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CHEMTRN USER'S MANUAL

C.W. Miller

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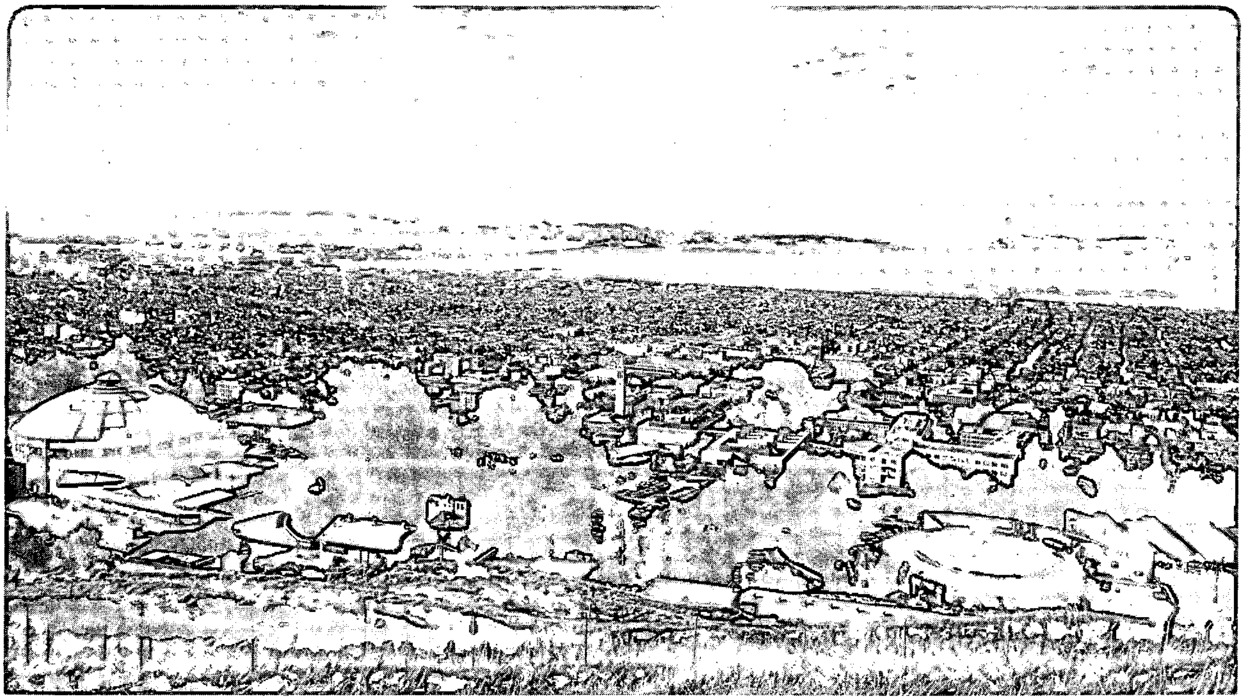

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CHEMTRN USER'S MANUAL

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March 1983

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TABLE OF CONTENTS

LIST OF FIGURES

ABSTRACT

A user's manual for operation of the chemical transport simulator CHEMTRN is presented. The manual includes descriptions of the basic equations to be solved, the solution procedure, information needed for the simulations, and the input parameters. Also included are four examples of simulations with their input and output listings, and a listing of the CHEMTRN source code with embedded comments.

CHEMTRN USER'S MANUAL

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INTRODUCTION

CHEMTRN is a computer code which simulates the transport of chemical species in groundwater systems. The program is based on thermodynamic principles. Equilibrium is assumed in all chemical reactions and thermodynamic activities of all reacting species are related by mass-action expressions. The solution procedure is flexible enough so that kinetic effects and effects of temperature gradients may be included with minor modifications. CHEMTRN can simulate either one-dimensional or purely radial flow in porous media using a grid with either a uniform or a variable spacing. The program includes the effects of dispersion/diffusion, advection, sorption via ion exchange or surface complexation, aqueous complexation, precipitation/dissolution of solids, and the dissociation of water. No data base is provided with the program; the user must supply the equilibrium constants and the stoichiometric coefficients for the reactions of interest.

This user's manual includes sections describing the basic equations solved, the solution procedure, a description of the different types of boundary conditions used in the program, the types of information needed for each problem, the input parameters, four different examples with sample input and output, an alphabetical listing of the input variables, and a listing of the program. The program listing includes comments which describe the input parameters and definitions of some of the variables used within the program.

BASIC EQUATIONS

CHEMTRN defines all reactions involving the formation of aqueous complexes, the sorption of aqueous species, and the formation of precipitates by mass-action relations. This procedure simplifies the problem formulation. The basic equations solved in CHEMTRN for chemical changes and transport of aqueous species are described below.

Aqueous phase complexation and formation of precipitates

Given the basis set of N_b species, $A_j^{n_j}$, the reactions for the formation of a complex $B_i^{n_{ci}}$ and a precipitate G_k are written,

$$\sum_{j=1}^{N_b} a_{ij} A_j^{n_j} \rightleftarrows B_i^{n_{ci}}, \tag{R1}$$

and

$$\sum_{j=1}^{N_b} s_{kj} A_j^{n_j} \rightleftarrows G_k, \tag{R2}$$

where a_{ij} and s_{kj} are the stoichiometric reaction coefficients, n_j is the charge of the basis species, and n_{c_i} is the charge of the complex. Assuming chemical equilibrium, mass action expressions can be written for each of these cases. For the formation of a complex,

$$K_i = \frac{\left[B_i^{n_{c_i}}\right]}{\prod_{j=1}^{N_b} [A_j^{n_j}]^{a_{ij}}}, \tag{1}$$

where the square brackets denote the thermodynamic activity of a species and K_i is the equilibrium constant. For the dissolution of a precipitate,

$$K_k = \prod_{j=1}^{N_b} [A_j^{n_j}]^{s_{kj}} \tag{2}$$

where K_k is the solubility product of the solid G_k. In CHEMTRN, the activity of a dissolved species is approximated by the relation,

$$[A_j^{n_j}] = \gamma_j m_j \tag{3}$$

where γ_j is an activity coefficient and m_j is the mass concentration of the species in moles per liter solution. Equation (1) then becomes

$$K_i = \frac{\gamma_{c_i} m_{c_i}}{\prod_{j=1}^{N_b} (\gamma_j m_j)^{a_{ij}}} \tag{4}$$

where m_{c_i} is the concentration of the complex $B_i^{n_{c_i}}$ in moles per liter.

The activity coefficients of the aqueous species (basis species and complexes) are functions of temperature, pressure, and chemical composition. In CHEMTRN, they are approximated using the Davies equation [*Stumm and Morgan*, 1970],

$$\log_{10} \gamma_j = -\frac{1}{2} n_j^2 \left(\frac{\sqrt{I}}{1 + \sqrt{I}} - 0.3I \right), \tag{5}$$

where I is the ionic strength defined by

$$I = \frac{1}{2}\left(\sum_{j=1}^{N_b} n_j^2 m_j + \sum_{i=1}^{N_c} n_{c_i}^2 m_{c_i}\right), \tag{6}$$

and N_c is the number of complexes in the the aqueous phase. The activity of water is taken to be unity. (Note that $0.3I$ has been used in the Davies equation instead of $0.2I$ as per footnote, p.83 of *Stumm and Morgan* [1970].)

Sorption via ion exchange

The mass transfer of ions and complexes from the aqueous phase to the solid phase is simulated by either ion exchange or surface complexation. For an ion exchange process, the charge on the solid surface and the number of sites available for exchange reactions are constant. Aqueous species are sorbed on the solid phase by displacing exchangeable ions. Because the charge on the solid matrix does not change, a species which is sorbed must displace an equivalent amount of charge. For species $A_1^{n_1}$ exchanging with species $A_2^{n_2}$,

$$n_2 A_1^{n_1}(aq) + n_1 \overline{A}_2 \rightleftarrows n_2 \overline{A}_1 + n_1 A_2^{n_2}(aq), \tag{R3}$$

where $\overline{A}_j$ denotes the sorbed component. This reaction is described by a thermodynamic equilibrium constant,

$$K_{eq} = \frac{[\overline{A}_1]^{n_2} [A_2^{n_2}]^{n_1}}{[A_1^{n_1}]^{n_2} [\overline{A}_2]^{n_1}}, \tag{7}$$

where the square brackets again denote activities. Because of the present lack of data for estimating activity coefficients for the surface phase, CHEMTRN approximates activities in the surface phase by an ideal solution model in which

$$[\overline{A}_j] = \frac{\overline{m}_j}{\overline{m}_T}, \tag{8}$$

where $\overline{m}_j$ is the concentration of species j on the surface phase, $\overline{m}_T$ is the total concentration sorbed in the surface phase given by

$$\overline{m}_T = \sum_{j=1}^{\overline{N}_b} \overline{m}_j + \sum_{i=1}^{\overline{N}_c} \overline{m}_{c_i}, \tag{9}$$

$\overline{N}_b$ is the number of sorbed basis species, $\overline{N}_c$ is the number of sorbed complexes, and $\overline{m}_{c_i}$ is the concentration of sorbed complexes. The units of $\overline{m}_j$, $\overline{m}_{c_i}$, and $\overline{m}_T$ are moles/ℓ solution. These units can be related to more conventional ones (moles/g solid) used for the sorbed phase by dividing $\overline{m}_j$ by $\rho_s(1-\phi)10^3/\phi$, where ρ_s is the the density of the solid phase in g/cm^3, and ϕ is the porosity of the porous medium. An effective equilibrium constant, K_1^2, is then used to model the ion exchange process and (7) is replaced by

$$K_1^2 = \frac{(\overline{m}_1/\overline{m}_T)^{n_2}}{(\gamma_1 m_1)^{n_2}} \frac{(\gamma_2 m_2)^{n_1}}{(\overline{m}_2/\overline{m}_T)^{n_1}}. \tag{10}$$

In addition, it is assumed that the number of equivalents of surface sites per ℓ solution, N_S, available for ion exchange is constant and given by,

$$N_S = \sum_{j=1}^{\overline{N}_b} n_j \overline{m}_j + \sum_{i=1}^{\overline{N}_c} n_{c_i} \overline{m}_{c_i}. \tag{11}$$

N_S can be evaluated from the cation exchange capacity, CEC (meq/g solid), by

$$N_S = (\mathrm{CEC})\rho_S \frac{1-\phi}{\phi}. \tag{12}$$

In the present version of CHEMTRN, the solid phase density, ρ_S, and the porosity, ϕ, are not input to the program. Therefore N_S must be evaluated and is input as the parameter **CECNS**.

Sorption via surface complexation

For a surface complexation model, a neutral surface site denoted by SOH can dissociate to give a negatively charged site, SO^-,

$$SOH \rightleftarrows SO^- + H_s^+ \tag{R4}$$

where the subscript s denotes that the ion is located at the so-called "surface-plane". SOH can also react with H^+ at the surface plane to give a positively charged site SOH_2^+,

$$SOH + H_s^+ \rightleftarrows SOH_2^+ . \tag{R5}$$

In contrast to the ion exchange model, the charge on the solid surface changes and both cations and anions can be sorbed. In addition, because of the variable surface charge, an ion does not necessarily have to displace an equal amount of charge when it forms a complex with the surface site. For example, in an ion exchange model, the sorption of Sr^{2+} on the solid phase would require a reaction with two surface sites,

$$2SOH + Sr_\beta^{2+} \rightleftarrows \left(\begin{matrix} SO^- \\ SO^- \end{matrix} > Sr^{2+} \right) + 2H_s^+ \tag{R6}$$

whereas in a surface complexation model, it is possible that a reaction may involve only one site,

$$SOH + Sr_\beta^{2+} \rightleftarrows SO^- Sr^{2+} + H_s^+ . \tag{R7}$$

The subscript β denotes the plane where the Sr^{2+} ion is located when it forms a complex with the surface site. In an ion exchange model, the s and β planes are not differentiated. In the surface complexation model, the β plane is displaced from the surface plane.

Following the discussion by *Davis et al.* [1978], the equilibrium constant for reaction R4 is

$$K = \frac{[\mathrm{SO}^-][\mathrm{H}_s^+]}{[\mathrm{SOH}]}. \tag{13}$$

The activity of H^+ at the surface plane is related to the activity in the bulk solution by

$$[\mathrm{H}_s^+] = [\mathrm{H}^+]\exp\left(-\frac{e\psi_i}{kT}\right), \tag{14}$$

where ψ_i is the change of electrical potential when a species moves from the bulk phase to the solid phase, k is the Boltzmann constant, T is the absolute temperature, and e is the electronic charge. In reactions R6 and R7, the sorbed Sr^{2+} ion resides at the β plane and moves through a potential difference of ψ_β. Therefore, the activity of Sr^{2+} at the β plane is equal to the activity in the bulk phase multiplied by $\exp(-2e\psi_\beta/kT)$. The factor of 2 is a result of the double positive charge of the strontium ion. CHEMTRN treats only reactions involving one surface site in the surface complexation model because these are expected to be more dominant; if reactions of the type of R6 are dominant, an ion exchange model must be used.

The potentials ψ_i and ψ_β are functions of the charge distribution developed between the bulk fluid and the solid surface and are defined in terms of this charge and the capacitances between the layers. A complete discussion of the surface complexation model for sorption is given in *Davis et al.* [1978].

Transport equations

All aqueous species are subject to transport by advection and dispersion/diffusion. In addition, they may undergo mass transfer reactions such as sorption and precipitation or dissolution. A mass balance can be written for the concentration of each species.

If W_j is the total concentration of species A_j in the aqueous phase, given by

$$W_j = m_j + \sum_{i=1}^{N_c} a_{ij} m_{c_i}, \tag{15}$$

and if $\overline{W}_j$ is the total concentration of the sorbed species $\overline{A}_j$, given by

$$\overline{W}_j = \overline{m}_j + \sum_{i=1}^{\overline{N}_c} a_{ij} \overline{m}_{c_i}, \qquad (16),$$

and if N_p is the total number of precipitates, then

$$\left(\frac{\partial}{\partial t} + v\frac{\partial}{\partial x} - D\frac{\partial^2}{\partial x^2}\right)W_j = -\frac{\partial}{\partial t}\overline{W}_j - \frac{\partial}{\partial t}\sum_{k=1}^{N_p} s_{kj} G_k \tag{17}$$

where v is the mean velocity of advective flow and D is the coefficient of hydrodynamic dispersion.

The number of unknowns is $N_b + \overline{N}_b + N_c + \overline{N}_c + N_p$. Therefore, an equal number of equations is needed for solution of this system. There are N_b equations of the type of (17). The mass action relations, (4), provide N_c equations for the complexes. There are $\overline{N}_b + \overline{N}_c - 1$ relationships of the form of (10) and (13), and N_p relations of the form of (2); (11) provides the final relationship needed. The activity coefficients are given by (5), and $\overline{m}_T$ is defined by (9). Therefore a sufficient number of equations exists to determine m_j, $\overline{m}_j$, m_{c_i}, m_p, and $\overline{m}_{c_i}$.

SOLUTION PROCEDURE

The partial differential equations (17) are discretized in space leading to a set of ordinary differential equations (ODE's). For a constant grid spacing, the ODE's have the form

$$\frac{d}{dt}W_{j,n} + \frac{d}{dt}\overline{W}_{j,n} + \frac{d}{dt}\sum_{k=1}^{N_p} s_{kj}G_k = \frac{D}{\Delta x^2}(W_{j,n+1} - 2W_{j,n} + W_{j,n-1}) - \frac{v}{\Delta x}(W_{j,n} - W_{j,n-1}) \tag{18}$$

where j denotes the species, n is the spatial position, and Δx is the grid spacing. The advection term has been expressed using an upwind differencing method.

Because aqueous species are transported at different rates, a uniformly spaced grid does not allow efficient tracking of different solute fronts. Errors propagated by an arbitary change in the grid spacing can become excessive. Therefore, a variable grid spacing is provided with this program with the grid locations dictated by the equation

$$x(i) = x_{\max}\frac{A^{(i-1)\Delta N/\Delta N_o} - 1}{A^{1/\Delta N_o} - 1} + x(1) \tag{19}$$

where $\Delta N = 1/$(number of grid points $- 1$), $x_{\max}$ is the position where the outer boundary condition is imposed, and A and ΔN_o are adjustable constants.

After replacing the spatial derivatives with finite difference approximations for a variable grid spacing, the transport equation can be written

$$\frac{d}{dt}W_{j,n} + \frac{d}{dt}\overline{W}_{j,n} + \frac{d}{dt}\sum_{k=1}^{N_p} s_{kj}G_k = -v\left(\frac{W_n^{\ell} - W_{n-1}^{\ell}}{x_n - x_{n-1}}\right) + \frac{D}{\frac{1}{2}(x_{n+1} - x_{n-1})}\left[\left(\frac{W_{n+1}^{\ell+1} - W_n^{\ell+1}}{x_{n+1} - x_n}\right) - \left(\frac{W_n^{\ell+1} - W_{n-1}^{\ell+1}}{x_n - x_{n-1}}\right)\right]. \tag{20}$$

Equations (2,4,10,11,13,14,18 or 20) form a set of differential/algebraic equations (DAE's) which fits the form

$$G(m,t)\frac{dm}{dt} + F(m,t) = 0, \tag{21}$$

where m is a vector which contains all the unknowns $(m_j, \overline{m}_j, m_{c_i}, \overline{m}_{c_i}, m_p)$ at all the nodes. The matrix G is singular because $g_{j,n} = 0$ when the mass action equations (2,4,10) and the site constraint equation (11) are cast in the form of (21).

A backward Euler method was used to discretize m in time:

$$G(m^{\ell+1}, t)\frac{(m^{\ell+1} - m^{\ell})}{\Delta t} + F(m^{\ell+1}, t) = 0, \tag{22}$$

where ℓ denotes the previous time level and $\ell + 1$ denotes the new time level. The finite difference approximation to the transport equation is then written as

$$\frac{W_{j,n}^{\ell+1} - W_{j,n}^{\ell}}{\Delta t} + \frac{\overline{W}_{j,n}^{\ell+1} - \overline{W}_{j,n}^{\ell}}{\Delta t} + \sum_{k=1}^{N_p} s_{kj}\frac{G_k^{\ell+1} - G_k^{\ell}}{\Delta t} = -v\left(\frac{W_n^{\ell} - W_{n-1}^{\ell}}{x_n - x_{n-1}}\right)$$
$$+ \frac{D}{\frac{1}{2}(x_{n+1} - x_{n-1})}\left[\left(\frac{W_{n+1}^{\ell+1} - W_n^{\ell+1}}{x_{n+1} - x_n}\right) - \left(\frac{W_n^{\ell+1} - W_{n-1}^{\ell+1}}{x_n - x_{n-1}}\right)\right]. \tag{23}$$

More sophisticated DAE solvers based on more than one previous time level are available, such as those of *Hindmarsh* [1980] and *Petzold* [1981]. However, CHEMTRN includes precipitation, and when precipitates form the number of unknowns increases. Methods based on using derivatives at several previous time steps would have to be restarted when the number of unknowns changes. Therefore, the simpler backward differencing method was used in CHEMTRN.

An advantage of using just two time levels is that it is possible to modify the backward Euler method slightly by evaluating the advection terms at the old time level using an upwind differencing method while still evaluating the diffusion terms at the new time level. Then the physical significance of the advection term is maintained: information is transported in the direction of the flow. The upwind differencing scheme used in CHEMTRN for the advection term does, however, introduce numerical diffusion with a coefficient of $(v\Delta x/2)(1 - c)$, where c is the Courant number equal to $v\Delta t/\Delta x$, and the equations are no longer unconditionally stable. The numerical dispersion can be thought of as contributing to the physical dispersion term; it is directly proportional to the velocity in the same manner in which the physical dispersion is formulated. The numerical dispersion can be minimized by using a time step such that $c = 1$ ($\Delta t = \Delta x/v$); however, this restriction can be rather stringent. In addition, for a variable grid spacing, one cannot necessarily have $c = 1$ thoughout the entire grid. In this case, if numerical dispersion is comparable to or greater than physical dispersion, alternate differencing methods [*Roache*, 1972] may have to be used for the advection term. As for the stability of the equations, the implicit form of the dispersion term offers greater stability than a purely explicit differencing scheme. No exact stability analysis has been done for the finite difference scheme. If the flow is mainly advective and if large oscillations begin to occur in the calculated concentrations, the time step should be reduced.

A Newton-Raphson iteration technique is used to solve the system of equations. Estimates of the values of the unknowns at the new time level are used to calculate the residues of all the equations for those estimates,

$$G(m^{\ell+1,k},t)\left(\frac{m^{\ell+1,k}-m^{\ell}}{\Delta t}\right)+F(m^{\ell+1,k},t)=R(m^{\ell+1,k},t), \tag{24}$$

where k denotes the iteration number and R is a matrix containing the residues of the equations. New estimates are obtained by first calculating the Jacobian, J, where $J = \partial R/\partial m$, and then using the Jacobian to predict the values of the unknowns at the new time level,

$$J\Delta m = J(m^{\ell+1,k+1} - m^{\ell+1,k}) = -R(m^{\ell+1,k}). \tag{25}$$

Since one-dimensional flow is being modeled, any component of the residue vector will be a function of m at that node and the neighboring nodes resulting in a block tridiagonal Jacobian matrix. The linear system of equations (25) is solved using LU

decomposition where the Jacobian is factored into lower and upper triangular matrices. A software package written by *Hindmarsh* [1977] was used both to perform the *LU* decomposition and to solve the set of equations. To save time, the Jacobian is not necessarily evaluated at every time step [*Kee and Miller*, 1980]. The iterations of (25) continue until the changes in the new values of m are less than the specified error tolerance. At present the convergence criterion used has been taken from *Kee and Miller* [1980]. In CHEMTRN the following norm,

$$\|\delta Q\| = \left[\sum_{n=1}^{N} \sum_{j=1}^{N_T} \left(\frac{m_{n,j}^{\ell+1,k+1} - m_{n,j}^{\ell+1,k}}{\max_j m_{n,j}^{\ell+1,k+1}} \right)^2 \right]^{\frac{1}{2}},$$

where N is the number of nodes and N_T is the total number of species, must be less than 10^{-4}. If convergence is not obtained in ten iterations, a new Jacobian is calculated. If convergence is still not obtained within five iterations, the time step is halved. When convergence is obtained within only five iterations, the time step is multiplied by 1.75. This criterion is set within the program.

Precipitation is only included in the set of equations when it occurs. One type of precipitate many form at one node while another type may form at a different node. After each time step, the activity product for each precipitate that is being considered is evaluated at each node. If the activity product exceeds the solubility product at a node, the total amount of each basis species is computed and a new distribution of species is calculated at that node. All the solubility products are considered when the new equilibrium distribution is calculated. From that time on, the solubility product is satisfied for any precipitate which has formed at the node and is included in the system of differential/algebraic equations which are solved simultaneously. Thus, the two-step procedure is only used at the time step when a precipitate first forms. The transport equation at a node with a precipitate henceforth includes an additional term representing the change in the amount of precipitate at that node. If complete dissolution occurs, the species concentration is forced to go to zero during the time step when the dissolution occurs. After this time step, the solubility product will no longer be satisfied at that node.

New chemical reactions are treated by calculating the residues of the new equations describing the reactions. The calculation of the Jacobian is done numerically and therefore is independent of the types of chemical reactions considered.

The matrix G is never stored; only the residues for each set of estimates are stored. The Jacobian, however, requires the calculation and the storage of the changes in residues of each equation with respect to the changes in all the unknowns at a node and at the two neighboring nodes. Although only the nonzero block matrices are stored, this storage requirement can be excessive for some computers. It is possible to break up the Jacobian matrix into several different blocks and then store these blocks separately. For example, this procedure helps to overcome some of the storage limitations of the CDC 7600 computer which was used for these calculations.

Boundary conditions

Different boundary conditions may be used with CHEMTRN. The flexibility is obtained by expressing the boundary conditions in the form of (19) and thus both time-dependent and steady-state boundary conditions can be simulated. At the inner boundary it is possible to specify a constant-concentration boundary condition,

$$m = m_b,$$

or a constant-flux boundary condition,

$$q_b = vm - D\frac{\partial m}{\partial x}.$$

The flux boundary condition is imposed at 0 if the flow is one-dimensional and at $x(1)/2$ if the flow is radial. At the outer boundary, either a constant concentration equal to that of the initial condition or a no-flux boundary condition can be imposed. An additional feature of CHEMTRN is that at the inner boundary, it is possible to impose a solubility product constraint for the equilibrium of a solid phase with the initial groundwater:

$$K_{12} = [A_1][A_2], \tag{26}$$

where K_{12} is an equilibrium solubility product. The equilibrium distribution of species is determined at this boundary from knowledge of the total amount of precipitate that has been added and from the additional condition that the increased amounts of each species making up the precipitate, A_1 and A_2 in this case, in the groundwater are in the same ratio as prescribed by the stoichiometry of the reaction forming the precipitate.

Water dissociation

To avoid convergence problems, CHEMTRN treats the dissociation of water by solving for a dummy variable, y, defined by

$$y = m_{H^+} - m_{OH^-}. \tag{27}$$

This method is employed because a mass balance equation for either H^+ or OH^- must include the concentration of water. Relatively large changes in concentrations of the former produce extremely small relative changes in the concentration of the latter. To solve for y, a slight modification must be made to the mass balance equations for H^+ and OH^-. The mass balance equation for the hydrogen ion is

$$L\left[m_{H^+} + \sum_i (a_{i,H^+}) m_{c_i}\right] + \frac{\partial}{\partial t}\overline{W}_{H^+} = -L(m_{H_2O}), \tag{28}$$

and for the hydroxyl ion,

$$L\left[m_{OH^-} + \sum_i (a_{i,OH^-}) m_{c_i}\right] = -L(m_{H_2O}), \tag{29}$$

where the operator L is defined by

$$L = \left(\frac{\partial}{\partial t} - D\frac{\partial^2}{\partial x^2} + v\frac{\partial}{\partial x}\right).$$

If (29) is subtracted from (28), the result is

$$L\left[y + \sum_i (a_{i,H^+} - a_{i.OH^-}) m_{c_i}\right] + \frac{\partial}{\partial t}\overline{W}_{H^+} = 0. \tag{30}$$

An additional relationship is obtained from the mass action equation for the dissociation of water:

$$[\mathrm{H}^+][\mathrm{OH}^-] = K_w\,, \tag{30}$$

where K_w has the value of $10^{-13.99}$ at 25 ° C.

PROBLEM FORMULATION

The user must supply the following items of information for the chemical reactions.

1. The stoichiometric coefficients of the basis species participating in the reactions which are being considered must be provided. These reactions include both aqueous phase complexation and the formation of precipitates. The reaction for the formation of a complex is written in terms of one mole of that complex. The basis species are the least number of species which can be used to define all other species present. The order of the stoichiometric coefficients is the same as that in which the information about the basis species is read

into the program. Because the program includes the dissociation of water, the hydroxyl complex (OH^-) is treated in a special manner which is explained below.

2. For each reaction, the equilibrium constant or solubility product must be provided and is expressed as the negative common logarithm of the equilibrium constant or solubility product (pK).

3. For sorption of aqueous species, it is necessary to specify whether the species will be sorbed by the solid and if it is, whether the sorption mechanism will be simple ion exchange or surface complexation.

4. The equilibrium constant must be provided for each sorption reaction expressed as —log (equilibrium constant). For ion exchange, every reaction must be written in terms of exchange with the same species: H^+ ion or else the first species sorbed. For surface complexation, the reactions are written in terms of a reaction with a SOH site.

5. For sorption via surface complexation, one must also specify how many H^+ species are displaced or additionally sorbed, e.g., a Sr^{2+} ion could displace one or two H^+ ions depending on whether it reacts with one or two SOH sites. At present, a species may react with only one surface site in the surface complexation model so the number of H^+ ions reacting is either -1 for sorption, 0 for the H^+ ion itself, or $+1$ for displacement of H^+.

As stated above, OH^- is treated differently than the other complexes. If dissociation of water is included, then the chemical reactions are written in terms of H^+ and OH^- instead of H^+ and H_2O, as if OH^- were a basis species. Because the concentration of OH^- can be obtained from H^+ and the equilibrium constant for dissociation of water, information read about this species will be like that read for a complex.

Because information about the basis species is read before the complexes, OH^- will be the first "complex" read and the stoichiometric coefficient for OH^- in any reaction will always be the last one in the list. For example, in a system composed of Na^+, Ca^{2+}, H^+, and CO_3^{2-}, with complexes NaOH, $NaCO_3^-$, HCO_3^-, H_2CO_3, $CaOH^+$, $CaCO_3$, $NaHCO_3$, $CaHCO_3^+$ and H_2O, the basis species for defining the reactions are Na^+, Ca^{2+}, H^+, CO_3^{2-}, and OH^-. Then for the reaction

$$Na^+ + OH^- \rightleftarrows NaOH$$

the stoichiometric coefficients are 1,0,0,0,1 and for the reaction

$$Ca^{2+} + H^+ + CO_3^{2-} \rightleftarrows CaHCO_3^+$$

they are 0,1,1,1,0. The equilibrium constants are read by providing —log K (pK) of the reactions. Because the reactions are expressed in terms of H^+ and OH^- instead of H^+ and H_2O, the pK's must be those for the reactions expressed in terms of OH^-.

In addition to providing the chemical reaction data, the user must specify the dispersivity, the fluid velocity and information on the grid spacing. Because a dispersion coefficient is usually written as av where a is the dispersivity and v is the velocity, the dispersion/diffusion coefficient is evaluated as $av + b$ where b is the diffusion coefficient. Therefore, the user can also specify pure diffusion if desired. Either a uniform or variable grid spacing is possible.

To initialize the system and to calculate the boundary conditions, the user must provide information about every basis species except OH^-. However, the information about each species does not have to be the same. For example, for H^+ the pH can be specified; for the Na^+ species, any one of the following can be specified: the total concentration of Na in the aqueous phase, the concentration of the Na^+ ion or the total concentration of Na in the aqueous phase plus the sorbed phase, etc. The exact form and order of the input data are given in the next section.

INPUT PARAMETERS

The following variables are listed in the order in which CHEMTRN reads them. The variable names, descriptions, units and read formats have been provided. The formats are either **F** or **I**; **E** format may be used instead of **F** as long as the value is correctly right justified in the field. For **Lines 2-12**, **13b**, **13c**, **14b**, **15b-d**, and **16b**, the first ten spaces have been left blank so that the user may use this space to identify the input line. Any consistent set of units may be used; in the variable descriptions, *L* indicates a unit of length and *t* a unit of time. Some of the input lines have been grouped in sets according to the type of information which they provide. Not all of the input is required for all simulations. An alphabetical list of the variables and their definitions appears in Appendix A.

Line 1a The title of the problem can be up to 80 characters long.

variable	**TITLE**
columns	1-80
format	20A4

TITLE	title information for the problem

Line 1b List of units of length and time used in calculations

variable	**ULENGTH**	**UTIME**
columns	1-10	11-20
format	**A10**	**A10**

ULENGTH	units of length
UTIME	units of time

Line 2 The user must provide an integer code for the type of flow, either one-dimensional or radial. In addition, the user should specify whether the program

should stop after calculating the equilibrium distributions for the initial and boundary conditions and whether the program or the user will provide the initial guesses for the concentrations.

variable	**ITYPE**	**IDYNAM**	**IG**
columns	11-20	21-30	31-40
format	**I10**	**I10**	**I10**

ITYPE	type of flow: 0 - one-dimensional flow; 1 - radial flow
IDYNAM	code to indicate whether the program should stop after calculating the equilibrium distribution for the initial and boundary conditions: 0 - stop; 1 - continue executing
IG	code to indicate whether the program or the user will provide initial guesses of the concentrations: 0 - user will; 1 - program will

Line 3 These parameters control the number of iterations performed, when calculating the equilibrium distribution of species, before intermediate calculations are printed. If the calculations converge slowly because of a poor initial guess, for example, then examining the old and new guesses will provide an idea of how the guess can be improved. To suppress printing intermediate calculations, values of 100 are recommended for all of these parameters. If the calculations do not converge after 100 iterations, the program will stop executing and print a message.

variable	**IN1**	**IN2**	**IN3**
columns	11-20	21-30	31-40
format	**I10**	**I10**	**I10**

IN1	number of iterations before printing when calculating the equilibrium distribution of the initial conditions
IN2	number of iterations before printing when calculating the equilibrium distribution at the grid point where the boundary condition is specified

IN3 number of iterations before printing when calculating the equilibrium distribution at a node where a new precipitate is forming

Line 4 The user must supply several parameters which control the grid spacing. For an evenly spaced grid (**DNO**=0), the grid spacing DX is equal to **XMAX** /(**NMAX**-1). For a variable grid, DX varies and is the difference between adjacent grid points $x(j)$ calculated from

$$x(j) = \mathbf{XMAX}\left[\frac{\mathbf{AK}^{(i-1)\Delta \mathbf{N}/\mathbf{DNO}} - 1}{\mathbf{AK}^{1/\mathbf{DNO}} - 1}\right] + x(1),$$

where $j = i$ for the concentration boundary condition, $j = i - 1$ for the flux boundary condition and one-dimensional flow, and ΔN = 1/(**NMAX**-1). This equation generates a spacing that is approximately exponential; **DNO** should be chosen less than 1 and **AK** should be chosen greater than 1 to have the smallest grid variation near $x = 0$.

If a concentration boundary condition is specified at the inner boundary (on **Line 8**, **IBND**(1)=0), it is imposed at the first grid point which is located at 0; **XMAX** is the location of the last grid point. If a flux boundary condition is specified at the inner boundary (**IBND**(1)=1 on **Line 8**) and if one-dimensional flow is specified, (**ITYPE**=0 on **Line 2**), the boundary condition is imposed at 0 and the program adjusts the grid spacing so that the new value of the first grid point is one-half of the old value of the first grid point; the last grid point is offset from **XMAX** by the same amount. If a flux boundary condition is specified at the inner boundary and if radial flow is specified (**ITYPE**=1 on **Line 2**), it is imposed at **RW** and the first grid point is at 2 X **RW** with the last grid point offset from **XMAX** by the same amount. If a no-flux boundary condition is specified at the outer boundary (**IBND**(2)=1 on **Line 8**), it is imposed midway between the last and next to last grid point.

variable	**NMAX**	**XMAX**	**DNO**	**AK**	**RW**
columns	11-20	21-30	31-40	41-50	51-60
format	**I10**	**F10.3**	**F10.3**	**F10.3**	**F10.3**

NMAX	number of grid points
XMAX	distance between the first and last grid points $[L]$
DNO	parameter used to calculate the grid spacing (see equation above); if **DNO**=0, then the grid spacing will be uniform and equal to **XMAX**/(**NMAX**-1)
AK	parameter used to calculate the grid spacing (see equation above)
RW	for the case of radial flow with a flux condition at the inner boundary, the first grid point is located at 2 × **RW** (can be left blank in other cases)

Line 5 The user must specify the number of times at which the results are to be printed, the size of the first time step and the size of the maximum time step allowed. The initial time step is usually between 10^{-4} and 10^{-5} (in units of time used for the flow velocity). To minimize numerical dispersion, the maximum time step should be approximately DX/**VO**, where DX is the grid spacing calculated from the grid parameters on **Line 4** and **VO** is the velocity on **Line 7**.

variable	**KMAX**	**DTINI**	**DTMAX**
columns	11-20	21-30	31-40
format	**I10**	**F10.3**	**F10.3**

KMAX	number of times at which the results are to be printed
DTINI	size of the initial time step $[t]$
DTMAX	size of the maximum time step permitted $[t]$

Line 6 The program will print the results at times nearest those specified. **KMAX** times, where **KMAX** was given on **Line 5**, are read, seven to a line.

variable	**TPRINT(K), K=1, KMAX**
columns	11-80
format	7F10.3

TPRINT	array which holds the times at which the results are to be printed $[t]$

Line 7 The hydrodynamic dispersion coefficient is calculated from the dispersivity, diffusion coefficient and fluid velocity given by the user (**DOA** × **VO** + **DOB**).

variable	**DOA**	**DOB**	**VO**
columns	11-20	21-30	31-40
format	F10.3	F10.3	F10.3

DOA	dispersivity $[L]$
DOB	diffusion coefficient $[L^2/t]$
VO	for one-dimensional flow (**ITYPE**=0 on **Line 2**), this is the mean fluid velocity (i.e., the specific discharge divided by the porosity) $[L/t]$; for radial flow (**ITYPE**=1 on **Line 2**), it is a constant of proportionality equal to the radial distance times the mean fluid velocity $[1/t]$

Line 8 The user must provide integer codes for the type of boundary conditions at both the inner and outer boundaries. At the inner boundary, either a concentration or a flux boundary condition is possible. At the outer boundary, either a concentration boundary where the fluid remains at the initial conditions or a no-flux boundary is possible.

variable	**IBND**(1)	**IBND**(2)
columns	11-20	21-30
format	I10	I10

IBND(1)	type of boundary condition to be imposed at the inner boundary: 0 - constant concentration; 1 - constant flux

IBND(2)	type of boundary condition to be imposed at the outer boundary: 0 - constant concentration equal to initial conditions; 1 - no flux

Line 9 There is an option in the program to allow a solid to leach into the groundwater; however, at this time, the option is limited to **one** solid located at the **first** grid point. The user must include the solid in the list of precipitates and give its position in that list on this line.

variable	**LEACH**	**NB**
columns	11-20	21-30
format	**I10**	**I10**

LEACH	position in the list of precipitates of the solid which is leaching: 0 - no leaching
NB	location of the solid which is leaching: 0 - no leaching; 1 - solid is leaching at the first grid point

Line 10 Integer data are read on this line: the number of basis species, the number of species which are sorbed following either an ion exchange mechanism or a surface complexation model, the number of aqueous complexes, the number of solid precipitates and the position of H^+ in the list of basis species which follows.

variable	**NUM**(1)	**NUM**(2)	**NUM**(3)	**NUM**(4)	**NUM**(5)	**LNH**
columns	11-20	21-30	31-40	41-50	51-60	61-70
format	**I10**	**I10**	**I10**	**I10**	**I10**	**I10**

NUM(1)	number of basis species (OH^- must be included in the count if the dissociation of water is to be incorporated in the model)
NUM(2)	number of species (both basis species and complexes) which are sorbed according to an ion exchange mechanism
NUM(3)	number of species (both basis species and complexes) which are sorbed according to a surface complexation model

NUM(4)	number of aqueous complexes
NUM(5)	number of solid precipitates
LNH	position of H^+ in the list of basis species: 0 - dissociation of water not included

Line 11 If any of the species are sorbed according to an ion exchange mechanism, then the user must specify the number of equivalents of sites per liter of solution that are available for sorption. This value is obtained from the cation exchange capacity (CEC), usually given in meq/g of solid, by multiplying the CEC by $10^{-3}\rho_s(1-\phi)/\phi$, where ϕ is the porosity and ρ_s is the solid density (g/cm^3). **This input line should be omitted if none of the species is sorbed according to an ion exchange mechanism.**

variable	**CECNS**
columns	11-20
format	**F10.3**

CECNS	concentration of sites in [equivalents $/l$ solution] available for sorption in ion exchange model

Line 12 If any of the species is sorbed according to the surface complexation model, then the user must specify the five parameters described below. **This line is omitted if none of the species is sorbed according to the surface complexation model.**

variable	**C1**	**C2**	**PK1**	**PK2**	**AREA**	**SOH**
columns	11-20	21-30	31-40	41-50	51-60	61-70
format	**F10.3**	**F10.3**	**F10.3**	**F10.3**	**F10.3**	**F10.3**

C1	capacitance between the surface plane and the beta plane $[\mu F/L^2]$
C2	capacitance between the beta plane and the diffuse layer $[\mu F/L^2]$
PK1	$-\log$ of the dissociation constant of the positively charged site SOH^{2+}

PK2	— log of the the dissociation constant of the neutral site SOH
AREA	sorption area $[L^2/l$ solution]
SOH	concentration of sites in [equivalents/l solution] available for forming complexes in surface complexation model

Lines 13a,b,c This set of input lines reads information about the basis species and constants involved in the processes of ion exchange or surface complexation. **Line 13a** is always read; both **Line 13b** and **Line 13c** are omitted if the basis species is not sorbed (**ISORPI**=**ISORPE**=0). **Line 13b** is read if the basis species is sorbed according to an ion exchange mechanism (**ISORPI**=1); **Line 13c** is read if the basis species is sorbed according to a surface complexation model (**ISORPE**=1). **GUESSI** and **GUESSB** can all be left blank if the program is to provide the guesses (**IG**=1 **on Line 2**).

