass balance equation (1) becomes

$$\frac{\partial \theta C}{\partial t} = -\nabla \cdot J + (\mu - k_d) \theta C - R_a \quad (11)$$

Based on the earlier discussion, the flux of bacteria, J , comprises Brownian diffusion, dispersion, convection, chemotaxis and gravitational settling. Therefore

$$J = -D \theta \nabla C + (v_f + v_m + v_g) \theta C = -D \theta \nabla C + u \theta C \quad (12)$$

where D , the coefficient of hydrodynamic dispersion, is the sum of Brownian diffusion, effective diffusivity due to tumbling of bacteria and mechanical dispersion coefficients; v_f is the water flow velocity; v_m is the chemotactic velocity; and v_g is the gravitational settling velocity. The term R_a in (11) representing the net mass transfer rate is given by (3).

The mass conservation equation for captured bacteria is obtained from (2), (7) and (9) as

$$\frac{\partial \rho \sigma}{\partial t} = (\mu - k_d) \rho \sigma + R_a \quad (13)$$

where σ is defined as the volume of captured bacteria in unit volume of bulk soil and ρ is the density of bacteria. In a saturated porous medium with deposition of suspended particles on soil grains,

$$\theta = n - \sigma \quad (14)$$

where n is the porosity of the medium.

The substrate, C_F , which is consumed by the microbes at a rate R_F , is assumed to be transported by convective dispersion. Thus the mass conservation equation for C_F in equilibrium with its adsorbed species S_F may be written as

$$\frac{\partial \theta C_F}{\partial t} + \frac{\partial \rho_s S_F}{\partial t} = -\nabla \cdot (-D_F \theta \nabla C_F + v_f \theta C_F) + R_F \quad (15)$$

where C_F is defined as mass of substrate per unit volume of

water and S_F as mass of adsorbed substrate per unit mass of soil grains. Hence ρ_s is bulk density of dry soil.

Assuming the existence of a stoichiometric ratio, Y , between mass of substrate utilized and microbes formed, the net rate of consumption of substrate becomes

$$R_F = -\frac{\mu}{Y} (\rho \sigma + \theta C) \quad (16)$$

where Y is called the yield coefficient. Experiments show Y to be constant. An equilibrium isotherm

$$S_F = k_a C_F^m \quad (17)$$

relates C_F and S_F . k_a and m are experimentally determined constants.

Equation (11) is modified for viruses with an equilibrium adsorption and no growth, as discussed previously. Assuming negligible pore volume change due to adsorbed viruses, i.e., $\theta = n$, (11) becomes

$$\frac{\partial \rho S}{\partial t} + \frac{\partial n C}{\partial t} = -\nabla \cdot J - k_d (nC + \rho S) \quad (18)$$

where J , the flux of viruses, includes hydrodynamic dispersion and convection. Therefore

$$\frac{\partial \rho S}{\partial t} + \frac{\partial n C}{\partial t} = -\nabla \cdot (-Dn \nabla C + v_f n C) - k_d (nC + \rho S) \quad (19)$$

A special case of (11) may be written for deep bed filtration without leaching substrate resulting in no growth, i.e., $\mu = 0$ and $u = v_f$:

$$\frac{\partial \theta C}{\partial t} = -\nabla \cdot J - k_d \theta C - R_a \quad (20)$$

where R_a is given by (3) and $J = -D \theta \nabla C + v_f \theta C$. The equation for adsorbed microbes remains as given by (13).

The model of Matthess and Pekdeger¹⁴ contains some of the terms of (11). The features missing are kinetically controlled deposition and resuspension, sedimentation, growth and chemotaxis. No solution of the equation is given.

The model of Sykes *et al.*⁵ predicts leachate organic concentration under sanitary landfills. An immobile microbial mass biodegrades the organics. These assumptions would reduce (11) and (15) to

$$\frac{\partial C}{\partial t} = \mu C - k_d C$$

$$\frac{\partial C_F}{\partial t} = -\nabla \cdot [-D_F \nabla C_F + v_f C_F] + R_F$$

A SURVEY OF MODEL PARAMETERS

The distinguishing feature of this type of mathematical model is the physical nature of the parameters. This implies experimental determination, in the laboratory or the field, although forbiddingly impractical for the latter in certain instances. A literature review was done to obtain reasonable estimates for the parameters of the model proposed.

The flow velocity, v_f , and Brownian and molecular diffusion coefficients, D_B , D_M , are readily available. Once these parameters are obtained, the effective dispersion coefficients are calculated from graphical relations (e.g., see p. 238, Bear³⁰) which relates the Peclet number ud/D_M , to the ratio of molecular and hydrodynamic dispersion coefficients.

Microbial growth parameters, μ_m , K_s , Y , k_d are available for heterogeneous populations in commercial use³¹. Sykes *et al.*⁵ present the following values of parameters for populations of organic leachates under sanitary landfills: $\mu_m = 0.144 - 0.072 \text{ day}^{-1}$, $K_s = 2000 - 4000 \text{ mg/l}$ of COD, $Y = 0.04$, $k_d = 0.015 \text{ day}^{-1}$. The leachate and microbial concentrations were estimated to be 1000 mg/l each in the landfill. This was used as a first kind boundary condition for their model.

Adsorption of substrate onto soil particles depends on parameters k_a and m as given in (17). Estimates from two sources are given as: $k_a = 0$ for landfill leachate by Sykes *et al.*⁵; $k_a = 0.2 \text{ mg/l}$, $m = 1$ for 2-4 D herbicide on sand, $k_a = 2.0 \text{ mg/l}$, $m = 1$ for 2-4 D herbicide on clay by Selim *et al.*³²

Filtration studies are a source for mass transfer coefficients, k_c and k_y as in (3). Experimenting with anaerobic filters composed of crushed stones of diameter 20 mm and 50% porosity, Polprasert and Hoang³³ determined $k_c = 1.06 \times 10^{-5} \text{ s}^{-1}$, $k_y \approx 0$ for fecal coliforms; $k_c = 6.25 \times 10^{-6} \text{ s}^{-1}$, $k_y \approx 0$ for bacteriophages. Based on experiments with latex suspensions (0.04 μm) filtered through glass beads (diameter 0.397 mm, porosity 0.35), Ring³⁴ used a similar rate expression to model adhesion and suspension. He obtained $k_c = 6.5 \times 10^{-3} \text{ s}^{-1}$, $k_y = 4.35 \times 10^{-4} \text{ s}^{-1}$ for negatively charged latex particles on glass beads.

The other parameters required are density of bacteria ρ as in (13) and bulk density of soil ρ_s as in (15). Bacteria were assumed neutrally buoyant for the purposes of this model, i.e., $\rho = 1 \text{ g/ml}$. ρ_s was taken as 1.75 g/ml.

