

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

David J. Kirkner, Howard W. Reeves, and Aaron A. Jennings

University of Notre Dame, Notre Dame, IN 46556

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

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

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

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

$$s_1 = x_T K_1 c_1 / (1$$

$$s_2 = x_T K_2 c_2 / (1$$

Precipitation-dissol

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

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 follows. Add (1) t yield,

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

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

$K_{13} = k_f/k_r$ 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 In order to isolate the effect possible, aqueous complex u_2, u_3 become simply c_1, c_2 solutes were fixed at the c_0 . The gradients of all downstream boundary, which beyond the column length L infinite domain. Zero in 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 is evident. A chromatogram the c_1 front displaces concentration. 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 solution below its source strength file is also altered concentration exhibits two zones; the source strength due to displacement due to competition. "competition zone" is not removed from solution by precipitation is effected by the precipitation, the initial condition solubility product, K_{23} .

The concentration of the Figure 5. As discussed

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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 concentration equal to its source strength. The physical and chemical constants used were: $P_e = 40, K_1 = 10.0, K_2 = 1.0, \alpha_T = 5.0$. To show the effect of precipitation the simulation was performed with $K_{23} = 1.2$ and $K_{23} = \infty$ (i.e., no precipitation) 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 profiles 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 profile 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 plateau 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 behavior is effected by the relative source strengths of the solutes, 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.

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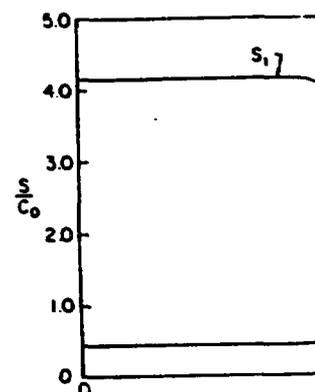


Figure 1. Sorbed

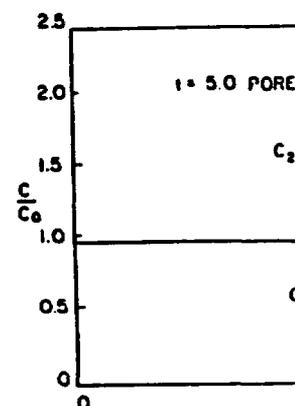


Figure 2. Solution

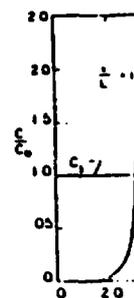


Figure 3. Break

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, the concentration decreased from approximately 40 to 0. The concentration 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 decreases as mobile solute. With an increase in the source strength, the concentration of the solute was significantly higher as an example of the effect of precipitation even in cases where the source strength is constant and the source strength is constant.

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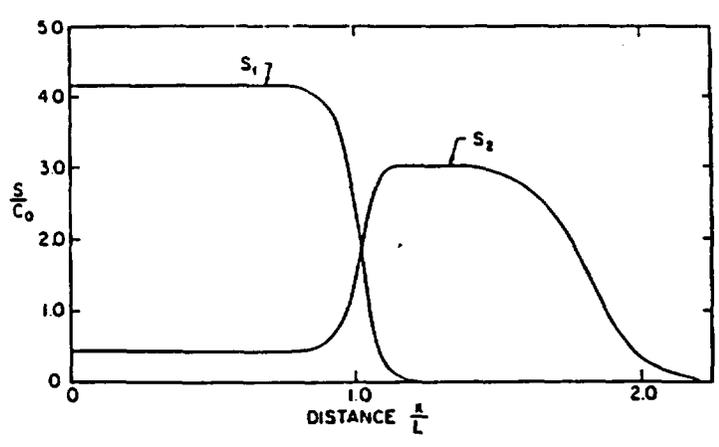


