

**FINITE ELEMENT ANALYSIS OF MULTICOMPONENT CONTAMINANT  
TRANSPORT INCLUDING PRECIPITATION-DISSOLUTION REACTIONS**

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**INTRODUCTION**

The determination of the fate of contaminants that enter groundwater systems pose difficult mathematical problems for the modeler. This is particularly true when complex multi component interactions occur among mobile and immobile species. The types of chemical reactions that can occur include; acid-base, adsorption-desorption, complex formation, ion exchange, oxidation-reduction and precipitation-dissolution. This paper will focus on the analysis of precipitation-dissolution reactions.

In multi-component transport systems, competition for sorptive sites can have unexpected results. Preferential ion-exchange or surface complexation can produce a concentration "spike" within the domain that exceeds the solute's source strength. This can occur whenever a rapidly moving component occupies surface sites and then is displaced by competition with some less mobile species. The concentration "spike" that develops in the neighborhood of the competition front will continue to grow as the solution penetrates further into the domain. Eventually this can grow until the solution's solubility constraints are violated. At this point a precipitate should form, and then dissolve once the concentration spike has passed. Therefore, to be successful, the mass transport model must be capable of accommodating both precipitation and dissolution reactions even for cases where the source strengths satisfy all solubility constraints.

In this paper, different formulations of the equations governing multicomponent mass transport with solution phase complexation, competitive adsorption and precipitation-dissolution are developed and their relative merits discussed. A finite element method of solution of one of the formulations is presented along with a sample simulation.

## MODEL PROBLEM

To avoid the complexity that often accompanies generality, the following model problem is considered. Let  $c_1, c_2$  be the concentrations (mass per unit volume of fluid) of two metals,  $c_3$  the concentration of a nonadsorbing ligand and  $c_{13}$  the concentration of a soluble complex formed by the reaction of constituents one and three. A mass balance on each species in solution yields

$$Lc_1 + \partial c_1 / \partial t + \partial s_1 / \partial t + r_1 = 0 \quad (1)$$

$$Lc_2 + \partial c_2 / \partial t + \partial s_2 / \partial t + \partial p / \partial t = 0 \quad (2)$$

$$Lc_3 + \partial c_3 / \partial t + \partial p / \partial t + r_3 = 0 \quad (3)$$

$$Lc_{13} + \partial c_{13} / \partial t + r_{13} = 0 \quad (4)$$

where the convection-diffusion operator in one dimension is

$$L(\cdot) = -\frac{1}{P_e} \partial^2(\cdot) / \partial x^2 + \partial(\cdot) / \partial x, \quad (5)$$

and  $P_e$  is the Peclet number. In the above system  $c_1$  and  $c_2$  are presumed to engage in competitive adsorption, thus  $s_1, s_2$  are the concentrations of the sorbed forms of  $c_1, c_2$  respectively. Also,  $r_1, r_3, r_{13}$  are the rates of accumulation of  $c_1, c_3, c_{13}$  due to reaction in solution. It is also presumed that a heterogeneous precipitation-dissolution reaction occurs between species two and three, and  $p$  is the concentration of the precipitate.

Each reaction occurring in the system (1) - (4) will be discussed separately.

Solution Phase Complexation. The reaction which forms the soluble complex is



where  $(\cdot)$  denotes moles of the indicated species, thus the symbol  $\hat{c}_1$ , for example, means one mole of species one. As noted above, the concentration of species one is  $c_1 \equiv [\hat{c}_1]$ . For ease in presentation, all stoichiometric coefficients are taken as one, and order corresponds to stoichiometry.