AN ANALYTICAL SOLUTION

An examination of the governing equations shows the complex nature of the model equations, with a high degree of non-linearity and coupling. It is very difficult, if not impossible, to obtain closed form solutions for C , σ , and C_F even for a one-dimensional space. Therefore, a numerical solution will be sought for a coupled solution of the governing equations. However, a simplified analytical solution is needed to test the validity of the numerical results. Therefore, we will solve the coupled set of equations (11), (3) and (13) as

$$\frac{\partial C^*}{\partial t} + R_a = D \frac{\partial^2 C^*}{\partial x^2} - u \frac{\partial C^*}{\partial x} + k C^* \quad (21)$$

$$\frac{\partial \sigma^*}{\partial t} - R_a = k \sigma^* \quad (22)$$

$$R_a = k_c C^* - k_y \sigma^* \quad (23)$$

where $C^* = \theta C$, $\sigma^* = \rho \sigma$ and $k = \mu - k_d$. The effective porosity, $\theta = n - \sigma$, flow velocity, u , and k are all assumed to be constants. We also assume $h = 1$ in (3). The equations

(21)–(23) are solved for a semi-infinite column ($0 \leq x \leq +\infty$) with boundary and initial conditions

$$C^* = C_0^* \quad \text{at } x = 0 \quad (24)$$

$$C^* = 0 \quad \text{at } x \rightarrow \infty \quad (25)$$

$$C^* = 0 \quad \text{at } t = 0 \quad (26)$$

$$\sigma^* = 0 \quad \text{at } t = 0 \quad (27)$$

The solution technique is similar to that of Ogata³⁵. Applying the Laplace transform on t to (21)–(27) we get

$$\bar{C} = A \exp \left[\left\{ u \pm \sqrt{u^2 - 4D[k - s - k_c/(1 + k_y/(s - k))]} \right\} \frac{x}{2D} \right] \quad (28)$$

where s is the Laplace transform variable and overbar denotes transformed quantities. Using (25) only the negative part of the argument is retained. Using (24) gives $A = C_0^*/s$ where C_0^* is a constant. Using the shifting property of the Laplace transform, and the convolution theorem, the inverse of (28) is obtained as

$$\begin{aligned} C^*/C_0^* = & \frac{2}{\sqrt{\pi}} \exp \left[\frac{ux}{2D} + kt \right] \int_{x/2\sqrt{D\tau}}^{\infty} \\ & \times \exp \left\{ -\xi^2 - \left(\frac{ux}{4D\xi} \right)^2 - \frac{x^2 k_c}{4D\xi^2} - k_y \left(t - \frac{x^2}{4D\xi^2} \right) \right\} \\ & \cdot \left\{ I_0 \left(\sqrt{\frac{x^2 k_c k_y (t - x^2/4D\xi^2)}{D\xi^2}} \right) \right. \\ & \left. + (k_y - k) \exp \left[-(k_y - k) \left(t - \frac{x^2}{4D\xi^2} \right) \right] \right. \\ & \left. \int_0^{(t - x^2/4D\xi^2)} \exp[-(k_y - k)\tau] I_0 \left(\sqrt{\frac{x^2 k_c k_y \tau}{D\xi^2}} \right) d\tau \right\} d\xi \end{aligned} \quad (29)$$

The solution (29) is computed and plotted in Figure 1.

NUMERICAL SOLUTIONS

The Galerkin Finite Element method was used to solve (11) and (15). The method involves the approximation of the solution with a known set of 'basis functions'³⁶. The rest of the model equations (3), (10), (13) and (14) were incorporated into the numerical technique as will be explained later.

The method is illustrated for (11) after substituting (12)

$$PC \equiv \frac{\partial \theta C}{\partial t} + R_a - \nabla \cdot (D \theta \nabla C - u \theta C) - (\mu - k_d) \theta C = 0 \quad (30)$$

where $u = v_f + v_m + v_g$ and P denotes an operator. The region of interest is $x \in \Omega$ with a boundary Γ . C and R_a in (30) are approximated as

$$C(x, t) \simeq \hat{C}(x, t) = \sum_{i=1}^n C_i(t) \phi_i(x) \quad (31)$$

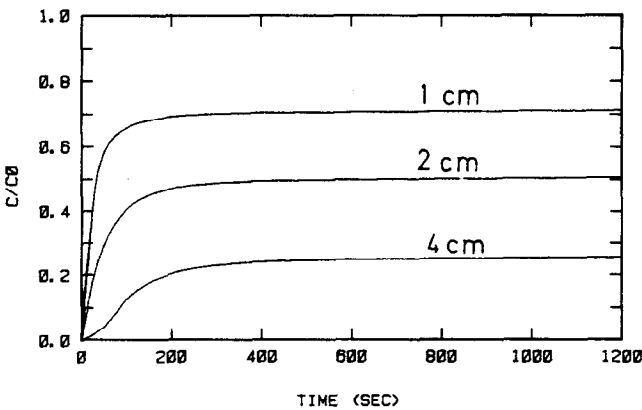
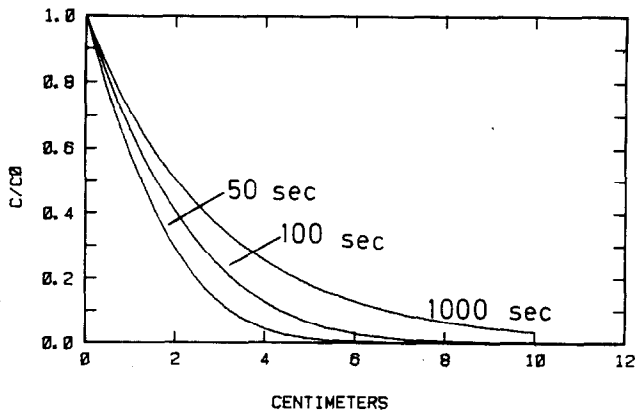


Fig. 1. Analytical solution with parameters: $D=0.04 \text{ cm}^2/\text{s}$, $u=0.003 \text{ cm/s}$, $k=-1 \times 10^{-6} \text{ s}^{-1}$, $k_c=6 \times 10^{-3} \text{ s}^{-1}$, $k_y=6 \times 10^{-5} \text{ s}^{-1}$

$$R_a(x, t) \simeq \hat{R}_a(x, t) = \sum_{i=1}^n R_{ai}(t) \phi_i(x) \quad (32)$$

where ϕ_i are known basis functions; overcaps denote approximate variables.

