A One-dimensional Model of Chemical Diffusion and Sorption in Saturated Soil and Aquatic Systems

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ABSTRACT

A one-dimensional model for chemical diffusion in saturated porous media systems is presented. The one-dimensional diffusion model provides for adsorption-desorption reactions either Freundlich or Langmuir, and both solid and liquid phase first-order chemical degradation under isothermal, water-saturated conditions. Finite-difference solutions to the model which simulate the one-dimensional diffusion of an inorganic/organic chemical from the sediment of an aquatic system into the overlying water are provided for a variety of initial and boundary conditions. Analogous applications to flow processes within a structured soil can be made for the diffusion of an inorganic/organic chemical into and out of saturated planar soil aggregates. The initial and boundary conditions are designed to simulate a variety of aquatic situations: ponds, lakes, streams, rivers and oceans. Both explicit and implicit (i.e., Crank-Nicholson) finite-difference schemes are presented for four different saturated systems. The model provides a means of assessing the physicochemical dynamics of chemical-sediment-water interactions and of assessing the pollution potential of chemicals to plants and animals as determined by their propensity to migrate to different compartments of the aquatic environment. The models can also determine the influence of diffusion processes within planar soil aggregates upon solute flow in saturated structured soils. Various simulations are presented for boron (B), diquat (1,1'-ethylene-2,2'-dipyridium dibromide), and bromacil (5-bromo-3-sec-butyl-6-methyluracil).

Additional Index Words: movement, finite-difference model, structured soils, soil aggregate.


Due to the adsorptive capacity of soil for various organic and inorganic chemicals (e.g., boron [B], pesticides) and to the "piggyback" transport of these adsorbed chemicals upon eroded soil particles, the sediments of some of our water bodies have become unintentional repositories for chemicals potentially harmful to plants and animals. Once these chemicals desorb from the sediment, they can diffuse into the overlying water resulting in a decrease in water quality which could threaten both plants and animals. Analogously, soil aggregates act as sinks or sources of chemicals to the flow process within structured soils due to the diffusion of the chemical into our out of the soil aggregates. This fact is evidenced by the asymmetric displacement patterns often observed for structured soils.

Since very low concentrations of some chemicals are known to be toxic to fish and other aquatic lifeforms, and since irrigation waters containing certain chemicals (e.g., B) are known to produce lower crop yields in certain instances, it is important to have a knowledge of the physicochemical dynamics of inorganic/organic chemical-sediment-water interactions to assess the hazard potential of these chemicals. Similarly, knowledge of the influence of soil aggregate diffusion processes upon solute transport in structured soils is needed to help provide an understanding of the transport of chemicals which may become potential groundwater pollutants, can retard or improve plant growth, or are involved in soil reclamation processes.

Since the aquatic compartment of our environment constitutes a potential sink for various chemicals, increased study of chemical-sediment-water interactions has developed over the years (Lotse et al., 1968; Nicolson and Hill, 1970; Veith and Lee, 1971; Weber, 1972; Pionke and Chesters, 1973; Karickhoff et al., 1979; Peck et al., 1980; Karickhoff, 1981; Goldberg, 1982; Corwin and Farmer, 1984a). In addition, various models describing simple aquatic systems have been presented as a means of assessing the relative importance of the various physico-chemical interactions (Corwin and Farmer, 1984b) and of assessing the pollution potential of hazardous chemicals (Corwin and Farmer, 1985). It is the purpose of this study to present finite-difference solutions to models representing a variety of more complicated aquatic systems such as ponds, lakes, oceans, streams, and rivers. These models also have analogous applications to diffusion within saturated planar soil aggregates of structured soils. The finite-difference schemes describe the one-dimensional diffusion under saturated conditions of any chemical undergoing Freundlich- or Langmuir-type adsorption-desorption reactions with consideration given to simultaneously occurring degradation reactions. A variety of initial and boundary conditions have been imposed to describe likely occurring aquatic systems. The models presented herein provide a means of assessing the pollution potential of chemicals to a variety of aquatic systems more sophisticated than that presented by Corwin and Farmer (1985). With regards to flow processes in structured soils, the models provide a means of determining the extent to which diffusion within planar soil aggregates acts as a source or a sink term to solute transport under saturated conditions.