Line 13a

variable	**DUM**	**VJ**	**INDEXI**	**BI**	**GUESSI**	**INDEXB**	**BC**	**GUESSB**
columns	1-10	11-20	21-25	26-35	36-45	46-50	51-60	61-70
format	**A10**	**F10.3**	**I5**	**F10.3**	**F10.3**	**I5**	**F10.3**	**F10.3**

Line 13a - continued

variable	**ISORPI**	**ISORPE**
columns	71-75	76-80
format	**I5**	**I5**

DUM	name of the species
VJ	charge of the species
INDEXI	type of initial condition: 0 - the total concentration of the species will be given (including sorbed phase, aqueous phase and precipitate); 1 - only the concentration of the basis species will be given; 2 - the combined concentration of the basis species and the aqueous complexes will be given; (if a species can form a precipitate, option 3 must be used instead of option 2 to allow for the inclusion of the solubility product if necessary)

	3 - the combined concentration of the basis species, aqueous complexes and precipitates will be given; 4 - the initial concentration will be determined from a charge balance;
BI	value of the initial concentration according to the value of **INDEXI** [moles/l]
GUESSI	guess for the initial concentration of the basis species [moles/l]; **can be left blank if the program is to provide the guess (IG=1 on Line 2)**
INDEXB	takes the same values as **INDEXI** and describes what type of concentration is being specified at the boundary
BC	value of the concentration at the boundary [moles/l] according to the value of **INDEXB** [moles/l]; if a solid is leaching into the groundwater at the inner boundary, the value of **BC** for the first species making up this solid is the amount of the solid while the value of **BC** need not be specified for the other species making up the solid
GUESSB	guess for the boundary concentration of the basis species [moles/l]; **can be left blank if the program is to provide the guess (IG=1 on Line 2)**
ISORPI	code to indicate whether the species is sorbed according to an ion exchange mechanism: 0 - is not sorbed; 1 - is sorbed
ISORPE	code to indicate whether the species is sorbed according to a surface complexation model: 0 - is not sorbed; 1 - is sorbed

Line 13b ion exchange

variable	**PKI**	**GUESSI**	**GUESSB**
columns	11-20	21-30	31-40
format	**F10.3**	**F10.3**	**F10.3**

PKI	— log of the equilibrium constant for the ion exchange between the basis species and H^+ (or another common species)
GUESSI	guess for the amount of this species which is sorbed initially [moles/l]; **can be left blank if the program is to provide the guess (IG=1 on Line 2)**
GUESSB	guess for the amount of this species which is sorbed initially at the boundary conditions [moles/l]; **can be left blank if the program is to provide the guess (IG=1 on Line 2)**

Line 13c surface complexation

variable	**PKE**	**GUESSI**	**GUESSB**	**AH**
columns	11-20	21-30	31-40	41-50
format	**F**10.3	**F**10.3	**F**10.3	**F**10.3

PKE	— log of the equilibrium constant for the surface complex reaction between the basis species and an SOH site
GUESSI	guess for the amount of this species which is sorbed initially [moles/l]; **can be left blank if the program is to provide the guess (IG=1 on Line 2)**
GUESSB	guess for the amount of this species which is sorbed initially at the inner boundary; [moles/l] **can be left blank if the program is to provide the guess (IG=1 on Line 2)**
AH	amount of charge which is displaced or sorbed for each surface complexation reaction with a SOH site: +1 - a H^+ ion is displaced, 0 - used for the H^+ ion, −1 - a H^+ ion is sorbed

Lines 14a,b These two lines are omitted if water dissociation is not included in the simulation (**LNH**=0 on **Line 10**). If water dissociation is allowed, information about OH must be read immediately after all of the information about the basis species has been read. OH must be included in the number of basis species (see **NUM**(1)) read on **Line 10**. If **Line 14a** is used, **Line 14b** must be included.

Line 14a

variable	**DUM**	**H2OK**
columns	1-10	11-20
format	**A**10	**F**10.3

DUM	name of the species
H2OK	— log of the dissociation constant of water

Line 14b

variable	**GUESSI**	**GUESSB**
columns	11-20	21-30
format	**F**10.3	**F**10.3

GUESSI	guess for the amount of this species which is sorbed initially [moles/l]; **can be left blank if the program is to provide the guess (IG=1 on Line 2)**
GUESSB	guess for the amount of this species which is sorbed initially at the boundary [moles/l]; **can be left blank if the program is to provide the guess (IG=1 on Line 2)**

Lines 15a,b,c,d These four lines are omitted if **NUM**(4) = 0 on **Line 10**, that is, if no aqueous complexes form. If the aqueous complex is sorbed according to an ion exchange mechanism, then **Lines 15a,b,c** are read; if the complex is sorbed according to a surface complexation reaction, then **Lines 15a,b,d** are read. If the complex is not sorbed, then only **Lines 15a,b** are read.

Line 15a

variable	**DUM**	**PK**	**S(J), J**=1,**NUM**(1)
columns	1-10	11-20	21-70,/,1-75
format	**A**10	**F**10.3	10**F**5.1,/,15**F**5.1

DUM	name of the complex
PK	— log of the equilibrium constant for the formation of the complex
S	array which holds the stoichiometric coefficients for the reaction, read in the same order in which the basis species are read

Line 15b

variable	**GUESSI**	**GUESSB**	**ISORPI**	**ISORPE**
columns	11-20	21-30	31-35	36-40
format	**F**10.3	**F**10.3	**I**5	**I**5

GUESSI	guess for the initial concentration of this complex [moles/l]; **can be left blank if the program is to provide the guess (IG=1 on Line 2)**
GUESSB	guess for the concentration of this complex at the boundary [moles/l]; **can be left blank if the program is to provide the guess(IG=1 on Line 2)**
ISORPI	code to indicate whether the complex is sorbed according to an ion exchange mechanism: 0 - is not sorbed; 1 - is sorbed
ISORPE	code to indicate whether the complex is sorbed according to a surface complexation model: 0 - is not sorbed; 1 - is sorbed

Line 15c ion exchange

variable	PKI	GUESSI	GUESSB
columns	11-20	21-30	31-40
format	F10.3	F10.3	F10.3

PKI	— log of the equilibrium constant for the ion exchange between the aqueous complex and H^+
GUESSI	guess for the amount of this complex which is sorbed initially [moles/l]; **can be left blank if the program is to provide the guess (IG=1 on Line 2)**
GUESSB	guess for the amount of the complex which is sorbed at the boundary conditions[moles/l]; **can be left blank if the program is to provide the guess (IG=1 on Line 2)**

Line 15d surface complexation

variable	PKE	GUESSI	GUESSB	AH
columns	11-20	21-30	31-40	41-50
format	F10.3	F10.3	F10.3	F10.3

PKE	— log of the equilibrium constant for the surface complex reaction between the complex and an SOH site
GUESSI	guess for the amount of this complex which is sorbed initially [moles/l]; **can be left blank if the program is to provide the guess (IG=1on Line 2)**
GUESSB	guess for the amount of this complex which is sorbed at the boundary [moles/l]; **can be left blank if the program is to provide the guess (IG=1 on Line 2)**

AH	amount of charge which is displaced or sorbed for each surface complexation reaction with a SOH site: +1 - a H^+ ion is displaced, 0 - used for the H^+ ion, −1 - a H^+ ion is sorbed

Lines 16a,b These two lines are omitted if **NUM**(5) = 0 on **Line 10**, that is, if no precipitates form. The concentration units for the precipitate are in *equivalent* moles/*l* of solution.

Line 16a

variable	**DUM**	**PK**	**SS(J), J=1NUM(1)**
columns	1-10	11-20	21-70,/,1-75
format	A10	F10.3	10F5.1,/,15F5.1

DUM	name of the precipitate
PK	— log of the solubility product
SS	array which holds the stoichiometric coefficients for the reaction, read in the same order in which the basis species are read

Line 16b

variable	**GUESSI**	**GUESSB**
columns	11-20	21-30
format	F10.3	F10.3

GUESSI	guess for the initial concentration of this precipitate [moles/*l*]; **can be left blank if the program is to provide the guess (IG=1 on Line 2)**
GUESSB	guess for the concentration of this precipitate at the boundary [moles/*l*]; **can be left blank if the program is to provide the guess (IG=1 on Line 2)**

EXAMPLES

Sample inputs and outputs for four different examples are given here. The examples incorporate (1) ion exchange only, (2) ion exchange and aqueous-phase complexation with water dissociation, (3) surface complexation, and (4) precipitation and dissolution of solids. All examples include advection and dispersion/diffusion.

(1) *Ion exchange case*

In this example, surface complexation is not considered (**NUM**(3)=0) and no complexes or precipitates form (**NUM**(4)=**NUM**(5)=0). The major species in the groundwater are Na^+, Mg^{2+}, Ca^{2+}, and Cl^- with other cations and anions making up the balance of the chemical species. This case is a simulation of a field test described by *Valocchi et al.* [1981] in which treated municipal wastewater effluent was injected into a shallow aquifer in the Palo Alto (California) Baylands region. The field data used for this simulation were obtained from *Valocchi et al.* [1981]. More data are available in *Roberts et al.* [1978] and *Charbeneau and Street* [1978], referenced by *Valocchi et al.* [1981].

The composition of the fluid arriving at well S23, 16 m from the injection site, is simulated. Pure radial flow is assumed so **ITYPE**=1. The initial composition of groundwater in this region consisted of 5700 mg/ℓ Cl^-, 1990 mg/ℓ Na^+, 436 mg/ℓ Mg^{2+}, and 444 mg/ℓ Ca^{2+}. However, because CHEMTRN requires concentrations in moles/ℓ solution, these values must be divided by 10^3 times the molecular weight of the species. For example, the initial value of Cl^- is 0moles/ℓ solution (**BI**=0.16, **INDEXI**=2). The effluent water was injected at an average rate of 21 m^3/hr and had an average composition of 320 mg/ℓ Cl^-, 216 mg/ℓ Na^+, 12 mg/ℓ Mg^{2+}, and 85 mg/ℓ Ca^{2+}. (Again the reported concentrations must be divided by 10^3 times the molecular weight of the species.) As given by *Valocchi et al.* [1981], the aquifer thickness was taken to be 2 m, the solid matrix density was 2500 g/ℓ, the CEC was 0.09 meq/g, and the porosity was 25 per cent. The concentration of sites available for sorption is then 0.67 equivalents per liter (**CECNS**). Assuming the flow to be radial with the fluid velocity equal to $Q/(2\pi b\phi r)$, where Q is the injection rate, ϕ is the porosity, and b is the aquifer thickness, then the velocity would be $6.8/r$ m/hr. However based on tracer tests, Valocchi suggested that the field had a permeability about 1.45 times greater in the direction of flow toward well S23. Therefore this velocity has been multiplied by 1.45 so **VO**=9.8. A dispersivity of 1.0 m is assumed (**DOA**=1.0 and **DOB**=0). Numerical dispersion contributes about an additional 20 per cent to the calculated dispersion coefficient because of the grid spacing used.

The number of basis species is 4 (**NUM**(1)) with 3 (**NUM**(2)) of them (Na^+, Ca^{2+}, and Mg^{2+}) being sorbed via ion exchange. For each of these three ions, **ISORPI**=1 and **ISORPE**=0. The negative log of the effective equilibrium constant used for the exchange reaction of Mg^{2+} replacing Na^+

$$\mathrm{Mg}^{2+}(aq) + 2\overline{\mathrm{Na}} \rightleftarrows \overline{\mathrm{Mg}} + 2\mathrm{Na}^{+}$$

is −0.35 (**PKI**) and that for Ca^{2+} replacing Na^+

$$\mathrm{Ca}^{2+}(aq) + 2\overline{\mathrm{Na}} \rightleftarrows \overline{\mathrm{Ca}} + 2\mathrm{Na}^{+}$$

is −0.6 (**PKI**). Note that the effective equilibrium constants in CHEMTRN are defined using a mole fraction convention for the sorbed phase instead of the equivalent fraction convention used by *Valocchi et al.* [1981] and incorporate activity coefficients for the aqueous phase species.

The input listing for this problem is given in Appendix B1. A uniform grid was used (**DNO**=0) with **NMAX**=40 and **XMAX**=64. The initial time step used was 10^{-4} hour (**DTINI**) with a maximum time step of 1.6 hours (**DTMAX**). Because the dissociation of water is not included **LNH** (position of the H^+ ion in the list of basis species) is 0. Also no solid is being leached into the groundwater so **LEACH**=0 and **NB**=0. For calculating the initial distribution of species, the concentrations of the basis species (**BI**) are given with **INDEXI**=2. (Since there are no complexes or precipitates, **INDEXI**=1, 2 or 3 represents the same initial condition.) For calculating the distribution of species in the injected fluid, **INDEXB**=1, 2 or 3 represents the same condition in this example. Intermediate printouts of the calculations of concentrations of species until an equilibrium distribution of species is determined are not desired so **IN1**=**IN2**=**IN3**=100. In addition, the initial estimates are being supplied so **IG**=0.

The treated wastewater is injected at a constant rate at the inner boundary so a flux boundary condition is used at this boundary (**IBND**(1)=1). The wastewater is assumed to be injected through a well of radius **RW**=0.5 m. This value of the well radius is large; however, if the grid variation is too drastic near the injection well, a stability problem occurs. Because a uniformly spaced grid is being used, the well radius was chosen to be more consistent with the grid spacing. At the outer boundary, a constant concentration equal to that of the initial groundwater is assumed (**IBND**(2)=0).

An example of the output for this problem follows the input listing in Appendix B1. The equilibrium distributions of species corresponding to the initial conditions and the inner boundary condition are given. Because there are no aqueous complexes or precipitates, the calculation gives the concentrations of the species sorbed on the solid matrix which must be in equilibrium with the given concentrations of the species in the groundwater. The output also lists the concentrations of the species as a function of distance from the inner boundary for two different times, 80 hours, and 800 hours. The number of printout times specified on input was fourteen but only two of them are reproduced here.

Figures 1 and 2 compare the results of the simulation with the field measurements at well S23 as functions of total injected volume. The figures show concentrations (in mg/ℓ) of the exchanging ions Ca^{2+} and Mg^{2+}, respectively, in the aqueous phase. The results of the simulation are encouraging given that purely radial flow with only longitudinal dispersion was assumed while the field did not seem to be purely radial from tracer tests. Additional data on the concentrations of SO_4^{2-}, HCO_3^-, CO_3^{2-}, and H^+ would be required to assess the effects of aqueous-phase complexation on the transport of Ca^{2+} and Mg^{2+}.

(2) *Ion exchange and aqueous-phase complexation*

This example considers the transport of strontium when solid $SrCO_3$ is placed in contact with the groundwater at the inner boundary. The groundwater is assumed to have a velocity of 0.1 m/yr (**VO**) and a dispersivity of 1.0 m (**DOA**). H_2O is allowed to dissociate (a nonzero value of **LNH**) and eleven complexes (**NUM**(4)=11) form from Na^+, Ca^{2+}, Sr^{2+}, H^+, CO_3^{2-}, and OH^-. To balance the charge of the cations, Cl^- has been included in the calculation making **NUM**(1)=7. The species Na^+, Ca^{2+}, Sr^{2+}, and H^+ are sorbed by ion exchange only (**NUM**(2)=4, **NUM**(3)=0). Two precipitates ($SrCO_3$ and $CaCO_3$) are considered in the calculation (**NUM**(5)=2). The concentration of sites available for sorption is 0.1 equivalents/ℓ solution (**CECNS**). The groundwater contains NaCl, Na_2CO_3 and $CaCl_2$ in concentrations such that the total initial concentrations of Na^+ and Ca^{2+} in the aqueous phase (**INDEXI**=2) are 1×10^{-3} and 5×10^{-4} moles/ℓ solution (**BI**) respectively. The initial concentration of CO_3^{2-} is 5×10^{-4} moles/ℓ and **INDEXI**=3 because CO_3^{2-} may be precipitated as $CaCO_3$ or $SrCO_3$. The concentration of Cl^- is determined from a charge balance

(**INDEXI**=4). The initial pH is 8 (**INDEXI**=1 for H^+) and the initial concentration of strontium is 1×10^{-8} (**INDEXI**=3, **BI**=1×10^{-8}). Dissociation of H_2O is included so the position of the H^+ ion must be given (**LNH**=4) with OH^- last in the list of basis species. At the inner boundary 6.95×10^{-5} *equivalent* moles/*l* solution of solid $SrCO_3$ is placed in contact with the groundwater (**LEACH**=1, **NB**=1). As Sr^{2+} and CO_3^{2-} are released into the groundwater, the pH of the water will change. Therefore, the concentration of H^+ at the inner boundary is now determined by a charge balance (**INDEXB**=4). The concentrations of Sr^{2+} and CO_3^{2-} in equilibrium with solid $SrCO_3$ at the inner boundary must be determined from the solubility product of $SrCO_3$ calculated from Equation 2 with $K_k = 9.25$ and the additional constraint that the amounts of Sr^{2+} and CO_3^2 released into the groundwater must be in the stoichiometric ratio for that solid. The value of **BC** given for the first basis species (Sr^{2+}) making up solid $SrCO_3$ must be equal to the total amount of the solid. No values of **BC** need be given for the other species (CO_3) which is leaching in from this solid so the field is left blank. For the other species present, a concentration boundary is imposed at the first node.

A nonuniform grid spacing is used with 40 grid points (**NMAX**). Node locations are determined from Equation 21 with **DNO**=0.2, **AK**=1.4 and **XMAX**=5.0 m and are listed in the output. The initial time step (**DTINI**) is 10^{-4} yr and the maximum time step (**DTMAX**) is 0.5 yr. One-dimensional flow is assumed (**ITYPE**=0) with a concentration boundary condition imposed at the inner boundary (**IBND(1)**=0) and a no-flux condition imposed at the outer boundary (**IBND(2)**=1).

The input listing for the problem is given in Appendix B2. Because the dissociation of water is included, the complexation reactions are written in terms of H^+ and OH^- and the pK values appropriate to these reactions are used. For example, the formation of $CaHCO_3^+$ is written as

$$Ca^{2+} + H^{+} + CO_3^{2-} \rightleftarrows CaHCO_3^{+},$$

and the pK (**PK**) used is —11.3. The stoichiometric coefficients for this reaction in terms of the listed basis species (Na^{+}, Sr^{2+}, Ca^{2+}, H^{+}, CO_3^{2-}, Cl^{-}, and OH^{-}) are 0,0,1,1,1,0,0 (**S(I,J)**). Initial estimates of concentrations are provided in the input deck so **IG**=0.

The output is listed in Appendix B2 and shows the calculation of the equilibrium distributions of species for the initial and boundary conditions as well as the concentrations of the species for two times. Figures 3 and 4 show the concentrations of the basis species and the associated complexes at 5.2 years.

(3) *Surface complexation and aqueous-phase complexation*

In this example, Pb^{2+} and $PbOH^{+}$ are sorbed on the solid γ-Al_2O_3 via a surface complexation model. The background electrolyte is $NaClO_4$ and both cations and anions can be sorbed. The basis species are Na^{+}, Pb^{2+}, H^{+}, ClO_4^{-}, and OH^{-} (**NUM**(1)=5) The total number of species being sorbed via surface complexation is 5 (**NUM**(3)); these species are Na^{+}, Pb^{2+}, H^{+}, ClO_4^{-}, and the complex, $PbOH^{+}$. No precipitates are being considered so **NUM**(5)=0.

Data for the reactions and the needed constants are taken from *Davis and Leckie* [1978]. The pK (**PKE**) values for sorption of Na^{+} and ClO_4^{-} are 9.2 and —7.9 respectively. The reactions in CHEMTRN are written in terms of the formation of the complex whereas the convention used by *Davis and Leckie* [1978] is to write the reactions in terms of release of H^{+}. The reactions for sorption of the background electrolyte are

$$SOH + Na^{+} \rightleftarrows (SO^{-} - Na^{+}) + H_s^{+}$$

and

$$SOH + ClO_4^- \rightleftarrows (SOH_2^+ - ClO_4^-) - H_s^+$$

A pK of 11.5 (**PK2**) is used for the dissociation of SOH (reaction R4) and a pK of 5.7 (**PK1**) is used for the dissociation of SOH_2^+ (reaction R5). The surface site density is 8 sites/nm^2, the surface area is 117 m^2/g, and the ratio of solid mass to fluid volume is 11 g/ℓ, giving a value of **SOH** of 0.017 equivalents/ℓ solution and a value of **AREA** of 1.37×10^7 cm^2/ℓ solution. The capacitances are 100 μF/cm^2 (**C1**) and 20 μF/cm^2 (**C2**).

Following the discussion of *Davis and Leckie* [1978], the Pb^{2+} forms a complex with one surface site and so the amount of charge displaced is 1 (**AH**). The pK values (**PKE**) for sorption of Pb^{2+} and $PbOH^+$ are 5.0 and 2.6, respectively. Although *Davis and Leckie* [1978] write the sorption of $PbOH^+$ in terms of Pb^{2+} in the aqueous phase, the reactions in CHEMTRN must be written in terms of the species that is actually forming the complex with the solid phase. Thus, the Pb^{2+} reacts first with OH^- to form $PbOH^+$ in the bulk solution; then $PbOH^+$ with a +1 charge moves through the potential field to form a bond with the surface rather than Pb^{2+} with a +2 charge. The value of 2.6 for the sorption of $PbOH^+$ was determined by correcting *Davis and Leckie's* [1978] data for the formation of $PbOH^+$ in the bulk solution. The pK value of −6.28 (**PK**) for the formation PbOH was taken from *Benson and Teague* [1981].

The total concentration of lead in the aqueous phase is assumed to be 2.9×10^{-4} moles/ℓ solution (**BI**) so **INDEXI**=2 and the pH of the solution is 7 (**INDEXI**=1 for H^+). A feed solution equivalent to the initial solution, but with a pH of 4.5 (**INDEXB**=1 for H^+), is introduced at $x = 0$ with a velocity of 0.1 m/hr (**VO**). The dispersivity of the porous medium is 0.3 m (**DOA**). The variable grid spacing given in the second example is used. The initial time step is 10^{-5} hr (**DTINI**) and the maximum time step permitted is 0.5 hr (**DTMAX**). The position of the H^+ ion is 3 (**LNH**) and **LEACH** and **NB** are both 0. The input and the output are listed in Appendix B3. The initial distribution of species, and the concentration profiles as functions of distance for two different times, are given.

Plotted in Figure 5 are the concentrations of aqueous Pb^{2+}, $PbOH^+$, H^+, sorbed lead in the forms of (SO^-Pb^{2+}) and (SO^-PbOH^+), and sorbed H^+ in the form of SOH at 5 hours. As seen in the figure, the concentration of the Pb^{2+} ion in the aqueous phase is approximately constant. The ratio of the total concentration of sorbed lead to the total aqueous phase concentration varies from 18 initially to approximately 1 at the boundary.

(4) *Precipitation/dissolution, ion exchange and aqueous-phase complexation*

In this example CHEMTRN is used to simulate precipitation of $CaCO_3$ when a Na^+-rich solution flows into a one-dimensional column of porous medium on which Ca^{2+} has previously been sorbed. Initially, the fluid in the column contains 1.5×10^{-3} $\underline{M}$ Ca^{2+} (**INDEXI**=3, **BI**=1.5×10^{-3}), 10^{-5} $\underline{M}$ Na^+ (**INDEXI**=2), 6.6×10^{-4} $\underline{M}$ CO_3^{2-} (**INDEXI**=3), and enough H^+ to give a pH of 8 (**INDEXI**=1). The program will calculate enough Cl^- (**INDEXI**=4) to balance the solution electrically. Then a solution that has a higher level of Na^+ (**BI**=1.1×10^{-2} $\underline{M}$, **INDEXB**=2) is fed into the column. The Ca^{2+} ion is displaced from the solid matrix. The initial concentrations in the fluid are such that the solubility product of $CaCO_3(s)$ (**NUM**(5)=1) is exceeded when the Na^+-rich fluid flows into the column. A constant-flux coundary condition (**IBND**(1)=1) is maintained at $x = 0$ and a boundary condition of constant concentration equal to that of the initial groundwater is maintained at the outflow boundary (**IBND**(2)=0). The dissociation of water (a nonzero value of **LNH**) and the formation of the complexes $NaCO_3^-$, $NaHCO_3^0$, $NaOH^0$, HCO_3^-, $H_2CO_3^0$, $CaCO_3^0$,

$CaHCO_3^+$, and $CaOH^+$ (**NUM**(4)=8) are included in the simulation. The position of H^+ in the list of basis species is 3 (**LNH**); OH is given last in the list of basis species.

The input and output listings for this example are given in Appendix B4. The output shows the initial distributions of species, the time at which a node begins to precipitate $CaCO_3$, and the concentration profile for two different times. Figure 6 is a plot of the time when $CaCO_3$ begins to precipitate along the column. Because $CaCO_3$ does not precipitate in the equilibrium distribution of species for the fluid flowing into the column, this precipitate will start to redissolve at the upstream boundary as the fluid approaches the inflow conditions.

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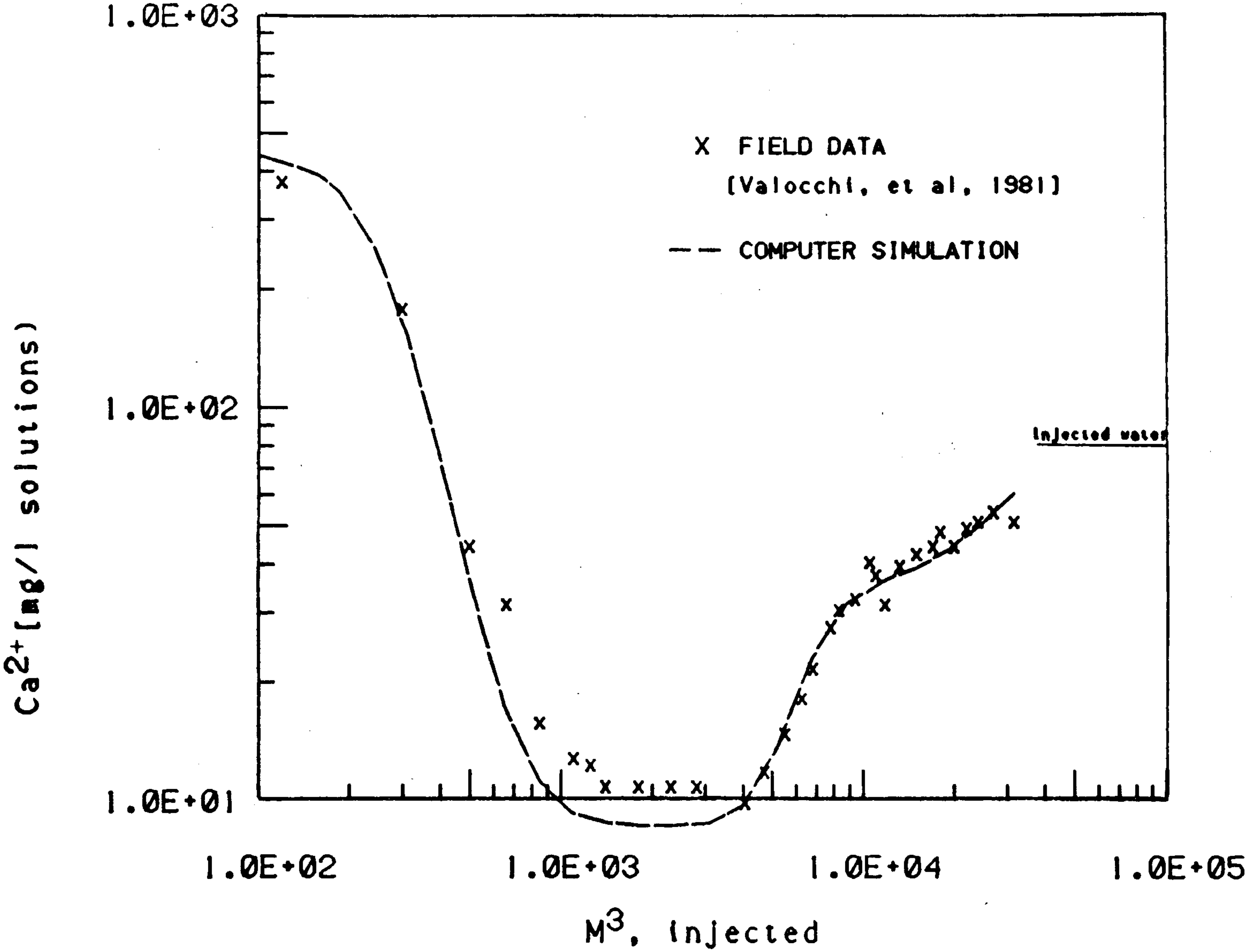

Figure 1. Example 1: Results of CHEMTRN simulations and field data [*Valocchi et al.*, 1981] for concentration of Ca^{2+} as a function of injected volume of treated wastewater.

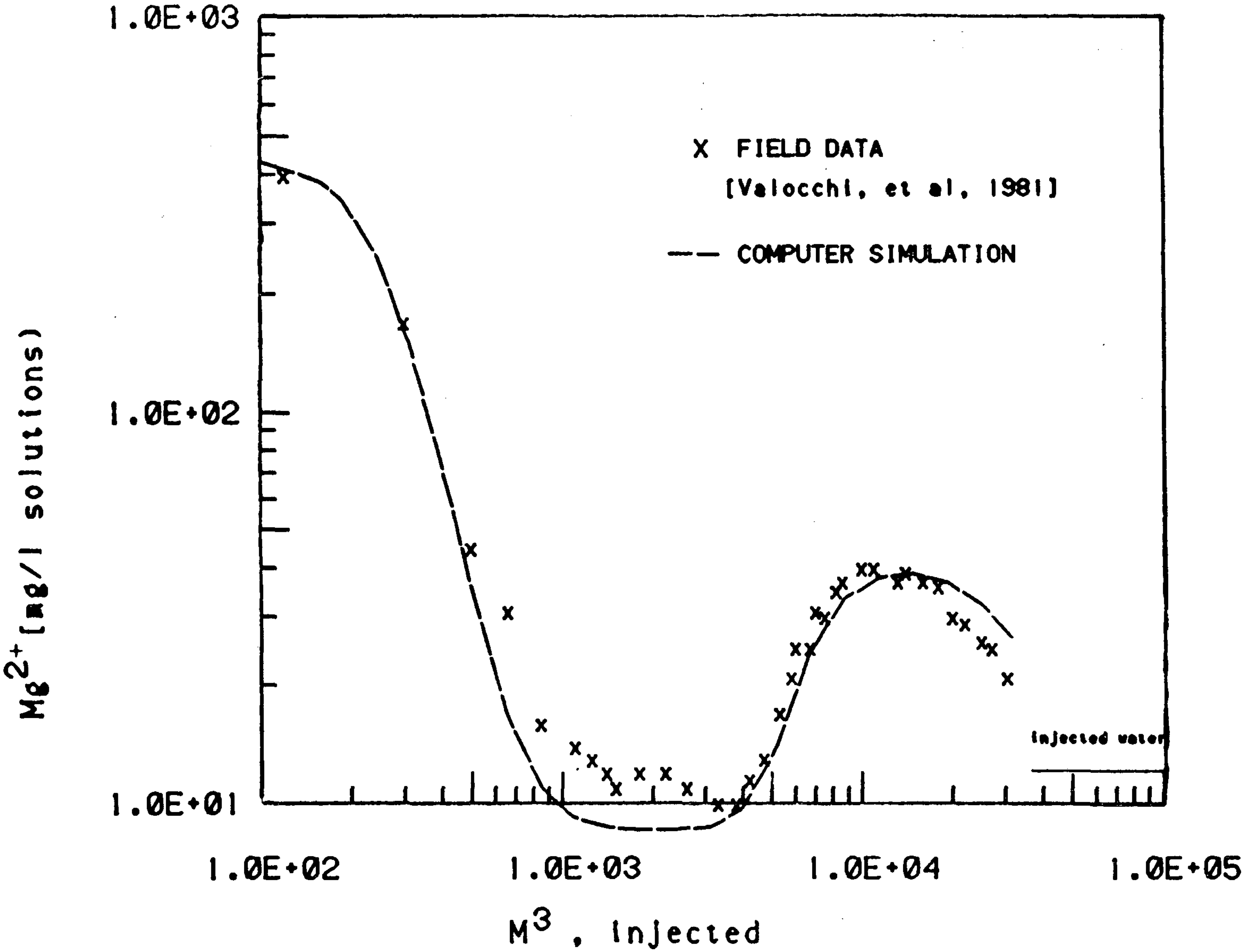

Figure 2. Example 1: Results of CHEMTRN simulations and field data [*Valocchi et al.*, 1981] for concentration of Mg^{2+} as a function of injected volume of treated wastewater.