The Galerkin method involves the orthogonality of $P\hat{C}$ to the space spanned by $\{\phi_i\}$, i.e.,

$$\langle P\hat{C}, \phi_j \rangle \equiv \int_{\Omega} P\hat{C} \cdot \phi_j \, dx = 0, \quad j=1, \dots, n \quad (33)$$

Using (30), (31) and (32) and employing Green's theorem, (33) becomes

$$\begin{aligned} \frac{d}{dt} \theta_i C \langle \phi_i, \phi_j \rangle + R_{ai} \langle \phi_i, \phi_j \rangle \\ = -D \theta_i C \langle \nabla \phi_i, \nabla \phi_j \rangle - u \theta_i C \langle \nabla \phi_i, \phi_j \rangle \\ + (\mu_i - k_d) \theta_i C \langle \phi_i, \phi_j \rangle + \int_{\Gamma} D \theta \nabla C \cdot \hat{n} \phi_j \, dx \\ \text{sum over } i \text{ for } j=1, \dots, n \end{aligned} \quad (34)$$

where D_i , θ_i , u_i and μ_i are assumed constant over an element and \hat{n} is the unit normal vector. Performing an

identical process on (15) after substituting (17) with $m=1$ yields

$$\begin{aligned} \frac{d}{dt} C_{Fi} [\theta_i + k_d \rho \sigma_i] \langle \phi_i, \phi_j \rangle \\ = -D_{Fi} \theta_i \langle \phi_i, \nabla \phi_j \rangle C_{Fi} - v_{Fi} \theta_i \langle \nabla \phi_i, \phi_j \rangle C_{Fi} \\ - \frac{\mu_i}{Y} (\theta_i C_i + \rho \sigma_i \langle \phi_i, \phi_j \rangle) + \int_{\Gamma} D_F \theta \nabla C_F \hat{n} \phi_j \, dx \end{aligned} \quad (35)$$

At each node (3) becomes with $h=1$

$$R_{ai} = k_c \theta_i C_i - k_y \rho \sigma_i \quad (36)$$

Similarly, (13), (10) and (14) can be written for each node as

$$\frac{d}{dt} \rho \sigma_i = (\mu_i - k_d) \rho \sigma_i + R_{ai} \quad (37)$$

$$\mu_i = \frac{\mu_m C_{Fi}}{K_s + C_{Fi}} \quad (38)$$

$$\theta_i = n - \sigma_i \quad (39)$$

The time derivatives in (34), (35) and (37) are replaced by a finite difference implicit scheme. We assume a uniform porosity distribution over the entire domain that is

$$n_i = n \quad (40)$$

One dimensional uncoupled solution

To compare the numerical schemes with the analytical solution given by (29), (34) is written for a one dimensional space as

$$\begin{aligned} \frac{d}{dt} \theta_i C \langle \phi_i, \phi_j \rangle + R_{ai} \langle \phi_i, \phi_j \rangle = -D \theta_i C_i \left\langle \frac{d\phi_i}{dx}, \frac{d\phi_j}{dx} \right\rangle \\ - u \theta_i C_i \left\langle \frac{d\phi_i}{dx}, \phi_j \right\rangle \\ + (\mu_i - k_d) \theta_i C_i \langle \phi_i, \phi_j \rangle \\ + D \theta \frac{dC}{dx} \phi_j \Big|_0^L \end{aligned} \quad (41)$$

θ_i and $\mu_i - k_d = k$ are taken to be constants for this uncoupled problem. The boundary conditions were $C=C_0$ at $x=0$ and $C=0$ at $x=L$. We should note that the particles larger than pore openings in treated sewage and septic tank effluent initiate the development of a filter cake at the soil surface $x=0$, so that C_0 is not constant with time, although it may become steady at a reduced value. In this case, particle concentration in the soil would substantially be reduced. The initial conditions were $C=0$, $\sigma=0$ at $t=0$. The basis functions were the Chapeau functions, shown in Fig. (2b). At each time step (41), (36) and (37) were solved in sequence. The process was repeated until the error between two iterations of C was less than 10^{-6} g/ml for the parameters used. The results are shown in Fig. 3 with the analytical solution for comparison. There is good agreement between the two solutions. The values of the parameters are given in the figure caption of Fig. 1.

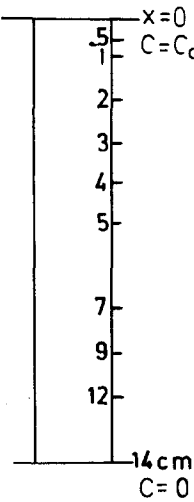


Fig. 2a. One dimensional column and finite elements

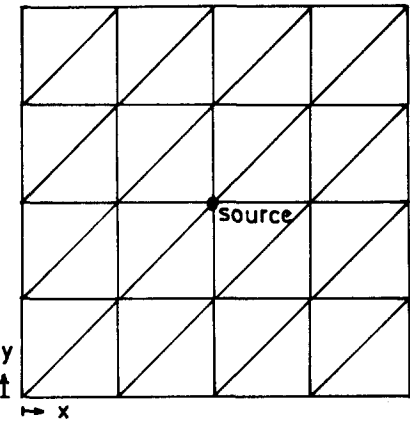


Fig. 2b. Two-dimensional finite elements

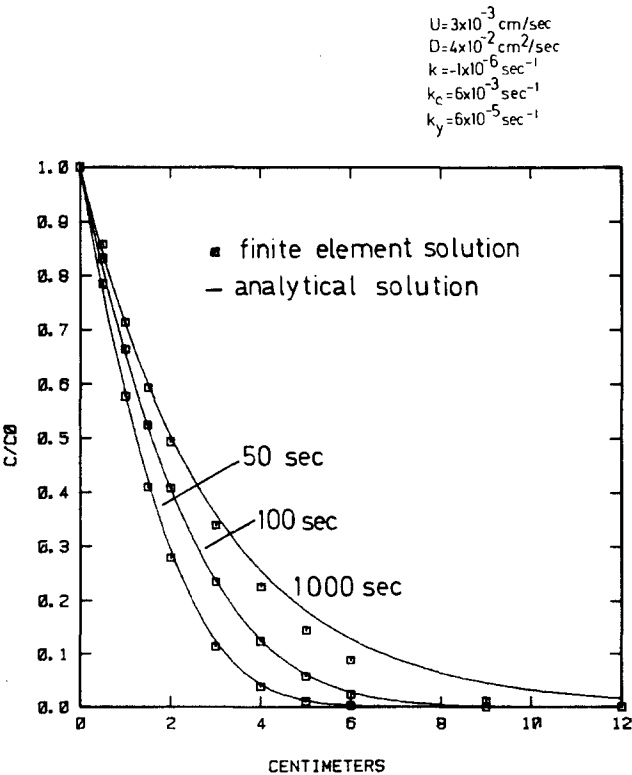


Fig. 3. Comparison of analytical and numerical solutions

One dimensional coupled solution

In addition to (41), the coupling equation (35) in a one dimensional space is given by

$$[\theta_i + k_a(1 - \theta_i)] \langle \phi_i, \phi_j \rangle \frac{d}{dt} C_{Fi} = -D_{Fi} \theta_i C_{Fi} \left\langle \frac{d\phi_i}{dx}, \frac{d\phi_j}{dx} \right\rangle - v_{Fi} \theta_i \left\langle \frac{d\phi_i}{dx}, \phi_j \right\rangle C_{Fi} - \frac{\mu_i}{Y} (\theta_i C_i + \rho \sigma_i) \langle \phi_i, \phi_j \rangle + D_F \theta \frac{d}{dx} C_F \theta_j \Big|_0 \quad (42)$$

Note that in this case θ_i and $\mu_i - k_d$ are variables. The basis functions were again Chapeau functions shown in Fig. 2b and the elements are shown in Fig. 2a. The scheme adopted is shown in Fig. 4. It involves the sequential solution of each equation and iteration until the value of C converges as per the criterion. For the parameters in Table 1, the largest time step was 60 seconds and the smallest time step was shown as 1 second. Steady state was achieved in approximately 20000 sec.