THEORY

The governing partial differential equation describing one-dimensional diffusion of a chemical under isothermal, water-saturated conditions within a sorbing porous medium is,

\[ \theta_r \frac{\partial C}{\partial t} + \eta \frac{\partial S}{\partial t} = D_p \frac{\partial^2 C}{\partial x^2} - \mu_s C - \mu_{v, s} S \]  

where \( C \) and \( S \) are the equilibrium solution and adsorbed concentrations, respectively, \( \theta \) is the volumetric water content, \( \eta \) is the bulk density, \( D_p \) is the porous diffusion coefficient (assumed constant), \( x \) is the distance, and \( t \) is the time. Negligible solid-phase diffusion is assumed. The coefficients \( \mu_s \) and \( \mu_{v, s} \) represent the degradation rates of first-order chemical de-
<table>
<thead>
<tr>
<th>Case</th>
<th>Aquatic system</th>
<th>Initial conditions</th>
<th>Boundary conditions</th>
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<tbody>
<tr>
<td>I</td>
<td>Well-mixed, fast-flowing rivers</td>
<td>( C(x, 0) = C_0 ) ( 0 &lt; x &lt; L )</td>
<td>( r(x) = 0 ) ( x = L, t &gt; 0 )</td>
</tr>
<tr>
<td>II</td>
<td>Lakes and oceans with low organic matter</td>
<td>( C(x, 0) = C_0 ) ( 0 &lt; x &lt; L )</td>
<td>If volatilization occurs, ( C(x, t) ) ( \frac{O}{Ox} C(x, t) ) ( 0 ) ( x = 0, t &gt; 0 ) If no volatilization occurs, ( D \frac{O}{Ox} C(x, t) = C(x, t) ) ( x = 0, t &gt; 0 )</td>
</tr>
<tr>
<td>III</td>
<td>Lakes and oceans with high organic matter</td>
<td>( C(x, 0) = C_0 ) ( 0 &lt; x &lt; L )</td>
<td>If volatilization occurs, ( C(x, t) ) ( \frac{O}{Ox} C(x, t) ) ( 0 ) ( x = 0, t &gt; 0 ) If no volatilization occurs, ( D \frac{O}{Ox} C(x, t) = C(x, t) ) ( x = 0, t &gt; 0 )</td>
</tr>
<tr>
<td>IV</td>
<td>Poorly-mixed, slow-moving</td>
<td>( C(x, 0) = C_0 ) ( 0 &lt; x &lt; L )</td>
<td>( \frac{O}{Ox} C(x, t) = 0 ) ( x = 0, t &gt; 0 )</td>
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Initial and boundary conditions were imposed which simulate those situations which would likely be found in many of our lakes, rivers, streams, and oceans as well as in planar soil aggregates of saturated structured soils. Four basic aquatic situations were envisioned and from these the initial and boundary conditions were drawn. Table 1 outlines the initial and boundary conditions of the four aquatic systems. In all cases an impermeable layer is assumed to exist at some finite depth, \( x = L \).
terial acts as an interface resistance due to its lower effective resistance to settled solids. The thin layer of undisturbed organic material surrounding the planar aggregates would be \( C_s \). The interface resistance would be due to an immobile water phase film which rounds the planar aggregates.

As in Case III, Case IV assumes that the concentration difference at their interface, but unlike Case III the rate of transfer between the two media is a function of the concentration difference and it is equated to a central-difference approximation to

\[
\frac{\partial C}{\partial t} = \frac{1}{\alpha x} \frac{\partial}{\partial x} \left( D \frac{\partial C}{\partial x} \right)
\]

representative of the conditions which would exist in saturated contaminated streams and rivers. Some small lakes may also fall into this category depending on the degree of mixing due to thermal currents. As in Case III, Case IV assumes that the fluid flowing through the macropores and cracks surrounding the planar aggregates would be \( C_s \). The interface resistance would be due to an immobile water phase film which rounds the planar aggregates.

The numerical solution for Case I was checked against the solution for Case II with the same boundary conditions and grid sizes. The agreement was excellent, and the results confirmed the accuracy of the numerical method. The overall computational time was short, and the method was stable; as a result, the overall computational time can be reduced.