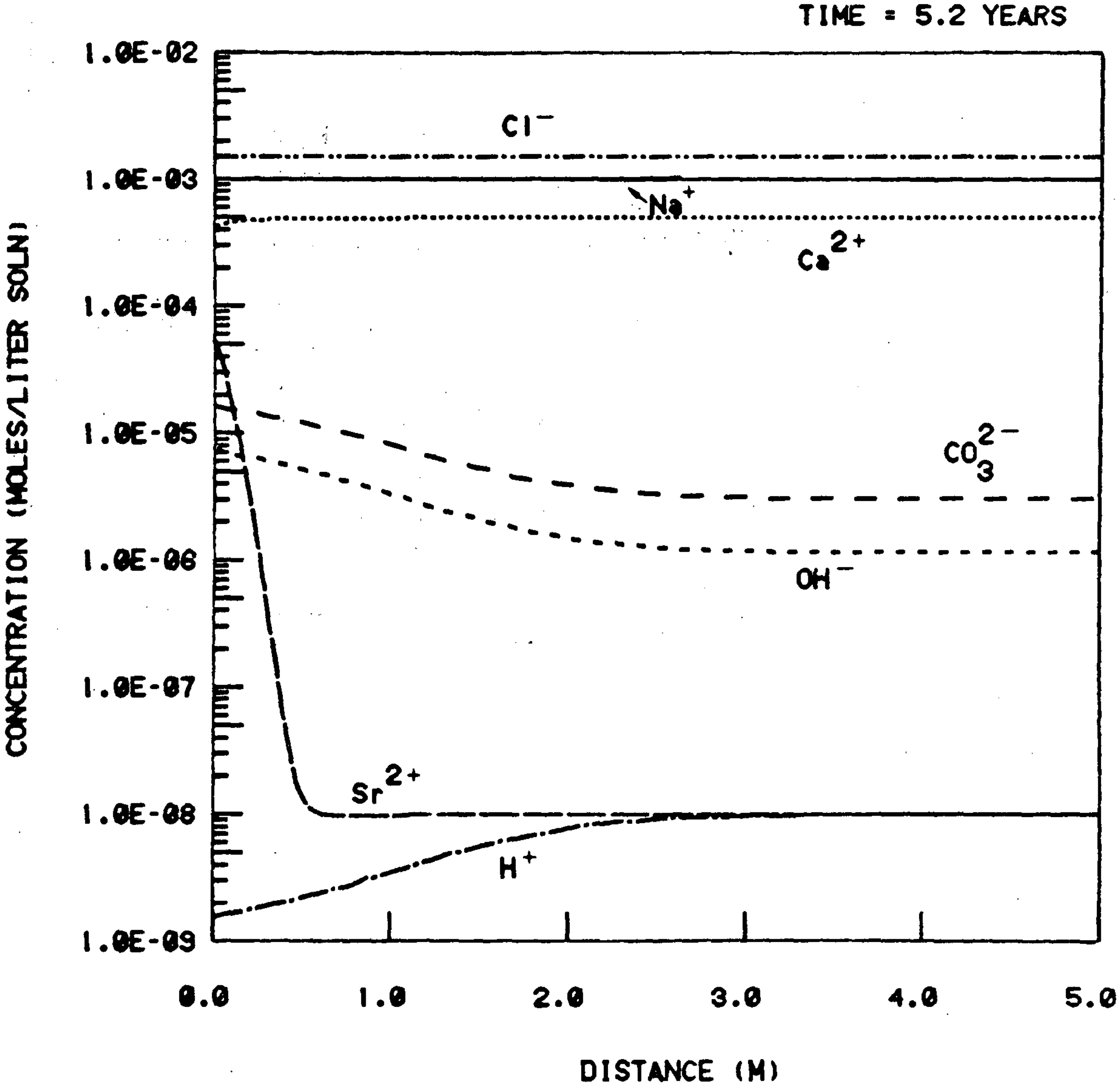

Figure 3. Example 2: Concentration of basis species at 5.2 years.

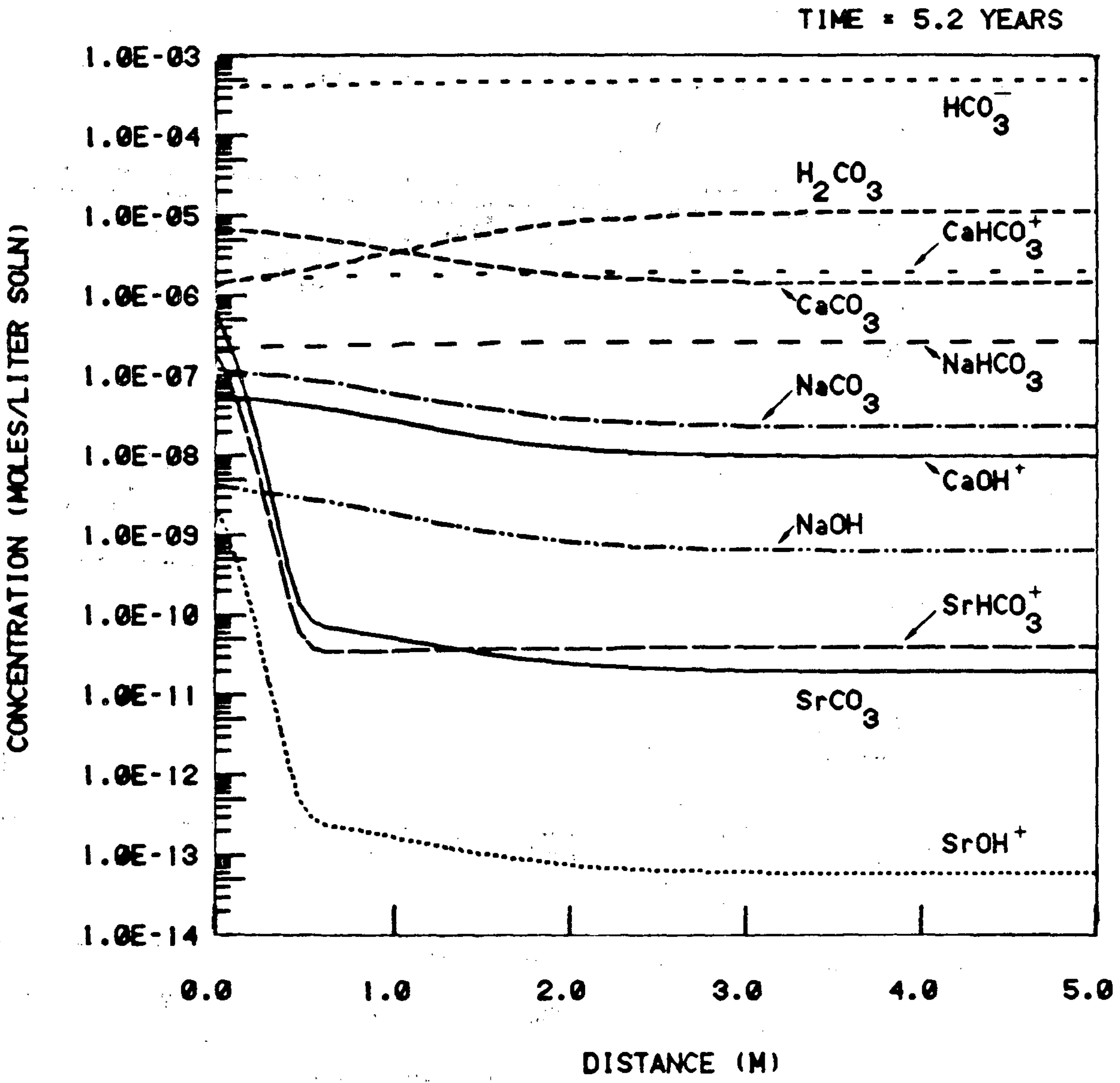

Figure 4. Example 2: Concentration of aqueous complexes at 5.2 years.

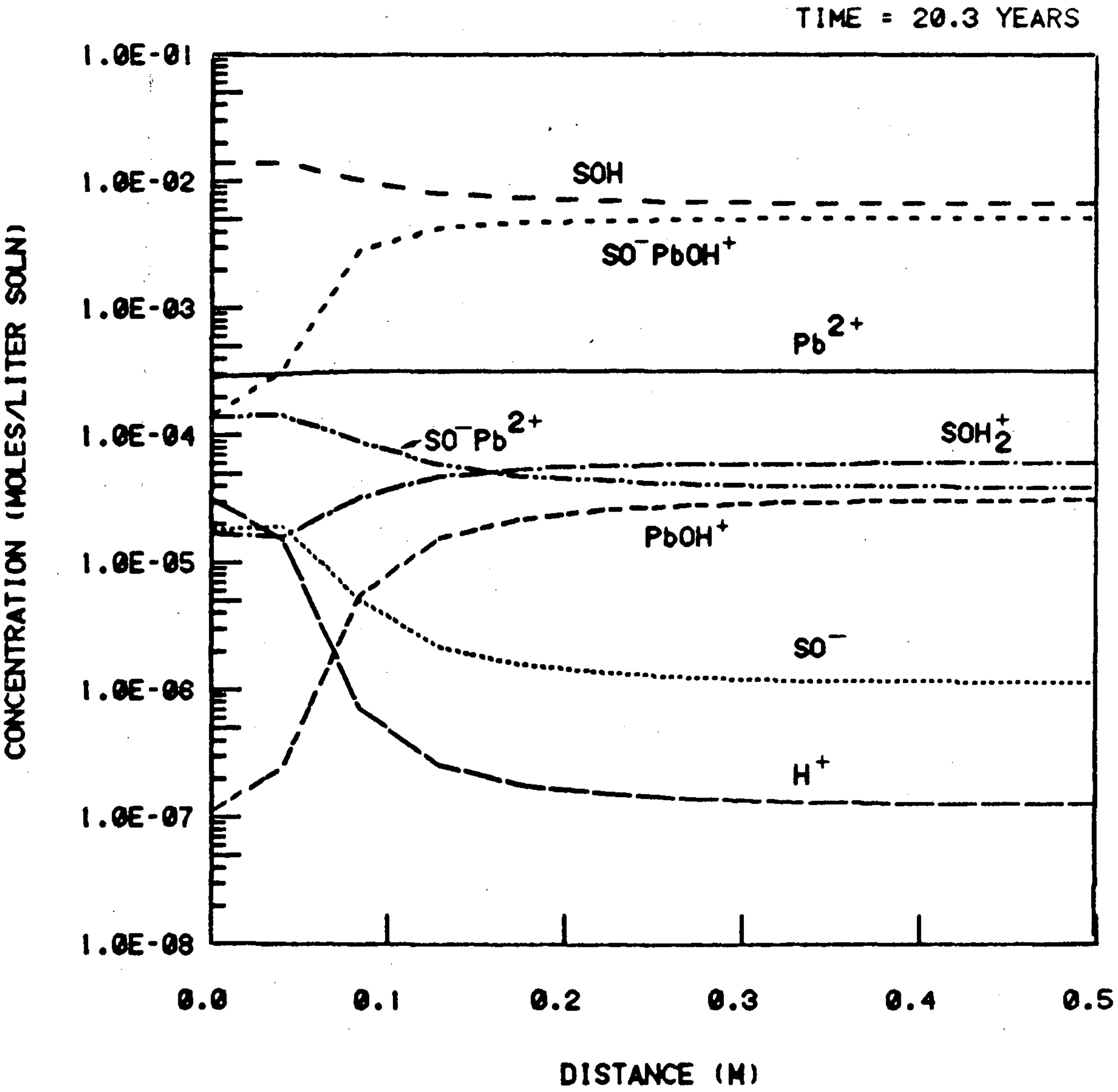

Figure 5. Example 3. Concentration of sorbed and aqueous species, H^+, Pb^{2+}, $PbOH^+$ at 20.3 years.

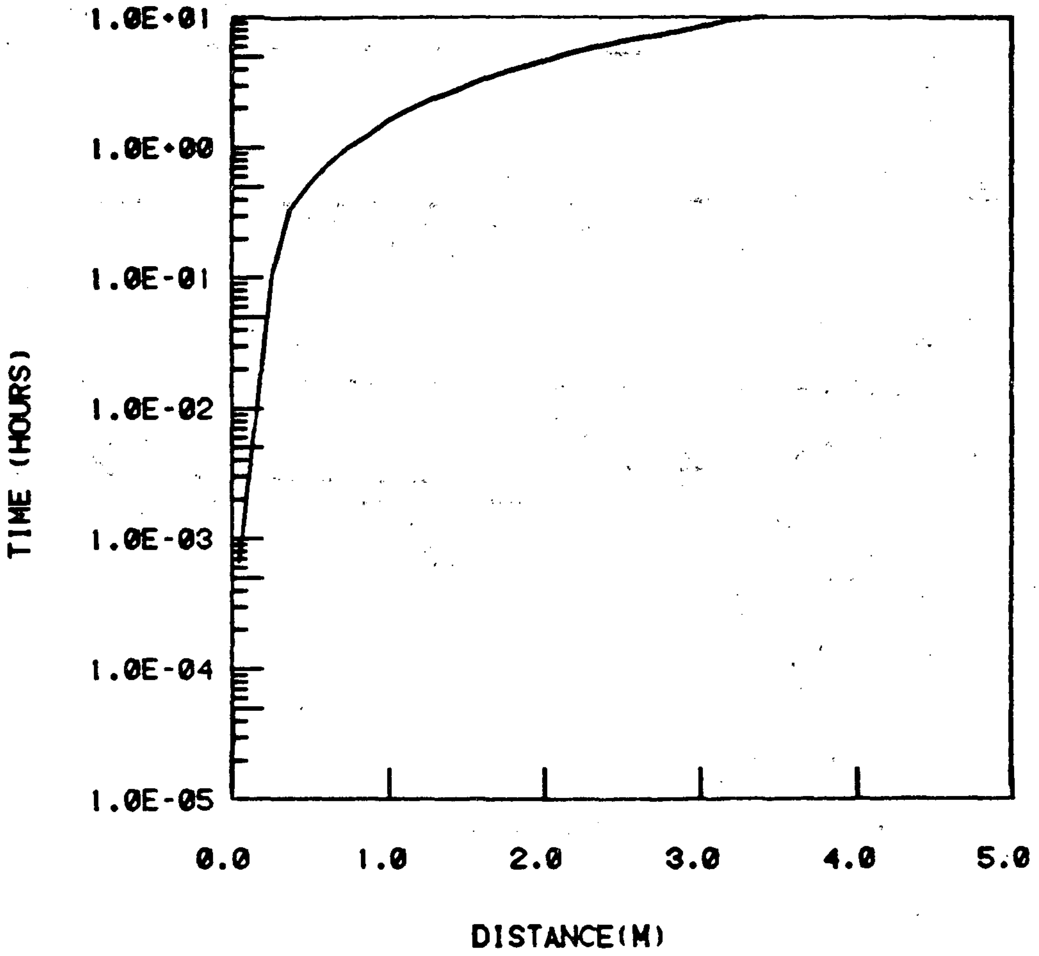

Figure 6. Example 4. Precipitation of $CaCO_{3(s)}$ along the column as a function of time.

APPENDIX A

An alphabetical list of the variables and their definitions in this appendix.

AH	amount of charge which is displaced or sorbed for each surface complexation reaction with a SOH site: **(Line 13c, Line 15b)** +1 - a H^+ ion is displaced, 0 - used for the H^+ ion, −1 - a H^+ ion is sorbed
AK	parameter used to calculate the grid spacing (Equation 19) **(Line 4)**
AREA	sorption area used in surface complexation model [L^2/l solution] **(Line 12)**
BC	value of the concentration at the boundary in [moles/l solution] according to the value of **INDEXB (Line 13a)**
BI	value of the initial concentration in [moles/l solution] according to the value of **INDEXI (Line 13a)**
CECNS	concentration of sites in [equivalents/l solution] available for sorption in ion exchange model **(Line 11)**
C1	capacitance between the surface plane and the beta plane in surface complexation model [$\mu F/L^2$] **(Line 12)**
C2	capacitance between the beta plane and the diffuse layer in surface complexation model [$\mu F/L^2$] **(Line 12)**
DOA	dispersivity [L] **(Line 7)**
DOB	diffusion coefficient [L^2/t] **(Line 7)**

DNO	parameter used to calculate the grid spacing (Equation 19); if **DNO** = 0, then the grid spacing will be uniform and equal to **XMAX/(NMAX—1)** **(Line 4)**
DTINI	size of the initial time step [t] **(Line 5)**
DTMAX	size of the maximum time step permitted [t] **(Line 5)**
DUM	name of the species **(Lines 13a, 14a, 15a, 16a)**
GUESSB	guess for the amount of the species which is sorbed initially at the boundary [moles/l solution] **(Lines 13b-c, 14b, 15c-d, 16b)**; **can be left blank if the program is to provide the quess (IG = 1 on Line 2)**
GUESSI	guess for the initial concentration of the species [moles/l solution] **(Lines 13b-c, 14b, 15c-d, 16b)** **can be left blank if the program is to provide the guess (IG = 1) on Line 2**
H2OK	— log of the dissociation constant of water **(Line 14a)**
IBND(1)	type of boundary condition to be imposed at the inner boundary **(Line 8)**: 0 - constant concentration; 1 - constant flux
IBND(2)	type of boundary condition to be imposed at the outer boundary **(Line 8)**: 0 - constant concentration equal to initial conditions; 1 - no flux
IDYNAM	code to indicate whether the program should stop after calculating the equilibrium distribution for the initial and boundary conditions **(Line 2)**: 0 - stop; 1 - continue executing
IG	code to indicate whether the program or the user will

	provide initial guesses of the concentrations (**Line 2**): 0 - user will; 1 - program will
IN1	number of iterations before printing when calculating the equilibrium distribution of the initial conditions (**Line 3**)
IN2	number of iterations before printing when calculating the equilibrium distribution at the grid point where the boundary condition is specified (**Line 3**)
IN3	number of iterations before printing when calculating the equilibrium distribution at a node point where a new precipitate is forming (**Line 3**)
INDEXB	type of condition specified for calculating distribution of species at the boundary conditions (**Line 13a**): 0 - the total concentration of the species will be given (including sorbed phase, aqueous phase and precipitate); 1 - only the concentration of the basis species will be given; 2 - the combined concentration of the basis species and the aqueous complexes will be given (if a species can form a precipitate, option 3 must be used instead of option 2 to allow for the inclusion of the solubility product if necessary); 3 - the combined concentration of the basis species, aqueous complexes and precipitates will be given; 4 - the initial concentration will be determined from a charge balance
INDEXI	takes the same values as **INDEXB** and describes what type of concentration is being specified as the initial conditions (**Line 13a**)
ISORPI	code to indicate whether the species is sorbed according to an ion exchange mechanism (**Lines 13a, 15a**): 0 - is not sorbed; 1 - is sorbed

ISORPE	code to indicate whether the species is sorbed according to a surface complexation model (**Lines 13a, 15a**): 0 - is not sorbed; 1 - is sorbed
ITYPE	type of flow (**Line 2**): 0 - one-dimensional flow; 1 - radial flow
KMAX	number of times at which the results are to be printed (**Line 5**)
LEACH	position in the list of precipitates of the solid which is leaching (**Line 9**): 0 - no leaching
LNH	position of H^+ in the list of basis species (**Line 10**): 0 - dissociation of water not included
NB	location of the solid which is leaching (**Line 9**): 0 - no leaching; 1 - solid is leaching at the first grid point
NMAX	number of grid points (**Line 4**)
NUM(1)	number of basis species (OH^- must be included in the count if the dissociation of water is to be incorporated in the model) (**Line 10**)
NUM(2)	number of species (both basis species and complexes) which are sorbed according to an ion exchange mechanism (**Line 10**)
NUM(3)	number of species (both basis species and complexes) which are sorbed according to a surface complexation model (**Line 10**)
NUM(4)	number of aqueous complexes (**Line 10**)
NUM(5)	number of solid precipitates (**Line 10**)

PK	— log of the equilibrium constant for the formation of a complex (**Line 15b**) or — log of the solubility product (**Line 16a**)
PK1	— log of the dissociation constant of the positively charged site SOH^{2+} (**Line 12**)
PK2	— log of the the dissociation constant of the neutral site SOH (**Line 12**)
PKI	— log of the equilibrium constant for the ion exchange between the aqueous complex and H^+ (or another common species) (**Lines 13b, 15c**)
PKE	— log of the equilibrium constant for the surface complex reaction between the aqueous species and an SOH site in the surface complexation reaction (**Lines 13c, 15d**)
RW	for the case of radial flow with a flux boundary condition, the first grid point is located at 2 × **RW** (can be left blank in other cases) (**Line 4**)
S	array which holds the stoichiometric coefficients for the reaction to form a complex; read in the same order in which the basis species are read (**Line 15a**)
SS	array which holds the stoichiometric coefficients for the reaction to form a precipitate; read in the same order in which the basis species are read (**Line 16a**)
SOH	number of sites in [equivalents/l solution] available for sorption in surface complexation model (**Line 12**)
TITLE	title information for the problem (**Line 1a**)
TPRINT	array which holds the times at which the results are to be printed [t] (**Line 6**)

VJ	charge of the species (**Line 13a**)
VO	for one-dimensional flow (**ITYPE** = 0 on **Line 2**), this is the mean fluid velocity (i.e., the specific discharge divided by the porosity) $[L/t]$; for radial flow (**ITYPE** = 1 on **Line 2**), it is a constant of proportionality equal to the radial distance times the mean fluid velocity $[1/t]$ (**Line 7**)
ULENGTH	unit of length used in calculations (**Line 1b**)
UTIME	unit of time used in calculations (**Line 1b**)
XMAX	distance between the first and last grid points $[L]$ (**Line 4**)

APPENDIX B1 - Example 1: Sample Input and Output

```
ION EXCHANGE WITH TRANSPORT
 METERS      HOURS
  TYPE             1         1         0
ITERATIONS       100       100       100
  GRID            40      64.0      0.00                 0.5
  TIME            14    1.0E-4      1.60
PRINT TIME       4.0      10.0      30.0      40.0      80.0     120.0      170.
PRINT TIME     300.      400.      600.       800.     1200.    1400.0    1500.0
PHYSICAL    1.000E+0       0.0   9.80E+0
BOUNDARY           1         0
  LEACH            0         0
NO.SPECIES         4         3         0         0         0         0
  CECNS         0.67
     NA     1.0    2   8.68E-2   8.68E-2    2   9.43E-3   9.43E-3    1    0
     NA        .0000    1.0E-3    1.0E-3
     MG     2.0    2   1.79E-2   1.79E-2    2   4.94E-4   4.94E-4    1    0
     MG       -0.350   1.00E-3   1.00E-3
     CA     2.0    2   1.11E-2   1.11E-2    2   2.12E-3   2.12E-3    1    0
     CA       -0.600   4.00E-2   4.90E-2
     CL    -1.0    2   1.60E-1   1.60E-1    2   9.04E-3   9.04E-3    0    0
```

```
1ION EXCHANGE WITH TRANSPORT

   UNIT OF LENGTH IS   METERS             UNIT OF TIME IS     HOURS

   INNER BOUNDARY IS CONSTANT FLUX        OUTER BOUNDARY IS CONSTANT INITIAL CONCENTRATION

   DISPERSION COEFFICIENT = 1.0 V +.0        FLUID VELOCITY =     9.800/ R     NUMBER OF GRID POINTS =   40


   NUMBER OF PRINT OUTS =   14
   GIVEN AT THE FOLLOWING TIMES = 4.000      10.00      30.00      40.00      80.00      120.0      170.0      300.0
                                  400.0      600.0      800.0      1200.      1400.      1500.

   NUMBER OF SITES(ION-EXCHANGE)     .6700           NUMBER OF SITES(EDL MODEL)    0.



    4      BARE IONS            3     SORBING IONS (IONEX)           0     SORBING IONS (EDL MODEL)


 COMPONENT  CHARGE        INITIAL CONDITIONS        BOUNDARY CONDITIONS        PK(IONEX)       PK(EDL)
                          TYPE       VALUE          TYPE       VALUE

    NA        1.            2      8.6800E-02         2      9.4300E-03        0.             ---
    MG        2.            2      1.7900E-02         2      4.9400E-04        -.350          ---
    CA        2.            2      1.1100E-02         2      2.1200E-03        -.600          ---
    CL       -1.            2      1.6000E-01         2      9.0400E-03         ---           ---

                                                    ** SPATIAL GRID **

    1.000         1.641         3.282         4.923         6.564         8.205         9.846         11.49         13.13         14.77
    16.41         18.05         19.69         21.33         22.97         24.62         26.26         27.90         29.54         31.18
    32.82         34.46         36.10         37.74         39.38         41.03         42.67         44.31         45.95         47.59
    49.23         50.87         52.51         54.15         55.79         57.44         59.08         60.72         62.36         64.00
```

```
1                                                INITIAL CONDITIONS


COMPONENT       TOTAL          BARE ION        SORBED CONCENTRATION         ACT. COEF.     KD(ION EX)        KD(EDL)
            AQUEOUS CONC.    CONCENTRATION      (IONEX)     (EDL)

   NA        .8680E-01        .8680E-01       .1305        0.                .7531          1.503           0.
   MG        .1790E-01        .1790E-01       .1283        0.                .3216          7.167           0.
   CA        .1110E-01        .1110E-01       .1415        0.                .3216          12.75           0.
   CL        .1600            .1600           0.           0.                .7531          0.              0.


  TO HAVE A NET BALANCE OF ZERO CHARGE, OTHER SPECIES MUST BE PRESENT (ALTHOUGH NOT PARTICIPATING IN THE
  CHEMICAL REACTIONS) WITH A TOTAL CONCENTRATION TIMES CHARGE OF   .152E-01


1                           BOUNDARY OR INFLUX CONDITIONS


COMPONENT       TOTAL          BARE ION        SORBED CONCENTRATION         ACT. COEF.     KD(ION EX)        KD(EDL)
            AQUEOUS CONC.    CONCENTRATION      (IONEX)     (EDL)

   NA        .9430E-02        .9430E-02       .3668E-01   0.                 .8801          3.890           0.
   MG        .4940E-03        .4940E-03       .3669E-01   0.                 .5999          74.26           0.
   CA        .2120E-02        .2120E-02       .2800       0.                 .5999          132.1           0.
   CL        .9040E-02        .9040E-02       0.          0.                 .8801          0.              0.


  TO HAVE A NET BALANCE OF ZERO CHARGE, OTHER SPECIES MUST BE PRESENT (ALTHOUGH NOT PARTICIPATING IN THE
  CHEMICAL REACTIONS) WITH A TOTAL CONCENTRATION TIMES CHARGE OF  -.562E-02


  CONVERGENCE IS OBTAINED IN LESS THAN 6 ITERATIONS SO TIME STEP IS INCREASED BY 1.75
  DELT=  1.7500E-04          AT TIME=  1.0000E-04

  CONVERGENCE IS OBTAINED IN LESS THAN 6 ITERATIONS SO TIME STEP IS INCREASED BY 1.75
  DELT=  3.0625E-04          AT TIME=  2.7500E-04
```

```
1    TIME=  80.39186          DELT=  1.6000E+00         CONCENTRATION OF SPECIES IN MOLES/LITER SOLUTION


                                                          DISTANCE(METERS)
      SPECIES         1.000        1.641        3.282        4.923        6.564        8.205        9.846       11.487       13.128

         NA        9.8941E-03   9.9319E-03   9.8211E-03   9.8904E-03   1.0646E-02   1.2046E-02   1.3181E-02   1.3467E-02   1.3514E-02
         MG        7.8272E-04   8.6396E-04   1.1274E-03   1.2640E-03   1.1659E-03   8.2980E-04   4.8488E-04   3.7327E-04   3.5327E-04
         CA        2.0203E-03   1.9250E-03   1.4136E-03   9.4147E-04   6.9995E-04   4.8545E-04   2.9189E-04   2.2884E-04   2.1746E-04
         CL        1.0017E-02   1.0028E-02   9.3241E-03   8.6263E-03   8.7148E-03   9.0616E-03   9.1284E-03   9.0558E-03   9.0375E-03

    SORBED(IONEX)

         NA        3.8110E-02   3.8645E-02   4.1350E-02   4.6199E-02   5.4801E-02   7.3729E-02   1.0396E-01   1.1991E-01   1.2342E-01
         MG        5.6518E-02   6.3615E-02   9.7322E-02   1.3418E-01   1.4877E-01   1.4612E-01   1.3669E-01   1.3159E-01   1.3047E-01
         CA        2.5943E-01   2.5206E-01   2.1700E-01   1.7772E-01   1.5883E-01   1.5201E-01   1.4633E-01   1.4346E-01   1.4282E-01


                                                          DISTANCE(METERS)
      SPECIES        14.769       16.410       18.051       19.692       21.333       22.974       24.615       26.256       27.897

         NA        1.3544E-02   1.3574E-02   1.3626E-02   1.3730E-02   1.3933E-02   1.4313E-02   1.4993E-02   1.6146E-02   1.7991E-02
         MG        3.5048E-04   3.5033E-04   3.5180E-04   3.5626E-04   3.6631E-04   3.8661E-04   4.2529E-04   4.9623E-04   6.2258E-04
         CA        2.1591E-04   2.1589E-04   2.1684E-04   2.1964E-04   2.2587E-04   2.3843E-04   2.6234E-04   3.0615E-04   3.8418E-04
         CL        9.0612E-03   9.0962E-03   9.1620E-03   9.2995E-03   9.5726E-03   1.0090E-02   1.1024E-02   1.2627E-02   1.5242E-02

    SORBED(IONEX)

         NA        1.2413E-01   1.2443E-01   1.2465E-01   1.2485E-01   1.2504E-01   1.2521E-01   1.2538E-01   1.2556E-01   1.2576E-01
         MG        1.3025E-01   1.3016E-01   1.3009E-01   1.3002E-01   1.2997E-01   1.2991E-01   1.2986E-01   1.2981E-01   1.2975E-01
         CA        1.4269E-01   1.4263E-01   1.4259E-01   1.4255E-01   1.4251E-01   1.4248E-01   1.4245E-01   1.4241E-01   1.4238E-01
```

DISTANCE(METERS)

SPECIES	29.538	31.179	32.821	34.462	36.103	37.744	39.385	41.026	42.667
NA	2.0761E-02	2.4643E-02	2.9710E-02	3.5863E-02	4.2812E-02	5.0140E-02	5.7402E-02	6.4174E-02	7.0129E-02
MG	8.4161E-04	1.2088E-03	1.7958E-03	2.6767E-03	3.9060E-03	5.4839E-03	7.3336E-03	9.3210E-03	1.1283E-02
CA	5.1948E-04	7.4637E-04	1.1093E-03	1.6545E-03	2.4160E-03	3.3942E-03	4.5417E-03	5.7752E-03	6.9930E-03
CL	1.9277E-02	2.5158E-02	3.3240E-02	4.3686E-02	5.6365E-02	7.0794E-02	8.6171E-02	1.0150E-01	1.1578E-01
SORBED(IONEX)									
NA	1.2601E-01	1.2635E-01	1.2680E-01	1.2737E-01	1.2802E-01	1.2866E-01	1.2923E-01	1.2968E-01	1.3001E-01
MG	1.2967E-01	1.2956E-01	1.2942E-01	1.2925E-01	1.2905E-01	1.2885E-01	1.2868E-01	1.2854E-01	1.2844E-01
CA	1.4233E-01	1.4226E-01	1.4218E-01	1.4207E-01	1.4194E-01	1.4182E-01	1.4171E-01	1.4162E-01	1.4156E-01

DISTANCE(METERS)

SPECIES	44.308	45.949	47.590	49.231	50.872	52.513	54.154	55.795	57.436
NA	7.5067E-02	7.8932E-02	8.1782E-02	8.3764E-02	8.5059E-02	8.5856E-02	8.6316E-02	8.6565E-02	8.6693E-02
MG	1.3066E-02	1.4563E-02	1.5726E-02	1.6564E-02	1.7127E-02	1.7478E-02	1.7683E-02	1.7794E-02	1.7852E-02
CA	8.1001E-03	9.0293E-03	9.7512E-03	1.0272E-02	1.0620E-02	1.0838E-02	1.0965E-02	1.1035E-02	1.1070E-02
CL	1.2822E-01	1.3833E-01	1.4601E-01	1.5146E-01	1.5507E-01	1.5732E-01	1.5862E-01	1.5933E-01	1.5969E-01
SORBED(IONEX)									
NA	1.3022E-01	1.3035E-01	1.3041E-01	1.3045E-01	1.3046E-01	1.3047E-01	1.3047E-01	1.3047E-01	1.3047E-01
MG	1.2837E-01	1.2833E-01	1.2831E-01	1.2830E-01	1.2830E-01	1.2829E-01	1.2829E-01	1.2829E-01	1.2829E-01
CA	1.4152E-01	1.4150E-01	1.4148E-01	1.4148E-01	1.4147E-01	1.4147E-01	1.4147E-01	1.4147E-01	1.4147E-01

DISTANCE(METERS)

SPECIES	59.077	60.718	62.359	64.000
NA	8.6754E-02	8.6781E-02	8.6793E-02	8.6800E-02
MG	1.7879E-02	1.7891E-02	1.7897E-02	1.7900E-02
CA	1.1087E-02	1.1095E-02	1.1098E-02	1.1100E-02
CL	1.5987E-01	1.5995E-01	1.5998E-01	1.6000E-01
SORBED(IONEX)				
NA	1.3047E-01	1.3047E-01	1.3047E-01	1.3047E-01
MG	1.2829E-01	1.2829E-01	1.2829E-01	1.2829E-01
CA	1.4147E-01	1.4147E-01	1.4147E-01	1.4147E-01

```
1    TIME= 800.39186          DELT=  1.6000E+00         CONCENTRATION OF SPECIES IN MOLES/LITER SOLUTION


                                                     DISTANCE(METERS)
   SPECIES          1.000        1.641        3.282        4.923        6.564        8.205        9.846       11.487       13.128

      NA         9.1864E-03   9.1884E-03   9.3708E-03   9.5396E-03   9.5137E-03   9.4325E-03   9.4264E-03   9.4568E-03   9.4766E-03
      MG         4.7219E-04   4.7460E-04   5.0756E-04   5.5623E-04   6.1145E-04   7.0495E-04   8.6880E-04   1.0902E-03   1.3141E-03
      CA         1.9967E-03   1.9950E-03   2.0694E-03   2.1209E-03   2.0472E-03   1.8996E-03   1.7235E-03   1.5077E-03   1.2801E-03
      CL         8.4208E-03   8.4247E-03   8.8855E-03   9.3136E-03   9.2407E-03   9.0211E-03   8.9850E-03   9.0338E-03   9.0481E-03

 SORBED(IONEX)

      NA         3.6716E-02   3.6728E-02   3.6767E-02   3.6869E-02   3.7086E-02   3.7493E-02   3.8167E-02   3.9108E-02   4.0161E-02
      MG         3.7166E-02   3.7361E-02   3.8376E-02   4.0686E-02   4.5508E-02   5.4603E-02   6.9761E-02   9.1188E-02   1.1526E-01
      CA         2.7948E-01   2.7927E-01   2.7824E-01   2.7588E-01   2.7095E-01   2.6165E-01   2.4616E-01   2.2426E-01   1.9966E-01


                                                     DISTANCE(METERS)
   SPECIES         14.769       16.410       18.051       19.692       21.333       22.974       24.615       26.256       27.897

      NA         9.4917E-03   9.5177E-03   9.5676E-03   9.6650E-03   9.8532E-03   1.0202E-02   1.0808E-02   1.1729E-02   1.2753E-02
      MG         1.4824E-03   1.5748E-03   1.6045E-03   1.5894E-03   1.5332E-03   1.4210E-03   1.2253E-03   9.2771E-04   5.9774E-04
      CA         1.1014E-03   9.9497E-04   9.4059E-04   9.0710E-04   8.6927E-04   8.0674E-04   6.9993E-04   5.3701E-04   3.5458E-04
      CL         9.0416E-03   9.0392E-03   9.0398E-03   9.0401E-03   9.0400E-03   9.0400E-03   9.0400E-03   9.0400E-03   9.0400E-03

 SORBED(IONEX)

      NA         4.1084E-02   4.1784E-02   4.2425E-02   4.3343E-02   4.5044E-02   4.8387E-02   5.5018E-02   6.8165E-02   9.1232E-02
      MG         1.3547E-01   1.4792E-01   1.5363E-01   1.5551E-01   1.5560E-01   1.5466E-01   1.5254E-01   1.4828E-01   1.4083E-01
      CA         1.7899E-01   1.6619E-01   1.6015E-01   1.5782E-01   1.5688E-01   1.5614E-01   1.5495E-01   1.5264E-01   1.4858E-01
```

```
                                                          DISTANCE(METERS)
  SPECIES        29.538      31.179      32.821      34.462      36.103      37.744      39.385      41.026      42.667

     NA       1.3329E-02  1.3504E-02  1.3545E-02  1.3554E-02  1.3558E-02  1.3560E-02  1.3562E-02  1.3563E-02  1.3565E-02
     MG       4.1320E-04  3.5735E-04  3.4431E-04  3.4123E-04  3.4017E-04  3.3953E-04  3.3899E-04  3.3850E-04  3.3806E-04
     CA       2.5127E-04  2.1971E-04  2.1231E-04  2.1056E-04  2.0996E-04  2.0959E-04  2.0928E-04  2.0900E-04  2.0875E-04
     CL       9.0400E-03  9.0400E-03  9.0400E-03  9.0400E-03  9.0400E-03  9.0400E-03  9.0401E-03  9.0402E-03  9.0405E-03

SORBED(IONEX)

     NA       1.1326E-01  1.2268E-01  1.2517E-01  1.2578E-01  1.2598E-01  1.2611E-01  1.2622E-01  1.2632E-01  1.2641E-01
     MG       1.3374E-01  1.3073E-01  1.2994E-01  1.2974E-01  1.2968E-01  1.2964E-01  1.2960E-01  1.2957E-01  1.2955E-01
     CA       1.4463E-01  1.4293E-01  1.4248E-01  1.4237E-01  1.4233E-01  1.4231E-01  1.4229E-01  1.4227E-01  1.4225E-01

                                                          DISTANCE(METERS)
  SPECIES        44.308      45.949      47.590      49.231      50.872      52.513      54.154      55.795      57.436

     NA       1.3567E-02  1.3570E-02  1.3575E-02  1.3587E-02  1.3617E-02  1.3694E-02  1.3890E-02  1.4374E-02  1.5501E-02
     MG       3.3767E-04  3.3736E-04  3.3721E-04  3.3746E-04  3.3873E-04  3.4290E-04  3.5605E-04  4.0143E-04  5.6935E-04
     CA       2.0852E-04  2.0835E-04  2.0828E-04  2.0844E-04  2.0924E-04  2.1181E-04  2.1982E-04  2.4706E-04  3.4641E-04
     CL       9.0413E-03  9.0435E-03  9.0491E-03  9.0641E-03  9.1038E-03  9.2084E-03  9.4849E-03  1.0215E-02  1.2143E-02

SORBED(IONEX)

     NA       1.2650E-01  1.2658E-01  1.2665E-01  1.2672E-01  1.2677E-01  1.2675E-01  1.2631E-01  1.2358E-01  1.1323E-01
     MG       1.2952E-01  1.2949E-01  1.2947E-01  1.2945E-01  1.2943E-01  1.2944E-01  1.2958E-01  1.3045E-01  1.3371E-01
     CA       1.4223E-01  1.4222E-01  1.4220E-01  1.4219E-01  1.4218E-01  1.4218E-01  1.4226E-01  1.4276E-01  1.4467E-01

                                                          DISTANCE(METERS)
  SPECIES        59.077      60.718      62.359      64.000
     NA       1.8111E-02  2.4659E-02  4.1752E-02  8.6800E-02
     MG       1.1288E-03  2.6983E-03  6.8701E-03  1.7900E-02
     CA       6.7721E-04  1.6303E-03  4.2213E-03  1.1100E-02
     CL       1.7235E-02  3.0683E-02  6.6200E-02  1.6000E-01

SORBED(IONEX)

     NA       9.6047E-02  8.7083E-02  9.6498E-02  1.3047E-01
     MG       1.3884E-01  1.4050E-01  1.3703E-01  1.2829E-01
     CA       1.4813E-01  1.5096E-01  1.4972E-01  1.4147E-01
```