The scheme was executed using a Fortran computer code. Plots of C , C_F and $(n - \sigma)$ for spatial and temporal variations are given in Figs 5–10. Table 1 gives the values of parameters used. As seen in Fig. 2a, there are ten space elements ranging from 0.5 to 2 cm.

Two dimensional coupled solution

The problem was solved in a two dimensional space with triangular elements. The basis functions are linear in x and y as shown in Fig. 2b.

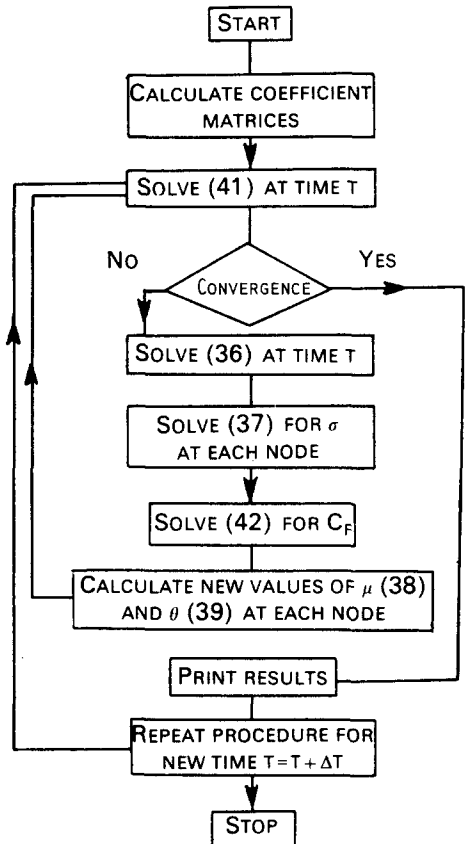


Fig. 4. Flow diagram of the coupled solution

Table 1. One-dimensional model parameters

Dispersion coefficients	$D = D_F = 4 \times 10^{-2} \text{ cm}^2/\text{s}$
Density of bacteria and dry soil	$\rho = 1 \text{ g/ml}; \rho_s = 1.74 \text{ g/ml}$
Clogging rate constant	$k_c = 6.5 \times 10^{-3} \text{ s}^{-1}$
Declogging rate constant	$k_y = 4.35 \times 10^{-4} \text{ s}^{-1}$
Specific decay constant	$k_d = 1 \times 10^{-6} \text{ s}^{-1}$
Monod half constant	$K_s = 2 \times 10^{-3} \text{ g/ml}$
Maximum growth rate	$\mu_m = 4.2 \times 10^{-5} \text{ s}^{-1}$
Maximum cell yield	$Y = 0.04$
Flow velocity	$u = 3 \times 10^{-2} \text{ cm/s}$
Porosity	$n = 0.6$
Surface bacteria concentration	$C_0 = 10^{-3} \text{ g/ml}$
Surface substrate concentration	$C_{F_0} = 10^{-3} \text{ g/ml}$

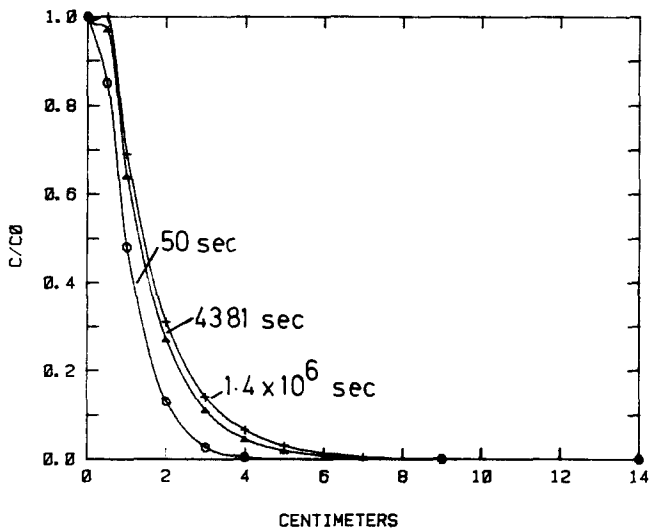


Fig. 5. Dimensionless microbial concentrations versus x for parameters given in Table 1

Equation (34) in a two dimensional space becomes

$$\begin{aligned}
 & \frac{d}{dt} \theta_i C_i \langle \phi_i, \phi_j \rangle + R_{ai} \langle \phi_i, \phi_j \rangle \\
 &= -D_i \theta_i C_i \left\{ \left\langle \frac{d\phi_i}{dx}, \frac{d\phi_j}{dx} \right\rangle + \left\langle \frac{d\phi_i}{dy}, \frac{d\phi_j}{dy} \right\rangle \right\} \\
 & - u_i \theta_i C_i \left\{ \left\langle \frac{d\phi_i}{dx}, \phi_j \right\rangle + \left\langle \frac{d\phi_i}{dy}, \phi_j \right\rangle \right\} \\
 & + (\mu_i - k_d) \theta_i C_i \langle \phi_i, \phi_j \rangle + \int_{\Gamma} D \nabla C \cdot \hat{n} \phi_j d\Gamma \\
 & \text{sum over } i \text{ for } j = 1, \dots, n \quad (43)
 \end{aligned}$$

Similarly (35) in two dimensions becomes

$$\begin{aligned}
 & \frac{d}{dt} C_{Fi} [\theta_i + k_a \rho_s] + \frac{\mu_i}{Y} (\theta_i C_i + \rho \sigma_i) \langle \phi_i, \phi_j \rangle \\
 &= D_{Fi} \theta_i C_{Fi} \left\{ \left\langle \frac{d\phi_i}{dx}, \frac{d\phi_j}{dx} \right\rangle + \left\langle \frac{d\phi_i}{dy}, \frac{d\phi_j}{dy} \right\rangle \right\} \\
 & - v_{ji} \theta_i C_{Fi} \left\{ \left\langle \frac{d\phi_i}{dx}, \phi_j \right\rangle + \left\langle \frac{d\phi_i}{dy}, \phi_j \right\rangle \right\} + \int_{\Gamma} D_F \nabla C_F \cdot \hat{n} \phi_j d\Gamma \\
 & \text{sum over } i \text{ for } j = 1, \dots, n \quad (44)
 \end{aligned}$$