The reaction rates for (6) are

$$r_1 = r_3 = -r_{13} = k_r c_{13} - k_f c_1 c_3 \quad (7)$$

For the analysis herein, the local equilibrium assumption is made. This means that  $k_r \rightarrow \infty$  and  $k_f \rightarrow \infty$  at a fixed ratio

$K_{13} = k_f/k_r$  while the bounded and not ident

$$c_{13} = K_{13} c_1 c_3$$

This is simply the la

Sorption. For the sy assumed to be surface ion exchange leads to reactions are

$$\hat{c}_1 + \hat{x} \rightleftharpoons \hat{c}_1 - \hat{x} \rightleftharpoons \dots$$

$$\hat{c}_2 + \hat{x} \rightleftharpoons \hat{c}_2 - \hat{x} \rightleftharpoons \dots$$

where  $\hat{x}$  indicates an assumed that the total sites (free plus occ

$$x + s_1 + s_2 = x_T$$

Again invoking local action for (9) and ( competitive Langmuir

$$s_1 = x_T K_1 c_1 / (1 + \dots)$$

$$s_2 = x_T K_2 c_2 / (1 + \dots)$$

Precipitation-dissol

$$\beta \equiv \hat{c}_2 - \hat{c}_3 \rightleftharpoons \hat{c}_2 + \dots$$

occurs to enforce th

$$c_2 c_3 < K_{23}$$

where  $K_{23}$  is the sol inequality constraint present only when ( $c_2 c_3 < K_{23}$ ).

PROBLEM FORMULATION

The rates  $r_1, r_3, r_{13}$  follows. Add (1) to yield,

$$L(c_1 + c_{13}) + \partial \dots$$

$$L(c_3 + c_{13}) + \partial \dots$$

$K_{13} = k_f/k_r$  while the rates  $r_1, r_3, r_{13}$  are assumed to be bounded and not identically zero. The condition for this is

$$c_{13} - K_{13} c_1 c_3 = 0. \quad (8)$$

This is simply the law of mass action for (6).

Sorption. For the system (1) - (4), the sorptive mechanism is assumed to be surface complexation (adsorption-desorption). Ion exchange leads to a similar mathematical system. The reactions are



where  $\bar{x}$  indicates an immobile surface site. It is further assumed that the total concentration of immobile surface sites (free plus occupied) is constant, i.e.,

$$x + s_1 + s_2 = x_T. \quad (11)$$

Again invoking local equilibrium, writing the law of mass action for (9) and (10) and using (11) leads to the familiar competitive Langmuir isotherms,

$$s_1 = x_T K_1 c_1 / (1 + K_1 c_1 + K_2 c_2) \quad (12)$$

$$s_2 = x_T K_2 c_2 / (1 + K_1 c_1 + K_2 c_2) \quad (13)$$

Precipitation-dissolution. The following reaction



occurs to enforce the constraint,

$$c_2 c_3 < K_{23}, \quad (15)$$

where  $K_{23}$  is the solubility product. In essence, (15) is an inequality constraint on the system (1) - (4), with the solid present only when (15) is satisfied but with  $p = 0$  if  $c_2 c_3 < K_{23}$ .

#### PROBLEM FORMULATION

The rates  $r_1, r_3, r_{13}$  may be eliminated as unknowns as follows. Add (1) to (4) and (3) to (4), utilizing (7) to yield,

$$L(c_1 + c_{13}) + \partial(c_1 + c_{13})/\partial t + \partial s_1/\partial t = 0 \quad (16)$$

$$L(c_3 + c_{13}) + \partial(c_3 + c_{13})/\partial t + \partial p/\partial t = 0. \quad (17)$$

The number of unknowns in the system is now seven;  $c_1, c_2, c_3, c_{13}, s_1, s_2, p$  and there are seven equations; (2), (16), (17), (18), (12), (13), (15). If  $c_2 c_3 < K_{23}$  there is one less equation, (15), and one less unknown,  $p$ . This approach to problem formulation has recently been taken by Miller and Benson (1983). Therein a finite difference approximation, in space and time, was used for equations (2) and (17). The total number of nonlinear algebraic equations to be solved every time step is then seven times the number of grid points, minus the number of specified degrees of freedom. An alternate formulation is obtained by introducing the total soluble concentration of each component as a primary unknown, i.e. let