APPENDIX B2 - Example 2: Sample Input and Output

```
ION EXCHANGE, AQUEOUS PHASE COMPLEXATION, WATER DISSOCIATION, TRANSPORT
  METERS       YEARS
   TYPE            0         1         0
ITERATIONS       100       100       100
   GRID           40     5.000       0.2       1.4
   TIME           10    1.0E-4      0.50
PRINT TIME   .000100    0.0020    0.4000      1.00       3.0       5.0       7.0
PRINT TIME      10.0      15.0      20.0
PHYSICAL        1.00       0.0   1.00E-1
BOUNDARY           0         1
  LEACH            1         1
NO.SPECIES         7         4         0        11         2         4
  CECNS         0.10
     NA     1.0    2    1.0E-3    1.0E-3    2   1.00E-3    1.0E-3    1    0
     NA        .1760    1.0E-3    1.0E-3
     SR     2.0    3   1.00E-8   1.00E-8    3   6.95E-5   6.95E-5    1    0
     SR        .3520   4.0E-10   8.00E-6
     CA     2.0    2   5.00E-4   5.00E-4    3   5.00E-4   5.00E-4    1    0
     CA        .3570   4.00E-2   4.00E-2
      H     1.0    1   1.00E-8   1.00E-8    4             2.00E-9    1    0
      H        .0000   1.00E-9   1.00E-9
    CO3    -2.0    3   5.00E-4   1.00E-6    3             6.95E-5    0    0
     CL    -1.0    4             1.00E-2                  1.00E-2    0    0
     OH       13.990
     OH      1.00E-6   1.00E-7
  SRCO3        -3.00  0.0  1.0  0.0  0.0  1.0  0.0  0.0
  SRCO3        0.000    0    0
 SRHCO3       -11.30  0.0  1.0  0.0  1.0  1.0  0.0  0.0
 SRHCO3        0.000    0    0
   SROH       -0.799  0.0  1.0  0.0  0.0  0.0  0.0  1.0
   SROH        0.000    0    0
  NACO3      -0.9600  1.0  0.0  0.0  0.0  1.0  0.0  0.0
  NACO3        0.000    0    0
 NAHCO3       -10.08  1.0  0.0  0.0  1.0  1.0  0.0  0.0
 NAHCO3        0.000    0    0
   NAOH         .213  1.0  0.0  0.0  0.0  0.0  0.0  1.0
   NAOH        0.000    0    0
   HCO3      -10.300  0.0  0.0  0.0  1.0  1.0  0.0  0.0
   HCO3        0.000    0    0
  H2CO3       -16.70  0.0  0.0  0.0  2.0  1.0  0.0  0.0
  H2CO3        0.000    0    0
  CACO3       -3.150  0.0  0.0  1.0  0.0  1.0  0.0  0.0
  CACO3        0.000    0    0
 CAHCO3        -11.3  0.0  0.0  1.0  1.0  1.0  0.0  0.0
 CAHCO3        0.000    0    0
   CAOH        -1.32  0.0  0.0  1.0  0.0  0.0  0.0  1.0
   CAOH        0.000    0    0
  SRCO3        9.250  0.0  1.0  0.0  0.0  1.0  0.0  0.0
  SRCO3       0.0000     0.000
  CACO3        8.350  0.0  0.0  1.0  0.0  1.0  0.0  0.0
  CACO3       0.0000     0.000
```

```
1ION EXCHANGE, AQUEOUS PHASE COMPLEXATION, WATER DISSOCIATION, TRANSPORT

    UNIT OF LENGTH IS    METERS            UNIT OF TIME IS       YEARS

    INNER BOUNDARY IS CONSTANT CONCENTRATION        OUTER BOUNDARY IS ZERO FLUX

    DISPERSION COEFFICIENT = 1.0 V +.0          FLUID VELOCITY =  .100          NUMBER OF GRID POINTS =   40


    NUMBER OF PRINT OUTS =   10
    GIVEN AT THE FOLLOWING TIMES = .1000E-03 .2000E-02 .4000     1.000     3.000     5.000     7.000     10.00
                                   15.00     20.00

    NUMBER OF SITES(ION-EXCHANGE)      .1000          NUMBER OF SITES(EDL MODEL)    0.



     6      BARE IONS              4     SORBING IONS (IONEX)            0     SORBING IONS (EDL MODEL)


  COMPONENT  CHARGE       INITIAL CONDITIONS      BOUNDARY CONDITIONS      PK(IONEX)       PK(EDL)
                          TYPE     VALUE          TYPE        VALUE


     NA        1.           2      1.0000E-03       2       1.0000E-03       .176           ---
     SR        2.           3      1.0000E-08       3       6.9500E-05       .352           ---
     CA        2.           2      5.0000E-04       3       5.0000E-04       .357           ---
      H        1.           1      1.0000E-08       4     -0.               0.              ---
    CO3       -2.           3      5.0000E-04       3     -0.               ---             ---
     CL       -1.           4    -0.               -0     -0.               ---             ---
```

```
 12    COMPLEXES              0     SORBING COMPLEXES(IONEX)          0     SORBING COMPLEXES (EDL MODEL)


 COMPLEX  CHARGE     EQUIL. CONSTANT       PK(IONEX)       PK(EDL)        STOICHIOMETRY

    OH      -1.          1.0233E-14           ---            ---        0.   0.   0.   0.   0.   0.   1.
  SRCO3      0.          1.0000E+03           ---            ---        0.   1.   0.   0.   1.   0.   0.
 SRHCO3      1.          1.9953E+11           ---            ---        0.   1.   0.   1.   1.   0.   0.
   SROH      1.          6.2951E+00           ---            ---        0.   1.   0.   0.   0.   0.   1.
  NACO3     -1.          9.1201E+00           ---            ---        1.   0.   0.   0.   1.   0.   0.
 NAHCO3      0.          1.2023E+10           ---            ---        1.   0.   0.   1.   1.   0.   0.
   NAOH      0.          6.1235E-01           ---            ---        1.   0.   0.   0.   0.   0.   1.
   HCO3     -1.          1.9953E+10           ---            ---        0.   0.   0.   1.   1.   0.   0.
  H2CO3      0.          5.0119E+16           ---            ---        0.   0.   0.   2.   1.   0.   0.
  CACO3      0.          1.4125E+03           ---            ---        0.   0.   1.   0.   1.   0.   0.
 CAHCO3      1.          1.9953E+11           ---            ---        0.   0.   1.   1.   1.   0.   0.
   CAOH      1.          2.0893E+01           ---            ---        0.   0.   1.   0.   0.   0.   1.



    2       SOLID PRECIPITATES

 PRECIPITATE  SOLUBILITY PRODUCT        STOICHIOMETRY

 SRCO3            5.6234E-10        0.   1.0  0.   0.   1.0  0.   0.
 CACO3            4.4668E-09        0.   0.   1.0  0.   1.0  0.   0.



                                   ** SPATIAL GRID **

   0.         .5034E-01   .1029     .1578     .2151     .2749     .3374     .4026     .4707     .5417
   .6160      .6935       .7744     .8589     .9471     1.039     1.135     1.236     1.340     1.450
  1.564       1.683       1.808     1.938     2.074     2.216     2.364     2.518     2.679     2.848
  3.024       3.207       3.399     3.599     3.808     4.027     4.254     4.492     4.741     5.000
```

```
1                                                  INITIAL CONDITIONS

COMPONENT     TOTAL          BARE ION       SORBED CONCENTRATION       ACT. COEF.     KD(ION EX)      KD(EDL)
           AQUEOUS CONC.   CONCENTRATION     (IONEX)     (EDL)

      NA     .1000E-02       .9997E-03      .2380E-02  0.                 .9475          2.381          0.
      SR     .1000E-07       .9942E-08      .9883E-06  0.                 .8060         99.41           0.
      CA     .5000E-03       .4967E-03      .4881E-01  0.                 .8060         98.27           0.
       H     .5065E-03       .1000E-07      .3570E-07  0.                 .9475          3.570          0.
     CO3     .5000E-03       .3000E-05      0.         0.                 .8060          0.             0.
      CL     .1505E-02       .1505E-02      0.         0.                 .9475          0.             0.
      OH     .1150E-05       .1140E-05      0.         0.                 .9475          0.             0.

COMPLEX       VALENCE        AQUEOUS CONC.   SORPTION(IO)     SORPTION(EDL)
  SRCO3        0.             .1938E-10      0.               0.
 SRHCO3        1.000          .3867E-10      0.               0.
   SROH        1.000          .5750E-13      0.               0.
  NACO3       -1.000          .2205E-07      0.               0.
 NAHCO3        0.             .2610E-06      0.               0.
   NAOH        0.             .6264E-09      0.               0.
   HCO3       -1.000          .4825E-03      0.               0.
  H2CO3        0.             .1088E-04      0.               0.
  CACO3        0.             .1368E-05      0.               0.
 CAHCO3        1.000          .1932E-05      0.               0.
   CAOH        1.000          .9534E-08      0.               0.


 PRECIPITATE   EQUIVALENT MOLES/LITER SOLUTION

  SRCO3      0.
  CACO3      0.


  TO HAVE A NET BALANCE OF ZERO CHARGE, OTHER SPECIES MUST BE PRESENT (ALTHOUGH NOT PARTICIPATING IN THE
  CHEMICAL REACTIONS) WITH A TOTAL CONCENTRATION TIMES CHARGE OF   0.
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1                                BOUNDARY OR INFLUX CONDITIONS

 COMPONENT       TOTAL          BARE ION       SORBED CONCENTRATION        ACT. COEF.    KD(ION EX)        KD(EDL)
              AQUEOUS CONC.   CONCENTRATION     (IONEX)      (EDL)

     NA        .1000E-02       .9997E-03      .2436E-02  0.                  .9481          2.437          0.
     SR        .5359E-04       .5286E-04      .5511E-02  0.                  .8080          104.3          0.
     CA        .4276E-03       .4199E-03      .4327E-01  0.                  .8080          103.1          0.
      H        .4057E-03       .1527E-08      .5581E-08  0.                  .9481          3.655          0.
    CO3        .4276E-03       .1630E-04      0.         0.                  .8080          0.             0.
     CL        .1505E-02       .1505E-02      0.         0.                  .9481          0.             0.
     OH        .7514E-05       .7455E-05      0.         0.                  .9481          0.             0.

 COMPLEX         VALENCE        AQUEOUS CONC.   SORPTION(IO)      SORPTION(EDL)
   SRCO3         0.              .5623E-08      0.                0.
  SRHCO3         1.000           .1713E-06      0.                0.
    SROH         1.000           .2004E-08      0.                0.
   NACO3        -1.000           .1200E-06      0.                0.
  NAHCO3         0.              .2172E-06      0.                0.
    NAOH         0.              .4102E-08      0.                0.
    HCO3        -1.000           .4012E-03      0.                0.
   H2CO3         0.              .1383E-05      0.                0.
   CACO3         0.              .6310E-05      0.                0.
  CAHCO3         1.000           .1361E-05      0.                0.
    CAOH         1.000           .5284E-07      0.                0.


  PRECIPITATE   EQUIVALENT MOLES/LITER SOLUTION

   SRCO3     .895E-04
   CACO3     .724E-04


    TO HAVE A NET BALANCE OF ZERO CHARGE, OTHER SPECIES MUST BE PRESENT (ALTHOUGH NOT PARTICIPATING IN THE
    CHEMICAL REACTIONS) WITH A TOTAL CONCENTRATION TIMES CHARGE OF   .763E-17
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1     TIME=   5.20169          DELT=  5.0000E-01          CONCENTRATION OF SPECIES IN MOLES/LITER SOLUTION



                                                                   DISTANCE
  SPECIES        0.           .050          .103          .158          .215          .275          .337          .403          .471

      NA      9.9966E-04    9.9891E-04    9.9810E-04    9.9726E-04    9.9641E-04    9.9557E-04    9.9476E-04    9.9402E-04    9.9338E-04
      SR      5.2858E-05    3.2856E-05    1.6740E-05    7.0211E-06    2.4567E-06    7.3093E-07    1.9153E-07    4.9309E-08    1.7190E-08
      CA      4.1987E-04    4.4010E-04    4.5686E-04    4.6764E-04    4.7333E-04    4.7625E-04    4.7802E-04    4.7942E-04    4.8072E-04
       H      1.5270E-09    1.6070E-09    1.6760E-09    1.7284E-09    1.7871E-09    1.8549E-09    1.9337E-09    2.0255E-09    2.1326E-09
     CO3      1.6296E-05    1.5546E-05    1.4977E-05    1.4604E-05    1.4211E-05    1.3761E-05    1.3313E-05    1.2805E-05    1.2258E-05
      CL      1.5054E-03    1.5054E-03    1.5054E-03    1.5054E-03    1.5054E-03    1.5054E-03    1.5054E-03    1.5054E-03    1.5054E-03
      OH      7.4554E-06    7.0840E-06    6.7923E-06    6.5869E-06    6.3708E-06    6.1382E-06    5.8884E-06    5.6218E-06    5.3398E-06

SORBED(IONEX)

      NA      2.4364E-03    2.4346E-03    2.4315E-03    2.4271E-03    2.4223E-03    2.4173E-03    2.4124E-03    2.4075E-03    2.4028E-03
      SR      5.5106E-03    3.4253E-03    1.7436E-03    7.2987E-04    2.5481E-04    7.5630E-05    1.9768E-05    5.0760E-06    1.7651E-06
      CA      4.3271E-02    4.5357E-02    4.7041E-02    4.8057E-02    4.8534E-02    4.8716E-02    4.8774E-02    4.8791E-02    4.8797E-02
       H      5.5813E-09    5.8738E-09    6.1232E-09    6.3083E-09    6.5153E-09    6.7543E-09    7.0324E-09    7.3568E-09    7.7358E-09

  COMPLEXES

    SRCO3     5.6234E-07    3.3347E-07    1.6367E-07    6.6930E-08    2.2784E-08    6.5726E-09    1.6634E-09    4.1181E-10    1.3741E-10
   SRHCO3     1.7133E-07    1.0692E-07    5.4733E-08    2.3081E-08    8.1240E-09    2.4325E-09    6.4177E-10    1.6643E-10    5.8467E-11
     SROH     2.0044E-09    1.1839E-09    5.7832E-10    2.3521E-10    7.9593E-11    2.2814E-11    5.7344E-12    1.4093E-12    4.6660E-13
    NACO3     1.2004E-07    1.1444E-07    1.1015E-07    1.0731E-07    1.0432E-07    1.0107E-07    9.7550E-08    9.3749E-08    8.9681E-08
   NAHCO3     2.1720E-07    2.1791E-07    2.1876E-07    2.1978E-07    2.2090E-07    2.2213E-07    2.2348E-07    2.2495E-07    2.2656E-07
     NAOH     4.1022E-09    3.8950E-09    3.7316E-09    3.6155E-09    3.4938E-09    3.3632E-09    3.2236E-09    3.0752E-09    2.9188E-09
     HCO3     4.0116E-04    4.0276E-04    4.0467E-04    4.0690E-04    4.0934E-04    4.1199E-04    4.1485E-04    4.1792E-04    4.2120E-04
    H2CO3     1.3831E-06    1.4614E-06    1.5314E-06    1.5879E-06    1.6516E-06    1.7252E-06    1.8109E-06    1.9108E-06    2.0275E-06
    CACO3     6.3096E-06    6.3096E-06    6.3096E-06    6.2969E-06    6.2007E-06    6.0492E-06    5.8641E-06    5.6557E-06    5.4279E-06
   CAHCO3     1.3609E-06    1.4322E-06    1.4938E-06    1.5373E-06    1.5653E-06    1.5849E-06    1.6017E-06    1.6181E-06    1.6351E-06
     CAOH     5.2842E-08    5.2632E-08    5.2384E-08    5.1994E-08    5.0897E-08    4.9336E-08    4.7499E-08    4.5477E-08    4.3307E-08

 PRECIPITATES

    SRCO3     6.9500E-05    0.            0.            0.            0.            0.            0.            0.            0.
    CACO3     7.2408E-05    1.2004E-04    8.1397E-06    0.            0.            0.            0.            0.            0.
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                                                DISTANCE

   SPECIES        .542         .616         .693         .774         .859         .947        1.039        1.135        1.236

       NA     9.9285E-04   9.9248E-04   9.9227E-04   9.9224E-04   9.9237E-04   9.9266E-04   9.9307E-04   9.9360E-04   9.9419E-04
       SR     1.0916E-08   9.8606E-09   9.7215E-09   9.7230E-09   9.7428E-09   9.7639E-09   9.7841E-09   9.8032E-09   9.8211E-09
       CA     4.8198E-04   4.8323E-04   4.8444E-04   4.8561E-04   4.8673E-04   4.8780E-04   4.8881E-04   4.8976E-04   4.9066E-04
        H     2.2577E-09   2.4039E-09   2.5751E-09   2.7753E-09   3.0094E-09   3.2822E-09   3.5983E-09   3.9614E-09   4.3731E-09
      CO3     1.1676E-05   1.1062E-05   1.0420E-05   9.7583E-06   9.0842E-06   8.4081E-06   7.7411E-06   7.0956E-06   6.4837E-06
       CL     1.5054E-03   1.5054E-03   1.5054E-03   1.5054E-03   1.5054E-03   1.5054E-03   1.5054E-03   1.5054E-03   1.5054E-03
       OH     5.0441E-06   4.7375E-06   4.4229E-06   4.1040E-06   3.7850E-06   3.4707E-06   3.1660E-06   2.8759E-06   2.6053E-06

SORBED(IONEX)

       NA     2.3985E-03   2.3945E-03   2.3911E-03   2.3882E-03   2.3859E-03   2.3840E-03   2.3826E-03   2.3816E-03   2.3809E-03
       SR     1.1180E-06   1.0074E-06   9.9070E-07   9.8850E-07   9.8825E-07   9.8824E-07   9.8826E-07   9.8827E-07   9.8827E-07
       CA     4.8800E-02   4.8802E-02   4.8803E-02   4.8805E-02   4.8806E-02   4.8807E-02   4.8808E-02   4.8808E-02   4.8809E-02
        H     8.1791E-09   8.6981E-09   9.3060E-09   1.0018E-08   1.0851E-08   1.1821E-08   1.2947E-08   1.4240E-08   1.5706E-08

  COMPLEXES

    SRCO3     8.3096E-11   7.1095E-11   6.6012E-11   6.1814E-11   5.7648E-11   5.3460E-11   4.9310E-11   4.5276E-11   4.1438E-11
   SRHCO3     3.7432E-11   3.4101E-11   3.3917E-11   3.4230E-11   3.4615E-11   3.5010E-11   3.5402E-11   3.5786E-11   3.6156E-11
     SROH     2.7987E-13   2.3742E-13   2.1850E-13   2.0275E-13   1.8735E-13   1.7214E-13   1.5734E-13   1.4319E-13   1.2994E-13
    NACO3     8.5368E-08   8.0836E-08   7.6123E-08   7.1276E-08   6.6354E-08   6.1426E-08   5.6571E-08   5.1875E-08   4.7424E-08
   NAHCO3     2.2830E-07   2.3017E-07   2.3217E-07   2.3428E-07   2.3648E-07   2.3875E-07   2.4104E-07   2.4332E-07   2.4555E-07
     NAOH     2.7557E-09   2.5870E-09   2.4146E-09   2.2403E-09   2.0663E-09   1.8951E-09   1.7294E-09   1.5717E-09   1.4246E-09
     HCO3     4.2469E-04   4.2836E-04   4.3219E-04   4.3616E-04   4.4022E-04   4.4433E-04   4.4844E-04   4.5247E-04   4.5636E-04
    H2CO3     2.1641E-06   2.3241E-06   2.5117E-06   2.7317E-06   2.9895E-06   3.2908E-06   3.6408E-06   4.0440E-06   4.5025E-06
    CACO3     5.1826E-06   4.9214E-06   4.6466E-06   4.3609E-06   4.0681E-06   3.7727E-06   3.4798E-06   3.1951E-06   2.9243E-06
   CAHCO3     1.6527E-06   1.6711E-06   1.6901E-06   1.7096E-06   1.7293E-06   1.7491E-06   1.7687E-06   1.7878E-06   1.8063E-06
     CAOH     4.1013E-08   3.8615E-08   3.6137E-08   3.3609E-08   3.1064E-08   2.8544E-08   2.6089E-08   2.3742E-08   2.1545E-08

 PRECIPITATES

    SRCO3     0.           0.           0.           0.           0.           0.           0.           0.           0.
    CACO3     0.           0.           0.           0.           0.           0.           0.           0.           0.
```

					DISTANCE				
SPECIES	1.340	1.450	1.564	1.683	1.808	1.938	2.074	2.216	2.364
NA	9.9483E-04	9.9547E-04	9.9610E-04	9.9670E-04	9.9725E-04	9.9773E-04	9.9816E-04	9.9852E-04	9.9881E-04
SR	9.8377E-09	9.8531E-09	9.8672E-09	9.8800E-09	9.8913E-09	9.9014E-09	9.9100E-09	9.9173E-09	9.9234E-09
CA	4.9149E-04	4.9226E-04	4.9296E-04	4.9360E-04	4.9417E-04	4.9467E-04	4.9510E-04	4.9546E-04	4.9577E-04
H	4.8317E-09	5.3311E-09	5.8607E-09	6.4052E-09	6.9471E-09	7.4682E-09	7.9522E-09	8.3862E-09	8.7623E-09
CO3	5.9165E-06	5.4030E-06	4.9488E-06	4.5559E-06	4.2232E-06	3.9468E-06	3.7212E-06	3.5402E-06	3.3973E-06
CL	1.5054E-03	1.5054E-03	1.5054E-03	1.5054E-03	1.5054E-03	1.5054E-03	1.5054E-03	1.5054E-03	1.5054E-03
OH	2.3582E-06	2.1374E-06	1.9444E-06	1.7791E-06	1.6404E-06	1.5260E-06	1.4331E-06	1.3590E-06	1.3007E-06
SORBED(IONEX)									
NA	2.3805E-03	2.3802E-03	2.3801E-03	2.3800E-03	2.3800E-03	2.3800E-03	2.3800E-03	2.3800E-03	2.3800E-03
SR	9.8828E-07	9.8828E-07	9.8828E-07	9.8828E-07	9.8829E-07	9.8829E-07	9.8829E-07	9.8829E-07	9.8829E-07
CA	4.8809E-02	4.8809E-02	4.8809E-02	4.8809E-02	4.8809E-02	4.8809E-02	4.8809E-02	4.8809E-02	4.8809E-02
H	1.7339E-08	1.9117E-08	2.1001E-08	2.2938E-08	2.4865E-08	2.6717E-08	2.8436E-08	2.9977E-08	3.1313E-08
COMPLEXES									
SRCO3	3.7870E-11	3.4630E-11	3.1758E-11	2.9270E-11	2.7159E-11	2.5404E-11	2.3970E-11	2.2818E-11	2.1909E-11
SRHCO3	3.6507E-11	3.6835E-11	3.7135E-11	3.7406E-11	3.7646E-11	3.7854E-11	3.8032E-11	3.8181E-11	3.8303E-11
SROH	1.1780E-13	1.0693E-13	9.7399E-14	8.9229E-14	8.2359E-14	7.6687E-14	7.2081E-14	6.8398E-14	6.5501E-14
NACO3	4.3299E-08	3.9563E-08	3.6256E-08	3.3395E-08	3.0971E-08	2.8956E-08	2.7311E-08	2.5990E-08	2.4948E-08
NAHCO3	2.4768E-07	2.4969E-07	2.5154E-07	2.5321E-07	2.5469E-07	2.5597E-07	2.5707E-07	2.5798E-07	2.5873E-07
NAOH	1.2902E-09	1.1701E-09	1.0651E-09	9.7508E-10	8.9951E-10	8.3715E-10	7.8653E-10	7.4609E-10	7.1428E-10
HCO3	4.6006E-04	4.6351E-04	4.6667E-04	4.6951E-04	4.7201E-04	4.7418E-04	4.7602E-04	4.7755E-04	4.7881E-04
H2CO3	5.0147E-06	5.5743E-06	6.1695E-06	6.7835E-06	7.3963E-06	7.9873E-06	8.5376E-06	9.0324E-06	9.4621E-06
CACO3	2.6724E-06	2.4438E-06	2.2411E-06	2.0655E-06	1.9166E-06	1.7927E-06	1.6916E-06	1.6103E-06	1.5461E-06
CAHCO3	1.8239E-06	1.8402E-06	1.8553E-06	1.8688E-06	1.8808E-06	1.8912E-06	1.9001E-06	1.9075E-06	1.9136E-06
CAOH	1.9533E-08	1.7730E-08	1.6150E-08	1.4795E-08	1.3656E-08	1.2716E-08	1.1952E-08	1.1341E-08	1.0861E-08
PRECIPITATES									
SRCO3	0.	0.	0.	0.	0.	0.	0.	0.	0.
CACO3	0.	0.	0.	0.	0.	0.	0.	0.	0.

```
                                                  DISTANCE
   SPECIES        2.518        2.679        2.848        3.024        3.207        3.399        3.599        3.808        4.027

       NA      9.9905E-04   9.9924E-04   9.9939E-04   9.9949E-04   9.9957E-04   9.9962E-04   9.9966E-04   9.9968E-04   9.9970E-04
       SR      9.9283E-09   9.9321E-09   9.9351E-09   9.9373E-09   9.9389E-09   9.9400E-09   9.9407E-09   9.9412E-09   9.9415E-09
       CA      4.9601E-04   4.9620E-04   4.9635E-04   4.9646E-04   4.9654E-04   4.9660E-04   4.9663E-04   4.9666E-04   4.9667E-04
        H      9.0771E-09   9.3316E-09   9.5305E-09   9.6804E-09   9.7895E-09   9.8660E-09   9.9176E-09   9.9512E-09   9.9721E-09
      CO3      3.2864E-06   3.2021E-06   3.1392E-06   3.0935E-06   3.0610E-06   3.0387E-06   3.0238E-06   3.0142E-06   3.0083E-06
       CL      1.5054E-03   1.5054E-03   1.5054E-03   1.5054E-03   1.5054E-03   1.5054E-03   1.5054E-03   1.5054E-03   1.5054E-03
       OH      1.2556E-06   1.2214E-06   1.1959E-06   1.1774E-06   1.1643E-06   1.1553E-06   1.1492E-06   1.1454E-06   1.1430E-06

SORBED(IONEX)

       NA      2.3801E-03   2.3801E-03   2.3801E-03   2.3801E-03   2.3801E-03   2.3801E-03   2.3801E-03   2.3801E-03   2.3801E-03
       SR      9.8829E-07   9.8829E-07   9.8829E-07   9.8829E-07   9.8829E-07   9.8829E-07   9.8829E-07   9.8829E-07   9.8829E-07
       CA      4.8809E-02   4.8809E-02   4.8809E-02   4.8809E-02   4.8809E-02   4.8809E-02   4.8809E-02   4.8809E-02   4.8809E-02
        H      3.2430E-08   3.3333E-08   3.4038E-08   3.4570E-08   3.4957E-08   3.5228E-08   3.5411E-08   3.5530E-08   3.5605E-08

   COMPLEXES

    SRCO3      2.1203E-11   2.0665E-11   2.0265E-11   1.9973E-11   1.9767E-11   1.9624E-11   1.9529E-11   1.9468E-11   1.9430E-11
   SRHCO3      3.8401E-11   3.8477E-11   3.8535E-11   3.8578E-11   3.8609E-11   3.8631E-11   3.8645E-11   3.8654E-11   3.8660E-11
     SROH      6.3260E-14   6.1557E-14   6.0290E-14   5.9369E-14   5.8717E-14   5.8267E-14   5.7968E-14   5.7775E-14   5.7656E-14
    NACO3      2.4139E-08   2.3523E-08   2.3064E-08   2.2730E-08   2.2493E-08   2.2330E-08   2.2221E-08   2.2151E-08   2.2108E-08
   NAHCO3      2.5933E-07   2.5980E-07   2.6016E-07   2.6042E-07   2.6061E-07   2.6074E-07   2.6083E-07   2.6088E-07   2.6092E-07
     NAOH      6.8967E-10   6.7098E-10   6.5708E-10   6.4697E-10   6.3982E-10   6.3489E-10   6.3160E-10   6.2949E-10   6.2818E-10
     HCO3      4.7981E-04   4.8059E-04   4.8118E-04   4.8162E-04   4.8194E-04   4.8216E-04   4.8230E-04   4.8240E-04   4.8246E-04
    H2CO3      9.8223E-06   1.0114E-05   1.0342E-05   1.0514E-05   1.0640E-05   1.0728E-05   1.0787E-05   1.0826E-05   1.0850E-05
    CACO3      1.4963E-06   1.4584E-06   1.4301E-06   1.4095E-06   1.3949E-06   1.3849E-06   1.3782E-06   1.3739E-06   1.3712E-06
   CAHCO3      1.9185E-06   1.9223E-06   1.9252E-06   1.9274E-06   1.9289E-06   1.9300E-06   1.9307E-06   1.9312E-06   1.9314E-06
     CAOH      1.0489E-08   1.0207E-08   9.9968E-09   9.8441E-09   9.7359E-09   9.6615E-09   9.6118E-09   9.5799E-09   9.5601E-09

  PRECIPITATES

    SRCO3      0.           0.           0.           0.           0.           0.           0.           0.           0.
    CACO3      0.           0.           0.           0.           0.           0.           0.           0.           0.
```

```
                                                    DISTANCE
   SPECIES        4.254       4.492       4.741       5.000
        NA     9.9971E-04  9.9971E-04  9.9971E-04  9.9971E-04
        SR     9.9417E-09  9.9418E-09  9.9418E-09  9.9418E-09
        CA     4.9668E-04  4.9668E-04  4.9669E-04  4.9689E-04
         H     9.9845E-09  9.9913E-09  9.9944E-09  9.9944E-09
       CO3     3.0048E-06  3.0028E-06  3.0020E-06  3.0020E-06
        CL     1.5054E-03  1.5054E-03  1.5054E-03  1.5054E-03
        OH     1.1416E-06  1.1408E-06  1.1404E-06  1.1404E-06

SORBED(IONEX)

        NA     2.3801E-03  2.3801E-03  2.3801E-03  2.3801E-03
        SR     9.8829E-07  9.8829E-07  9.8829E-07  9.8829E-07
        CA     4.8809E-02  4.8809E-02  4.8809E-02  4.8809E-02
         H     3.5649E-08  3.5673E-08  3.5684E-08  3.5684E-08

   COMPLEXES

     SRCO3     1.9408E-11  1.9396E-11  1.9390E-11  1.9390E-11
    SRHCO3     3.8664E-11  3.8666E-11  3.8666E-11  3.8666E-11
      SROH     5.7585E-14  5.7546E-14  5.7529E-14  5.7529E-14
     NACO3     2.2082E-08  2.2068E-08  2.2061E-08  2.2061E-08
    NAHCO3     2.6094E-07  2.6095E-07  2.6096E-07  2.6096E-07
      NAOH     6.2740E-10  6.2698E-10  6.2678E-10  6.2678E-10
      HCO3     4.8249E-04  4.8251E-04  4.8252E-04  4.8252E-04
     H2CO3     1.0864E-05  1.0872E-05  1.0875E-05  1.0875E-05
     CACO3     1.3696E-06  1.3687E-06  1.3683E-06  1.3683E-06
    CAHCO3     1.9316E-06  1.9317E-06  1.9318E-06  1.9318E-06
      CAOH     9.5483E-09  9.5419E-09  9.5390E-09  9.5390E-09

  PRECIPITATES

     SRCO3     0.          0.          0.          0.
     CACO3     0.          0.          0.          0.
```

```
1    TIME=  10.20169          DELT=  5.0000E-01         CONCENTRATION OF SPECIES IN MOLES/LITER SOLUTION


                                                                   DISTANCE
   SPECIES        0.           .050         .103         .158         .215         .275         .337         .403         .471

        NA    9.9966E-04   9.9915E-04   9.9860E-04   9.9799E-04   9.9736E-04   9.9670E-04   9.9604E-04   9.9536E-04   9.9469E-04
        SR    5.2858E-05   3.8843E-05   2.5598E-05   1.4930E-05   7.6519E-06   3.4341E-06   1.3507E-06   4.6902E-07   1.4755E-07
        CA    4.1987E-04   4.3384E-04   4.4720E-04   4.5823E-04   4.6611E-04   4.7108E-04   4.7396E-04   4.7567E-04   4.7686E-04
         H    1.5270E-09   1.5807E-09   1.6329E-09   1.6774E-09   1.7114E-09   1.7413E-09   1.7747E-09   1.8132E-09   1.8577E-09
       CO3    1.6296E-05   1.5770E-05   1.5298E-05   1.4930E-05   1.4679E-05   1.4476E-05   1.4257E-05   1.4011E-05   1.3736E-05
        CL    1.5054E-03   1.5054E-03   1.5054E-03   1.5054E-03   1.5054E-03   1.5054E-03   1.5054E-03   1.5054E-03   1.5054E-03
        OH    7.4554E-06   7.2017E-06   6.9715E-06   6.7865E-06   6.6520E-06   6.5377E-06   6.4150E-06   6.2789E-06   6.1289E-06

 SORBED(IONEX)

        NA    2.4364E-03   2.4357E-03   2.4344E-03   2.4324E-03   2.4295E-03   2.4262E-03   2.4226E-03   2.4189E-03   2.4151E-03
        SR    5.5106E-03   4.0512E-03   2.6701E-03   1.5566E-03   7.9692E-04   3.5714E-04   1.4024E-04   4.8617E-05   1.5268E-05
        CA    4.3271E-02   4.4731E-02   4.6113E-02   4.7227E-02   4.7988E-02   4.8430E-02   4.8648E-02   4.8742E-02   4.8777E-02
         H    5.5813E-09   5.7789E-09   5.9699E-09   6.1311E-09   6.2518E-09   6.3567E-09   6.4733E-09   6.6083E-09   6.7642E-09

   COMPLEXES

     SRCO3    5.6234E-07   3.9993E-07   2.5568E-07   1.4554E-07   7.3329E-08   3.2451E-08   1.2569E-08   4.2886E-09   1.3225E-09
    SRHCO3    1.7133E-07   1.2613E-07   8.3303E-08   4.8711E-08   2.5039E-08   1.1275E-08   4.4507E-09   1.5515E-09   4.9020E-10
      SROH    2.0044E-09   1.4229E-09   9.0774E-10   5.1540E-10   2.5890E-10   1.1419E-10   4.4067E-11   1.4976E-11   4.5987E-12
     NACO3    1.2004E-07   1.1611E-07   1.1258E-07   1.0980E-07   1.0788E-07   1.0631E-07   1.0463E-07   1.0275E-07   1.0066E-07
    NAHCO3    2.1720E-07   2.1749E-07   2.1784E-07   2.1826E-07   2.1877E-07   2.1936E-07   2.2002E-07   2.2074E-07   2.2154E-07
      NAOH    4.1022E-09   3.9608E-09   3.8321E-09   3.7281E-09   3.6518E-09   3.5866E-09   3.5189E-09   3.4398E-09   3.3552E-09
      HCO3    4.0116E-04   4.0189E-04   4.0274E-04   4.0377E-04   4.0498E-04   4.0636E-04   4.0786E-04   4.0949E-04   4.1126E-04
     H2CO3    1.3831E-06   1.4344E-06   1.4849E-06   1.5293E-06   1.5649E-06   1.5976E-06   1.6342E-06   1.6763E-06   1.7248E-06
     CACO3    6.3096E-06   6.3096E-06   6.3096E-06   6.3096E-06   6.3096E-06   6.2880E-06   6.2300E-06   6.1437E-06   6.0373E-06
    CAHCO3    1.3609E-06   1.4088E-06   1.4553E-06   1.4950E-06   1.5252E-06   1.5466E-06   1.5617E-06   1.5736E-06   1.5842E-06
      CAOH    5.2842E-08   5.2746E-08   5.2633E-08   5.2500E-08   5.2343E-08   5.1989E-08   5.1321E-08   5.0411E-08   4.9326E-08

  PRECIPITATES

     SRCO3    6.9500E-05   0.           0.           0.           0.           0.           0.           0.           0.
     CACO3    7.2408E-05   1.7282E-04   9.6117E-05   4.6543E-06   2.1030E-06   0.           0.           0.           0.
```