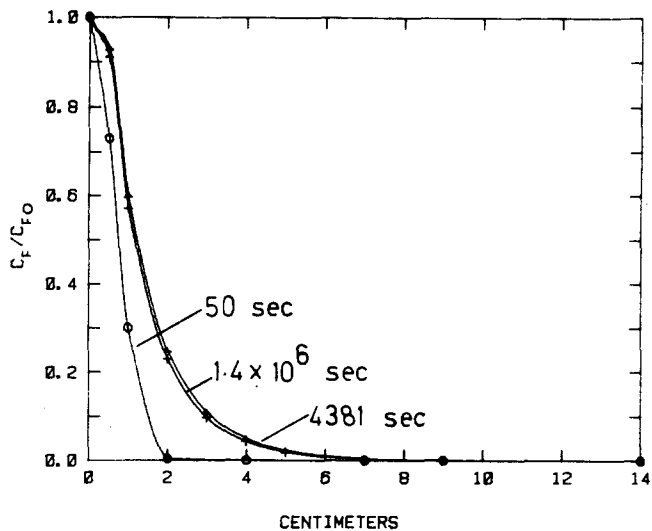


Fig. 6. Dimensionless substrate concentration versus x for parameters given in Table 1

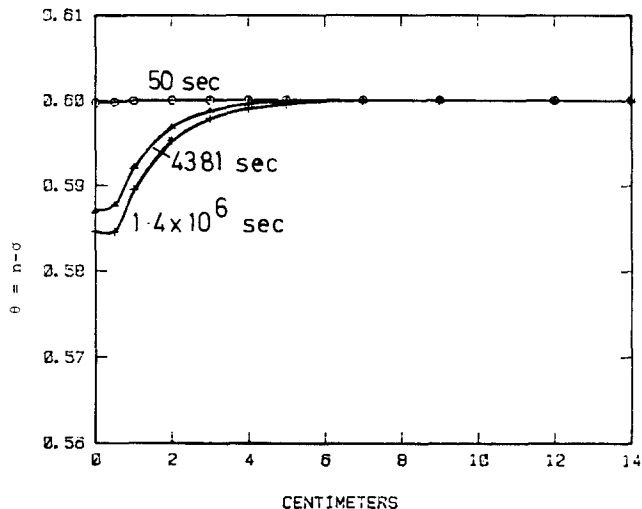


Fig. 7. Effective porosity versus x for parameters given in Table 1

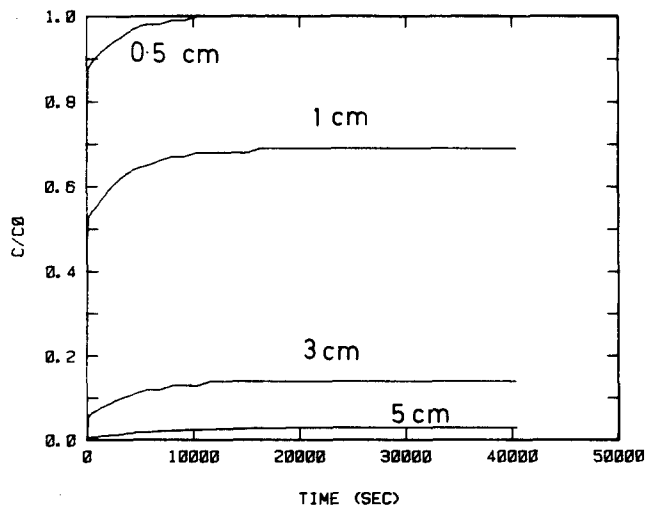


Fig. 8. Dimensionless microbial concentration versus time for parameters given in Table 1

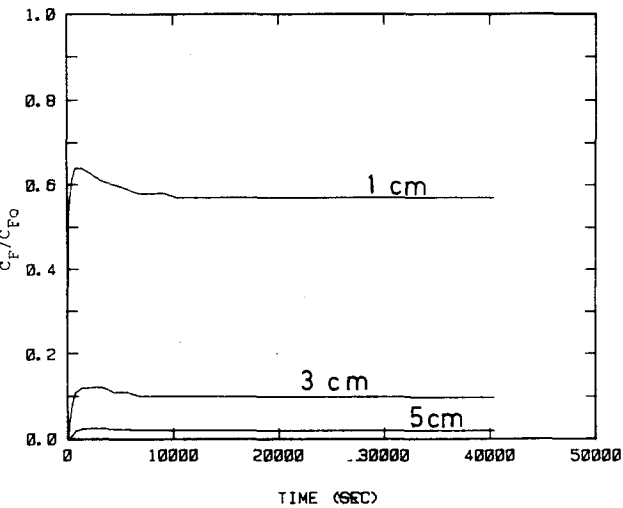


Fig. 9. Dimensionless substrate concentration versus time for parameters given in Table 1

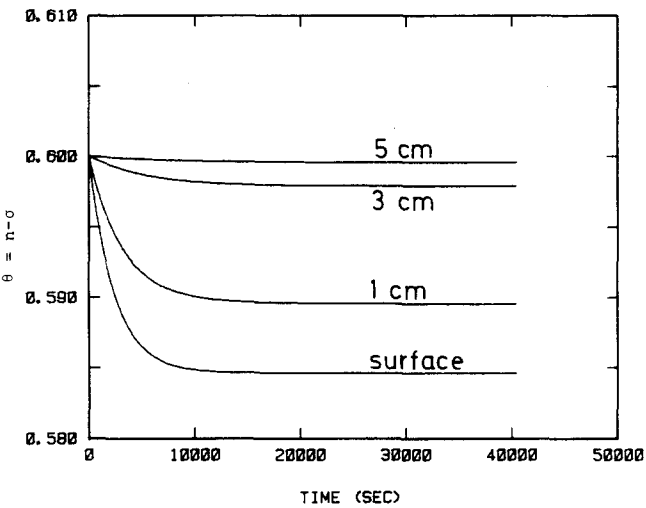


Fig. 10. Effective porosity versus time for parameters given in Table 1

The other governing numerical equations are given by (36) to (39). Boundary conditions were $C = 0$ and $C_F = 0$ on the outer boundaries with $C = C_0$ and $C_F = C_{F0}$ at the central node. Initial conditions were $C = 0$, $C_F = 0$, and $\sigma = 0$ at $t = 0$.

The solution procedure was identical to the one-dimensional one. Results for parameters given in Table 2 are shown graphically in Figs 11–13.

Two dimensional coupled solution interacting with one dimensional coupled solution

The problem solved is identical to the one in two-dimensional space except the source of pollutant and the source of substrate are time dependent. The source concentration was taken to be the solution of the one dimensional coupled problem at $x = 3$ cm. It is postulated that this problem represents an infiltrating pollutant reaching the groundwater table located at a depth of 3 cm.