$$u_1 = c_1 + c_{13} \quad (18)$$

$$u_2 \equiv c_2 \quad (19)$$

$$u_3 = c_3 + c_{13} \quad (20)$$

Equations (2), (16) and (17) then become,

$$Lu_1 + \partial u_1 / \partial t + \partial s_1 / \partial t = 0 \quad (21)$$

$$Lu_2 + \partial u_2 / \partial t + \partial s_2 / \partial t + \partial p / \partial t = 0 \quad (22)$$

$$Lu_3 + \partial u_3 / \partial t + \partial p / \partial t = 0 \quad (23)$$

This has simply added three additional equations and three additional unknowns to the system. Note however that (8), the law of mass action for the solution phase reaction, may be substituted into (18) through (20) and that system inverted to yield,

$$c_i = \bar{c}_i(u_1, u_3) \quad i = 1, 3 \quad (24)$$

In (24), the distinction between a function,  $\bar{c}_i$ , and its value,  $c_i$ , is made. The fact that an equation like (24) may be written even for a more general system is guaranteed by the implicit function theorem. Equation (24), in the general case, may be implicit, but since a numerical solution is anticipated this is acceptable.

Equation (24) can now be substituted into (12), (13) and (15) to yield,

$$s_i = \bar{s}_i(u_1, u_2, u_3) \quad i = 1, 2 \quad (25)$$

$$\bar{c}_2 \bar{c}_3 = K_{23} \quad (26)$$

Equation (25) is now substituted into (21) and (22) to yield

$$Lu_1 + \partial u_1 / \partial t + \partial \bar{s}_1 / \partial t = 0 \quad (27)$$

$$Lu_2 + \partial u_2 / \partial t +$$

In essence the number is four;  $u_1, u_2, u_3$  and (26). For large unknowns, from the dramatic.

The fundamental difference present in the system of accumulation of always be expressed concentration of all surface sites. Thus, considered a nonlinear term, however is concentrations, in "constraint" equation formulation the solid retained as a primary

Note that the total actually been reduced still must be evaluated process. However, discrete points in than expanding the primary unknowns as discussed.

In equations (28) the relation of  $u_2$  to  $u_3$  due to stoichiometry of the differentiates the problem of a system where this ratio is "constraint surface" another formulation is removed as a primary (28) to yield

$$L(u_2 - u_3) + \partial$$

The primary unknown equations: (26), stoichiometric coefficients of (23) and (28) will be calculated during done using (23) or available.

If there is no sorption difference,  $u_2 - u_3$  quantity can be in

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(21) and (22) to yield

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$$Lu_2 + \partial u_2 / \partial t + \partial s_2 / \partial t + \partial p / \partial t = 0 \quad (28)$$

In essence the number of primary unknowns has been reduced to four;  $u_1, u_2, u_3$  and  $p$  with four equations; (27), (28), (23) and (26). For larger systems the reduction in primary unknowns, from the formulation discussed above, is even more dramatic.

The fundamental difference between the two types of solids present in the system should perhaps be noted here. The rate of accumulation of a particular component due to sorption can always be expressed as a function of the total soluble concentration of all components engaged in competition for surface sites. Thus, in effect, the sorption term can be considered a nonlinear source/sink term. The precipitation term, however is clearly not a function of the solution phase concentrations, in essence because  $p$  does not appear in the "constraint" equation (26). Therefore in the second formulation the solid accumulated due to precipitation is retained as a primary unknown.

Note that the total number of unknowns in the system has not actually been reduced; the secondary unknowns  $c_{13}, s_1, s_2$  still must be evaluated during the course of the solution process. However, the solution of (24), (25) and (8) at discrete points in space and time is certainly less effort than expanding the total system to include these variables as primary unknowns as is done in the first formulation discussed.