	DISTANCE								
SPECIES	.542	.616	.693	.774	.859	.947	1.039	1.135	1.238
NA	9.9403E-04	9.9340E-04	9.9282E-04	9.9231E-04	9.9188E-04	9.9156E-04	9.9135E-04	9.9127E-04	9.9131E-04
SR	4.6001E-08	1.8064E-08	1.1348E-08	9.9403E-09	9.6929E-09	9.6679E-09	9.6805E-09	9.6984E-09	9.7168E-09
CA	4.7786E-04	4.7881E-04	4.7976E-04	4.8071E-04	4.8167E-04	4.8263E-04	4.8359E-04	4.8452E-04	4.8545E-04
H	1.9088E-09	1.9675E-09	2.0350E-09	2.1124E-09	2.2013E-09	2.3036E-09	2.4213E-09	2.5571E-09	2.7137E-09
CO3	1.3431E-05	1.3096E-05	1.2732E-05	1.2337E-05	1.1912E-05	1.1458E-05	1.0977E-05	1.0470E-05	9.9401E-06
CL	1.5054E-03	1.5054E-03	1.5054E-03	1.5054E-03	1.5054E-03	1.5054E-03	1.5054E-03	1.5054E-03	1.5054E-03
OH	5.9650E-06	5.7871E-06	5.5955E-06	5.3906E-06	5.1730E-06	4.9436E-06	4.7035E-06	4.4540E-06	4.1971E-06
SORBED(IONEX)									
NA	2.4113E-03	2.4075E-03	2.4038E-03	2.4002E-03	2.3969E-03	2.3937E-03	2.3909E-03	2.3885E-03	2.3864E-03
SR	4.7511E-06	1.8622E-06	1.1676E-06	1.0208E-06	9.9340E-07	9.8891E-07	9.8827E-07	9.8821E-07	9.8822E-07
CA	4.8790E-02	4.8794E-02	4.8797E-02	4.8799E-02	4.8801E-02	4.8802E-02	4.8804E-02	4.8805E-02	4.8806E-02
H	6.9440E-09	7.1510E-09	7.3890E-09	7.6627E-09	7.9775E-09	8.3400E-09	8.7578E-09	9.2400E-09	9.7969E-09
COMPLEXES									
SRCO3	4.0311E-10	1.5433E-10	9.4233E-11	7.9973E-11	7.5285E-11	7.2218E-11	6.9262E-11	6.6173E-11	6.2932E-11
SRHCO3	1.5352E-10	6.0586E-11	3.8262E-11	3.3707E-11	3.3067E-11	3.3194E-11	3.3462E-11	3.3761E-11	3.4075E-11
SROH	1.3952E-12	5.3151E-13	3.2281E-13	2.7240E-13	2.5488E-13	2.4293E-13	2.3140E-13	2.1952E-13	2.0723E-13
NACO3	9.8351E-08	9.5833E-08	9.3103E-08	9.0161E-08	8.7013E-08	8.3664E-08	8.0125E-08	7.6410E-08	7.2540E-08
NAHCO3	2.2242E-07	2.2339E-07	2.2445E-07	2.2562E-07	2.2690E-07	2.2829E-07	2.2980E-07	2.3142E-07	2.3315E-07
NAOH	3.2632E-09	3.1637E-09	3.0571E-09	2.9435E-09	2.8234E-09	2.6972E-09	2.5655E-09	2.4291E-09	2.2890E-09
HCO3	4.1318E-04	4.1526E-04	4.1750E-04	4.1990E-04	4.2248E-04	4.2523E-04	4.2815E-04	4.3122E-04	4.3444E-04
H2CO3	1.7805E-06	1.8444E-06	1.9179E-06	2.0022E-06	2.0992E-06	2.2109E-06	2.3398E-06	2.4886E-06	2.6606E-06
CACO3	5.9150E-06	5.7782E-06	5.6275E-06	5.4630E-06	5.2846E-06	5.0925E-06	4.8873E-06	4.6697E-06	4.4411E-06
CAHCO3	1.5948E-06	1.6059E-06	1.6176E-06	1.6301E-06	1.6432E-06	1.6571E-06	1.6716E-06	1.6867E-06	1.7024E-06
CAOH	4.8104E-08	4.6758E-08	4.5296E-08	4.3721E-08	4.2037E-08	4.0249E-08	3.8366E-08	3.6399E-08	3.4361E-08
PRECIPITATES									
SRCO3	0.	0.	0.	0.	0.	0.	0.	0.	0.
CACO3	0.	0.	0.	0.	0.	0.	0.	0.	0.

```
                                                        DISTANCE
 SPECIES         1.340       1.450       1.564       1.683       1.808       1.938       2.074       2.216       2.364

    NA       9.9148E-04  9.9177E-04  9.9217E-04  9.9265E-04  9.9320E-04  9.9380E-04  9.9443E-04  9.9506E-04  9.9568E-04
    SR       9.7348E-09  9.7523E-09  9.7694E-09  9.7859E-09  9.8019E-09  9.8173E-09  9.8321E-09  9.8462E-09  9.8594E-09
    CA       4.8635E-04  4.8722E-04  4.8807E-04  4.8890E-04  4.8970E-04  4.9047E-04  4.9121E-04  4.9191E-04  4.9257E-04
     H       2.8946E-09  3.1033E-09  3.3437E-09  3.6197E-09  3.9346E-09  4.2906E-09  4.6880E-09  5.1243E-09  5.5939E-09
   CO3       9.3917E-06  8.8299E-06  8.2611E-06  7.6929E-06  7.1338E-06  6.5930E-06  6.0794E-06  5.6013E-06  5.1651E-06
    CL       1.5054E-03  1.5054E-03  1.5054E-03  1.5054E-03  1.5054E-03  1.5054E-03  1.5054E-03  1.5054E-03  1.5054E-03
    OH       3.9350E-06  3.6706E-06  3.4068E-06  3.1472E-06  2.8954E-06  2.6554E-06  2.4304E-06  2.2235E-06  2.0370E-06

SORBED(IONEX)

    NA       2.3846E-03  2.3832E-03  2.3822E-03  2.3814E-03  2.3808E-03  2.3804E-03  2.3802E-03  2.3801E-03  2.3800E-03
    SR       9.8824E-07  9.8825E-07  9.8826E-07  9.8827E-07  9.8828E-07  9.8828E-07  9.8828E-07  9.8828E-07  9.8828E-07
    CA       4.8807E-02  4.8807E-02  4.8808E-02  4.8808E-02  4.8809E-02  4.8809E-02  4.8809E-02  4.8809E-02  4.8809E-02
     H       1.0440E-08  1.1183E-08  1.2040E-08  1.3023E-08  1.4145E-08  1.5412E-08  1.6828E-08  1.8381E-08  2.0052E-08

 COMPLEXES

  SRCO3      5.9559E-11  5.6086E-11  5.2554E-11  4.9013E-11  4.5516E-11  4.2124E-11  3.8893E-11  3.5879E-11  3.3124E-11
 SRHCO3      3.4397E-11  3.4728E-11  3.5062E-11  3.5399E-11  3.5733E-11  3.6061E-11  3.6380E-11  3.6684E-11  3.6970E-11
   SROH      1.9463E-13  1.8186E-13  1.6907E-13  1.5643E-13  1.4414E-13  1.3239E-13  1.2134E-13  1.1116E-13  1.0196E-13
  NACO3      6.8544E-08  6.4456E-08  6.0322E-08  5.6195E-08  5.2135E-08  4.8207E-08  4.4475E-08  4.1000E-08  3.7828E-08
 NAHCO3       2.3497E-07  2.3688E-07  2.3885E-07  2.4087E-07  2.4289E-07  2.4490E-07  2.4686E-07  2.4873E-07  2.5051E-07
   NAOH       2.1464E-09  2.0026E-09  1.8593E-09  1.7184E-09  1.5817E-09  1.4514E-09  1.3292E-09  1.2168E-09  1.1154E-09
   HCO3       4.3779E-04  4.4124E-04  4.4476E-04  4.4831E-04  4.5185E-04  4.5533E-04  4.5870E-04  4.6192E-04  4.6494E-04
  H2CO3       2.8597E-06  3.0899E-06  3.3557E-06  3.6615E-06  4.0112E-06  4.4076E-06  4.8512E-06  5.3398E-06  5.8669E-06
  CACO3       4.2030E-06  3.9580E-06  3.7087E-06  3.4588E-06  3.2121E-06  2.9727E-06  2.7447E-06  2.5320E-08  2.3375E-06
 CAHCO3       1.7185E-06  1.7350E-06  1.7517E-06  1.7685E-06  1.7852E-06  1.8016E-06  1.8175E-06  1.8327E-06  1.8470E-06
   CAOH       3.2272E-08  3.0155E-08  2.8034E-08  2.5939E-08  2.3901E-08  2.1951E-08  2.0120E-08  1.8432E-08  1.6907E-08

PRECIPITATES

  SRCO3       0.          0.          0.          0.          0.          0.          0.          0.          0.
  CACO3       0.          0.          0.          0.          0.          0.          0.          0.          0.
```

```
                                                   DISTANCE
  SPECIES         2.518       2.679       2.848       3.024       3.207       3.399       3.599       3.808       4.027

      NA       9.9628E-04  9.9684E-04  9.9734E-04  9.9780E-04  9.9820E-04  9.9854E-04  9.9882E-04  9.9905E-04  9.9923E-04
      SR       9.8718E-09  9.8832E-09  9.8935E-09  9.9027E-09  9.9108E-09  9.9177E-09  9.9235E-09  9.9282E-09  9.9319E-09
      CA       4.9319E-04  4.9376E-04  4.9427E-04  4.9473E-04  4.9514E-04  4.9548E-04  4.9577E-04  4.9601E-04  4.9619E-04
       H       6.0872E-09  6.5917E-09  7.0928E-09  7.5754E-09  8.0256E-09  8.4320E-09  8.7863E-09  9.0842E-09  9.3242E-09
     CO3       4.7754E-06  4.4342E-06  4.1410E-06  3.8937E-06  3.6887E-06  3.5217E-06  3.3883E-06  3.2838E-06  3.2043E-06
      CL       1.5054E-03  1.5054E-03  1.5054E-03  1.5054E-03  1.5054E-03  1.5054E-03  1.5054E-03  1.5054E-03  1.5054E-03
      OH       1.8720E-06  1.7288E-06  1.6067E-06  1.5044E-06  1.4200E-06  1.3516E-06  1.2971E-06  1.2546E-06  1.2223E-06

SORBED(IONEX)

      NA       2.3800E-03  2.3800E-03  2.3800E-03  2.3800E-03  2.3800E-03  2.3800E-03  2.3800E-03  2.3801E-03  2.3801E-03
      SR       9.8829E-07  9.8829E-07  9.8829E-07  9.8829E-07  9.8829E-07  9.8829E-07  9.8829E-07  9.8829E-07  9.8829E-07
      CA       4.8809E-02  4.8809E-02  4.8809E-02  4.8809E-02  4.8809E-02  4.8809E-02  4.8809E-02  4.8809E-02  4.8809E-02
       H       2.1808E-08  2.3602E-08  2.5383E-08  2.7098E-08  2.8698E-08  3.0140E-08  3.1398E-08  3.2455E-08  3.3307E-08

  COMPLEXES

   SRCO3       3.0658E-11  2.8496E-11  2.6636E-11  2.5065E-11  2.3762E-11  2.2700E-11  2.1851E-11  2.1186E-11  2.0680E-11
  SRHCO3       3.7236E-11  3.7478E-11  3.7694E-11  3.7885E-11  3.8051E-11  3.8190E-11  3.8306E-11  3.8400E-11  3.8473E-11
    SROH       9.3814E-14  8.6730E-14  8.0684E-14  7.5611E-14  7.1426E-14  6.8029E-14  6.5322E-14  6.3209E-14  6.1604E-14
   NACO3       3.4992E-08  3.2507E-08  3.0371E-08  2.8568E-08  2.7073E-08  2.5855E-08  2.4881E-08  2.4119E-08  2.3539E-08
  NAHCO3       2.5215E-07  2.5365E-07  2.5499E-07  2.5617E-07  2.5718E-07  2.5804E-07  2.5875E-07  2.5933E-07  2.5977E-07
    NAOH       1.0256E-09  9.4761E-10  8.8111E-10  8.2535E-10  7.7936E-10  7.4205E-10  7.1233E-10  6.8913E-10  6.7151E-10
    HCO3       4.6773E-04  4.7026E-04  4.7252E-04  4.7451E-04  4.7621E-04  4.7766E-04  4.7884E-04  4.7980E-04  4.8055E-04
   H2CO3       6.4223E-06  6.9920E-06  7.5595E-06  8.1075E-06  8.6200E-06  9.0836E-06  9.4887E-06  9.8299E-06  1.0105E-05
   CACO3       2.1635E-06  2.0109E-06  1.8797E-06  1.7688E-06  1.6769E-06  1.6019E-06  1.5420E-06  1.4951E-06  1.4593E-06
  CAHCO3       1.8603E-06  1.8724E-06  1.8832E-06  1.8927E-06  1.9010E-06  1.9080E-06  1.9138E-06  1.9184E-06  1.9221E-06
    CAOH       1.5556E-08  1.4381E-08  1.3378E-08  1.2537E-08  1.1843E-08  1.1280E-08  1.0831E-08  1.0481E-08  1.0215E-08

 PRECIPITATES

   SRCO3       0.          0.          0.          0.          0.          0.          0.          0.          0.
   CACO3       0.          0.          0.          0.          0.          0.          0.          0.          0.
```

```
                                                DISTANCE
  SPECIES        4.254      4.492      4.741      5.000
      NA      9.9936E-04 9.9946E-04 9.9951E-04 9.9951E-04
      SR      9.9346E-09 9.9365E-09 9.9375E-09 9.9375E-09
      CA      4.9633E-04 4.9642E-04 4.9647E-04 4.9647E-04
       H      9.5070E-09 9.6335E-09 9.7016E-09 9.7016E-09
     CO3      3.1464E-06 3.1076E-06 3.0870E-06 3.0870E-06
      CL      1.5054E-03 1.5054E-03 1.5054E-03 1.5054E-03
      OH      1.1989E-06 1.1831E-06 1.1748E-06 1.1748E-06

SORBED(IONEX)

      NA      2.3801E-03 2.3801E-03 2.3801E-03 2.3801E-03
      SR      9.8829E-07 9.8829E-07 9.8829E-07 9.8829E-07
      CA      4.8809E-02 4.8809E-02 4.8809E-02 4.8809E-02
       H      3.3955E-08 3.4404E-08 3.4646E-08 3.4646E-08

  COMPLEXES

   SRCO3      2.0310E-11 2.0063E-11 1.9932E-11 1.9932E-11
  SRHCO3      3.8527E-11 3.8564E-11 3.8583E-11 3.8583E-11
    SROH      6.0436E-14 5.9653E-14 5.9240E-14 5.9240E-14
   NACO3      2.3116E-08 2.2832E-08 2.2683E-08 2.2683E-08
  NAHCO3      2.6010E-07 2.6033E-07 2.6045E-07 2.6045E-07
    NAOH      6.5869E-10 6.5010E-10 6.4556E-10 6.4556E-10
    HCO3      4.8110E-04 4.8148E-04 4.8168E-04 4.8168E-04
   H2CO3      1.0315E-05 1.0460E-05 1.0539E-05 1.0539E-05
   CACO3      1.4333E-06 1.4158E-06 1.4066E-06 1.4066E-06
  CAHCO3      1.9248E-06 1.9266E-06 1.9276E-06 1.9276E-06
    CAOH      1.0021E-08 9.8913E-09 9.8228E-09 9.8228E-09

 PRECIPITATES

   SRCO3      0.         0.         0.         0.
   CACO3      0.         0.         0.         0.
```

APPENDIX B3 - Example 3: Sample Input and Output

```
SURFACE COMPLEXATION, WATER DISSOCIATION WITH TRANSPORT
 METERS        HOURS
  TYPE             0         1         0
ITERATIONS       100       100       100
  GRID            40      5.00       0.2       1.5
  TIME             6    .00001       0.5
PRINT TIME       1.0       2.0       4.0       8.0      10.0      20.0
PHYSICAL       0.300      0.00   1.00E-1
BOUNDARY           0         1
  LEACH            0         0
NO.SPECIES         5         0         5         1         0         3
SURF.COMP.    1.00E2     2.0E1     5.700    11.500    1.37E7    .01700
     NA     1.0    2   1.00E-1   1.00E-1    2    1.0E-1    1.0E-1    0    1
     NA        9.200   4.19E-6   3.52E-5  1.0
     PB     2.0    2   2.90E-4   2.90E-4    2  2.900E-4   2.90E-4    0    1
     PB        5.000   3.50E-5   9.50E-5  1.0
      H     1.0    1   1.00E-7   1.00E-7    1   3.16E-5   3.16E-5    0    1
      H       0.0000   6.00E-3   1.40E-2  0.0
   CL04    -1.0    2   1.00E-1   1.00E-1    2   1.00E-1   1.00E-1    0    1
   CL04        -7.90   5.50E-3   2.72E-3 -1.0
     OH        13.99  0.0  0.0  0.0  0.0  1.0
     OH      1.00E-7   3.1E-10    0    0
   PBOH       -6.280  0.0  1.0  0.0  0.0  1.0
   PBOH      5.00E-5   5.06E-7    0    1
   PBOH        2.600   5.00E-3   7.19E-5  1.0
```

```
1SURFACE COMPLEXATION, WATER DISSOCIATION WITH TRANSPORT

    UNIT OF LENGTH IS   METERS             UNIT OF TIME IS       HOURS


    DISPERSION COEFFICIENT =  .3 V +.0         FLUID VELOCITY =  .100         NUMBER OF GRID POINTS =   40
    INNER BOUNDARY IS CONSTANT CONCENTRATION          OUTER BOUNDARY IS ZERO FLUX

    NUMBER OF PRINT OUTS =    6
    GIVEN AT THE FOLLOWING TIMES = 1.000     2.000     4.000     8.000     10.00     20.00

    NUMBER OF SITES(ION-EXCHANGE)    0.              NUMBER OF SITES(EDL MODEL)     .0170



     4      BARE IONS             0     SORBING IONS (IONEX)            4     SORBING IONS (EDL MODEL)


  COMPONENT  CHARGE       INITIAL CONDITIONS        BOUNDARY CONDITIONS       PK(IONEX)       PK(EDL)
                          TYPE        VALUE         TYPE        VALUE

     NA       1.           2      1.0000E-01         2      1.0000E-01          ---            9.200
     PB       2.           2      2.9000E-04         2      2.9000E-04          ---            5.000
      H       1.           1      1.0000E-07         1      3.1600E-05          ---            0.
   CLO4      -1.           2      1.0000E-01         2      1.0000E-01          ---           -7.900



     2     COMPLEXES             0       SORBING COMPLEXES(IONEX)            1     SORBING COMPLEXES (EDL MODEL)

   COMPLEX   CHARGE     EQUIL. CONSTANT          PK(IONEX)        PK(EDL)         STOICHIOMETRY

     OH      -1.           1.0233E-14              ---             ---          0.   0.   0.   0.   1.
   PBOH       1.           1.9055E+06              ---           2.600          0.   1.   0.   0.   1.

                                                ** SPATIAL GRID **

     0.           .4046E-01    .8308E-01   .1280       .1753       .2251       .2775       .3328       .3910       .4524
     .5170        .5850        .6567       .7322       .8117       .8955       .9837       1.077       1.175       1.278
     1.386        1.501        1.621       1.748       1.882       2.023       2.171       2.328       2.492       2.666
     2.848        3.041        3.244       3.457       3.682       3.919       4.169       4.431       4.708       5.000
```

```
1                                                    INITIAL CONDITIONS

COMPONENT       TOTAL          BARE ION        SORBED CONCENTRATION        ACT. COEF.     KD(ION EX)         KD(EDL)
             AQUEOUS CONC.   CONCENTRATION      (IONEX)     (EDL)

      NA         .1000          .1000          0.         .4186E-05           .7846         0.             .4186E-04
      PB         .2900E-03      .2589E-03      0.         .3301E-04           .3789         0.             .1275
       H         .1000E-06      .1000E-06      0.         .6563E-02           .7846         0.             .6563E+05
    CLO4         .1000          .1000          0.         .5158E-02           .7846         0.             .5158E-01
      OH         .3124E-04      .1662E-06      0.         0.                  .7846         0.             0.

COMPLEX       VALENCE        AQUEOUS CONC.   SORPTION(IO)     SORPTION(EDL)
   PBOH         1.000           .3108E-04    0.              .5178E-02


    SIGO= 2.745E-02     SIGB= 6.378E-01     SIGD=-6.652E-01
    PSIO= 4.264E-02     PSIBETA= 4.236E-02     PSID= 9.101E-03

   SO- =  1.0916E-06          SOH2+ =  6.2538E-05

   TO HAVE A NET BALANCE OF ZERO CHARGE, OTHER SPECIES MUST BE PRESENT (ALTHOUGH NOT PARTICIPATING IN THE
   CHEMICAL REACTIONS) WITH A TOTAL CONCENTRATION TIMES CHARGE OF  -.549E-03
```

```
1                          BOUNDARY OR INFLUX CONDITIONS


COMPONENT       TOTAL        BARE ION      SORBED CONCENTRATION      ACT. COEF.    KD(ION EX)      KD(EDL)
            AQUEOUS CONC.  CONCENTRATION    (IONEX)     (EDL)

      NA       .1000         .1000        0.          .3271E-04         .7845        0.            .3271E-03
      PB       .2900E-03     .2899E-03    0.          .1380E-03         .3788        0.            .4760
       H       .3160E-04     .3160E-04    0.          .1375E-01         .7845        0.            435.2
    CL04       .1000         .1000        0.          .2898E-02         .7845        0.            .2898E-01
      OH       .1106E-06     .5262E-09    0.          0.                .7845        0.            0.

COMPLEX        VALENCE       AQUEOUS CONC.  SORPTION(IO)     SORPTION(EDL)
   PBOH        1.000          .1101E-06     0.                .1434E-03


   TO HAVE A NET BALANCE OF ZERO CHARGE, OTHER SPECIES MUST BE PRESENT (ALTHOUGH NOT PARTICIPATING IN THE
   CHEMICAL REACTIONS) WITH A TOTAL CONCENTRATION TIMES CHARGE OF  -.611E-03



    SIGO= 1.819E+01      SIGB=-1.723E+01      SIGD=-9.643E-01
    PSIO= 2.432E-01      PSIBETA= 6.133E-02      PSID= 1.311E-02

   SO-  =   1.7856E-05          SOH2+ =   1.6789E-05
```

```
1    TIME=  20.29697          DELT=  5.0000E-01          CONCENTRATION OF SPECIES IN MOLES/LITER SOLUTION


                                                           DISTANCE
   SPECIES       0.            .040         .083         .128         .175         .225         .278         .333         .391

       NA      1.0000E-01   1.0000E-01   1.0000E-01   1.0000E-01   1.0000E-01   1.0000E-01   1.0000E-01   1.0000E-01   1.0000E-01
       PB      2.8989E-04   3.0678E-04   3.2166E-04   3.2235E-04   3.2253E-04   3.2258E-04   3.2256E-04   3.2247E-04   3.2234E-04
        H      3.1600E-05   1.5109E-05   7.1773E-07   2.5520E-07   1.7908E-07   1.5009E-07   1.3653E-07   1.2993E-07   1.2683E-07
     CLO4      1.0000E-01   1.0000E-01   1.0000E-01   1.0000E-01   1.0000E-01   1.0000E-01   1.0000E-01   1.0000E-01   1.0000E-01
       OH      5.2616E-10   1.1005E-09   2.3168E-08   6.5160E-08   9.2857E-08   1.1079E-07   1.2179E-07   1.2798E-07   1.3111E-07

   SORBED(EDL)

       SO      1.7856E-05   1.8779E-05   5.0346E-06   2.1298E-06   1.5655E-06   1.3418E-06   1.2353E-06   1.1831E-06   1.1588E-06
     SOH2      1.6789E-05   1.5722E-05   3.2343E-05   4.8043E-05   5.3950E-05   5.6860E-05   5.8397E-05   5.9191E-05   5.9575E-05
        H      1.3753E-02   1.3649E-02   1.0136E-02   8.0350E-03   7.3000E-03   6.9383E-03   6.7466E-03   6.6473E-03   6.5997E-03
       NA      3.2712E-05   3.3104E-05   1.3232E-05   6.9398E-06   5.4155E-06   4.7649E-06   4.4442E-06   4.2845E-06   4.2095E-06
       PB      1.3799E-04   1.4220E-04   8.8856E-05   5.7901E-05   4.7995E-05   4.3357E-05   4.0966E-05   3.9743E-05   3.9154E-05
     CLO4      2.8980E-03   2.8204E-03   3.8915E-03   4.6625E-03   4.9318E-03   5.0635E-03   5.1330E-03   5.1688E-03   5.1859E-03
     PBOH      1.4337E-04   3.2110E-04   2.8329E-03   4.1875E-03   4.6593E-03   4.8919E-03   5.0154E-03   5.0795E-03   5.1103E-03

   COMPLEXES

     PBOH      1.1009E-07   2.4365E-07   5.3777E-06   1.5157E-05   2.1611E-05   2.5788E-05   2.8347E-05   2.9780E-05   3.0494E-05
```

SPECIES	DISTANCE .452	.517	.585	.657	.732	.812	.895	.984	1.077
NA	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
PB	3.2216E-04	3.2193E-04	3.2166E-04	3.2133E-04	3.2094E-04	3.2047E-04	3.1990E-04	3.1922E-04	3.1841E-04
H	1.2548E-07	1.2492E-07	1.2466E-07	1.2449E-07	1.2433E-07	1.2414E-07	1.2392E-07	1.2365E-07	1.2333E-07
CLO4	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
OH	1.3252E-07	1.3311E-07	1.3339E-07	1.3357E-07	1.3375E-07	1.3395E-07	1.3419E-07	1.3448E-07	1.3483E-07
SORBED(EDL)									
SO	1.1484E-06	1.1444E-06	1.1430E-06	1.1424E-06	1.1420E-06	1.1416E-06	1.1411E-06	1.1406E-06	1.1399E-06
SOH2	5.9743E-05	5.9812E-05	5.9842E-05	5.9861E-05	5.9878E-05	5.9898E-05	5.9921E-05	5.9948E-05	5.9981E-05
H	6.5794E-03	6.5718E-03	6.5694E-03	6.5687E-03	6.5685E-03	6.5684E-03	6.5684E-03	6.5683E-03	6.5682E-03
NA	4.1778E-06	4.1661E-06	4.1624E-06	4.1615E-06	4.1613E-06	4.1615E-06	4.1616E-06	4.1619E-06	4.1622E-06
PB	3.8893E-05	3.8783E-05	3.8730E-05	3.8693E-05	3.8657E-05	3.8616E-05	3.8566E-05	3.8507E-05	3.8436E-05
CLO4	5.1931E-03	5.1957E-03	5.1964E-03	5.1965E-03	5.1963E-03	5.1961E-03	5.1958E-03	5.1954E-03	5.1949E-03
PBOH	5.1235E-03	5.1286E-03	5.1303E-03	5.1310E-03	5.1314E-03	5.1317E-03	5.1321E-03	5.1326E-03	5.1331E-03
COMPLEXES									
PBOH	3.0805E-05	3.0922E-05	3.0960E-05	3.0971E-05	3.0974E-05	3.0975E-05	3.0976E-05	3.0977E-05	3.0979E-05

	DISTANCE								
SPECIES	1.175	1.278	1.386	1.501	1.621	1.748	1.882	2.023	2.171
NA	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
PB	3.1744E-04	3.1629E-04	3.1494E-04	3.1335E-04	3.1151E-04	3.0937E-04	3.0693E-04	3.0418E-04	3.0111E-04
H	1.2295E-07	1.2250E-07	1.2197E-07	1.2134E-07	1.2062E-07	1.1978E-07	1.1882E-07	1.1774E-07	1.1653E-07
CLO4	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
OH	1.3525E-07	1.3574E-07	1.3633E-07	1.3703E-07	1.3786E-07	1.3882E-07	1.3994E-07	1.4122E-07	1.4268E-07
SORBED(EDL)									
SO	1.1392E-06	1.1382E-06	1.1371E-06	1.1359E-06	1.1344E-06	1.1327E-06	1.1307E-06	1.1285E-06	1.1260E-06
SOH2	6.0021E-05	6.0068E-05	6.0123E-05	6.0189E-05	6.0265E-05	6.0353E-05	6.0454E-05	6.0569E-05	6.0698E-05
H	6.5682E-03	6.5681E-03	6.5680E-03	6.5678E-03	6.5677E-03	6.5675E-03	6.5673E-03	6.5671E-03	6.5668E-03
NA	4.1625E-06	4.1629E-06	4.1634E-06	4.1639E-06	4.1646E-06	4.1654E-06	4.1662E-06	4.1673E-06	4.1684E-06
PB	3.8352E-05	3.8252E-05	3.8133E-05	3.7994E-05	3.7831E-05	3.7643E-05	3.7427E-05	3.7183E-05	3.6909E-05
CLO4	5.1944E-03	5.1937E-03	5.1930E-03	5.1920E-03	5.1910E-03	5.1898E-03	5.1883E-03	5.1867E-03	5.1849E-03
PBOH	5.1338E-03	5.1346E-03	5.1355E-03	5.1366E-03	5.1379E-03	5.1395E-03	5.1412E-03	5.1432E-03	5.1454E-03
COMPLEXES									
PBOH	3.0980E-05	3.0982E-05	3.0984E-05	3.0987E-05	3.0990E-05	3.0993E-05	3.0997E-05	3.1001E-05	3.1006E-05

	DISTANCE								
SPECIES	2.328	2.492	2.666	2.848	3.041	3.244	3.457	3.682	3.919
NA	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
PB	2.9774E-04	2.9411E-04	2.9027E-04	2.8630E-04	2.8229E-04	2.7837E-04	2.7464E-04	2.7123E-04	2.6822E-04
H	1.1521E-07	1.1379E-07	1.1228E-07	1.1072E-07	1.0915E-07	1.0761E-07	1.0615E-07	1.0482E-07	1.0364E-07
CLO4	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01	1.0000E-01
OH	1.4432E-07	1.4612E-07	1.4808E-07	1.5016E-07	1.5232E-07	1.5450E-07	1.5662E-07	1.5861E-07	1.6041E-07
SORBED(EDL)									
SO	1.1233E-06	1.1203E-06	1.1172E-06	1.1140E-06	1.1107E-06	1.1075E-06	1.1045E-06	1.1017E-06	1.0993E-06
SOH2	6.0840E-05	6.0994E-05	6.1158E-05	6.1328E-05	6.1502E-05	6.1673E-05	6.1836E-05	6.1987E-05	6.2120E-05
H	6.5665E-03	6.5662E-03	6.5659E-03	6.5655E-03	6.5652E-03	6.5649E-03	6.5645E-03	6.5642E-03	6.5640E-03
NA	4.1696E-06	4.1710E-06	4.1725E-06	4.1741E-06	4.1757E-06	4.1773E-06	4.1788E-06	4.1802E-06	4.1815E-06
PB	3.6606E-05	3.6279E-05	3.5930E-05	3.5568E-05	3.5200E-05	3.4837E-05	3.4491E-05	3.4171E-05	3.3889E-05
CLO4	5.1829E-03	5.1807E-03	5.1783E-03	5.1759E-03	5.1733E-03	5.1708E-03	5.1684E-03	5.1662E-03	5.1642E-03
PBOH	5.1479E-03	5.1505E-03	5.1534E-03	5.1564E-03	5.1595E-03	5.1625E-03	5.1655E-03	5.1682E-03	5.1706E-03
COMPLEXES									
PBOH	3.1012E-05	3.1018E-05	3.1024E-05	3.1030E-05	3.1037E-05	3.1044E-05	3.1050E-05	3.1055E-05	3.1060E-05

```
                                                        DISTANCE
SPECIES          4.169       4.431       4.708       5.000
    NA       1.0000E-01  1.0000E-01  1.0000E-01  1.0000E-01
    PB       2.6572E-04  2.6380E-04  2.6261E-04  2.6261E-04
     H       1.0266E-07  1.0191E-07  1.0144E-07  1.0144E-07
  CLO4       1.0000E-01  1.0000E-01  1.0000E-01  1.0000E-01
    OH       1.6194E-07  1.6314E-07  1.6388E-07  1.6388E-07

SORBED(EDL)

    SO       1.0972E-06  1.0956E-06  1.0947E-06  1.0947E-06
  SOH2       6.2232E-05  6.2318E-05  6.2371E-05  6.2371E-05
     H       6.5637E-03  6.5636E-03  6.5635E-03  6.5635E-03
    NA       4.1826E-06  4.1834E-06  4.1839E-06  4.1839E-06
    PB       3.3653E-05  3.3471E-05  3.3358E-05  3.3358E-05
  CLO4       5.1625E-03  5.1612E-03  5.1604E-03  5.1604E-03
  PBOH       5.1726E-03  5.1742E-03  5.1752E-03  5.1752E-03

COMPLEXES

  PBOH       3.1065E-05  3.1068E-05  3.1070E-05  3.1070E-05
```