Results for parameters given in Table 3 are illustrated in Figs 14–16.

DISCUSSION OF RESULTS

One dimensional uncoupled solution

As seen in Fig. 3, the difference between the analytical and numerical solutions increases at larger times. This is explained by the boundary condition at $x = 14$ cm for the numerical solution which forces the solution to zero at all times while the analytical solution for a semi-infinite column attains a non-zero value at every x at larger times.

It was also noted that the numerical solution encounters instability as the element Peclet number, $Pe = ul/D$ where l is the element length, becomes large compared with unity. This is a common feature with the usual finite element solution of the convective dispersion equation.

Table 2. Two-dimensional model parameters

Dispersion coefficients in x and y directions	$D = D_F = 4 \times 10^{-2} \text{ cm}^2/\text{s}$
Flow velocity in x and y directions	$u = 3 \times 10^{-3} \text{ cm/s}$
Density of bacteria and dry soil	$\rho = 1 \text{ g/ml}; \rho_s = 1.74 \text{ g/ml}$
Clogging rate constant	$k_c = 6.5 \times 10^{-3} \text{ s}^{-1}$
Declogging rate constant	$k_d = 4.35 \times 10^{-4} \text{ s}^{-1}$
Specific decay constant	$k_d = 1 \times 10^{-6} \text{ s}^{-1}$
Monod half constant	$K_s = 2 \times 10^{-3} \text{ g/ml}$
Maximum cell yield	$Y = 0.04$
Maximum growth rate	$\mu_m = 4.2 \times 10^{-5} \text{ s}^{-1}$
Porosity	$n = 0.5$
Surface concentrations	$C_0 = 10^{-3} \text{ gm/ml};$ $C_{F0} = 10^{-3} \text{ g/ml}$

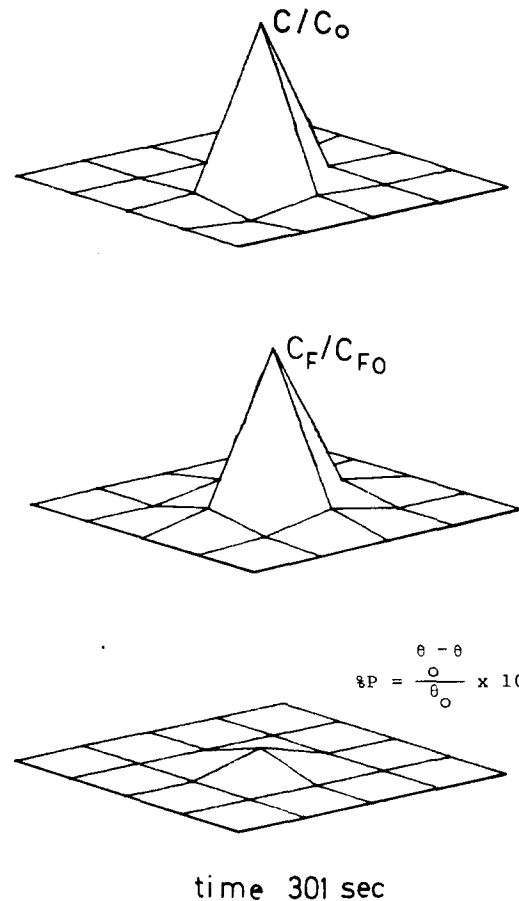


Fig. 11. Three dimensional representation of dimensionless microbial and substrate concentrations and percent reduction of porosity for parameters given in Table 2 at 301 seconds

Table 3. Model parameters for a two-dimensional solution interacting with one-dimensional coupled solution

One dimensional solution	
Dispersion coefficients	$D = D_F = 4 \times 10^{-2} \text{ cm}^2/\text{s}$
Flow velocity	$u = 3 \times 10^{-2} \text{ cm/s}$
Porosity	$n = 0.6$
Two dimensional solution	
Dispersion coefficients in x and y directions	$D = D_F = 4 \times 10^{-2} \text{ cm}^2/\text{s}$
Flow velocity in x and y directions	$u = 3 \times 10^{-3} \text{ cm/s}$
Porosity	$n = 0.5$

All other parameters are common with Table 1

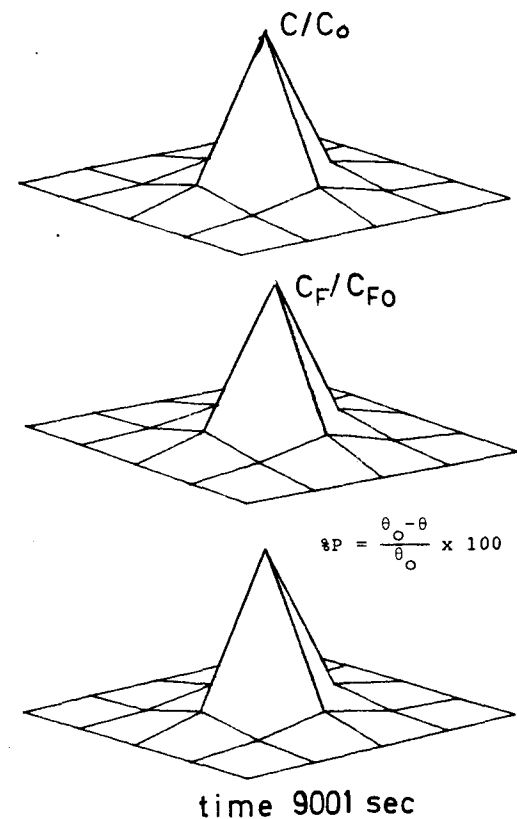


Fig. 12. Three dimensional representation of dimensionless microbial and substrate concentrations and percent reduction of porosity for parameters given in Table 2 at 9001 seconds

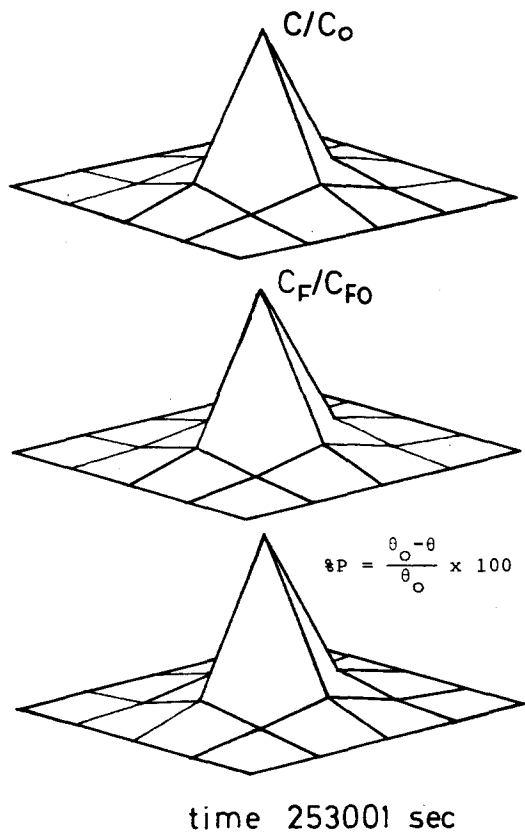


Fig. 13. Three dimensional representation of dimensional microbial and substrate concentrations and percent reduction of porosity for parameters given in Table 2 at 253001 seconds