In equations (28) and (23) the ratio of the rate of accumulation of  $u_2$  to  $u_3$  due to precipitation is fixed by the stoichiometry of the reaction (14). It is this fact which differentiates the system considered here from the classic problem of a system subjected to an inequality constraint, where this ratio is determined by the orientation of the "constraint surface"; Dorny (1975). This fact also allows another formulation to be developed where the precipitate  $p$  is removed as a primary unknown. Simply subtract (23) from (28) to yield

$$L(u_2 - u_3) + \partial(u_2 - u_3) / \partial t + \partial s_2 / \partial t = 0 \quad (29)$$

The primary unknowns are now three;  $u_1, u_2, u_3$  with three equations: (26), (27) and (29). In the case where the stoichiometric coefficients are not one, a linear combination of (23) and (28) will still eliminate  $p$ . Again  $p$  must still be calculated during the solution process, but this is easily done using (23) or (28) once the primary unknowns are available.

If there is no sorbed form of  $u_2$  then (29) indicates that the difference,  $u_2 - u_3$  is transported conservatively and this quantity can be introduced as a primary unknown. This type of

problem has been recently discussed by Rubin (1983). This approach cannot be taken with sorption, however, since  $s_2$  is not a function of the difference  $u_2 - u_3$ .

It would seem that this last formulation is the most attractive having the fewest number of primary unknowns. However there are other considerations, such as; ease in programming, efficiency, and ease in generalizing to a larger system. Space does not allow a complete comparison of these alternatives here. Rather, a numerical procedure and sample problem will be presented for one formulation; the primary system governed by (27), (28), (23) and (26), which retains  $p$  as an unknown.

#### NUMERICAL SOLUTION

The unknown functions in (27), (28), (23) and (26) are interpolated as follows

$$u_i(x,t) = \underline{\phi}(x) \cdot \underline{u}_i, \quad (30)$$

$$s_i(x,t) = \underline{\phi}(x) \cdot \underline{s}_i, \quad (31)$$

$$p(x,t) = \underline{\psi}(x) \cdot \underline{p}, \quad (32)$$

where, for example,  $\underline{u}_i$  is a vector whose components are concentrations,  $u_i$  at the nodal points, i.e.,

$$\underline{u}_i = (u_{i1}, u_{i2}, \dots, u_{iN}) \quad (33)$$

In the example to follow, the vector of shape functions,  $\underline{\phi}$  are the "hat" functions, Strang and Fix (1973). Since  $p$  may exhibit discontinuities it should not be interpolated with  $C^0$  shape functions. Here a vector of Dirac delta functions centered at the nodal points is used. Thus

$$p(x,t) = \begin{cases} p_i & \text{if } x = x_i \text{ (ith nodal point)} \\ 0 & \text{if } x \neq x_i. \end{cases} \quad (34)$$

Employing a standard weighted residual approach then requires that the solubility constraint be satisfied only at the nodal points and precipitate is only accumulated at the nodal points. The weighted residual formulation reduces (27), (28), (23) and (26) to a set of coupled ordinary differential and algebraic equations. The ordinary differential equations are converted to algebraic equations by a finite difference approximation. Herein the backward difference scheme is used. The resulting set of nonlinear algebraic equations are solved iteratively using Newton's method and the solution is marched through time. The constraint, (26), is presumed not to be in effect

initially, and it is checked is either "turned-on" or

#### RESULTS

A simulation was performed above and the results are shown. In order to isolate the effects as possible, aqueous complexing solutes  $u_2, u_3$  become simply  $c_1, c_2$  solutes were fixed at the  $c_0$ . The gradients of all species beyond the column length  $L$  are infinite domain. Zero initial  $c_1, c_2$  and  $p$  while  $c_3$  was concentration equal to its source chemical constants used were  $K_{23} = 5.0$ . To show the effect was performed with  $K_{23} = 5.0$  (tion) and the results compared

Figures 1 and 4 show the adsorbed solids  $s_1$  and  $s_2$  respectively. While precipitation the results of sorption are evident. A chromatogram the  $c_1$  front displaces  $c_2$  solution. It is the greatest which causes the concentration strength. Figures 2 and 3 files at 5.0 pore volumes. Without precipitation  $c_3$  condition equals the source strong chromatographic effect

Concentration profiles for are given in Figure 5. constant. There is a zone above its source strength aqueous phase as the solid below its source strength file is also altered concentration exhibits two zones; the source strength due to decrease due to competition. "competition zone" is not removed from solution by behavior is effected by the species, the initial condition solubility product,  $K_{23}$ .