APPENDIX B4 - Example 4: Sample Input and Output

```
PRECIPITATION AND DISSOLUTION OF CACO3
  METERS       HOURS
  TYPE             0         1         0
ITERATIONS       100       100       100
  GRID            40      10.0       0.2       1.4
  TIME            14   1.00E-5      1.00
PRINT TIME     0.001      0.01       0.1       0.5       1.0       1.5       2.0
PRINT TIME     3.000       4.0       5.0       6.0       8.0       9.0      10.0
PHYSICAL         1.0        0.   1.00E-1
BOUNDARY           1         0
  LEACH            0         0
NO.SPECIES         6         2         0         8         1         3
  CECNS         0.10
     NA     1.0    2   1.00E-5   1.00E-5    2   1.10E-2    1.1E-2    1    0
     NA        .1760  1.0E-12   1.00E-1
     CA     2.0    3   1.50E-3   5.00E-4    3 4.000E-4   4.00E-4    1    0
     CA        .3570   4.00E-2   4.90E-3
      H     1.0    1   1.00E-8   1.00E-8    4             2.0E-12    0    0
    CO3    -2.0    3   0.66E-3   2.00E-4    3   3.00E-5   3.00E-5    0    0
     CL    -1.0    4             2.35E-3                  2.35E-3    0    0
     OH       13.990
     OH      1.00E-6   1.00E-9
  NACO3      -0.9600  1.0  0.0  0.0  1.0  0.0  0.0
  NACO3         0.00     0.000    0    0
 NAHCO3     -10.0800  1.0  0.0  1.0  1.0  0.0  0.0
 NAHCO3        0.000     0.000    0    0
   NAOH        .2130  1.0  0.0  0.0  0.0  0.0  1.0
   NAOH       0.0000     0.000    0    0
   HCO3     -10.3000  0.0  0.0  1.0  1.0  0.0  0.0
   HCO3       0.0000     0.000    0    0
  H2CO3     -16.7000  0.0  0.0  2.0  1.0  0.0  0.0
  H2CO3       0.0000     0.000    0    0
  CACO3      -3.1500  0.0  1.0  0.0  1.0  0.0  0.0
  CACO3       0.0000     0.000    0    0
 CAHCO3      -11.330  0.0  1.0  1.0  1.0  0.0  0.0
 CAHCO3       0.0000     0.000    0    0
   CAOH       -1.320  0.0  1.0  0.0  0.0  0.0  1.0
   CAOH       0.0000     0.000    0    0
  CACO3        8.350  0.0  1.0  0.0  1.0  0.0  0.0
  CACO3       0.0000     0.000
```

```
1PRECIPITATION AND DISSOLUTION OF CACO3

   UNIT OF LENGTH IS    METERS           UNIT OF TIME IS       HOURS


   DISPERSION COEFFICIENT = 1.0 V +.0        FLUID VELOCITY =  .100         NUMBER OF GRID POINTS =   40
   INNER BOUNDARY IS CONSTANT FLUX          OUTER BOUNDARY IS CONSTANT INITIAL CONCENTRATION

   NUMBER OF PRINT OUTS =   14
   GIVEN AT THE FOLLOWING TIMES = .1000E-02 .1000E-01 .1000     .5000     1.000     1.500     2.000     3.000
                                  4.000     5.000     6.000     8.000     9.000     10.00

   NUMBER OF SITES(ION-EXCHANGE)     .1000         NUMBER OF SITES(EDL MODEL)    0.



    5      BARE IONS             2    SORBING IONS (IONEX)          0     SORBING IONS (EDL MODEL)

 COMPONENT  CHARGE         INITIAL CONDITIONS      BOUNDARY CONDITIONS       PK(IONEX)      PK(EDL)
                           TYPE      VALUE         TYPE       VALUE

    NA        1.            2      1.0000E-05       2      1.1000E-02         .176          ---
    CA        2.            3      1.5000E-03       3      4.0000E-04         .357          ---
     H        1.            1      1.0000E-08       4     -0.                 ---           ---
   CO3       -2.            3      6.6000E-04       3      3.0000E-05         ---           ---
    CL       -1.            4     -0.              -0     -0.                 ---           ---
```

```
  9     COMPLEXES             0       SORBING COMPLEXES(IONEX)            0     SORBING COMPLEXES (EDL MODEL)


 COMPLEX   CHARGE     EQUIL. CONSTANT         PK(IONEX)       PK(EDL)        STOICHIOMETRY

    OH      -1.           1.0233E-14            ---             ---        0.   0.   0.   0.   0.   1.
  NACO3     -1.           9.1201E+00            ---             ---        1.   0.   0.   1.   0.   0.
 NAHCO3      0.           1.2023E+10            ---             ---        1.   0.   1.   1.   0.   0.
   NAOH      0.           6.1235E-01            ---             ---        1.   0.   0.   0.   0.   1.
   HCO3     -1.           1.9953E+10            ---             ---        0.   0.   1.   1.   0.   0.
  H2CO3      0.           5.0119E+16            ---             ---        0.   0.   2.   1.   0.   0.
  CACO3      0.           1.4125E+03            ---             ---        0.   1.   0.   1.   0.   0.
 CAHCO3      1.           2.1380E+11            ---             ---        0.   1.   1.   1.   0.   0.
   CAOH      1.           2.0893E+01            ---             ---        0.   1.   0.   0.   0.   1.


   1       SOLID PRECIPITATES

 PRECIPITATE  SOLUBILITY PRODUCT          STOICHIOMETRY

 CACO3           4.4668E-09            0.   1.0  0.   1.0  0.   0.

                                                 ** SPATIAL GRID **

   .5034E-01   .2561      .3659      .4805      .6001      .7251      .8555      .9917      1.134      1.282
   1.437       1.599      1.768      1.944      2.129      2.321      2.522      2.731      2.950      3.179
   3.417       3.666      3.926      4.198      4.482      4.778      5.087      5.409      5.746      6.098
   6.465       6.849      7.249      7.667      8.104      8.559      9.035      9.532      10.05      10.59
```

```
1                                              INITIAL CONDITIONS


 COMPONENT      TOTAL          BARE ION        SORBED CONCENTRATION        ACT. COEF.     KD(ION EX)       KD(EDL)
            AQUEOUS CONC.   CONCENTRATION    (IONEX)      (EDL)

        NA     .1000E-04      .9996E-05     .1399E-04  0.                .9317          1.399          0.
        CA     .1500E-02      .1487E-02     .4999E-01  0.                .7537          33.61          0.
         H     .6646E-03      .1000E-07    0.          0.                .9317         0.              0.
       CO3     .6600E-03      .4186E-05    0.          0.                .7537         0.              0.
        CL     .2353E-02      .2353E-02    0.          0.                .9317         0.              0.
        OH     .1206E-05      .1179E-05    0.          0.                .9317         0.              0.

 COMPLEX       VALENCE        AQUEOUS CONC.   SORPTION(IO)      SORPTION(EDL)
   NACO3       -1.000          .2876E-09      0.                 0.
  NAHCO3        0.             .3292E-08      0.                 0.
    NAOH        0.             .6264E-11      0.                 0.
    HCO3       -1.000          .6295E-03      0.                 0.
   H2CO3        0.             .1373E-04      0.                 0.
   CACO3        0.             .4996E-05      0.                 0.
  CAHCO3        1.000          .7562E-05      0.                 0.
    CAOH        1.000          .2761E-07      0.                 0.


  PRECIPITATE   EQUIVALENT MOLES/LITER SOLUTION

   CACO3     0.


   TO HAVE A NET BALANCE OF ZERO CHARGE, OTHER SPECIES MUST BE PRESENT (ALTHOUGH NOT PARTICIPATING IN THE
   CHEMICAL REACTIONS) WITH A TOTAL CONCENTRATION TIMES CHARGE OF   0.
```

```
1                              BOUNDARY OR INFLUX CONDITIONS


COMPONENT       TOTAL          BARE ION       SORBED CONCENTRATION       ACT. COEF.     KD(ION EX)        KD(EDL)
           AQUEOUS CONC.    CONCENTRATION     (IONEX)    (EDL)

      NA     .1100E-01      .1095E-01      .3116E-01  0.                  .8960          2.846          0.
      CA     .4000E-03      .3512E-03      .3442E-01  0.                  .6446          98.00          0.
       H     .4139E-06      .1372E-11      0.         0.                  .8960          0.             0.
     CO3     .3000E-04      .2329E-04      0.         0.                  .6446          0.             0.
      CL     .2353E-02      .2353E-02      0.         0.                  .8960          0.             0.
      OH     .9387E-02      .9293E-02      0.         0.                  .8960          0.             0.

COMPLEX        VALENCE       AQUEOUS CONC.   SORPTION(IO)     SORPTION(EDL)
   NACO3      -1.000          .1499E-05      0.              0.
  NAHCO3       0.             .2176E-08      0.              0.
    NAOH       0.             .5002E-04      0.              0.
    HCO3      -1.000          .4108E-06      0.              0.
   H2CO3       0.             .1136E-11      0.              0.
   CACO3       0.             .4800E-05      0.              0.
  CAHCO3       1.000          .9965E-09      0.              0.
    CAOH       1.000          .4396E-04      0.              0.


 PRECIPITATE   EQUIVALENT MOLES/LITER SOLUTION

  CACO3     0.


  TO HAVE A NET BALANCE OF ZERO CHARGE, OTHER SPECIES MUST BE PRESENT (ALTHOUGH NOT PARTICIPATING IN THE
  CHEMICAL REACTIONS) WITH A TOTAL CONCENTRATION TIMES CHARGE OF  -.102E-15
```

```
 PRECIPITATION AT NODE    1     FOR SPECIES  CACO3   AT TIME  6.569E-04

THE ACTIVITY PRODUCT IS 4.568E-09     WHICH NOW EXCEEDS THE SOLUBILITY PRODUCT OF 4.467E-09



 PRECIPITATION AT NODE    2     FOR SPECIES  CACO3   AT TIME  1.049E-01

THE ACTIVITY PRODUCT IS 6.304E-09     WHICH NOW EXCEEDS THE SOLUBILITY PRODUCT OF 4.467E-09

 PRECIPITATION AT NODE    3     FOR SPECIES  CACO3   AT TIME  3.359E-01

THE ACTIVITY PRODUCT IS 7.158E-09     WHICH NOW EXCEEDS THE SOLUBILITY PRODUCT OF 4.467E-09


PRECIPITATION AT NODE    4     FOR SPECIES  CACO3   AT TIME  5.128E-01

THE ACTIVITY PRODUCT IS 5.800E-09     WHICH NOW EXCEEDS THE SOLUBILITY PRODUCT OF 4.467E-09
```

```
1    TIME=   1.06544         DELT=  7.7376E-02         CONCENTRATION OF SPECIES IN MOLES/LITER SOLUTION


                                                               DISTANCE
   SPECIES            .050         .256         .366         .480         .600         .725         .855         .992        1.134

         NA       2.5836E-03   1.0545E-03   5.7772E-04   2.8386E-04   1.2546E-04   5.3751E-05   2.5050E-05   1.4628E-05   1.1253E-05
         CA       1.3727E-03   1.4207E-03   1.3639E-03   1.2689E-03   1.1698E-03   1.2637E-03   1.3652E-03   1.4242E-03   1.4567E-03
          H       4.0130E-12   7.6273E-12   1.2325E-11   2.5347E-11   1.3370E-10   2.3097E-09   5.0056E-09   7.2872E-09   8.6706E-09
        CO3       6.4326E-06   5.8057E-06   5.8359E-06   6.0608E-06   6.3857E-06   5.9911E-06   5.1715E-06   4.5789E-06   4.3437E-06
         CL       2.3533E-03   2.3533E-03   2.3533E-03   2.3533E-03   2.3533E-03   2.3533E-03   2.3533E-03   2.3533E-03   2.3533E-03
         OH       3.0236E-03   1.5640E-03   9.5922E-04   4.6244E-04   8.6663E-05   5.0552E-06   2.3425E-06   1.6132E-06   1.3576E-06

SORBED(IONEX)

         NA       3.8158E-03   1.5189E-03   8.4555E-04   4.2890E-04   1.9670E-04   8.1222E-05   3.6497E-05   2.0892E-05   1.5902E-05
         CA       4.8092E-02   4.9241E-02   4.9577E-02   4.9786E-02   4.9902E-02   4.9959E-02   4.9982E-02   4.9990E-02   4.9992E-02

   COMPLEXES

      NACO3       1.0780E-07   4.1089E-08   2.3035E-08   1.1958E-08   5.6498E-09   2.2558E-09   8.9978E-10   4.6288E-10   3.3685E-10
     NAHCO3       4.8095E-10   3.5441E-10   3.2394E-10   3.4883E-10   8.7756E-10   6.0197E-09   5.1814E-09   3.8708E-09   3.3470E-09
       NAOH       4.0341E-06   8.6635E-07   2.9371E-07   7.0175E-08   5.8562E-09   1.4582E-10   3.1358E-11   1.2578E-11   8.1322E-12
       HCO3       3.6633E-07   6.5019E-07   1.0751E-06   2.3361E-06   1.3176E-05   2.1207E-04   3.9335E-04   5.0449E-04   5.6785E-04
      H2CO3       3.1142E-12   1.0686E-11   2.8810E-11   1.2985E-10   3.7065E-09   1.0783E-06   4.3162E-06   8.0386E-06   1.0751E-05
      CACO3       6.3096E-06   6.3096E-06   6.3096E-06   6.3096E-06   6.3096E-06   6.3096E-06   5.7841E-06   5.2893E-06   5.1036E-06
     CAHCO3       3.8324E-09   7.2840E-09   1.1771E-08   2.4207E-08   1.2768E-07   2.2057E-06   4.3822E-06   5.8339E-06   6.6977E-06
       CAOH       6.1676E-05   3.4163E-05   2.0476E-05   9.3434E-06   1.6380E-06   1.0252E-07   5.0886E-08   3.6373E-08   3.1223E-08

 PRECIPITATES

      CACO3       9.2566E-04   7.9861E-04   6.8931E-04   6.4665E-04   4.7485E-04   4.0460E-05   0.           0.           0.
```

```
                                                    DISTANCE
  SPECIES        1.282         1.437         1.599         1.768         1.944         2.129         2.321         2.522         2.731

       NA      1.0291E-05    1.0053E-05    1.0004E-05    9.9966E-06    9.9960E-06    9.9962E-06    9.9964E-06    9.9964E-06    9.9964E-06
       CA      1.4735E-03    1.4816E-03    1.4852E-03    1.4866E-03    1.4872E-03    1.4873E-03    1.4874E-03    1.4874E-03    1.4874E-03
        H      9.3939E-09    9.7429E-09    9.8992E-09    9.9636E-09    9.9880E-09    9.9964E-09    9.9990E-09    9.9998E-09    9.9999E-09
      CO3      4.2519E-06    4.2138E-06    4.1974E-06    4.1905E-06    4.1878E-06    4.1869E-06    4.1865E-06    4.1865E-06    4.1864E-06
       CL      2.3533E-03    2.3533E-03    2.3533E-03    2.3533E-03    2.3533E-03    2.3533E-03    2.3533E-03    2.3533E-03    2.3533E-03
       OH      1.2540E-06    1.2095E-06    1.1906E-06    1.1830E-06    1.1801E-06    1.1792E-06    1.1788E-06    1.1788E-06    1.1787E-06

SORBED(IONEX)

       NA      1.4465E-05    1.4095E-05    1.4011E-05    1.3993E-05    1.3990E-05    1.3990E-05    1.3990E-05    1.3990E-05    1.3990E-05
       CA      4.9993E-02    4.9993E-02    4.9993E-02    4.9993E-02    4.9993E-02    4.9993E-02    4.9993E-02    4.9993E-02    4.9993E-02

  COMPLEXES

    NACO3      3.0112E-10    2.9132E-10    2.8868E-10    2.8795E-10    2.8774E-10    2.8767E-10    2.8765E-10    2.8765E-10    2.8765E-10

   NAHCO3      3.2391E-09    3.2490E-09    3.2707E-09    3.2835E-09    3.2890E-09    3.2910E-09    3.2916E-09    3.2918E-09    3.2919E-09
     NAOH      6.8645E-12    6.4659E-12    6.3327E-12    6.2868E-12    6.2712E-12    6.2660E-12    6.2645E-12    6.2640E-12    6.2639E-12
     HCO3      6.0135E-04    6.1766E-04    6.2493E-04    6.2789E-04    6.2899E-04    6.2937E-04    6.2948E-04    6.2951E-04    6.2952E-04
    H2CO3      1.2326E-05    1.3126E-05    1.3491E-05    1.3643E-05    1.3700E-05    1.3719E-05    1.3725E-05    1.3727E-05    1.3728E-05
    CACO3      5.0388E-06    5.0139E-06    5.0034E-06    4.9988E-06    4.9969E-06    4.9962E-06    4.9960E-06    4.9959E-06    4.9959E-06
   CAHCO3      7.1643E-06    7.3937E-06    7.4965E-06    7.5385E-06    7.5541E-06    7.5594E-06    7.5610E-06    7.5615E-06    7.5616E-06
     CAOH      2.9131E-08    2.8232E-08    2.7849E-08    2.7694E-08    2.7636E-08    2.7616E-08    2.7609E-08    2.7607E-08    2.7607E-08

 PRECIPITATES

    CACO3      0.            0.            0.            0.            0.            0.            0.            0.            0.
```

```
                                               DISTANCE
   SPECIES       2.950      3.179      3.417      3.666      3.926      4.198      4.482      4.778      5.087

      NA      9.9964E-06 9.9964E-06 9.9964E-06 9.9964E-06 9.9964E-06 9.9964E-06 9.9964E-06 9.9964E-06 9.9964E-06
      CA      1.4874E-03 1.4874E-03 1.4874E-03 1.4874E-03 1.4874E-03 1.4874E-03 1.4874E-03 1.4874E-03 1.4874E-03
       H      1.0000E-08 1.0000E-08 1.0000E-08 1.0000E-08 1.0000E-08 1.0000E-08 1.0000E-08 1.0000E-08 1.0000E-08
     CO3      4.1864E-06 4.1864E-06 4.1864E-06 4.1864E-06 4.1864E-06 4.1864E-06 4.1864E-06 4.1864E-06 4.1864E-06
      CL      2.3533E-03 2.3533E-03 2.3533E-03 2.3533E-03 2.3533E-03 2.3533E-03 2.3533E-03 2.3533E-03 2.3533E-03
      OH      1.1787E-06 1.1787E-06 1.1787E-06 1.1787E-06 1.1787E-06 1.1787E-06 1.1787E-06 1.1787E-06 1.1787E-06

SORBED(IONEX)

      NA      1.3990E-05 1.3990E-05 1.3990E-05 1.3990E-05 1.3990E-05 1.3990E-05 1.3990E-05 1.3990E-05 1.3990E-05
      CA      4.9993E-02 4.9993E-02 4.9993E-02 4.9993E-02 4.9993E-02 4.9993E-02 4.9993E-02 4.9993E-02 4.9993E-02

   COMPLEXES

   NACO3      2.8765E-10 2.8765E-10 2.8765E-10 2.8765E-10 2.8765E-10 2.8765E-10 2.8765E-10 2.8765E-10 2.8765E-10
  NAHCO3      3.2919E-09 3.2919E-09 3.2919E-09 3.2919E-09 3.2919E-09 3.2919E-09 3.2919E-09 3.2919E-09 3.2919E-09
    NAOH      6.2639E-12 6.2639E-12 6.2639E-12 6.2639E-12 6.2639E-12 6.2639E-12 6.2639E-12 6.2639E-12 6.2639E-12
    HCO3      6.2952E-04 6.2952E-04 6.2952E-04 6.2952E-04 6.2952E-04 6.2952E-04 6.2952E-04 6.2952E-04 6.2952E-04
   H2CO3      1.3728E-05 1.3728E-05 1.3728E-05 1.3728E-05 1.3728E-05 1.3728E-05 1.3728E-05 1.3728E-05 1.3728E-05
   CACO3      4.9959E-06 4.9959E-06 4.9959E-06 4.9959E-06 4.9959E-06 4.9959E-06 4.9959E-06 4.9959E-06 4.9959E-06
  CAHCO3      7.5616E-06 7.5616E-06 7.5616E-06 7.5616E-06 7.5616E-06 7.5616E-06 7.5616E-06 7.5616E-06 7.5616E-06
    CAOH      2.7607E-08 2.7607E-08 2.7607E-08 2.7607E-08 2.7607E-08 2.7607E-08 2.7607E-08 2.7607E-08 2.7607E-08

 PRECIPITATES

   CACO3      0.         0.         0.         0.         0.         0.         0.         0.         0.
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                                                    DISTANCE
   SPECIES        5.409       5.746       6.098       6.465       6.849       7.249       7.667       8.104       8.559

      NA       9.9964E-06  9.9964E-06  9.9964E-06  9.9964E-06  9.9964E-06  9.9964E-06  9.9964E-06  9.9964E-06  9.9964E-06
      CA       1.4874E-03  1.4874E-03  1.4874E-03  1.4874E-03  1.4874E-03  1.4874E-03  1.4874E-03  1.4874E-03  1.4874E-03
       H       1.0000E-08  1.0000E-08  1.0000E-08  1.0000E-08  1.0000E-08  1.0000E-08  1.0000E-08  1.0000E-08  1.0000E-08
     CO3       4.1864E-06  4.1864E-06  4.1864E-06  4.1864E-06  4.1864E-06  4.1864E-06  4.1864E-06  4.1864E-06  4.1864E-06
      CL       2.3533E-03  2.3533E-03  2.3533E-03  2.3533E-03  2.3533E-03  2.3533E-03  2.3533E-03  2.3533E-03  2.3533E-03
      OH       1.1787E-06  1.1787E-06  1.1787E-06  1.1787E-06  1.1787E-06  1.1787E-06  1.1787E-06  1.1787E-06  1.1787E-06

SORBED(IONEX)

      NA       1.3990E-05  1.3990E-05  1.3990E-05  1.3990E-05  1.3990E-05  1.3990E-05  1.3990E-05  1.3990E-05  1.3990E-05
      CA       4.9993E-02  4.9993E-02  4.9993E-02  4.9993E-02  4.9993E-02  4.9993E-02  4.9993E-02  4.9993E-02  4.9993E-02

   COMPLEXES

    NACO3      2.8765E-10  2.8765E-10  2.8765E-10  2.8765E-10  2.8765E-10  2.8765E-10  2.8765E-10  2.8765E-10  2.8765E-10
   NAHCO3      3.2919E-09  3.2919E-09  3.2919E-09  3.2919E-09  3.2919E-09  3.2919E-09  3.2919E-09  3.2919E-09  3.2919E-09

     NAOH      6.2639E-12  6.2639E-12  6.2639E-12  6.2639E-12  6.2639E-12  6.2639E-12  6.2639E-12  6.2639E-12  6.2639E-12
     HCO3      6.2952E-04  6.2952E-04  6.2952E-04  6.2952E-04  6.2952E-04  6.2952E-04  6.2952E-04  6.2952E-04  6.2952E-04
     H2CO3     1.3728E-05  1.3728E-05  1.3728E-05  1.3728E-05  1.3728E-05  1.3728E-05  1.3728E-05  1.3728E-05  1.3728E-05
    CACO3      4.9959E-06  4.9959E-06  4.9959E-06  4.9959E-06  4.9959E-06  4.9959E-06  4.9959E-06  4.9959E-06  4.9959E-06
   CAHCO3      7.5616E-06  7.5616E-06  7.5616E-06  7.5616E-06  7.5616E-06  7.5616E-06  7.5616E-06  7.5616E-06  7.5616E-06
     CAOH      2.7607E-08  2.7607E-08  2.7607E-08  2.7607E-08  2.7607E-08  2.7607E-08  2.7607E-08  2.7607E-08  2.7607E-08

 PRECIPITATES

    CACO3      0.          0.          0.          0.          0.          0.          0.          0.          0.
```

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                                                    DISTANCE
   SPECIES          9.035       9.532      10.050      10.592
        NA      9.9964E-06  9.9964E-06  9.9964E-06  9.9964E-06
        CA      1.4874E-03  1.4874E-03  1.4874E-03  1.4874E-03
         H      1.0000E-08  1.0000E-08  1.0000E-08  1.0000E-08
       CO3      4.1864E-06  4.1864E-06  4.1864E-06  4.1864E-06
        CL      2.3533E-03  2.3533E-03  2.3533E-03  2.3533E-03
        OH      1.1787E-06  1.1787E-06  1.1787E-06  1.1787E-06

SORBED(IONEX)

        NA      1.3990E-05  1.3990E-05  1.3990E-05  1.3990E-05
        CA      4.9993E-02  4.9993E-02  4.9993E-02  4.9993E-02

   COMPLEXES

     NACO3      2.8765E-10  2.8765E-10  2.8765E-10  2.8765E-10
    NAHCO3      3.2919E-09  3.2919E-09  3.2919E-09  3.2919E-09
      NAOH      6.2639E-12  6.2639E-12  6.2639E-12  6.2639E-12
      HCO3      6.2952E-04  6.2952E-04  6.2952E-04  6.2952E-04
     H2CO3      1.3728E-05  1.3728E-05  1.3728E-05  1.3728E-05
     CACO3      4.9959E-06  4.9959E-06  4.9959E-06  4.9959E-06
    CAHCO3      7.5616E-06  7.5616E-06  7.5616E-06  7.5616E-06
      CAOH      2.7607E-08  2.7607E-08  2.7607E-08  2.7607E-08

 PRECIPITATES

     CACO3      0.          0.          0.          0.
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1    TIME=  10.19828          DELT=  4.1469E-01         CONCENTRATION OF SPECIES IN MOLES/LITER SOLUTION

                                                               DISTANCE
   SPECIES           .050         .256         .366         .480         .600         .725         .855         .992        1.134

        NA       6.8941E-03   5.7870E-03   5.2198E-03   4.6510E-03   4.0876E-03   3.5374E-03   3.0083E-03   2.5084E-03   2.0455E-03
        CA       1.2801E-03   1.5220E-03   1.6359E-03   1.7412E-03   1.8350E-03   1.9143E-03   1.9763E-03   2.0182E-03   2.0378E-03
         H       1.7505E-12   1.9058E-12   2.0039E-12   2.1199E-12   2.2583E-12   2.4247E-12   2.6268E-12   2.8751E-12   3.1845E-12
       CO3       8.0792E-06   6.7102E-06   6.1956E-06   5.7698E-06   5.4199E-06   5.1360E-06   4.9109E-06   4.7395E-06   4.6183E-06
        CL       2.3533E-03   2.3533E-03   2.3533E-03   2.3533E-03   2.3533E-03   2.3533E-03   2.3533E-03   2.3533E-03   2.3533E-03
        OH       7.2109E-03   6.6026E-03   6.2674E-03   5.9113E-03   5.5351E-03   5.1405E-03   4.7297E-03   4.3054E-03   3.8714E-03

 SORBED(IONEX)

        NA       1.0700E-02   8.2437E-03   7.1714E-03   6.1910E-03   5.2962E-03   4.4827E-03   3.7471E-03   3.0869E-03   2.5004E-03
        CA       4.4650E-02   4.5878E-02   4.6414E-02   4.6905E-02   4.7352E-02   4.7759E-02   4.8126E-02   4.8457E-02   4.8750E-02

   COMPLEXES

     NACO3       3.3384E-07   2.3421E-07   1.9580E-07   1.6319E-07   1.3541E-07   1.1168E-07   9.1407E-08   7.4095E-08   5.9356E-08
    NAHCO3       6.2453E-10   4.7851E-10   4.2143E-10   3.7241E-10   3.3001E-10   2.9308E-10   2.6070E-10   2.3215E-10   2.0682E-10
      NAOH       2.4678E-05   1.9027E-05   1.6322E-05   1.3748E-05   1.1342E-05   9.1418E-06   7.1763E-06   5.4670E-06   4.0249E-06
      HCO3       1.8545E-07   1.6875E-07   1.6445E-07   1.6273E-07   1.6367E-07   1.6748E-07   1.7461E-07   1.8580E-07   2.0218E-07
     H2CO3       6.6106E-13   6.5693E-13   6.7445E-13   7.0762E-13   7.6003E-13   8.3743E-13   9.4896E-13   1.1092E-12   1.3423E-12
     CACO3       6.3096E-06   6.3096E-06   6.3096E-06   6.3096E-06   6.3096E-06   6.3096E-06   6.3096E-06   6.3096E-06   6.3096E-06
    CAHCO3       1.6717E-09   1.8200E-09   1.9137E-09   2.0245E-09   2.1566E-09   2.3155E-09   2.5085E-09   2.7457E-09   3.0412E-09
      CAOH       1.2674E-04   1.3885E-04   1.4221E-04   1.4339E-04   1.4222E-04   1.3858E-04   1.3249E-04   1.2406E-04   1.1355E-04

  PRECIPITATES

     CACO3       1.0315E-03   8.1874E-04   7.0481E-04   6.6507E-04   6.3207E-04   6.2668E-04   5.8444E-04   5.8756E-04   5.7668E-04
```

	DISTANCE								
SPECIES	1.282	1.437	1.599	1.768	1.944	2.129	2.321	2.522	2.731
NA	1.6264E-03	1.2568E-03	9.4037E-04	6.7857E-04	4.7029E-04	3.1189E-04	1.9744E-04	1.1942E-04	6.9598E-05
CA	2.0336E-03	2.0050E-03	1.9527E-03	1.8787E-03	1.7862E-03	1.6799E-03	1.5655E-03	1.4492E-03	1.3374E-03
H	3.5763E-12	4.0822E-12	4.7516E-12	5.6643E-12	6.9582E-12	8.8920E-12	1.2010E-11	1.7673E-11	3.0472E-11
CO3	4.5455E-06	4.5204E-06	4.5438E-06	4.6169E-06	4.7414E-06	4.9187E-06	5.1488E-06	5.4277E-06	5.7468E-06
CL	2.3533E-03	2.3533E-03	2.3533E-03	2.3533E-03	2.3533E-03	2.3533E-03	2.3533E-03	2.3533E-03	2.3533E-03
OH	3.4318E-03	2.9918E-03	2.5567E-03	2.1326E-03	1.7257E-03	1.3421E-03	9.8755E-04	6.6701E-04	3.8461E-04
SORBED(IONEX)									
NA	1.9860E-03	1.5418E-03	1.1659E-03	8.5536E-04	6.0617E-04	4.1325E-04	2.7016E-04	1.6932E-04	1.0242E-04
CA	4.9007E-02	4.9229E-02	4.9417E-02	4.9572E-02	4.9697E-02	4.9793E-02	4.9865E-02	4.9915E-02	4.9949E-02
COMPLEXES									
NACO3	4.6870E-08	3.6375E-08	2.7650E-08	2.0504E-08	1.4769E-08	1.0287E-08	6.9016E-09	4.4548E-09	2.7809E-09
NAHCO3	1.8423E-10	1.6401E-10	1.4589E-10	1.2970E-10	1.1545E-10	1.0339E-10	9.4273E-11	9.0093E-11	9.7536E-11
NAOH	2.8497E-06	1.9292E-06	1.2401E-06	7.5067E-07	4.2352E-07	2.1979E-07	1.0302E-07	4.2343E-08	1.4312E-08
HCO3	2.2547E-07	2.5848E-07	3.0565E-07	3.7445E-07	4.7807E-07	6.4163E-07	9.1843E-07	1.4423E-06	2.6637E-06
H2CO3	1.6887E-12	2.2208E-12	3.0730E-12	4.5132E-12	7.1208E-12	1.2288E-11	2.3905E-11	5.5579E-11	1.7802E-10
CACO3	6.3096E-06	6.3096E-06	6.3096E-06	6.3096E-06	6.3096E-06	6.3096E-06	6.3096E-06	6.3096E-06	6.3096E-06
CAHCO3	3.4153E-09	3.8985E-09	4.5377E-09	5.4093E-09	6.6450E-09	8.4918E-09	1.1469E-08	1.6877E-08	2.9101E-08
CAOH	1.0136E-04	8.7982E-05	7.4009E-05	6.0070E-05	4.6770E-05	3.4634E-05	2.4046E-05	1.5219E-05	8.1928E-06
PRECIPITATES									
CACO3	5.5810E-04	5.4369E-04	5.1771E-04	4.9389E-04	5.0526E-04	4.9010E-04	4.7453E-04	4.3803E-04	4.4473E-04

	DISTANCE								
SPECIES	2.950	3.179	3.417	3.666	3.926	4.198	4.482	4.778	5.087
NA	3.9988E-05	2.3856E-05	1.5997E-05	1.2389E-05	1.0842E-05	1.0239E-05	1.0033E-05	9.9793E-06	9.9744E-06
CA	1.2380E-03	1.2176E-03	1.2932E-03	1.3540E-03	1.3986E-03	1.4305E-03	1.4524E-03	1.4668E-03	1.4759E-03
H	8.0197E-11	8.4528E-10	2.6108E-09	4.4227E-09	6.2848E-09	7.6755E-09	8.6069E-09	9.1967E-09	9.5554E-09
CO3	6.0808E-06	6.1512E-06	5.8731E-06	5.3113E-06	4.7078E-06	4.4258E-06	4.2985E-06	4.2403E-06	4.2128E-06
CL	2.3533E-03	2.3533E-03	2.3533E-03	2.3533E-03	2.3533E-03	2.3533E-03	2.3533E-03	2.3533E-03	2.3533E-03
OH	1.4538E-04	1.3776E-05	4.4757E-06	2.6494E-06	1.8682E-06	1.5319E-06	1.3674E-06	1.2805E-06	1.2330E-06
SORBED(IONEX)									
NA	6.1007E-05	3.6675E-05	2.3905E-05	1.8118E-05	1.5617E-05	1.4593E-05	1.4199E-05	1.4057E-05	1.4010E-05
CA	4.9969E-02	4.9982E-02	4.9988E-02	4.9991E-02	4.9992E-02	4.9993E-02	4.9993E-02	4.9993E-02	4.9993E-02
COMPLEXES									
NACO3	1.7083E-09	1.0335E-09	6.5710E-10	4.5766E-10	3.5360E-10	3.1303E-10	2.9736E-10	2.9137E-10	2.8911E-10
NAHCO3	1.5851E-10	1.0121E-09	1.9805E-09	2.3302E-09	2.5533E-09	2.7566E-09	2.9334E-09	3.0694E-09	3.1632E-09
NAOH	3.1245E-09	1.7685E-10	3.8394E-11	1.7552E-11	1.0810E-11	8.3589E-12	7.3048E-12	6.7994E-12	6.5409E-12
HCO3	7.4952E-06	8.0117E-05	2.3462E-04	3.5745E-04	4.4842E-04	5.1338E-04	5.5805E-04	5.8746E-04	6.0594E-04
H2CO3	1.3252E-09	1.4949E-07	1.3474E-06	3.4679E-06	6.1697E-06	8.6143E-06	1.0490E-05	1.1792E-05	1.2632E-05
CACO3	6.3096E-06	6.3096E-06	6.3096E-06	5.9082E-06	5.3663E-06	5.1306E-06	5.0398E-06	5.0082E-06	4.9985E-06
CAHCO3	7.6588E-08	8.0723E-07	2.4933E-06	3.9550E-06	5.1047E-06	5.9604E-06	6.5654E-06	6.9712E-06	7.2291E-06
CAOH	2.8966E-06	2.7064E-07	9.2740E-08	5.7159E-08	4.1467E-08	3.4678E-08	3.1368E-08	2.9629E-08	2.8682E-08
PRECIPITATES									
CACO3	4.1575E-04	1.4951E-04	1.1096E-06	0.	0.	0.	0.	0.	0.

```
                                                     DISTANCE
   SPECIES         5.409       5.746       6.098       6.465       6.849       7.249       7.667       8.104       8.559

      NA        9.9810E-06  9.9877E-06  9.9920E-06  9.9944E-06  9.9956E-06  9.9961E-06  9.9963E-06  9.9964E-06  9.9964E-06
      CA        1.4813E-03  1.4843E-03  1.4859E-03  1.4868E-03  1.4871E-03  1.4873E-03  1.4874E-03  1.4874E-03  1.4874E-03
       H        9.7649E-09  9.8819E-09  9.9438E-09  9.9748E-09  9.9894E-09  9.9958E-09  9.9985E-09  9.9995E-09  9.9998E-09
     CO3        4.1994E-06  4.1927E-06  4.1894E-06  4.1878E-06  4.1870E-06  4.1866E-06  4.1865E-06  4.1865E-06  4.1864E-06
      CL        2.3533E-03  2.3533E-03  2.3533E-03  2.3533E-03  2.3533E-03  2.3533E-03  2.3533E-03  2.3533E-03  2.3533E-03
      OH        1.2068E-06  1.1927E-06  1.1853E-06  1.1817E-06  1.1800E-06  1.1792E-06  1.1789E-06  1.1788E-06  1.1788E-06

 SORBED(IONEX)

      NA        1.3995E-05  1.3991E-05  1.3990E-05  1.3990E-05  1.3990E-05  1.3990E-05  1.3990E-05  1.3990E-05  1.3990E-05
      CA        4.9993E-02  4.9993E-02  4.9993E-02  4.9993E-02  4.9993E-02  4.9993E-02  4.9993E-02  4.9993E-02  4.9993E-02

   COMPLEXES

    NACO3       2.8825E-10  2.8791E-10  2.8776E-10  2.8770E-10  2.8767E-10  2.8765E-10  2.8765E-10  2.8765E-10  2.8765E-10
   NAHCO3       3.2221E-09  3.2564E-09  3.2749E-09  3.2843E-09  3.2887E-09  3.2906E-09  3.2914E-09  3.2917E-09  3.2918E-09
     NAOH       6.4048E-12  6.3332E-12  6.2965E-12  6.2784E-12  6.2700E-12  6.2663E-12  6.2648E-12  6.2642E-12  6.2640E-12
     HCO3       6.1697E-04  6.2320E-04  6.2651E-04  6.2818E-04  6.2896E-04  6.2930E-04  6.2944E-04  6.2950E-04  6.2952E-04
    H2CO3       1.3141E-05  1.3431E-05  1.3586E-05  1.3664E-05  1.3701E-05  1.3717E-05  1.3724E-05  1.3726E-05  1.3727E-05
    CACO3       4.9961E-06  4.9957E-06  4.9958E-06  4.9959E-06  4.9959E-06  4.9959E-06  4.9959E-06  4.9959E-06  4.9959E-06
   CAHCO3       7.3841E-06  7.4720E-06  7.5190E-06  7.5425E-06  7.5536E-06  7.5585E-06  7.5605E-06  7.5612E-06  7.5615E-06
     CAOH       2.8162E-08  2.7882E-08  2.7737E-08  2.7665E-08  2.7631E-08  2.7616E-08  2.7610E-08  2.7608E-08  2.7607E-08

  PRECIPITATES

    CACO3       0.          0.          0.          0.          0.          0.          0.          0.          0.
```

	DISTANCE			
SPECIES	9.035	9.532	10.050	10.592
NA	9.9964E-06	9.9964E-06	9.9964E-06	9.9964E-06
CA	1.4874E-03	1.4874E-03	1.4874E-03	1.4874E-03
H	1.0000E-08	1.0000E-08	1.0000E-08	1.0000E-08
CO3	4.1864E-06	4.1864E-06	4.1864E-06	4.1864E-06
CL	2.3533E-03	2.3533E-03	2.3533E-03	2.3533E-03
OH	1.1787E-06	1.1787E-06	1.1787E-06	1.1787E-06
SORBED(IONEX)				
NA	1.3990E-05	1.3990E-05	1.3990E-05	1.3990E-05
CA	4.9993E-02	4.9993E-02	4.9993E-02	4.9993E-02
COMPLEXES				
NACO3	2.8765E-10	2.8765E-10	2.8765E-10	2.8765E-10
NAHCO3	3.2919E-09	3.2919E-09	3.2919E-09	3.2919E-09
NAOH	6.2639E-12	6.2639E-12	6.2639E-12	6.2639E-12
HCO3	6.2952E-04	6.2952E-04	6.2952E-04	6.2952E-04
H2CO3	1.3728E-05	1.3728E-05	1.3728E-05	1.3728E-05
CACO3	4.9959E-06	4.9959E-06	4.9959E-06	4.9959E-06
CAHCO3	7.5616E-06	7.5616E-06	7.5616E-06	7.5616E-06
CAOH	2.7607E-08	2.7607E-08	2.7607E-08	2.7607E-08
PRECIPITATES				
CACO3	0.	0.	0.	0.