To ensure stability and convergence in the explicit method, the stability and convergence requirements are

\[
\begin{align*}
\text{Stability:} & \quad \left| \frac{\partial C}{\partial t} \right| < \frac{\alpha x}{D} \left[ \left| \frac{\partial C}{\partial x} \right| \right] \\
\text{Convergence:} & \quad \left| \frac{\partial C}{\partial x} \right| < \frac{\alpha x}{D} \left[ \left| \frac{\partial C}{\partial x} \right| \right]
\end{align*}
\]

Using the method of explicit finite-differences which are

\[
\frac{C_{i+1} - C_i}{\Delta t} = \frac{D}{\alpha x} \left( \frac{C_{i+1} - C_i}{\Delta x} \right)
\]

One advantage of the Crank-Nicolson method is that it is stable for any positive value of \( B \) and \( r \), although small values of \( B \) and \( r \) are necessary to ensure stability. The truncation error for the Crank-Nicolson method is

\[
e = 0(\Delta t) + 0(\Delta x)^2
\]

To maintain stability and avoid the occurrence of oscillations, the truncation error must be kept small. One way to achieve this is by selecting \( \Delta t \) and \( \Delta x \) such that

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\frac{1}{\Delta t} \frac{D}{\alpha x} \left( \frac{\Delta x}{\Delta t} \right) = \frac{1}{\Delta t} \frac{D}{\alpha x} \left( \frac{\Delta x}{\Delta t} \right) < 1
\]

This ensures that the system is stable. In the Crank-Nicolson method, the system is tridiagonal so it is possible to use a LU method and then solve by back-substitution.

The overall mass balance error after 10 iterations was never exceeded 2% and all subsequent iterations were < 1%. The overall mass balance error after 10 iterations was never exceeded 2% and all subsequent iterations were < 1%. Using space and time grids of 0.5 cm and 0.1 d, respectively, the method was stable and accurate. The overall mass balance error after 10 iterations was never exceeded 2% and all subsequent iterations were < 1%

Note that the new equilibrium solution concentration, \( C_{+1} \), is

\[
C_{+1} = \frac{1}{1 + (B/\alpha)} C_i
\]

This requires a solution to a set of simultaneous equations at each time step. Fortunately, the system is tridiagonal so it is possible to use a LU method and then solve by back-substitution.

The simplicity of the explicit method is counteracted by the necessity of taking so many time steps that the amount of computation can become unreasonable. For this reason, the method is usually abandoned in favor of the Crank-Nicolson method.

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Representative inorganic and organic chemicals are used to demonstrate the models. Representative adsorption and sediment property parameters are shown. Degradation rates were taken from the literature. The four models. Representative adsorption and sediment property parameters are shown. Degradation rates were taken from the literature.

EXPERIMENTAL PROCEDURE

Table 2 summarizes the chemical and physical parameters used in the four models. Degradation rates were taken from the literature. Some small lakes may also fall into this category depending on the degree of mixing due to thermal currents. As in Case III, Case IV assumes that the fluid flowing through the macropores and cracks surrounding the planar aggregates would be \( C_s \). The interface resistance would be due to an immobile water phase film which rounds the planar aggregates.

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the porous diffusion coefficient can be determined from the molecular diffusion coefficient relationship (Millington and Quirk, 1961) which under saturated conditions results in a value for bromacil and diquat. This value has been used in previous models (Jury et al., 1983). Using the Millington-Quirk relationship accounts for the implicit finite-difference scheme since larger time steps are possible. In all cases, the solution cone is justified although less computational time is needed for the implicit approach.

Since similar molecular weight organic chemicals (i.e., pesticides) vary only slightly in the magnitude of their molecular diffusion coefficients, and a porous diffusion coefficient for bromacil was obtained from papers by Elrashidi and O'Connor (1982) and Sulaiman and Kay (1972), respectively. For diquat, diquat was assumed to be degraded by microorganisms after 1 yr. For these reasons, diquat was assumed to be present in a solution phase, and a porous diffusion coefficient for bromacil was obtained from papers by Elrashidi and O'Connor (1982) and Sulaiman and Kay (1972), respectively. For diquat, diquat was assumed to be degraded by microorganisms after 1 yr. For these reasons, diquat was assumed to be present in a solution phase, and a porous diffusion coefficient for bromacil was obtained from papers by Elrashidi and O'Connor (1982) and Sulaiman and Kay (1972), respectively.

As a cationic herbicide, diquat is strongly adsorbed by sorbents to a greater extent than by anionic herbicides (Buckman and Brady, 1969). The representative porous diffusion coefficient has been calculated using the Millington-Quirk relationship for bromacil and diquat. This value has been used in previous models (Jury et al., 1983). Using the Millington-Quirk relationship accounts for the implicit finite-difference scheme since larger time steps are possible. In all cases, the solution cone is justified although less computational time is needed for the implicit approach.