The concentration of the Figure 5. As discussed

by Rubin (1983). This  
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initially, and it is checked at each node every iteration and  
 is either "turned-on" or "turned-off" appropriately.

RESULTS

A simulation was performed for the model problem introduced  
 above and the results are summarized in Figures 1 through 6.  
 In order to isolate the effects of precipitation as much as  
 possible, aqueous complexation was not considered. Thus  $u_1$ ,  
 $u_2$ ,  $u_3$  become simply  $c_1$ ,  $c_2$ ,  $c_3$ . The source strength of all  
 solutes were fixed at the upstream boundary and taken equal to  
 $c_0$ . The gradients of all solutes were set to zero at the  
 downstream boundary, which was located a sufficient distance  
 beyond the column length that the model simulates a semi  
 infinite domain. Zero initial conditions were specified for  
 $c_1$ ,  $c_2$  and p while  $c_3$  was given a constant initial con-  
 centration equal to its source strength. The physical and  
 chemical constants used were:  $P_e = 40$ ,  $K_1 = 10.0$ ,  $K_2 = 1.0$ ,  
 $x_T = 5.0$ . To show the effect of precipitation the simulation  
 was performed with  $K_{23} = 1.2$  and  $K_{23} = \infty$  (i.e., no precipita-  
 tion) and the results compared.

Figures 1 and 4 show the concentration profiles for the  
 adsorbed solids  $s_1$  and  $s_2$ , without and with precipitation  
 respectively. While precipitation has very little effect on  
 the results of sorption the driving force for the precipitation  
 is evident. A chromatographic effect is seen as the arrival of  
 the  $c_1$  front displaces  $c_2$  from the surface and thus back into  
 solution. It is the greater affinity of the  $c_1$  for adsorption  
 which causes the concentration of  $c_2$  to rise above its source  
 strength. Figures 2 and 5 show the soluble concentration pro-  
 files at 5.0 pore volumes, without and with precipitation.  
 Without precipitation  $c_3$  is conservative and since the initial  
 condition equals the source strength,  $c_3$  remains constant. The  
 strong chromatographic effect is clearly displayed in Figure 2.

Concentration profiles for the simulation with precipitation  
 are given in Figure 5. The concentration of  $c_3$  is no longer  
 constant. There is a zone where the concentration is elevated  
 above its source strength due to the addition of  $c_3$  to the  
 aqueous phase as the solid dissolves. Beyond this zone  $c_3$  is  
 below its source strength due to precipitation. The  $c_2$  pro-  
 file is also altered considerably from Figure 2. It also  
 exhibits two zones; the first shows a small increase over the  
 source strength due to dissolution and the second higher pla-  
 teau due to competition. The concentration in this  
 "competition zone" is not as high as in Figure 2 because  $c_2$  is  
 removed from solution by precipitation. This two stage beha-  
 vior is effected by the relative source strengths of the solu-  
 tes, the initial conditions, adsorption, as well as the  
 solubility product,  $K_{23}$ .

The concentration of the precipitate, p, is also given in  
 Figure 5. As discussed in the previous section the solubility

constraint was imposed pointwise at the nodes, and thus precipitate was only accumulated at the nodes. For graphical purposes, an average concentration was computed at each node and these values then interpolated. This was done in order to show the relative amount and position of the precipitate to the aqueous components. Breakthrough curves for the simulations without and with precipitation are presented in Figures 3 and 6 respectively. Figure 6 shows clearly the lowering of the  $c_2$  peak. A second zone where  $c_2$  is greater than the source strength due to dissolution is exhibited from approximately six to ten pore volumes. The precipitation and dissolution zones are also clearly displayed in the  $c_3$  curve. For comparative purposes the precipitate breakthrough is also given.