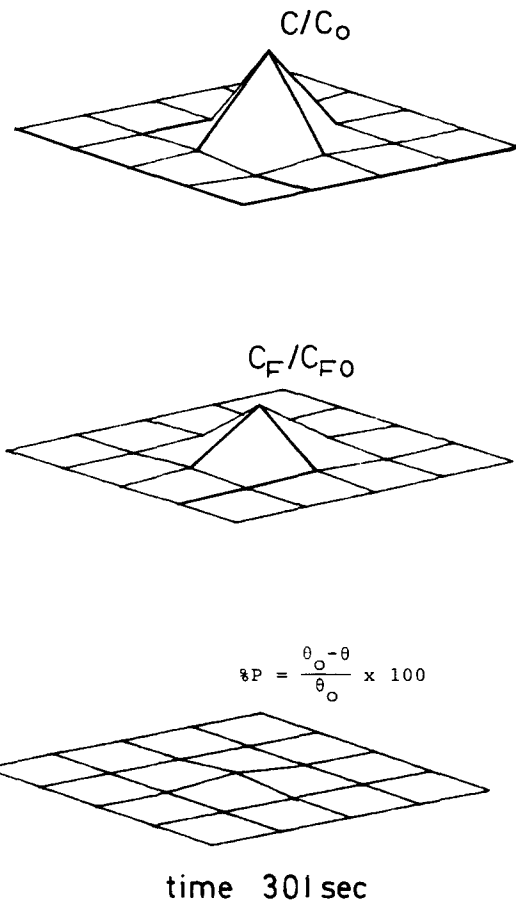


Fig. 14. Three dimensional representation of solution with time dependent source. Time = 301 sec. Parameters given in Table 3

One dimensional coupled solution

The soil column is initially free of bacteria. When steady state values are achieved, the bacterial concentration is seen to be negligible beyond 7 cm. The deposited bacteria reduced the porosity on the surface about 3% at 1.4×10^6 sec. The clogging of the soil is negligible after a depth of 6 cm. As shown again in Fig. 17, for a smaller declogging rate constant, substrate concentration values will have larger values. Also, when the velocity and dispersion coefficients were taken as a tenth of the values in Table 1, all other parameters being the same, as seen in Fig. 18 a larger time is required to reach the steady state values.

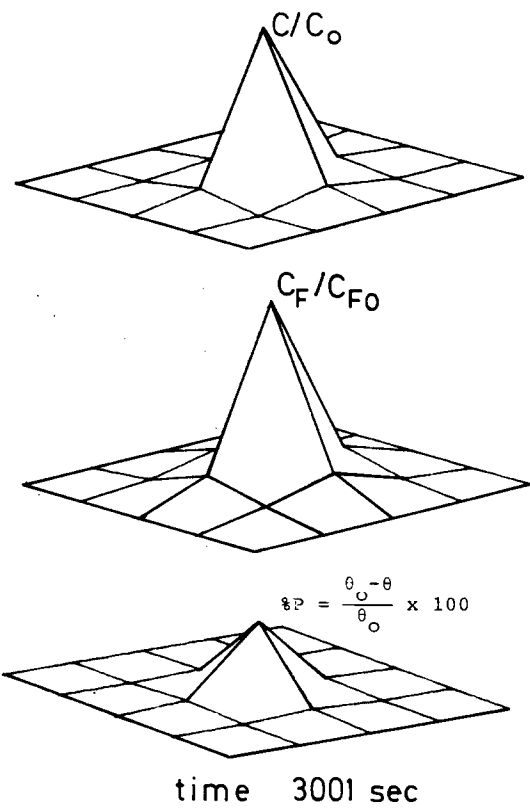


Fig. 15. Three dimensional representation of solution with time dependent source. Time=3001 sec. Parameters given in Table 3

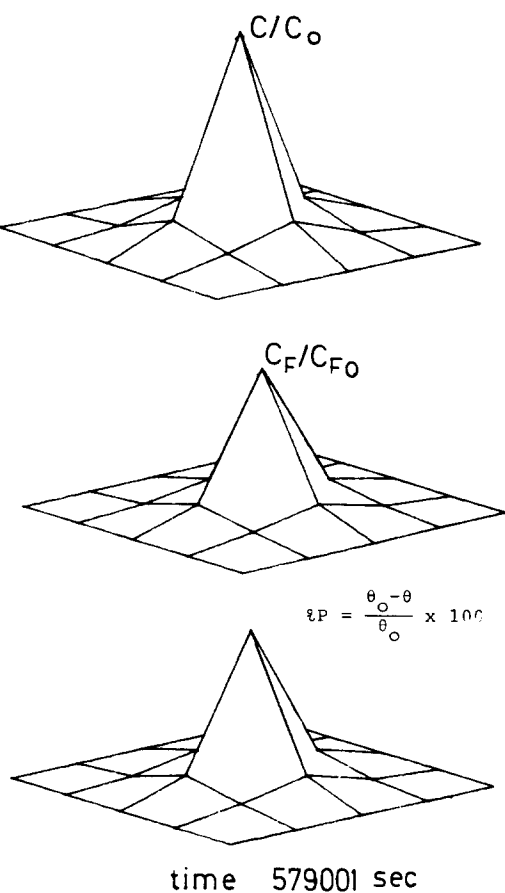


Fig. 16. Three dimensional representation of solution with time dependent source. Time=579001 sec. Parameters given in Table 3

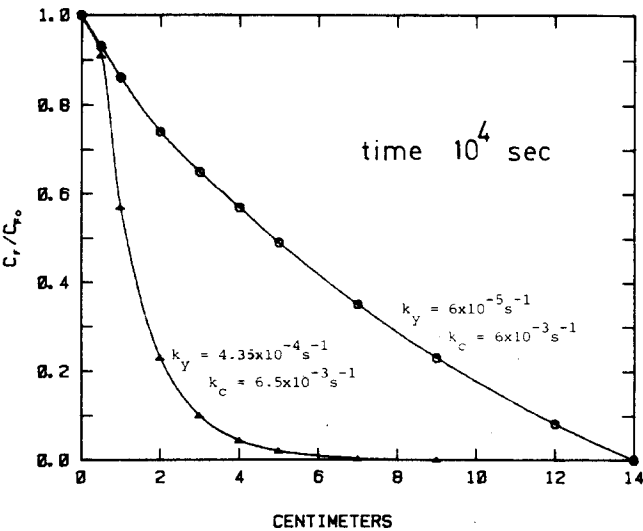


Fig. 17. Comparison of the substrate concentrations with two different values of declogging rate constants