Results from the implicit approach were performed using both the explicit and implicit approaches. They were selected so that a spatial mesh within both the water and the sediment of a particular aquatic system has been previously modelled (Corwin and Farmer, 1984a; Corwin and Farmer, 1984b). Using an explicit finite-difference approach, simulations involving bromacil and diquat diffusion through a representative sediment (Corwin and Farmer, 1984a; Corwin and Farmer, 1984b) were performed. Simulations were run on a DECStation 3100 computer and figures were produced using a color computer graphics system. Simulations involving bromacil and diquat diffusion through a representative sediment (Corwin and Farmer, 1984a; Corwin and Farmer, 1984b) were performed. Simulations were run on a DECStation 3100 computer and figures were produced using a color computer graphics system.

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The porous diffusion coefficient for bromacil has been found to have a different value than that for diquat. This value has been used in previous models (Jury et al., 1983). Using the Millington-Quirk relationship accounts for the implicit finite-difference scheme since larger time steps are possible. In all cases, the solution cone is justified although less computational time is needed for the implicit approach.

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Figures 1a and 1b provide the equilibrium distributions of the two chemically dissimilar herbicides. The drastically different physicochemical dynamics involved, due to the radically different adsorption behavior of diquat and bromacil, are apparent from the illustrations. Figures 1c and 1d illustrate the simulated diffusion of B for two dissimilar soils, R-30 and Glendale clay. Since the same physical parameters were assumed for each soil (i.e., same $D_p$, $O_v$, and $O_b$), the sharply different diffusion rates indicated by the equilibrium solution concentration curves are once again the result of differences in retardation effects due to adsorption capacity and binding strength differences.

Since this particular aquatic system has been previously discussed at length (Corwin and Farmer, 1984b; Corwin and Farmer, 1985), there is no need for further discussion. Case I is presented primarily as a reference for comparison to the other aquatic systems and as part of a compendium of aquatic systems.
logically inactive state such as when diquat is adsorbed for a longer period of time. The persistence may be in a bio-degradation rate is significantly less for the adsorbed phase than the liquid phase, then the adsorptive ability of a sediment not only retains the chemical, but it provides a means by which a chemical may persist for a longer time within the sediment and permits continued accumulation of chemical in the “stagnant” water layer. This, of course, is due to the tortuous diffusion path which exists within the sediment. The more adsorptive and tortuous that the media is, then the more slowly the chemical moves into the overlying water body. Furthermore, if the sediment would be characteristically low in organic matter so that a thin organic matter layer would not exist at the sediment-water interface. Nevertheless, this retention and inactivation process. The complete removal of the chemical at the air-water interface acts as a driving force to remove the chemical from the sediment due to the larger concentration gradient which is maintained within the system.

The sediment would be characteristically low in organic matter so that a thin organic matter layer would not exist at the sediment-water interface. The air-water interface acts as a quasi-barrier since it retards but does not completely stop the migration of the chemical into the overlying water which increases the residence time within the sediment and permits continued accumulation of chemical in the “stagnant” water layer. This is the result of the lower rate of migration of a chemical into the water body. The “clean” layer of sediment is sandwiched between two “clean” sediment layers. Figures 4a-c illustrate the equilibrium solution concentration distributions for diffusion at the sediment-water interface, or (iii) a contaminated sediment layer is buried beneath a thin layer of “clean” sediment, (ii) a thin contaminated layer exists above the “clean” sediment, and (iii) an advective process is occurring. These figures show that as the chemical passes into the overlying water from the sediment, adsorption equilibrium adjustments occur so that additional chemical is desorbed from the sediment until depletion or until a system equilibrium is reached in Fig. 3c and 3d, approximately 8.7% and 0.15% of the initial mass of diquat is attributable to desorption from the adsorbed phase. This is especially apparent in Fig. 3b since the adsorptive capacity for diquat is so high. More specifically, as the chemical diffuses into the overlying “stagnant” water, the adsorbed phase serves as an additional source of chemical. In comparison to diffusion from a sediment into a fast-flowing water body maintained at zero concentration slowly decreases as it diffuses through the sediment and it is depleted from the equilibrium solution of the system. This is especially apparent in Case II since no adsorption and no degradation are occurring in Fig. 2, the concentration gradient through the sediment is less. The concentration gradient for Case II is significantly slower due to the fact that the migration rate is reduced due to the retardation effect upon the diffusion process. The complete removal of the chemical at the air-water interface [i.e., (O/Ox)C,(L,) = 0, (Case II)] without adsorption and without volatilization, shows the effect of volatilization on the diffusion process. The same solutions for Case II diffusion can be varied to describe situations where (i) a contaminated sediment layer is buried beneath a thin layer of “clean” sediment, (ii) a thin contaminated layer exists above the “clean” sediment, (iii) an advective process is occurring, these figures show that as the chemical reaches a system equilibrium, the net effect is that less chemical is transferred into the overlying water which increases the residence time within the sediment and permits continued accumulation of chemical in the “stagnant” water layer. The accumulated chemical in the “stagnant” water layer is strongly influenced by the retardation effect upon the diffusion process and due to the more complicated diffusion by the adsorption process. Due to the retardation effect upon the diffusion process, the net effect is that less chemical is transferred into the overlying water which increases the residence time within the sediment and permits continued accumulation of chemical in the “stagnant” water layer. The complete removal of the chemical at the air-water interface acts as a driving force to remove the chemical from the sediment due to the larger concentration gradient which is maintained within the system. The retardation effect upon the diffusion process and due to the more complicated diffusion by the adsorption process.
CASE II Equilibrium Solution Concentration (g/L)