```
      PROGRAM CHEMTRN(INPUT,OUTPUT,TAPE6=OUTPUT,TAPE5=INPUT,FILM,DEBUG=
     1OUTPUT)
C
C
C  CHEMTRN SOLVES A MULTI-COMPONENT-CHEMICAL-TRANSPORT-MODEL.  THIS VERSION
C  OF CHEMTRN WAS COMPLETED JAN. 1983.
C
C  AUTHOR         C. W. MILLER
C                 EARTH SCIENCES DIVISION
C                 GEOCHEMISTRY GROUP
C                 LAWRENCE BERKELEY LAB
C                 BERKELEY, CA 94720
C
C  DESCRIPTION    CHEMTRN SIMULATES SOLUTE TRANSPORT FOR STEADY ONE-DIMENSIONAL
C                 FLUID FLOW BY CONVECTION AND DIFFUSION/DISPERSION IN A
C                 SATURATED POROUS MEDIUM BASED ON THE ASSUMPTION OF LOCAL
C                 CHEMICAL EQUILIBRIUM.  THE CHEMICAL INTERACTIONS INCLUDED
C                 IN THE MODEL ARE AQUEOUS-PHASE COMPLEXATION, SOLID-PHASE
C                 ION EXCHANGE OF BARE IONS AND COMPLEXES, SOLID-PHASE
C                 SORPTION OF BARE IONS AND COMPLEXES USING THE SURFACE
C                 COMPLEXATION MODEL, AND PRECIPITATION/DISSOLUTION OF
C                 SOLIDS.
C
C  SOLUTION       THE NONLINEAR PARTIAL DIFFERENTIAL EQUATIONS USED BY CHEMTRN
C  PROCEDURE      ARE DISCRETIZED IN SPACE BY FINITE DIFFERENCES AND COMBINED
C                 WITH THE ALGEBRAIC EQUATIONS TO FORM A SET OF
C                 ORDINARY DIFFERENTIAL AND ALGEBRAIC EQUATIONS.  THIS  SYSTEM
C                 IS SOLVED USING A NEWTON-RAPHSON ITERATION METHOD
C
C
C
C
C   DESCRIPTION OF INPUT VARIABLES
C
C          TITLE = TITLE OF RUN UP TO 80 CHARACTERS
C
C          ULENGTH = UNIT OF LENGTH USED IN THE PROBLEM
C          UTIME   =  UNIT OF TIME USED IN THE PROBLEM
C
C          ITYPE  = 0 IF ONE-DIMENSIONAL FLOW IS MODELLED
C                 = 1 IF RADIAL FLOW IS MODELLED
C          IDYNAM = 0   STATIC DISTRIBUTION OF SPECIES CALCULATED
C                 = 1   DYNAMIC TRANSPORT CALCULATION
C          IG     =  0 USER PROVIDES THE INITIAL GUESSES
C                 =  1 PROGRAM PROVIDES THE INITIAL GUESSES
C
C          IN1, IN2, IN3 = NUMBER OF ITERATIONS DONE IN EQUILIBRIUM SPECIATION
C                 SUBROUTINE UNTIL PRINTOUT IS DESIRED.  IF THE SPECIATION CALCULATION
C                 CONCLUDES BEFORE THIS VALUE IS OBTAINED, THERE IS NO PRINTOUT;
C                 IN1 IS FOR THE INITIALIZATION CALCULATION, IN2 IS FOR THE SPECIATION
C                 CALCULATION FOR THE BOUNDARY OR INFLUX CONDITIONS, AND IN3 IS WHEN
C                 THERE IS AN EQUILIBRIUM SPECIATION CALCULATION WHEN A NEW PRECIPITATE
C                 FORMS.  IF THE VALUES ARE SET TO 100 OR GREATER, NO PRINTOUT
```

```
C                 WILL OCCUR HERE.
C
C          NMAX = MAXIMUM NUMBER OF GRID POINTS. LIMITED TO 100 POINTS AT
C                 PRESENT
C          XMAX = SPATIAL DISTANCE OVER WHICH PROBLEM IS SOLVED
C          DNO AND AK =  CONSTANTS IN THE MESH GENERATING EQUATION.
C                        IF DNO = 0, A UNIFORM GRID IS GENERATED OF SPACING
C                        1/(NMAX-1)
C          RW   =  POSITION WHERE A FLUX BOUNDARY CONDITION IS IMPOSED FOR
C                 THE RADIAL FLOW PROBLEM WITH A FLUX CONDITION AT THE INNER
C                 BOUNDARY
C
C          KMAX = NUMBER OF PRINTOUTS DESIRED
C          DTINI  = FIRST TIME STEP USED, USUALLY ABOUT 1.E-4 OR 1.E-5 TO ALLOW
C                   FOR THE INITIAL LARGE CHANGES WHICH USUALLY OCCUR
C          DTMAX    = MAXIMUM TIME STEP DESIRED.  IF CONVERGENCE IS WITHIN 4 ITERATIONS
C                    TIME STEP IS MULTIPLIED BY 1.75 EACH TIME.  HOWEVER, THERE ARE
C                    OTHER CRITERIA SUCH AS NUMERICAL DISPERSION WHICH MUST BE
C                    CONSIDERED. USUALLY THERE IS A MAXIMUM TIME STEP WHICH SHOULD
C                    BE USED.
C
C          TPRINT = ARRAY CONTAINING PRINTOUT TIMES
C
C          DOA = DISPERSIVITY (IT IS MULTIPLIED BY THE VELOCITY
C                IN THE PROGRAM)
C          DOB = DIFFUSION COEFFICIENT
C          VO = AVERAGE FLUID VELOCITY
C
C          IBND(1) = 0  CONSTANT CONCENTRATION AT INNER BOUNDARY
C                  = 1  CONSTANT FLUX AT INNER BOUNDARY
C          IBND(2) = 0  CONSTANT CONCENTRATION EQUAL TO INITIAL CONDITIONS AT
C                       OUTER BOUNDARY
C                    1  NO FLUX AT OUTER BOUNDARY
C
C          LEACH =  POSITION IN THE LIST OF PRECIPITATES OF THE SOLID WHICH
C                  HAS BEEN PUT IN CONTACT WITH THE GROUNDWATER.  THE EQUILIBRIUM
C                  CONDITION USED IS THAT THE TOTAL CONCENTRATION OF THIS
C                  PRECIPITATE IS GIVEN AND THAT THE SPECIES MAKING UP THIS
C                  PRECIPITATE ARE ENTERING THE GROUNDWATER EQUIVALENT TO THE
C                  STOICHIOMETRIC COEFFICIENTS; EQUALS 0 IF NO LEACHING
C          NB   = THE NUMBER OF THE NODE WHERE THE SOLID WAS PLACED IN CONTACT
C                 WITH THE GROUNDWATER.  IN THIS VERSION IT MUST BE AT NODE 1.
C                 IF NO SOLID IS PUT IN CONTACT WITH THE GROUNDWATER, NB = 0.
C
C          NUM(1) = NUMBER OF BASIS SPECIES (MUST INCLUDE HYDROXYL ION IF WATER
C                   DISSOCIATION IS INCLUDED)
C          NUM(2) = NUMBER OF CATIONS AND COMPLEXES WHICH ARE SORBED BY ION EXCHANGE
C          NUM(3) = NUMBER OF IONS AND COMPLEXES WHICH ARE SORBED BY SURFACE
C                    COMPLEXATION MODEL (VALUE IS INCREASED BY 2 IN PROGRAM TO
C                   ALLOW FOR INCLUSION OF NEGATIVELY CHARGED SURFACE SITE AND
C                   POSITIVELY CHARGED SURFACE SITE)
C          NUM(4) = NUMBER OF AQUEOUS COMPLEXES
C          NUM(5) = NUMBER OF PRECIPITATES THAT COULD FORM
```

```
C          LNH= THE POSITION OF THE H ION IN THE BASIS SPECIES LIST.
C                  EQUALS 0 IF WATER DISSOCIATION IS NOT INCLUDED.
C
C          CECNS = CONCENTRATION OF SITES AVAILABLE FOR SORPTION IN ION EXCHANGE
C                  MODEL; EXPRESSED IN EQUIVALENTS/LITER SOLUTION
C
C          C1  = CAPACITANCE BETWEEN THE SURFACE PLANE AND THE BETA PLANE FOR
C                SURFACE COMPLEXATION MODEL (MICROFARADS/LENGTH**2)
C          C2  = CAPACITANCE BETWEEN THE BETA PLANE AND THE DIFFUSE LAYER FOR SURFACE
C                COMPLEXATION MODEL (MICROFARADS/LENGTH**2)
C          PK1  = NEGATIVE LOG OF THE EQUILIBRIUM CONSTANT FOR THE DISSOCIATION OF
C                 POSITIVELY CHARGE SITE FOR SURFACE COMPLEXATION
C          PK2 = NEGATIVE LOG OF THE EQUILIBRIUM CONSTANT FOR THE FORMATION OF THE
C                NEGATIVELY CHARGE SITE FOR SURFACE COMPLEXATION
C          AREA = AREA OF SITES FOR SORPTION IN SURFACE COMPLEXATION IN
C                 LENGTH**2/LITER SOLUTION
C          SOH  = CONCENTRATION OF SITES FOR FORMING COMPLEXES IN SURFACE
C                 COMPLEXATION MODEL; IN EQUIVALENTS/LITER SOLUTION
C
C          DUM  = ARRAY CONTAINING THE NAMES OF THE BASIS SPECIES, COMPLEXES AND
C                 THE PRECIPITATES
C          VJ = ARRAY CONTAINING ION VALENCES AND COMPLEX VALENCES; THE COMPLEX
C              VALANCES ARE COMPUTED FROM THE VALENCES OF THE BASIS SPECIES
C          INDEXI = ARRAY GIVING TYPE OF INITIAL CONDITIONS USED FOR
C                   EACH PARTICULAR SPECIES
C                   VALUE OF 0 MEANS TOTAL CONCENTRATION IS SPECIFIED
C                   VALUE OF 1 MEANS BASIS SPECIES CONCENTRATION IS GIVEN
C                   VALUE OF 2 MEANS TOTAL AQUEOUS CONCENTRATION IS
C                   GIVEN EXCLUDING ANY PRECIPITATES (HOWEVER, IF A SPECIES MAY
C                   FORM A PRECIPITATE, THE VALUE OF 3 SHOULD BE USED INSTEAD OF
C                   2 TO ALLOW FOR THE INCLUSION OF THE SOLUBILITY PRODUCT IF
C                   NECESSARY);
C                   VALUE OF 3 MEANS TOTAL AQUEOUS CONCENTRATION PLUS
C                   ANY PRECIPITATES IS GIVEN
C                   VALUE OF 4 MEANS THAT THE CONCENTRATION OF THIS
C                   SPECIES COMES FROM A CHARGE BALANCE
C          BI = ARRAY OF INITIAL CONDITIONS
C          GUESSI = GUESS OF EQUILIBRATED INITIAL CONDITIONS
C                   FOR ALL THE SPECIES
C          INDEXB = ARRAY GIVING TYPE OF CONDITIONS USED TO DETERMINE
C                   BOUNDARY OR INFLUX CONDITIONS; VALUES OF 0 TO 4 ARE USED;
C                   SAME AS GIVEN IN INDEXI ABOVE
C          BC = ARRAY OF BOUNDARY CONDITIONS
C          GUESSB = GUESS OF EQUILIBRATED BOUNDARY OR INFLUX CONDITIONS
C                   FOR ALL THE SPECIES
C          ISORPI  = ARRAY CONTAINING INFORMATION ABOUT WHETHER THE BASIS SPECIES
C                    OR THE COMPLEX SORBS VIA ION EXCHANGE;
C                    0 - NO SORPTION
C                    1 - SORPTION
C          ISORPE  = ARRAY CONTAINING INFORMATION ABOUT WHETHER THE BASIS SPECIES
C                    OR COMPLEX SORBS VIA SURFACE COMPLEXATION
C                    0 - NO SORPTION
C                    1 - SORPTION
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```
C          PKI  = ARRAY CONTAINING NEGATIVE LOG OF THE EQUILIBRIUM CONSTANTS FOR
C                 MASS ACTION EQUATIONS DESCRIBING SORPTION VIA ION EXCHANGE
C          PKE  = ARRAY CONTAINING NEGATIVE LOG OF THE EQUILIBRIUM CONSTANTS FOR
C                 MASS ACTION EQUATIONS DESCRIBING SORPTION VIA SURFACE COMPLEXATION
C
C          S(J,I) = THE STOICHIOMETRIC COEFFICIENTS FOR THE AQUEOUS
C                   PHASE COMPLEXES; GIVEN FOR 1 MOLE OF THE COMPLEX AND READ IN
C                   SAME ORDER AS THE BASIS SPECIES ARE GIVEN
C
C          PK    =  NEGATIVE LOG OF THE FORMATION OF ONE MOLE OF A COMPLEX FROM
C                   THE BASIS SPECIES
C
C          H2OK  =  NEGATIVE LOG OF THE DISSOCIATION OF WATER
C
C          SS(J,I) = STOICHIOMETRIC COEFFICIENTS FOR PRECIPITATES; GIVEN IN
C                    SAME ORDER AS THE LIST OF THE BASIS SPECIES
C
C          AH(I)    =  NUMBER OF H IONS RELEASED OR TAKEN UP BY THE SURFACE
C                      IN SURFACE COMPLEXATION MODEL
C                      +1 - IF H+ ION IS RELEASED
C                       0 - SPECIAL CASE FOR H+ ION
C                      -1 - IF H+ ION IS SORBED
C
C
C   DESCRIPTION OF OTHER IMPORTANT VARIABLES USED IN THE PROGRAM
C
C         CN(J)  = ARRAY CONTAINING ALL THE UNKNOWN SPECIES. THE ORDER IS FIRST
C                  THOSE IN NODE 1, THEN THOSE IN NODE 2, ETC. THE ORDER OF THE SPECIES
C                  AT EACH NODE IS FIRST THE BASIS SPECIES (THE LAST BASIS SPECIES
C                  IS ALWAYS OH IF WATER DISSOCIATION IS INCLUDED), THEN SORBED
C                  BASIS SPECIES AND COMPLEXES VIA SIMPLE ION EXCHANGE, THEN SORBED
C                  BASIS SPECIES AND COMPLEXES VIA SURFACE COMPLEXATION, THEN COMPLEXES
C                  AND THE LAST ARE THE PRECIPITATES.
C         CO(J)  = ARRAY CONTAINING ALL THE OLD VALUES OF THE SPECIES IN THE SAME
C                  ORDER AS LISTED FOR CN(J)
C         R(I,N)  = RESIDUES FROM THE EQUATIONS ARE STORED HERE.  N IS THE NODE, AND
C                   I IS THE NUMBER OF THE EQUATION.  THE ORDER OF THE EQUATIONS
C                   AT EACH NODE IS (1)TRANSPORT EQUATIONS, (2)THE SITE CONCENTRATION FOR
C                   ION EXCHANGE (3)MASS ACTION EQUATIONS FOR SORPTION VIA ION EXCHANGE,
C                   (4) SITE CONSTRAINT FOR SORPTION VIA SURFACE COMPLEXATION, (5) MASS
C                   ACTION EQUATIONS FOR SURFACE COMPLEXATION, (6) MASS ACTION EQUATIONS
C                   FOR FORMATION OF COMPLEXES IN THE AQUEOUS PHASE, AND (7) SOLUBILITY
C                   PRODUCTS
C         AC(I,N)  =  ACTIVITIES OF THE BASIS SPECIES AND COMPLEXES IN THE AQUEOUS
C                    PHASE ARE STORED HERE; I IS THE SPECIES, N IS THE NODE
C         EQCONST(J)  =  ARRAY CONTAINING THE EQUILIBRIUM CONSTANTS
C                        FIRST FOR SORBED SPECIES VIA ION EXCHANGE,
C                       THEN FOR SPECIES SORBED VIA SURFACE COMPLEXATION,
C                       THEN FOR AQUEOUS PHASE COMPLEXATION,
C                       THEN SOLUBILITY PRODUCTS
C         A(I,J,N)  = THE DIAGONAL MATRIX OF THE BLOCK TRIDIAGONAL JACOBIAN MATRIX
C                     IT IS CHANGE IN RESIDUE(I) DIVIDED BY THE CHANGE IN CONCENTRATION
C                     AT THE NODE N
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```
C         B(I,J,N)  = OFF DIAGONAL MATRIX OF THE BLOCK TRIDIAGONAL JACOBIAN MATIRX
C         C(I,J,N)  = OFF DIAGONAL MATRIX OF THE BLOCK TRIDIAGONAL JACOBIAN MATIRX
C
      DIMENSION CN(3000),CO(3000),DUM(20),TITLE(20),PKI(30),PKE(30)
      DIMENSION CM(25),WCONST(25),BI(25),BC(25),TPRINT(25),NUM(20),
     1INDEX1(10),INDEX2(25),INDEXB(25),CMAX(25),IBND(2),BC2(25),
     2IIP(3000),GUESSI(30),GUESSB(30),INDEXI(25)
      COMMON/AB/VJ(75),AC(75,100),EQCONST(100),
     1S(25,25),SS(25,25),AH(25),
     2 ILBLI(25),ILBLE(25)
      COMMON/EDL/C1,C2,AREA,SOH
      COMMON/EDL2/SIGO,SIGB,SIGD,PSIO,PSIBETA,PSID
      COMMON/NJ/ISORPI(30),ISORPE(30),IION,IEION
      COMMON/AD/X(200),DELT,DOA,DOB,VO,CECNS,H2OK
      COMMON/CONST/REL,ABSV
      COMMON/LCM/A(25,25,100),B(25,25,100)
      COMMON/LCM1/R(25,100)
      COMMON/LCM2/C(25,25,100)
      COMMON/SPEC/LEACH1(5),NB,PINI(5)
      LEVEL 2,A,B,C,R
      MDIM=25
C **************************
C READ IN INPUT PARAMETERS
C **************************
      READ(5,1000) TITLE
         WRITE(6,999) TITLE
      READ 1010, ULENGTH,UTIME
         WRITE (6,1011) ULENGTH,UTIME
      READ 910, ITYPE,IDYNAM,IG
      READ 910,IN1,IN2,IN3
      READ 920,NMAX,XMAX,DNO,AK,RW
      READ 920, KMAX,DTINI,DTMAX
      READ 900, (TPRINT(K),K=1,KMAX)
      READ 900, DOA,DOB,VO
      READ 910, IBND(1),IBND(2)
      READ 910,LEACH,NB
      READ 910, (NUM(I),I=1,5),LNH
         NUM(10)=NUM(1)+NUM(4)
         NUM(11)=NUM(10)+NUM(5)
         IF (NUM(2).EQ.0) CECNS=0.
      IF (NUM(2).GT.0) READ 900, CECNS
         IF (NUM(3).EQ.0) SOH=0.
         IF (NUM(3).EQ.0) GO TO 5
      READ 900, C1,C2,PK1,PK2,AREA,SOH
         EQCONST(NUM(2)+1)=10.**(-PK1)
         EQCONST(NUM(2)+2)=10.**(-PK2)
         NUM(3)=NUM(3)+2
         DUM(NUM(11)+1)=2HSO
         DUM(NUM(11)+2)=4HSOH2
         ILBLE(1)=NUM(11)+1
         ILBLE(2)=NUM(11)+2
    5 CONTINUE
         NUM(6)=NUM(1)+NUM(2)
```

```
         NUM(7)=NUM(6)+NUM(3)
         NUM(8)=NUM(7)+NUM(4)
         NUM(9)=NUM(8)+NUM(5)
         NUM(12)=NUM(2)+NUM(3)
         NUM(14)=NMAX
         NTOTP=NUM(9)
         LEACH1(1)=LEACH
         IF (LEACH1(1).NE.0) GO TO 7
      DO 6 I=2,5
    6 LEACH1(I)=0
    7 IF (LNH.EQ.0) GO TO 8
      S0=0
      S1=1
    8 CONTINUE
C  ************************************
C  WRITE OUT SOME OF THE CONSTANTS USED
C  ************************************
      IF ((IBND(1).EQ.0).AND.(IBND(2).EQ.1)) WRITE(6,2060)
      IF ((IBND(1).EQ.1).AND.(IBND(2).EQ.1)) WRITE(6,2061)
      IF ((IBND(1).EQ.0).AND.(IBND(2).EQ.0)) WRITE(6,2062)
      IF ((IBND(1).EQ.1).AND.(IBND(2).EQ.0)) WRITE(6,2063)
      IF (ITYPE.EQ.0) WRITE(6,600) DOA,DOB,VO,NMAX
      IF (ITYPE.EQ.1) WRITE(6,601) DOA,DOB,VO,NMAX
      WRITE(6,610) KMAX,(TPRINT(I),I=1,KMAX)
      WRITE(6,611) CECNS,SOH
         II=0
         IE=3
         LI=0
         LB=0
C  *****************************************************
C  READ IN INFORMATION ON BARE IONS AND TYPE OF SORPTION
C  *****************************************************
         M1=NUM(1)
         NSPECM=NUM(1)
         IF (LNH.GT.0) NSPECM=NUM(1)-1
      DO 17 J=1,NSPECM
      READ 950, DUM(J),VJ(J),INDEXI(J),BI(J),GUESSI(J),INDEXB(J),
     1          BC(J),GUESSB(J),ISORPI(J),ISORPE(J)
         IF (INDEXI(J).EQ.4) LI=J
         IF (INDEXB(J).EQ.4) LB=J
C
C  IF THE SPECIES IS SORBED VIA ION EXCHANGE, READ IN EQUILIBRIUM CONSTANT,
C  AND GUESSES IF THEY ARE BEING PROVIDED
C
         IF (ISORPI(J).EQ.0) GO TO 15
         II=II+1
         ILBLI(II)=J
         K=II+NUM(1)
      READ 960,PKI(II),GUESSI(K),GUESSB(K)
         EQCONST(II)=10.**(-PKI(II))
C
C  IF THE SPECIES IS SORBED VIA SURFACE COMPLEXATION, READ IN EQUILIBRIUM
C  CONSTANT AND NUMBER OF H IONS SORBED OR RELEASED FROM THE SURFACE, AND
```

```
C  GUESSES IF BEING PROVIDED
C
  15     IF (ISORPE(J).EQ.0) GO TO 17
         IF (J.EQ.LNH) IEJ=3
         IF (J.EQ.LNH) GO TO 16
         IE=IE+1
         IEJ=IE
  16     CONTINUE
         ILBLE(IEJ)=J
         K=IEJ+NUM(6)
      READ 960, PKE(IEJ),GUESSI(K),GUESSB(K),AH(IEJ)
         EQCONST(NUM(2)+IEJ)=10.**(-PKE(IEJ))
  17 CONTINUE
C
C  ***********************************************
C  WRITE OUT THE CONDITIONS ON THE BASIS SPECIES
C  ***********************************************
       IIE=IE-2
       IF (NUM(3).EQ.0) IIE=0
      WRITE (6,800) NSPECM,II,IIE
       IION=II
       IEION=IE
       II=0
       IE=3
C
      DO 20 J=1,NSPECM
       IF (ISORPI(J).EQ.1) II=II+1
       IF (J.EQ.LNH.AND.ISORPE(J).EQ.1) IEK=3
       IF (J.EQ.LNH.AND.ISORPE(J).EQ.1) GO TO 19
       IF (ISORPE(J).EQ.1) IE=IE+1
       IEK=IE
  19 CONTINUE
       IF (ISORPI(J).EQ.0.AND.ISORPE(J).EQ.0) WRITE (6,805) DUM(J),
     1VJ(J),INDEXI(J),BI(J),INDEXB(J),BC(J)
       IF (ISORPI(J).EQ.1.AND.ISORPE(J).EQ.0) WRITE (6,806) DUM(J),
     1VJ(J),INDEXI(J),BI(J),INDEXB(J),BC(J),PKI(II)
       IF (ISORPI(J).EQ.0.AND.ISORPE(J).EQ.1) WRITE (6,807) DUM(J),
     1VJ(J),INDEXI(J),BI(J),INDEXB(J),BC(J),PKE(IEK)
       IF (ISORPI(J).EQ.1.AND.ISORPE(J).EQ.1) WRITE (6,808) DUM(J),
     1VJ(J),INDEXI(J),BI(J),INDEXB(J),BC(J),PKI(II),PKE(IEK)
  20 CONTINUE
C
       NCMPLXP=NUM(4)
C  ***************************************************************
C  IF WATER DISSOCIATION IS CONSIDERED, NEED TO READ AND WRITE OUT
C  INFORMATION ABOUT THE OH ION
C  ***************************************************************
       IF (LNH.EQ.0) GO TO 21
      READ 970,DUM(NUM(1)),H2OK
       H2OK=10.**(-H2OK)
       VJ(NUM(1))=-1.0
       INDEXI(NUM(1))=1
       INDEXB(NUM(1))=1
```

```
      READ 980,GUESSI(NUM(1)),GUESSB(NUM(1)),ISORPI(NUM(1)),
     1         ISORPE(NUM(1))
       NCMPLXP=NUM(4)+1
       BI(NUM(1))=GUESSI(NUM(1))
       BC(NUM(1))=GUESSB(NUM(1))
   21 IF (NUM(4).EQ.0) GO TO 35
C  *****************************************************
C  READ IN INFORMATION ON COMPLEXES AND TYPE OF SORPTION
C  *****************************************************
       M4=NUM(4)
C
      DO 27 I=1,M4
       KK=I+NUM(1)
      READ 970, DUM(KK),PK,(S(J,I),J=1,M1)
       EQCONST(NUM(12)+I)=10.**(-PK)
       VJ(KK)=0.
         DO 22 J=1,M1
   22    VJ(KK)= VJ(KK)+(S(J,I)*VJ(J))
       IC=KK+NUM(12)
      READ 980, GUESSI(IC),GUESSB(IC),ISORPI(KK),ISORPE(KK)
C
C  IF COMPLEX IS SORBED VIA ION EXCHANGE NEED TO READ IN EQUILIBRIUM CONSTANT
C
       IF (ISORPI(KK).EQ.0) GO TO 25
       II=II+1
       K=II+NUM(1)
      READ 960,PKI(II),GUESSI(K),GUESSB(K)
       ILBLE(II)=IC
       EQCONST(II)=10.**(-PKI(II) )
C
C  IF COMPLEX IS SORBED VIA SURFACE COMPLEXATION NEED TO READ IN EQUILIBRIUM
C  CONSTANT AND NUMBER OF H IONS SORBED OR RELEASED BY THE SURFACE
C
   25  IF (ISORPE(KK).EQ.0) GO TO 27
       IE=IE+1
       ILBLE(IE)=IC
       K=IE+NUM(6)
      READ 960,PKE(IE),GUESSI(K),GUESSB(K),AH(IE)
       EQCONST(NUM(2)+IE)=10.**(-PKE(IE) )
   27 CONTINUE
C
C
C  WRITE OUT INFORMATION ABOUT THE COMPLEXES
C
       ICMPLX=II-IION
       IECMPLX=IE-IEION
      WRITE (6,802) NCMPLXP,ICMPLX,IECMPLX
       IF (II.NE.NUM(2)) WRITE (6,990) II,NUM(2),IE,NUM(3)
       II=IION
       IE =IEION
       IF (LNH.GT.0) WRITE (6,820) DUM(NUM(1)),VJ(NUM(1)),H2OK,
     1 (SO, J=1,NSPECM), S1
C
```

```
      DO 30 I=1,M4
       IF (ISORPI(I).EQ.1) II=II+1
       IF (ISORPE(I).EQ.1) IE=IE+1
       KK=I+NUM(1)
       INP=NUM(12)+I
       IF (ISORPI(KK).EQ.0.AND.ISORPE(KK).EQ.0) WRITE (6,820) DUM(KK),
     1     VJ(KK),EQCONST(INP),(S(J,I),J=1,M1)
       IF (ISORPI(KK).EQ.1.AND.ISORPE(KK).EQ.0) WRITE (6,821) DUM(KK),
     1     VJ(KK),EQCONST(INP),PKI(II),(S(J,I),J=1,M1)
       IF (ISORPI(KK).EQ.0.AND.ISORPE(KK).EQ.1) WRITE (6,822) DUM(KK),
     1     VJ(KK),EQCONST(INP),PKE(IE),(S(J,I),J=1,M1)
       IF (ISORPI(KK).EQ.1.AND.ISORPE(KK).EQ.1) WRITE (6,823) DUM(KK),
     1     VJ(KK),EQCONST(INP),PKI(II),PKE(IE),(S(J,I),J=1,M1)
   30 CONTINUE
C
   35 CONTINUE
C  ***********************************
C  READ IN INFORMATION ON PRECIPITATES
C  ***********************************
       IF (NUM(5).EQ.0) GO TO 41
      WRITE (6,840) NUM(5)
       M5=NUM(5)
C
      DO 40 I=1,M5
       KK=NUM(10)+I
       KL=KK+NUM(12)
      READ 970, DUM(KK),PK,(SS(J,I),J=1,M1)
       EQCONST(NUM(12)+NUM(4)+I)=10.**(-PK)
      READ 960,GUESSI(KL),GUESSB(KL)
C
C  IF A SOLID IS BEING PLACED IN CONTACT WITH THE INITIAL GROUNDWATER
C  NEED TO DETERMINE THE SPECIES MAKING UP THIS SOLID
C
       IF (I.NE.LEACH1(1)) GO TO 39
       ILEACH=1
         DO 38 J=1,m1
         IF (SS(J,I).EQ.0) gO TO 38
         ILEACH=ILEACH+1
         LEACH1(ILEACH)=J
   38    CONTINUE
C  ********************************************
C  WRITE OUT INFORMATION ABOUT THE PRECIPITATES
C  ********************************************
   39 WRITE (6,971) DUM(KK),EQCONST(NUM(12)+NUM(4)+I),(SS(J,I),J=1,M1)
   40 CONTINUE
   41 CONTINUE
      REL=0.01
      ABSV=1.E-12
      DELT=DTINI
      NTOT=NUM(8)
      NEQ=NUM(9)*NMAX
C  ************
C  SET UP GRID
```

```
C  ************
      CALL SETUP(XMAX,DNO,AK,NMAX,ITYPE,IBND,RW)
      INDEX=0
C  ******************************
C  EQUILIBRATE INITIAL CONDITIONS
C  ******************************
      M9=NUM(9)
C
C  DETERMINE HERE WHETHER THE PROGRAM OR THE USER IS
C  PROVIDING THE FIRST GUESSES
C
      IF (IG.EQ.1) CALL IGUESS(CM,BI,NUM,LNH)
      DO 50 J=1,M9
      AC(J,2)=1.0
      IF (IG.EQ.1) GO TO 50
      CM(J)=GUESSI(J)
   50 CONTINUE
      IF ((NUM(3).EQ.0).OR.(IG.EQ.1) ) GO TO 51
      CM(NUM(6)+1)=EQCONST(NUM(2)+2)*SOH/CM(LNH)
      CM(NUM(6)+2)=CM(LNH)*SOH/EQCONST(NUM(2)+1)
      CM(NUM(6)+2)=CM(NUM(6)+2)/10.
   51 CONTINUE
C
      CTOT=0.
C  *******************************************************************
C  DETERMINE THE EQUILIBRIUM CONCENTRATIONS FOR THE INITIAL CONDITIONS
C  *******************************************************************
      CALL EQLIB(CM,BI,INDEX1,INDEXI,NUM,2,SS,EQCONST,CTOT,AC,
     1LI,LNH,IN1)
C  ******************************
C  WRITE OUT INITIAL CONDITIONS
C  ******************************
      WRITE (6,760)
      WRITE (6,780)
      II=0
      IE=0
      ILEACH=2
C
C  CALCULATE CONVENTIONAL KD'S HERE, THE TOTAL AMOUNT OF THE
C  SPECIES IN THE AQUEOUS PHASE
C
      DO 80 J=1,M1
      CMTOTAQ=CM(J)
      IF (ISORPI(J).EQ.0) SORB=0.
      IF (ISORPI(J).EQ.0) GO TO 55
      II=II+1
      SORB=CM(II+NUM(1))
   55 DK=SORB/CM(J)
      CONTINUE
      IF (ISORPE(J).EQ.0) SORBE=0.
      IF (ISORPE(J).EQ.0) GO TO 56
      IE=IE+1
      SORBE=CM(IE+NUM(6)+3)
```

```
      IF (J.EQ.LNH) SORBE=CM(3+NUM(6))
      IF (J.EQ.LNH) IE=IE-1
   56 DKE=SORBE/CM(J)
      CONTINUE
      IF (NUM(4).EQ.0) GO TO 61
      DO 60 I=1,M4
   60 CMTOTAQ=CMTOTAQ+S(J,I)*CM(NUM(7)+I)
C
C  IF A SOLID IS GOING TO BE PLACED IN CONTACT WITH THE GROUNDWATER,
C  NEED TO CALCULATE HOW MUCH OF EACH SPECIES THAT MAKES UP THIS
C  SOLID ALREADY EXISTS IN THE GROUNDWATER
C
   61 IF (LEACH1(1).EQ.0) GO TO 79
      IF (J.NE.LEACH1(ILEACH)) GO TO 70
      PINI(ILEACH-1)=CMTOTAQ
      INDEXB(J)=3
      ILEACH=ILEACH+1
   70 CONTINUE
   79 IF (INDEXI(J).EQ.4) INDEXB(J)=2
      IF (INDEXI(J).EQ.4) BC(J)=CMTOTAQ
C
C  WRITE OUT THIS INFORMATION
C
   80 WRITE (6,700) DUM(J),CMTOTAQ,CM(J),SORB,SORBE,AC(J,2),DK,DKE
C
      IF (NUM(4).EQ.0) GO TO 91
      WRITE (6,740)
C
      DO 90 I=1,M4
      KK=I+NUM(1)
      IF (ISORPI(KK).EQ.0) SORB=0.
      IF (ISORPI(KK).EQ.0) GO TO 85
      II=II+1
      SORB=CM(II+NUM(1))
   85 CONTINUE
      IF (ISORPE(KK).EQ.0) SORBE=0.
      IF (ISORPE(KK).EQ.0) GO TO 86
      IE=IE+1
      SORBE=CM(IE+NUM(6)+3)
   86 CONTINUE
      IK=I+NUM(7)
C
C  WRITE OUT INFORMATION ABOUT THE AQUEOUS PHASE COMPLEXES
C
   90 WRITE (6,750) DUM(KK),VJ(KK),CM(IK),SORB,SORBE
C
   91 DO 110 N=1,NMAX
      DO 110 J=1,M9
      CN((N-1)*NUM(9)+J)=CM(J)
      AC(J,N)=AC(J,2)
  110 CONTINUE
C
      IF (LI.NE.0) GO TO 141
```

```
C
C  A SPECIES AT THE BOUNDARY MAY BE CALCULATED FROM A CHARGE BALANCE
C  THEREFORE IT IS NECESSARY TO KNOW THE CHARGE THAT
C  IS NOT BEING CONSIDERED IN THESE CALCULATIONS AND WHICH IS BEING
C  MADE UP BY SPECIES NOT PARTICIPATING IN THE CHEMICAL CHANGES
C
      CTOT=0.
      CTOT1=-CTOT
      DO 130 J=1,M1
  130 CTOT=CM(J)*VJ(J)+CTOT
C
      IF (NUM(4).EQ.0) GO TO 141
C
      DO 140 I=1,M4
  140 CTOT=CTOT+CM(NUM(7)+I)*VJ(NUM(1)+I)
C
  141 IF (NUM(5).EQ.0) GO TO 160
C
      WRITE (6,841)
C
      DO 150 I=1,M5
      II=NUM(10)+I
      WRITE (6,845) DUM(II),CM(II+NUM(12))
C
C  IF A SOLID IS BEING PLACED IN CONTACT WITH THE INITIAL GROUNDWATER
C  NEED TO CALCULATE HOW MUCH OF EACH PARTICULAR SPECIES IN THIS
C  SOLID WAS INITIALLY IN THE GROUNDWATER; THIS CALCULATION INCLUDES
C  THE AQUEOUS PHASE COMPLEXES
C
      IF (LEACH1(1).EQ.0) GO TO 150
      ILEACH=2
C
      DO 145 J=1,NSPEC
      IF (SS(J,I).EQ.0) GO TO 145
      IF (J.NE.LEACH1(ILEACH)) GO TO 145
      PINI(ILEACH-1)=PINI(ILEACH-1)+SS(J,I)*CM(NUM(8)+I)
      ILEACH=ILEACH+1
  145 CONTINUE
C
  150 CONTINUE
  160 CONTINUE
C
C  IF A SURFACE COMPLEXATION MODEL IS USED FOR SORPTION,
C  THEN WRITE OUT THE CHARGES DEVELOPED AT THE LAYERS AND
C  THE POTENTIALS BETWEEN THESE LAYERS
C
      IF (NUM(3).EQ.0) GO TO 161
      WRITE (6,597) SIGO,SIGB,SIGD,PSIO,PSIBETA,PSID
      WRITE (6,598) CM(NUM(6)+1),CM(NUM(6)+2)
  161 CONTINUE
      WRITE (6,596)  CTOT1
C  ********************************
C  EQUILIBRATE BOUNDARY CONDITIONS
```