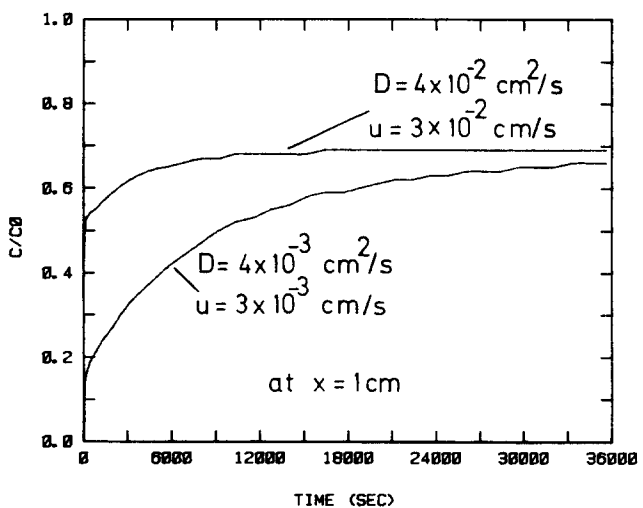


Fig. 18. One dimensional numerical solution for two sets of velocities and dispersion coefficients

An interesting feature of the substrate concentration is that the maximum is attained at an early time and then a gradual decrease to steady state. [See Fig. 9.] This is because of consumption by micro organisms.

Two dimensional coupled solution

Steady state conditions were attained in about 9000 seconds. The graphs, Figs 11–13, are self explanatory.

Two dimensional coupled solution interacting with one dimensional coupled solution

The concentrations are much smaller than that of two-dimensional problem, since the maximum concentration of the time dependent source is only about 15% of that in 2-D. It should be noted, however, that this approach to an infiltrating pollutant reaching a horizontal water table is an idealization. The trend in the variations of C , C_F and σ are similar to the two-dimensional case. The previous comments are valid here also. A numerical comparison at the centre node is given in Table 4.

Table 4. Numerical results of two-dimensional model at the centre node

Two-dimensional coupled solution				
	C/C_0	C_F/C_{F_0}	% pore volume clogged	Related figure number
$t = 301$ sec	1.00	1.00	0.370	11
$t = 9001$ sec	1.00	1.00	3.109	12
$t = 253\,001$ sec	1.00	1.00	3.179	13
Two-dimensional solution interacting with one-dimensional solution				
	C/C_0	C_F/C_{F_0}	% pore volume clogged	Related figure number
$t = 301$ sec	0.058	0.033	0.017	14
$t = 3001$ sec	0.099	0.120	0.183	15
$t = 579\,001$ sec	0.140	0.097	0.421	16

CONCLUSIONS

In this study, we presented a fully coupled mathematical model to predict the transport and fate of biological pollutants entering soil and groundwater from various sources like septic tanks, land application of municipal wastewaters, artificial recharge of sewage water, and landfills.

The governing equation for microbial transport is coupled with another transport equation for the bacterial nutrient present in the seeping wastewater. Additional mechanisms considered include the clogging, declogging, growth and decay of the pathogens. Fully coupled numerical solutions of the governing equations have been obtained by the finite element technique. The governing equations have been discretized by the Galerkin formulation. The set of basis functions are assumed to be standard piecewise linear functions. The time derivatives in this set of first order differential equations are finite differenced in a fully implicit form. Each of the discretized equations is solved separately in sequence at a particular time step. Using the values obtained, the process is repeated until a specified convergence criterion has been satisfied. The solution then moves to the time step. The convergence criterion is specified on the maximum error between two iterations of the value of the microbial concentration.

The results obtained are given in graphical form. The model parameters used to obtain these results are given in Tables 1–3. The soil column is assumed to be free of bacteria and substrate initially. As seen in these figures, the soil surface is 3% clogged on the surface after 1.4×10^6 seconds. At this time, the bacteria are almost totally removed in the upper 7 centimeters of soil, although the substrate in the seeping wastewater travels up to 9 cm. The clogging of the soil is negligible after a depth of 6 cm. Another interesting feature is that the substrate concentration has a peak value at an early time and then decreases gradually due to bacterial consumption. Similar results have been obtained for two-dimensional soils.

The model approach presented here can be applied to planning of future sanitary landfills and cesspools, determining the suitability of septic tank locations, and studying the efficiency of removal of biological pathogens

by filtering. The ultimate goal is that the removal of suspended microorganisms leaving the septic tank or landfill must occur during the soil percolation process before reaching the groundwater.

NOMENCLATURE

C	concentration of micro-organism [ML^{-3}]
C_F	substrate concentration [ML^{-3}]
D	effective dispersion coefficient
D_B	Brownian diffusion coefficient of micro-organisms
D_F	hydrodynamic dispersion coefficient for substrate
D_T	diffusivity coefficient due to random tumbling
d	micro-organism particle diameter
d_g	grain diameter
h	the power term in the kinetic equation
J	specific mass discharge of particles [$\text{ML}^{-2} \text{T}^{-1}$]
J_B	specific mass discharge of micro-organisms due to Brownian motion
J_{CT}	specific mass discharge of micro-organisms due to chemotactic movement
K_s	Monod half constant
k	first order growth or decay constant in analytical solution
k_a	adsorption isotherm constant
k_b	Boltzman's constant
k_c	clogging rate constant
k_d	specific decay rate
k_F	adsorption isotherm constant
k_m	migration rate constant (or chemotactic coefficient)
k_y	declogging rate constant
m	the power term in adsorption isotherm
n	porosity
P	an operator
$\%P$	percent reduction in porosity due to deposition
R_a	rate of deposition of micro-organisms [$\text{ML}^{-3} \text{T}^{-1}$]
R_d	rate of decay
R_g	rate of growth
S	concentration of adsorbed phase
s	Laplace transform variable
t	time
u	flow velocity
v_f	velocity of water flow
v_g	gravitational settling velocity
v_m	velocity of the micro-organisms due to chemotactic movement
Y	growth yield coefficient, mass of micro-organisms per unit mass of substrate utilized
μ	specific growth rate
μ_w	viscosity of water
ρ	density of micro-organisms
ρ_s	bulk density of dry soil
ρ_w	density of water
θ	volume occupied by the suspension per unit volume of total porous medium
σ	volume of deposited micro-organisms per unit volume of total porous medium [L^3/L^3]
ϕ	basis function
τ, ξ	dummy integration variables

Superscripts

- (overbar); transformed quantities in the Laplace space
- ^ (hat) indicates perturbation from average
- * (star) indicates new variable defined for analytical solution

Subscripts

- f indicates liquid state
- i, j indicates variable discretized variables and nodes in finite element solution
- 0 indicates initial state
- s indicates deposited state

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