#### CONCLUSION

Several formulations of the equations governing multicomponent mass transport with chemical interactions including precipitation-dissolution reactions were presented. A finite element solution algorithm was presented with a sample simulation. The simulation was for a system where the concentration of one component rises significantly above its source strength due to competitive adsorption with a less mobile solute. With the imposition of a solubility constraint this increase of soluble concentration above the source strength was significantly reduced. This simulation serves as an example of the importance of modeling precipitation-dissolution even in cases where there is no solid initially present and the source strengths satisfy all solubility constraints.

#### ACKNOWLEDGEMENT

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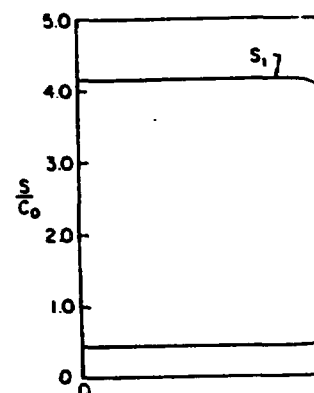


Figure 1. Sorbed

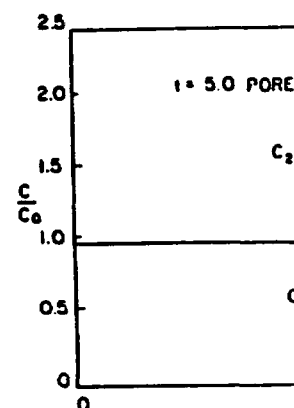


Figure 2. Solution

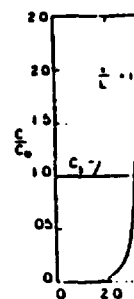


Figure 3. Break



nodes, and thus precise. For graphical purposes, the concentration was computed at each node and was done in order to show the precipitate to the nodes for the simulations presented in Figures 3 and 4. By the lowering of the concentration greater than the source strength from approximately 40 to 30, the concentration and dissolution curve is  $c_3$  curve. For comparison, the breakthrough curve is also given.

governing multicomponent systems including precipitation are presented. A finite difference method was used with a sample simulation where the concentration of the solute above its source strength is mobile solute. With this increase of concentration, the strength was significant as an example of the dissolution even in cases where the source strength is constant and the source is constrained.

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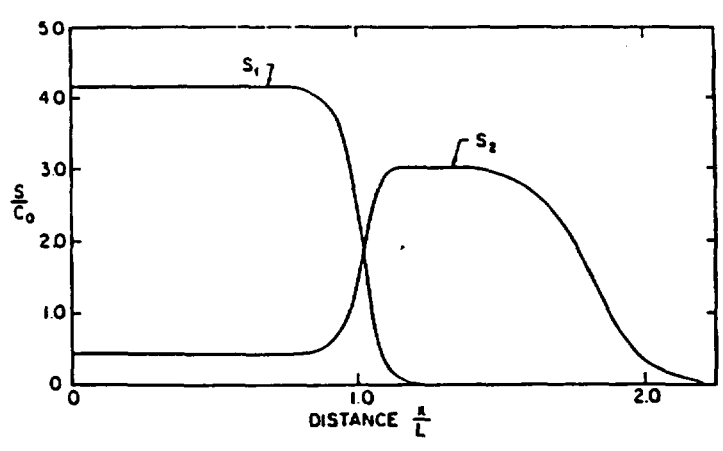