Figure 1. Sorbed Form Profiles without Precipitation

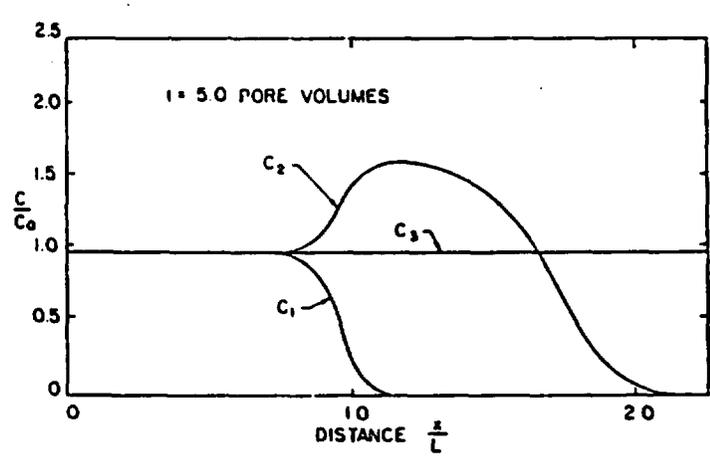


Figure 2. Solute Profiles without Precipitation

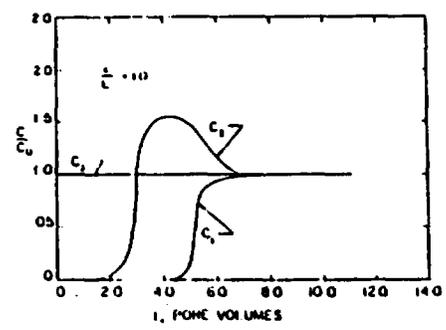


Figure 3. Breakthrough Curves without Precipitation

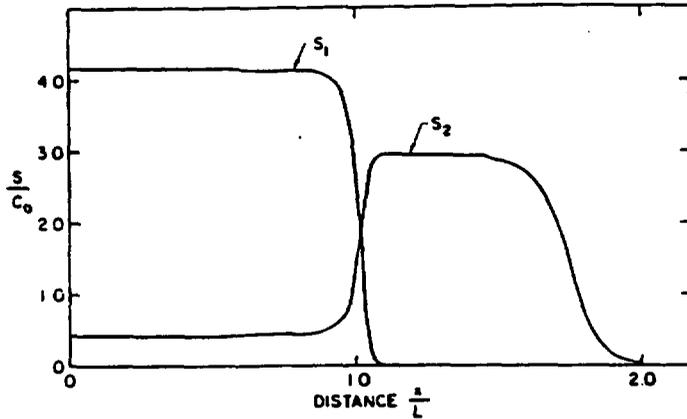


Figure 4. Sorbed Form Profiles with Precipitation

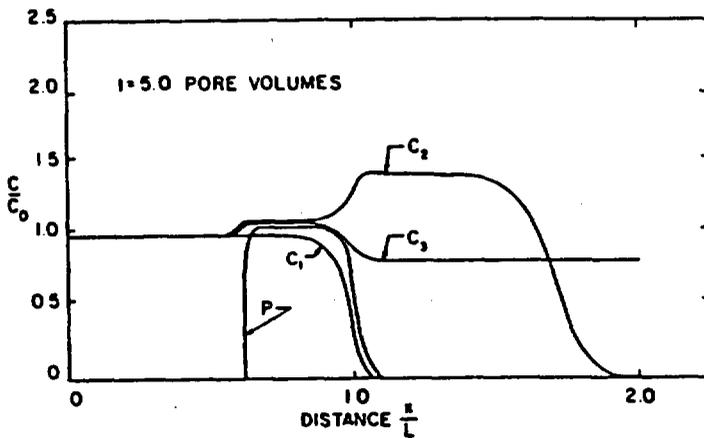


Figure 5. Solute Profiles with Precipitation

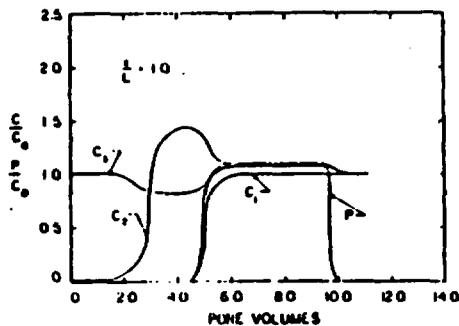


Figure 6. Breakthrough Curves with Precipitation

GROUNDWATER FLOW AND MASS
PARAMETRIC STUDY

A. Pandit and S. C. Anand

Assistant Professor, Florida
Professor, Clemson Univer

INTRODUCTION

The subject of saltwater :
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MATHEMATICAL FORMULATION

The mathematical model is
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