(a) Bromacil
- 0.20
- 0.15
- 0.10
- 0.05
- 0.00

(b) Diquat

(c) Boron

(d) Boron

Fig. 3. Equilibrium solution concentration distributions for the Case II diffusion of (a) bromacil, (b) diquat, and (c) and (d) B (R-30 sand and Glendale clay): Co = 0.01 g/L, L1 = -0.2 m, and L2 = 0.1 m = equivalent depth of water in the sediment.

CASE II Equilibrium Solution Concentration

(a) Day
(b) Day
(c) Day

Fig. 4. Equilibrium solution concentration distributions for the Case II diffusion of bromacil using the respective initial conditions outlined in Table 5: Co = 0.01 g/L. (a) "Clean" sediment overlying contaminated sediment: L1 = -0.2 m, L2 = 0.025 m, and L3 = 0.1 m. (b) Contaminated sediment overlying "clean" sediment: L1 = -0.2 m, L2 = 0.025 m, and L3 = 0.1 m. (c) Contaminated sediment sandwiched between "clean" sediment: L1 = -0.2 m, L2 = 0.05 m, L3 = 0.075 m, and L4 = 0.1 m.

Composite media. In high organic matter sediments a thin film of organic matter suspension often exists at the sediment-water interface (Gschwend and Wu, 1985). This film would not have an effective diffusion coefficient similar to either the water or the sediment since as a suspension the pathway through the film is not as tortuous as through the sediment, yet there are still numerous sites for adsorption by the organic material. A means of modeling this essentially dimensionless film is to treat it as an interface resistance between the water...
Fig. 5. Equilibrium solution concentration distributions for Case III diffusion without adsorption and without degradation: $C_i = \text{g/L}, \, \theta = 1.0, \, D = 5.0 \times 10^{-10} \, \text{m}^2/\text{s}, \, \lambda = -0.2 \, \text{m}, \, \text{and} \, \mu = 0.1 \, \text{m}$: (a) No volatilization, $(\partial/\partial x)C_i(0, t) = 0$, and sediment. By doing so, the flux of material across a unit area of the interface is proportional to the difference between the surface concentration of the sediment and the concentration in the "stagnant" water immediately across the film,

$$(\partial/\partial x)C_i(0, t) = \alpha (C_i - C_s)$$

where $\alpha = h/D_p$, $h$ (in meters per second) is some empirically determined proportionality factor analogous to the coefficient of heat transfer in heat conduction problems having a radiation boundary condition, and $C_i$ and $C_s$ are the equilibrium solution concentrations in the "stagnant" water and the sediment, respectively.

The presence of the thin organic matter film creates a discontinuous concentration at the sediment-water interface so that concentrations on either side of the interface are no longer the same (see Fig. 5a and 5b). The net effect of the interface resistance imposed by the organic matter film upon the diffusion process is to further retard the diffusion of the chemical into the water body (compare Fig. 2 and 5). As $\alpha$ decreases the discontinuity of concentration at the sediment-water interface increases which is expected since the resistance across the film has increased (i.e., $h$ is lower) due primarily to greater adsorption, thereby reducing the rate at which the chemical diffuses across the interface into the "stagnant" water (Fig. 6).