Figure 1. Sorbed Form Profiles without Precipitation

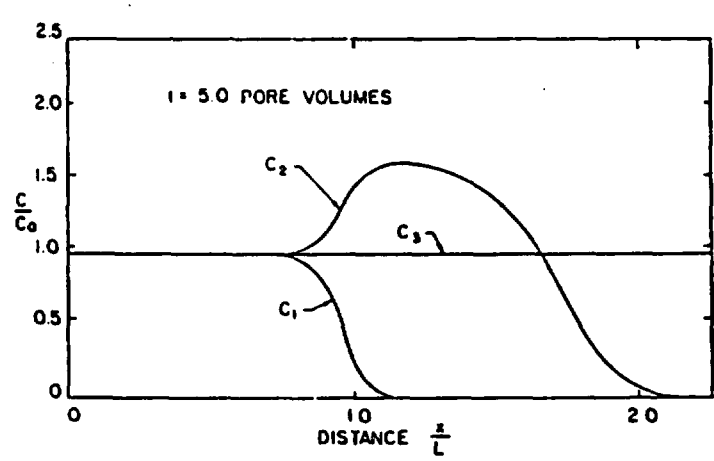


Figure 2. Solute Profiles without Precipitation

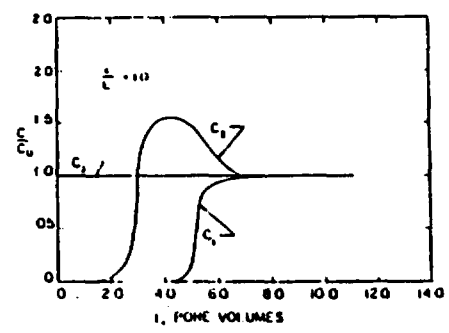


Figure 3. Breakthrough Curves without Precipitation

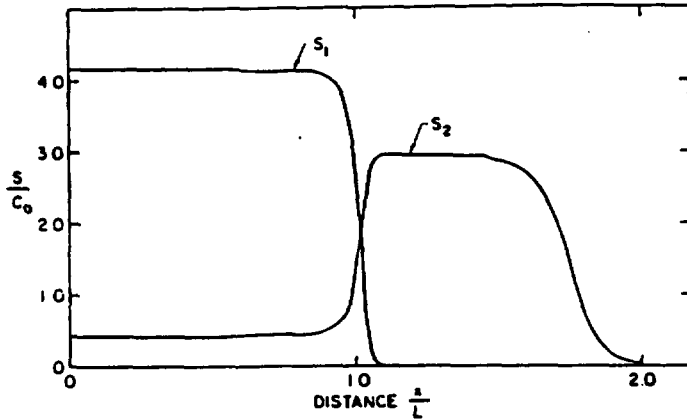


Figure 4. Sorbed Form Profiles with Precipitation

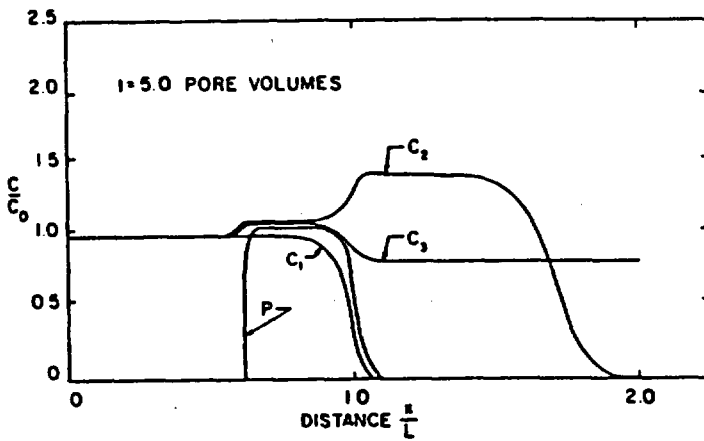


Figure 5. Solute Profiles with Precipitation

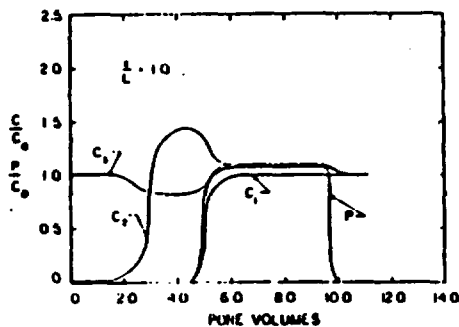


Figure 6. Breakthrough Curves with Precipitation

GROUNDWATER FLOW AND MASS  
PARAMETRIC STUDY

A. Pandit and S. C. Anand

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INTRODUCTION

The subject of saltwater :  
been receiving wide atten  
(1960) was the first inve  
solution for the coupled  
an idealized, rectangular  
Fourier-Galerkin double s  
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MATHEMATICAL FORMULATION

The mathematical model is  
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ity and density terms.

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