Case IV described the diffusion of a solute from a sediment into a "well-stirred" solution which is analogous to a perfect conductor of heat in heat conduction problems. In heat conduction problems, however, the most usual situation is not that the two media at the interface are held at the same temperature, but that heat is lost by

Fig. 6. The effect of $\mu$ upon Case III diffusion assuming no adsorption by the sediment, no volatilization, and no degradation. $C_o = 0.01 \, \text{g/L}, \, D = 5.0 \times 10^{-10} \, \text{m}^2/\text{s}, \, \lambda = 0.2$ (solid line), and $\alpha = 5.0$ (dashed line).

Fig. 7. Sediment equilibrium solution concentration distributions for Case IV diffusion of 11 from (a) R-30 sand, and (b) Glendale clay.
Fig. 8. Sediment equilibrium solution concentration distributions for Case IV diffusion of B into (a) R-30 sand, and (b) Glendale clay. Co = 0.001 g/L, and Cs = 0.01 g/L.

Since B is often found in the drainage water and sometimes in the soils of the arid southwest, it is likely to exhibit Case IV type of diffusion in irrigation and drainage canals. Figures 7a and 7b illustrate the simulated results of a situation where B is diffusing from the irrigation canal sediment into irrigation water which is at a lower B concentration than that of the sediment equilibrium solution. Diffusion curves for both low (R-30) and high (Glendale clay) adsorptive capacity media with assumed equivalent porous diffusion coefficients are shown in Fig. 7. As expected, B diffuses from the high adsorptive capacity soil more slowly. Agricultural drainage waters are often very high in B; as a result, they produce an opposite situation where boron gradually diffuses into the sediment equilibrium solution which is at a lower B concentration (see Fig. 8a and 8b).

The cycling of high and low B concentration irrigation waters yields interesting equilibrium solution concentration distribution curves for diffusion in sediments of irrigation canals. Figure 9 shows a set of curves for Glendale clay. For the first 200 d the B concentration of the surrounding fluid is maintained at 0.01 g/L, after which it is decreased to 0.001 g/L. Since the initial B concentration in the sediment equilibrium solution is 0.001 g/L, B gradually diffuses into the sediment. As soon as the B concentration of the surrounding fluid (Cs) is decreased to 0.001 g/L there is a quick decrease in B within the sediment solution nearest to the sediment-water interface. The B concentration of the sediment near the sediment-water interface continues to decrease and to approach Cs, while at the impermeable layer interface there is initially an increase in concentration due to the redistribution of B from the upper sediment.
ment region (0.015-0.04 m). Gradually a uniform sediment solution of C concentration of Cs is approached. As mentioned, this particular model has application to diffusion in soil aggregates. A simulation of diffusion of B through a planar soil aggregate sheet of thickness 2L where L = 0.001 m shows that as different quality irrigation waters are applied to soils the aggregates can act as reservoirs or sources of B to the soil solution of the large pores and cracks surrounding the aggregates. So, even though a system may appear to be at steady state the diffusion of B into or out of soil aggregates of a structured soil could result in continuing fluctuations in B concentration over extended time periods. This effect has definite ramifications for the agricultural reclamation of high B soils.

**SUMMARY**

Since organisms within the aquatic environment are often very sensitive to certain organic pesticides and since surface waters serve as irrigation water for crops, it is important to have an understanding of the physicochemical dynamics of chemical-sediment-water systems and of aggregated soil systems. The four models presented provide a means of assessing the various interactions involved in diffusion in simplified aquatic and structured soil systems, as well as a means of assessing the potential threat that a chemical will pose to different compartments of the aquatic and soil environments by providing information concerning their migratory propensity.

As the future demand for water increases, the increased potential for the reuse of high B drainage water as a source of agricultural irrigation water becomes more likely. In order to manage these drainage waters in a way that maximizes their use yet minimizes their deleterious effects to plants, an understanding of the distribution and movement of boron in soils is essential. The modeling of the physical process of solute flow in one-dimension for homogeneous, unstructured porous media is well understood, but aggregated soils present additional complexities as revealed by the asymmetric displacement patterns which are often found in structured soils. In structured soils the bulk of the flow of water and transport of chemicals generally occurs through the cracks between the soil aggregates. The exchange of solutes between the aggregates and these cracks is controlled by diffusion processes. These models, particularly the Case IV model, can assist in determining the contribution which diffusion makes to solute flow in structured soils.