```
C  ********************************
C
C  DECIDE IF THE PROGRAM IS SUPPLYING THE FIRST GUESSES
C  FOR THE SPECIES CONCENTRATIONS
C
      IF (IG.EQ.1) CALL IGUESS(CM,BC,NUM,LNH)
      DO 170 J=1,M9
      AC(J,1)=1.0
      IF (IG.EQ.1) GO TO  170
      CM(J)=GUESSB(J)
  170 CONTINUE
      IF ((NUM(3).EQ.0).OR.(IG.EQ.1)) GO TO 171
      CM(NUM(6)+1)=EQCONST(NUM(2)+2)*SOH/CM(LNH)
      CM(NUM(6)+2)=CM(LNH)*SOH/EQCONST(NUM(2)+1)
      CM(NUM(6)+2)=CM(NUM(6)+2)/1000.
  171 CONTINUE
C  ******************************************************************
C  DETERMINE THE EQUILIBRIUM DISTRIBUTION OF SPECIES FOR THE BOUNDARY
C  OR INFLUX CONDITIONS
C  ******************************************************************
      CALL EQLIB(CM,BC,INDEX1,INDEXB,NUM,1,SS,EQCONST,CTOT,AC,
     1LB,LNH,IN2)
      WRITE (6,790)
      WRITE (6,780)
      II=0
      IE=0
      NEND=(NMAX-1)*NUM(9)
C  ******************************************
C  WRITE OUT THE BOUNDARY OR INFLUX CONDITIONS
C  ******************************************
C
C  ALSO CALCULATE CONVENTIONAL KD'S, AND THE TOTAL AQUEOUS
C  PHASE CONCENTRATION OF THE SPECIES
C
      DO 180 J=1,M1
      IF (IBND(2).EQ.0) BC2(J)=CN(NEND+J)
      CMTOTAQ=CM(J)
      IF (ISORPI(J).EQ.0) SORB=0.
      IF (ISORPI(J).EQ.0) GO TO 172
      II=II+1
      SORB=CM(II+NUM(1))
  172 DK=SORB/CM(J)
      CONTINUE
      IF (ISORPE(J).EQ.0) SORBE=0.
      IF (ISORPE(J).EQ.0) GO TO 173
      IE=IE+1
      SORBE=CM(IE+NUM(6)+3)
      IF (J.EQ.LNH) SORBE=CM(NUM(6)+3)
      IF (J.EQ.LNH) IE=IE-1
  173 DKE=SORBE/CM(J)
      CONTINUE
      IF (NUM(4).EQ.0) GO TO 176
      DO 175 I=1,M4
```

```
  175 CMTOTAQ=CMTOTAQ+S(J,I)*CM(NUM(7)+I)
  176 BBC=CMTOTAQ
      IF (NUM(5).EQ.0) GO TO 179
      DO 177 I=1,M5
      BBC=BBC+SS(J,I)*CM(NUM(8)+I)
  177 CONTINUE
C  ******************************************
C  SET INNER BOUNDARY CONDITION
C  ******************************************
C
C  SET UP THE ACTUAL BOUNDARY CONDITIONS FOR THE INNER
C  BOUNDARY
C
  179 IF (IBND(1).EQ.0) BC(J)=BBC
      IF (IBND(1).EQ.1 ) BC(J)=V0*CMTOTAQ
      IF((IBND(1).EQ.1).AND.(ITYPE.EQ.1)) BC(J)=V0*CMTOTAQ/X(1)
      INDEX2(J)=0
  180 WRITE (6,700) DUM(J),CMTOTAQ,CM(J),SORB,SORBE,AC(J,1),DK,DKE
C
C  DO CALCULATIONS FOR THE COMPLEXES
C
      IF (NUM(4).EQ.0) GO TO 191
      WRITE (6,740)
C
      DO 190 I=1,M4
      KK=I+NUM(1)
      IF (ISORPI(KK).EQ.0) SORB=0.
      IF (ISORPI(KK).EQ.0) GO TO 192
      II=II+1
      SORB=CM(II+NUM(1))
  192 CONTINUE
      IF (ISORPE(KK).EQ.0) SORBE=0
      IF (ISORPE(KK).EQ.0) GO TO 193
      IE=IE+1
      SORBE=CM(NUM(6)+IE+3)
  193 CONTINUE
      IK=I+NUM(7)
  190 WRITE (6,750) DUM(KK),VJ(KK),CM(IK),SORB,SORBE
C
  191 CONTINUE
C  ******************************************************
C  IF FLUX CONDTION IS USED, THEN FIRST GRID IS THE SAME
C  AS THE REST OF THE GRIDS
C  *******************************************************
      IF (IBND(1).EQ.1) GO TO 201
      N=1
C
      DO 200 J=1,M9
      CN((N-1)*NUM(9)+J)=CM(J)
  200 CONTINUE
C
  201  CONTINUE
C
```

```
C  WRITE OUT INFORMATION ABOUT THE PRECIPITATES
C
      IF (NUM(5).EQ.0) GO TO 210
      WRITE (6,841)
C
      DO 205 I=1,M5
      II=NUM(10)+I
      WRITE (6,845) DUM(II),CM(II+NUM(12))
  205 CONTINUE
C
  210 CONTINUE
      CTOT1=0.
C
C   DO A CHECK OF THE CHARGE BALANCE
C
      DO 215 J=1,M1
  215 CTOT1=CM(J)*VJ(J)+CTOT1
C
      IF (NUM(4).EQ.0) GO TO 221
C
      DO 220 I=1,M4
  220 CTOT1=CTOT1+CM(NUM(7)+I)*VJ(NUM(1)+I)
      CTOT1=-CTOT1
  221 WRITE (6,596) CTOT1
C
C  IF SURFACE COMPLEXATION IS USED FOR SORPTION,  WRITE
C  OUT THE CHARGES DEVELOPED AT THE SURFACES AND THE
C  POTENTIALS BETWEEN THE SURFACES FOR THE BOUNDARY CONDITIONS
C
      IF (NUM(3).EQ.0) GO TO 231
      WRITE (6,597) SIGO,SIGB,SIGD,PSIO,PSIBETA,PSID
      WRITE (6,598) CM(NUM(6)+1),CM(NUM(6)+2)
  231 CONTINUE
      TIME=0.
      K1=1
      DELT=DTINI
      IF (IDYNAM.EQ.0) GO TO 500
C  **************************************************************
C  CALCULATE NEW VALUES OF THE CONCENTRATION AS A FUNCTION OF TIME
C  **************************************************************
C
C  SET OLD VALUES OF CONCENTRATION = TO NEW VALUES
C
  235 DO 240 N=1,NMAX
      DO 240 J=1,M9
  240 CO((N-1)*NUM(9)+J)=CN((N-1)*NUM(9)+J)
C
      TIME=TIME+DELT
  250 ITER=0
      ITER2=0
C
C  CALCULATE THE RESIDUES OF THE EQUATIONS FOR THE NEW GUESS OF
C  CONCENTRATIONS AT THIS TIME
```

```
C
      CALL RES(CN,CO,BC,BC2,R,NUM,MDIM,LNH,IBND,ITYPE)
C
C  CALCULATE THE JACOBIAN
C
  260 CALL JACOBI(A,B,C,CO,CN,BC,BC2,NUM,R,MDIM,LNH,IBND,ITYPE)
      ITER =0
C  THE SUBROUTINES DECBT AND SOLBT INVERT THE JACOBIAN
C
  263 CALL DECBT(NUM(9),NMAX,MDIM,A,B,C,IIP,IER)
  270 CONTINUE
      ITER=ITER+1
      CALL SOLBT(NUM(9),NMAX,MDIM,A,B,C,R,IIP)
C
      DO 280 I=1,M9
  280 CMAX(I)=0.
C
C  ****************************************************************
C  DETERMINE THE NEW VALUE OF THE CONCENTRATIONS FROM THE OLD VALUES
C  AND THE INVERSION OF THE JACOBIAN
C  ****************************************************************
      DO 291 N=1,NMAX
      DO 290 J=1,M9
      COLD=CN((N-1)*NUM(9)+J)
      CN((N-1)*NUM(9)+J)=CN((N-1)*NUM(9)+J)-R(J,N)
      IF (CN((N-1)*NUM(9)+J).LT.0.) CN((N-1)*NUM(9)+J)=COLD/10.
      NPNSNE=NUM(7)+1
      IF((J.GT.NUM(6)).AND.(J.LT.NPNSNE).AND.
     1(CN((N-1)*NUM(9)+J).gt.SOH)) CN((N-1)*NUM(9)+J)=SOH
      CMAX(J)=AMAX1(CN((N-1)*NUM(9)+J),CMAX(J)  )
  290 CONTINUE
  291 CONTINUE
C
C  ******************************************************************
C  DETERMINE IF THE CHANGES IN THE CONCENTRATIONS ARE WITHIN THE ERROR
C  RANGE
C  ******************************************************************
      ERR=0.
C
      DO 300 N=1,NMAX
      DO 300 I=1,M9
      AAA=R(I,N)
      BBB=CMAX(I)
      IF (BBB.LT.1.E-30) GO TO 300
      AAA=AAA/BBB
      ERR=ERR + AAA*AAA
  300 CONTINUE
      ERR=SQRT(ERR)
C
      IF (ERR.LT.1.E-3) GO TO 310
C  ***********************************************************************
C  IF CONVERGENCE IS NOT OBTAINED CALCULATE THE RESIDUES FOR THE NEXT GUESS
C  ***********************************************************************
```

```
      CALL RES(CN,CO,BC,BC2,R,NUM,MDIM,LNH,IBND,ITYPE)
      IF (ITER.LT. 10) GO TO 270
  301 CONTINUE
      ITER2=ITER2+1
      IF (ITER2.LT.3) GO TO 260
C  ***********************************************************************
C  IF CONVERGENCE IS NOT OBTAINED WITHIN 10 ITERATIONS REDUCE THE TIME STEP
C  ***********************************************************************
      TIME=TIME-DELT
      DELT=DELT/2.0
      WRITE (6,2022) DELT
      K6=1
C
C  SET NEW VALUES EQUAL TO OLD VALUES AND START THIS TIME STEP OVER
C
      DO 306 N=1,NMAX
      DO 306 J=1,M9
  306 CN((N-1)*NUM(9)+J)=CO((N-1)*NUM(9)+J)
      TIME=TIME+DELT
      GO TO 250
C
C  CONVERGENCE IS OBTAINED, SO START NEXT TIME STEP
C
  310 CONTINUE
C  **********************************************************************
C  CHECK TO SEE IF THERE IS A NEW SOLID WHICH IS STARTING TO PRECIPITATE
C  OR DISSOLVE AT ANY POINT.
C  IF THERE IS, RE-EQUILIBRIATE THE SPECIES.
C  **********************************************************************
      DO 400 N=1,NMAX
      IF (NUM(5).EQ.0) GO TO 400
        DO 390 I=1,M5
        AKSOL=1.0
          DO 320 J=1,M1
  320     AKSOL=AKSOL*(AC(J,N)*CN((N-1)*NUM(9)+J))**SS(J,I)
        INDEX1(I)=0
        IJ=NUM(12)+NUM(4)+I
        EK=0.01*EQCONST(IJ)
        IF ((AKSOL-EQCONST(IJ)).GT.EK) GO TO 325
        KK=(N-1)*NUM(9)+NUM(8)+I
        IF((CN(KK).GT.1.E-30).AND.((EQCONST(IJ)-AKSOL).GT.EK))GO TO
     1  325
        IF((CO((N-1)*NUM(9)+NUM(8)+I).GT.0.).AND.(CN((N-1)*NUM(9)
     1 +NUM(8)+I).LE.1.E-16)) GO TO 389
        GO TO 390
C
C  CALCULATE THE TOTAL CONCENTRATON OF EACH SPECIES AT A NODE POINT
C  AND DO A REDISTRIBUTION OF SPECIES WHEN A NEW PRECIPITATE STARTS
C  TO FORM AT A NODE POINT
C
  325   CONTINUE
        KI=NUM(10)+I
        WRITE(6,2021)N,DUM(KI),TIME
```

```
        WRITE (6,2000) AKSOL,EQCONST(NUM(12)+NUM(4)+I)
          II=0
          IE=3
          DO 330 J=1,M9
  330       CM(J)=CN((N-1)*NUM(9)+J)
          DO 375 J=1,M1
            WCONST(J)=CM(J)
            IF (ISORPI(J).EQ.0) GO TO 350
            II=II+1
            WCONST(J)=WCONST(J)+CM(NUM(1)+II)
  350       CONTINUE
            IF (ISORPE(J).EQ.0) GO TO 355
            IE=IE+1
            IEJ=IE
            IF (J.EQ.LNH) IEJ=3
            IF (J.EQ.LNH) IE=IE-1
            WCONST(J)=WCONST(J)+CM(NUM(6)+IEJ)
            IF (J.EQ.LNH) WCONST(J)=WCONST(J)+2.*CM(NUM(6)+2)
  355   CONTINUE
            IF (NUM(4).EQ.0) GO TO 362
              DO 360 K=1,M4
                KK=K+NUM(1)
                IF (ISORPI(KK).EQ.0) GO TO 356
                II=II+1
                WCONST(J)=WCONST(J)+S(J,K)*CM(NUM(1)+II)
  356         CONTINUE
                 IF (ISORPE(KK).EQ.0) GO TO 360
                 IE=IE+1
                 WCONST(J)=WCONST(J)+S(J,K)*CM(NUM(6)+IE)
  360           WCONST(J)=WCONST(J)+CM(NUM(7)+K)*S(J,K)
  362        DO 370 K=1,M5
                WCONST(J)=WCONST(J)+SS(J,K)*CM(NUM(8)+K)
  370         CONTINUE
  375   CONTINUE
C  ************************************************************
C  DO AN EQUILIBRIUM SPECIATION IF A NEW PRECIPITATE IS FORMING
C  ************************************************************
      CALL EQLIB(CM,WCONST,INDEX1,INDEX2,NUM,N,SS,EQCONST,CTOT,AC,
     10,LNH,IN3)
          DO 380 J=1,M9
  380       CN((N-1)*NUM(9)+J)=CM(J)
        GO TO 390
  389   CONTINUE
      TMINUS=TIME-DELT
      WRITE(6,2050)N,DUM(NUM(10)+I),TMINUS,CO((N-1)*NUM(9)+NUM(8)+I),
     1 TIME,CN((N-1)*NUM(9)+NUM(8)+I)
  390 CONTINUE
  400 CONTINUE
C
      IF ((TIME-TPRINT(K1)).GT.0.) GO TO 401
      IF (ITER.LT.6) DELT=DELT*1.75
      IF (DELT.GT.DTMAX) DELT=DTMAX
      IF ((ITER.LT.6).AND.(DELT.LT.DTMAX)) WRITE (6,2023) DELT,TIME
```

```
      GO TO 235
  401 CONTINUE
C  ********************************************************
C  WRITE OUT THE SPECIES CONCENTRATIONS
C  ********************************************************
      K1=K1+1
      WRITE (6,530) TIME,DELT
      NPRI=NMAX/9
      I1=1
      I5=1
      I4=9
      K2P=0
      I3=0
  405 CONTINUE
      K1P=K2P+1
      K2P=K1P+(I4-1)
      I2=I3
      I3=I2+NUM(9)*I4
      WRITE (6,620) (X(K),K=K1P,K2P)
C
C  BASIS SPECIES
C
      DO 410 J=1,M1
      I22=I2+J
      WRITE (6,625) DUM(J),(CN(K),K=I22,I3,M9)
  410 CONTINUE
C
C  SORBED SPECIES VIA ION EXCHANGE
C
      IF (NUM(2).EQ.0) GO TO 420
      WRITE (6,621)
      M2=NUM(2)
C
      DO 415 J=1,M2
      I22=I2+NUM(1)+J
      KK=ILBLI(J)
      WRITE (6,625) DUM(KK),(CN(K),K=I22,I3,M9)
  415 CONTINUE
C
C  SORBED SPECIES VIA SURFACE COMPLEXATION
C
  420 IF (NUM(3).EQ.0) GO TO 435
      WRITE (6,622)
      M3=NUM(3)
C
      DO 430 J=1,M3
      I22=I2+NUM(6)+J
      KK=ILBLE(J)
      IF (KK.GT.NUM(1)) KK=KK-NUM(2)-NUM(3)
      IF ((J.EQ.1).OR.(J.EQ.2)) KK=ILBLE(J)
      WRITE (6,625) DUM(KK),(CN(K),K=I22,I3,M9)
  430 CONTINUE
C
```

```
C  AQUEOUS PHASE COMPLEXES
C
  435 IF (NUM(4).EQ.0) GO TO 445
      WRITE(6,623)
C
      DO 440 I=1,M4
      I22=I2+NUM(7)+I
      KK=I+NUM(1)
      WRITE (6,625) DUM(KK),(CN(K),K=I22,I3,M9)
  440 CONTINUE
C
C  PRECIPITATES
C
  445 IF (NUM(5).EQ.0) GO TO 470
      WRITE (6,624)
C
      DO 460 I=1,M5
      KK=NUM(10)+I
      I22=I2+NUM(8)+I
      WRITE (6,625) DUM(KK),(CN(K),K=I22,I3,M9)
  460 CONTINUE
C
  470 CONTINUE
      I1=I1+1
      IF (I1.LE.NPRI) GO TO 405
      NPRI2=NPRI*9
      IF (NPRI2.EQ.NMAX) GO TO 490
      I4=NMAX-NPRI2
      IF (I5.EQ.5) GO TO 490
      I5=5
      GO TO 405
  490 IF (K1.GT.KMAX) GO TO 500
      GO TO 235
  500 CONTINUE
      STOP
C
C  FORMAT STATEMENTS FOR THE MAIN PROGRAM
C
  530 FORMAT (*1*,4X,*TIME=*,F10.5,10X,*DELT=*,1PE12.4,10X,
     1*CONCENTRATION OF SPECIES IN MOLES/LITER SOLUTION*,/)
  596 FORMAT (//,4X,*TO HAVE A NET BALANCE OF ZERO CHARGE, OTHER *
     1*SPECIES MUST BE PRESENT (ALTHOUGH NOT PARTICIPATING IN THE*,/,
     2 4X, *CHEMICAL REACTIONS) WITH A TOTAL CONCENTRATION TIMES *,
     2 *CHARGE OF *,G10.3,/)
  597 FORMAT (///,5X,*SIGO=*,(1PE10.3),5X,*SIGB=*,(1PE10.3),5X,*SIGD=*,
     1 (1PE10.3),/,5X,*PSIO=*,(1PE10.3),5X,*PSIBETA=*,(1PE10.3),5X,
     2*PSID=*,(1PE10.3),/)
  598 FORMAT (4X,*SO- =*,1PE12.4,10X,*SOH2+ =*,1PE12.4,//)
  600 FORMAT(//,4X,*DISPERSION COEFFICIENT =*,F4.1,* V +*,G6.2,5x,
     1*FLUID VELOCITY =*,G10.3,5x, *NUMBER OF GRID POINTS =*,I5,/)
  601 FORMAT(//,4X,*DISPERSION COEFFICIENT =*,F4.1,* V +*,G6.2,5x,
     1*FLUID VELOCITY =*,F10.3,*/ R*,5x,
     2 #NUMBER OF GRID POINTS =#,I5,/)
```

```
610 FORMAT(/,4X,#NUMBER OF PRINT OUTS =#,I5,/,4X,
   1#GIVEN AT THE FOLLOWING TIMES =#,8G10.4,/,34X,8G10.4)
611 FORMAT (/,4X,*NUMBER OF SITES(ION-EXCHANGE)*,F10.4,10X,
   1*NUMBER OF SITES(EDL MODEL)*,F10.4)
620 FORMAT (//,4X,55X,*DISTANCE*,/,4X,*SPECIES*,1X,9F12.3,/)
622 FORMAT (/,4X,*SORBED(EDL)*,/)
623 FORMAT(/,4X,*COMPLEXES*,/)
621 FORMAT(/,1X,*SORBED(IONEX)*,/)
624 FORMAT(/,2X,*PRECIPITATES*,/)
625 FORMAT (3X,A10,2X,9(1PE12.4))
700 FORMAT(# #A10,2G15.4,4X,2G11.4,6X,3G15.4)
740 FORMAT(/# COMPLEX        VALENCE       AQUEOUS CONC.   SORPTION(IONEX
   1)      SORPTION(EDL)#)
750 FORMAT(# #A10,5G15.4)
760 FORMAT(*1*,60X,*INITIAL CONDITIONS*,//)
780 FORMAT(# COMPONENT#5X#  TOTAL    #5X
   1#BARE ION    #5X#SORBED CONCENTRATION#,8X#ACT. COEF.#5X
   2#KD(ION EX)        KD(EDL)    #,/,13X,#AQUEOUS CONC.#4X,
   3 #CONCENTRATION#,3X,#  (IONEX)     (EDL) #,/)
790 FORMAT(*1*,30X,* BOUNDARY or influx conditions*,//)
800 FORMAT (////,2X,I4,#      BARE IONS#,10X,I4,5X,#SORBING IONS#,
   1 # (IONEX)#,10X,I4,5X,#SORBING IONS (EDL MODEL)#,///,
   2# COMPONENT  CHARGE  #,
   35X,#INITIAL CONDITIONS#,7X,#BOUNDARY CONDITIONS#,7X,#PK(IONEX)#,
   47X,#PK(EDL) #,/,
   525X,#TYPE#,7X,#VALUE#,9X,#TYPE#,7X,#VALUE#,/)
802 FORMAT (///,2X,I4,#     COMPLEXES#,10X,I4,7X,#SORBING COMPLEXES#,
   1#(IONEX)#,10X,I4,5X,#SORBING COMPLEXES (EDL MODEL)#,///,
   2#   COMPLEX   CHARGE  #,
   33X,#EQUIL. CONSTANT#,9X,#PK(IONEX)#,7X,#PK(EDL)#,10X,
   4#STOICHIOMETRY#,/)
805 FORMAT(A10,F6.0,6X,I5,4X,1PE12.4,4X,I5,4X,1PE12.4,10X,#---#,12X,
   1#---#)
806 FORMAT(A10,F6.0,6X,I5,4X,1PE12.4,4X,I5,4X,E12.4,4X,0PF10.3,11X,
   1#---#)
807 FORMAT(A10,F6.0,6X,I5,4X,1PE12.4,4X,I5,4X,1PE12.4,11X,#---#,6X,
   10PF10.3)
808 FORMAT(A10,F6.0,6X,I5,4X,1PE12.4,4X,I5,4X,1PE12.4,9X,0PF10.3,9X,
   10PF10.3)
820 FORMAT (A10,F6.0,9X,1PE12.4,15X,#---#,10X,#---#,7X,10(0PF5.0))
821 FORMAT (A10,F6.0,9X,1PE12.4,8X,0PF10.3,10X,#---#,7X,10F5.0)
822 FORMAT (A10,F6.0,9X,1PE12.4,15X,#---#,4X,0PF10.3,6X,10F5.0)
823 FORMAT (A10,F6.0,9X,1PE12.4,8X,0PF10.3,4X,F10.3,6X,10F5.0)
840 FORMAT (///,2X,I5,7X,*SOLID PRECIPITATES*,//,2X,*PRECIPITATE*,
   12X,*SOLUBILITY PRODUCT*,10X,*STOICHIOMETRY*,/)
841 FORMAT (//,2X,*PRECIPITATE*,3X,*EQUIVALENT MOLES*,
   1*/LITER SOLUTION*,/)
845 FORMAT (1X,A10,G10.3)
900 FORMAT (10X,7F10.3)
910 FORMAT (10X,7I10)
920 FORMAT (10X,I10,6F10.3)
950 FORMAT(A10,F5.0,I5,2F10.3,I5,2F10.3,2I5)
960 FORMAT(10X,3F10.3,F5.1)
```

```
 970 FORMAT (A10,F10.3,10F5.1,/,20F5.1)
 971 FORMAT (A10,6X,1PE12.4,9X,10(0PF5.1))
 980 FORMAT (10X,2F10.3,2I5)
 990 FORMAT (/,4X,*YOUR NUMBER OF SORBING IONS INPUT DOES NOT EQUAL THE
    1 NUMBER THAT WAS LISTED INITIALLY*,2I5,10X,2I5)
 999 FORMAT (*1*,20A4)
1000 FORMAT (20A4)
1001 FORMAT (10X,5(1PE12.4,/))
1010 FORMAT (2A10)
1011 FORMAT (/,4X,*UNIT OF LENGTH IS*,2X,A10,10X,*UNIT OF TIME IS*
    1,2X,A10)
2000 FORMAT (/,4X,*THE ACTIVITY PRODUCT IS*,1PE10.3,5X,
    1*WHICH NOW EXCEEDS THE SOLUBILITY PRODUCT OF*,1PE10.3)
2021 FORMAT (//,4X,*PRECIPITATION AT NODE*,I5,5X,*FOR SPECIES*,A10,
    1 *AT TIME*,1PE11.3)
2022 FORMAT (/,4X,*CONVERGENCE IS NOT OBTAINED, SO TIME STEP IS *
    1 , *DIVIDED BY 2,    DELT=*,1PE12.4)
2023 FORMAT (/,4X,*CONVERGENCE IS OBTAINED IN LESS THAN 6 *,
    1*ITERATIONS SO TIME STEP IS INCREASED BY 1.75*,/,4X,*DELT=*,
    11PE12.4,10X, *AT TIME=*,1PE12.4)
2050 FORMAT (/,4X,*AT NODE*,I5,4X,*SPECIES*,A10,*HAS REDISSOLVED*,/,
    1*  THE CONCENTRATION OF THIS SPECIES AT TIME* 1PE8.2,4x, *IS*,
    2 E12.4,/,*AND THE CONCENTRATION OF THIS SPECIES AT TIME*,E8.2,
    3 4x,*IS*, E12.4)
2060 FORMAT (/,4X,*INNER BOUNDARY IS CONSTANT CONCENTRATION*,10X,
    1*OUTER BOUNDARY IS ZERO FLUX*)
2061 FORMAT (/,4X,*INNER BOUNDARY IS CONSTANT FLUX*,10X,*OUTER*,
    1* BOUNDARY IS ZERO FLUX*)
2062 FORMAT (/,4X,*INNER BOUNDARY IS CONSTANT CONCENTRATION*,10X,
    1*OUTER BOUNDARY IS CONSTANT INITIAL CONCENTRATION*)
2063 FORMAT (/,4X,*INNER BOUNDARY IS CONSTANT FLUX*,10X,*OUTER*
    1* BOUNDRY IS CONSTANT INITIAL CONCENTRATION*)
     END
```

```
      SUBROUTINE ACTIVE(NUM,CN,VJ,AC,ELCONC,MDIM,NBEGIN,NEND)
C  **********************************************************
C  CALCULATES THE ACTIVITIES BASED ON THE DAVIES EQUATION
C  THE IONIC STRENGTH AT EACH NODE POINT IS STORED IN ELCONC,
C  THE ACTIVITIES ARE IN THE MATRIX AC(I,N)
C  **********************************************************
      DIMENSION NUM(1),CN(1),VJ(1),AC(MDIM,1),ELCONC(1)
      M1=NUM(1)
      M4=NUM(4)
      NTOT=NUM(9)
      IF (NBEGIN.EQ.NEND) NTOT=0
      DO 50 N=NBEGIN,NEND
C
C  CALCULATION OF IONIC STRENGTH
C
      CTOT=0.
      SI=0.
      DO 10 J=1,M1
      IF (CN((N-1)*NTOT+J) .LT.0.) GO TO 60
      CTOT=CTOT+VJ(J)*CN((N-1)*NTOT+J)
   10 SI=SI+VJ(J)**2*CN((N-1)*NTOT+J)
      IF (NUM(4).EQ.0) GO TO 16
      DO 15 I=1,M4
      IF (CN((N-1)*NTOT+NUM(7)+I).LT.0) GO TO 60
      CTOT=CTOT+VJ(NUM(1)+I)*CN((N-1)*NTOT+NUM(7)+I)
   15 SI=SI+VJ(NUM(1)+I)**2*CN((N-1)*NTOT+NUM(7)+I)
   16 CONTINUE
C
C  ALTHOUGH THE NET CHARGE OF THE SPECIES BEING CONSIDERED IS IN THE
C  CALCULATIONS MAY NOT BE EQUAL TO ZERO, FOR AN ACCURATE CALCULATION
C  OF THE IONIC STRENGTH, ALL THE CHEMICAL SPECIES MUST BE CONSIDERED
C  THEREFORE, IT IS ASSUMED HERE THAT THE BALANCE OF THE CHARGE IS MADE
C  UP BY A CHEMICAL SPECIES OF A +1 OR -1 CHARGE AND A CONCENTRATION
C  OF CTOT.  IF THIS IS NOT REASONABLE, THEN THE ACTUAL CALCULATION
C  SHOULD BE DONE WITH A NET CHARGE OF 0.
C
      SI=SI+ABS(CTOT)
      CIONST=0.5*SI
      ELCONC(N)=CIONST
      SI=SQRT(CIONST)
      FI=0.5*(SI/(1.+SI)-0.3*CIONST)
C
C  CALCULATION OF ACTIVITY COEFFICIENTS
C
      DO 20 J=1,M1
      G=FI*VJ(J)**2
   20 AC(J,N)=10.**(-G)
      IF (NUM(4).EQ.0) GO TO 50
      DO  25 I=1,M4
      GCX=FI*VJ(NUM(1)+I)**2
   25 AC(NUM(1)+I,N)=10.**(-GCX)
   50 CONTINUE
      RETURN
```

```
 60 WRITE (6,100)
100 FORMAT (/,4X,*THE CONCENTRATION IS LESS THAN ZERO WHICH IS NOT*
   1 * ALLOWED, THEREFORE THE PROGRAM HAS STOPPED*,/)
    RETURN
    END
```

```
      SUBROUTINE ALGEBRC(NUM,CN,R,N1,N2,MDIM,ELCONC,LNH,K1)
C
C  **********************************************************
C  CALCULATES THE RESIDUE FOR THE SITE CONSTRAINT EQUATIONS
C  AND THE MASS ACTION EQUATIONS DESCRIBING THE SORPTION
C  REACTIONS AND THE FORMATION OF COMPLEXES AND PRECIPITATES
C  **********************************************************
C
      DIMENSION NUM(1),CN(1),R(MDIM,1),RESIDUE(25),ELCONC(1)
      LEVEL2,R
      COMMON/AB/VJ(75),AC(75,100),EQCONST(100)
     1,S(25,25),SS(25,25),AH(25)
     2,ILBLI(25),ILBLE(25)
      COMMON/NJ/ISORPI(30),ISORPE(30),IION,IEION
      COMMON/AD/X(200),DELT,DOA,DOB,VO,CECNS,H2OK
      M1=NUM(1)
      M2=NUM(2)
      M3=NUM(3)
      M4=NUM(4)
      M5=NUM(5)
      KK=K1
C
C  FOR SORPTION VIA ION EXCHANGE, SITE CONSTRAINT EQUATION
C
      DO 200 N=N1,N2
      NSTART=(N-1)*NUM(9)
      IF (KK.EQ.1) NSTART=0
      IF (NUM(2).EQ.0) GO TO 45
      R(NUM(1)+1,N)=CECNS
      AMTOTAL=0.
      DO 35 J=1,M2
      JJ=ILBLI(J)
      R(NUM(1)+1,N)=R(NUM(1)+1,N)-VJ(JJ)*CN(NSTART+NUM(1)+J)
   35 AMTOTAL=AMTOTAL+CN(NSTART+NUM(1)+J)
C
C  MASS ACTION EQUATIONS DESCRIBING SORPTION VIA ION EXCHANGE
C
      IF (NUM(2).EQ.1) GO TO 45
      J1=ILBLI(1)
      DO 40 J=2,M2
      JJ=ILBLI(J)
      AJ=(CN(NSTART+NUM(1)+J)/AMTOTAL)**VJ(J1)
      A1=(CN(NSTART+NUM(1)+1)/AMTOTAL)**VJ(JJ)
      IF (CN(NSTART+JJ).LT.1.E-16) GO TO 36
      R(NUM(1)+J,N)=EQCONST(J)**VJ(J1)*A1/AJ-EQCONST(1)**VJ(JJ)*
     1(CN(NSTART+J1)*AC(J1,N))**VJ(JJ)/(CN(NSTART+JJ)*AC(JJ,N))**VJ(J1)
      GO TO 40
   36 R(NUM(1)+J,N)=(EQCONST(J)*CN(NSTART+JJ)*AC(JJ,N))**VJ(J1)*
     1A1-(EQCONST(1)*CN(NSTART+J1)*AC(J1,N))**VJ(JJ)*AJ
   40 CONTINUE
   45 CONTINUE
      IF (NUM(3).EQ.0) GO TO 52
C
```

```
C  FOR SOPTION VIA SURFACE COMPLEXATION, MASS ACTION EQUATIONS
C  ARE SOLVED IN SUBROUTINE REDL
C
      CALL REDL(CN,RESIDUE,NSTART,ELCONC(N),LNH,NUM)
      DO 50 I=1,M3
      R(NUM(6)+I,N)=RESIDUE(I)
   50 CONTINUE
   52 CONTINUE
      IF (NUM(4).EQ.0) GO TO  58
C
C  MASS ACTIONS EQUATIONS FOR FORMATION OF COMPLEXES IN THE AQUEOUS
C  PHASE
C
      DO 56 I=1,M4
      CM=EQCONST(NUM(12)+I)
      DO 54 J=1,M1
      IF (S(J,I).EQ.0) GO TO 54
      CM=CM*(AC(J,N)*CN(NSTART+J))**S(J,I)
   54 CONTINUE
   56 R(NUM(7)+I,N)=AC(NUM(1)+I,N)*CN(NSTART+NUM(7)+I)-CM
   58 CONTINUE
      IF (NUM(5).EQ.0) GO TO 170
C
C  SOLUBILITY PRODUCT EQUATIONS FOR THE FORMATIONS OF PRECIPITATES
C
      DO 168 I=1,M5
      KK=NSTART+NUM(8)+I
      KN=NUM(8)+I
      IF (CN(KK).LT.1.E-11) GO TO 167
      AKSOL=1.0
      DO 162 J=1,M1
      IF (SS(J,I).LT.1.E-15) GO TO 162
      AKSOL=AKSOL*(AC(J,N)*CN(NSTART+J))**SS(J,I)
  162 CONTINUE
      R(KN,N)=AKSOL-EQCONST(NUM(12)+NUM(4)+I)
      GO TO 168
  167 R(KN,N)=CN(KK)
  168 CONTINUE
  170 CONTINUE
  200 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE EQLIB(CM,WCONST,INDEX1,INDEX2,NUM,N,SS,EQCONST,CTOT,
     1AC,LCHRG,LNH,IN)
C *************************************************************************
C THIS SUBROUTINE CALCULATES THE EQUILIBRIUM DISTRIBUTION OF SPECIES.  IT
C CALLS THE SUBROUTINE RESEQ WHICH CALCULATES THE RESIDUES OF THE EQUILIBRIUM
C EQUATIONS.  THE EQUILIBRIUM DISTRIBUTION OF SPECIES IS CALCULATED GIVEN
C THE TYPE OF CONDITIONS SET FOR EACH SPECIES, I.E. TOTAL CONCENTRATION OF THE
C SPECIES, BARE ION CONCENTRATION, ETC.  THIS SET OF CONDITIONS MUST EQUAL
C THE NUMBER OF BASIS SPECIES. THE MASS ACTION EXPRESSIONS, SOLUBILITY PRODUCT
C EQUATIONS, AND THE SITE CONSTRAINT EQUATION ARE USED TO CALCULATE THE
C CONCENTRATIONS OF THE REST OF THE SPECIES.
C *************************************************************************
      DIMENSION CM(1),WCONST(1),Z(25,25),Y(25),INDEX1(1),INDEX2(1)
     1,SS(25,1),EQCONST(1),AC(75,1),ITERP(35),NUM(1)
      COMMON/EDL/C1,C2,AREA,SOH
      COMMON/SPEC/LEACH1(5),NB,PINI(5)
C
      MDIM=25
      NTOT=NUM(8)
C
      IF (NUM(3).EQ.0) SOH=20.
      ITER=1
      IF (NUM(5).EQ.0) GO TO 2
      M5=NUM(5)
      DO 1 I=1,M5
    1 ITERP(I)=1
    2 ITER=ITER+1
C
C IF CONVERGENCE IS NOT OBTAINED WITHIN 100 ITERATIONS, THE
C CALCULATIONS ARE STOPPED
C
      IF (ITER.GT.100) GO TO 90
      NSOL=0
C
C THE SOLUBILITY PRODUCT FOR A PRECIPITATE IS ONLY INCLUDED WHEN
C THE PRODUCT OF THE ACTIVITIES OF THE SPECIES MAKING UP THAT
C PRECIPITATE EXCEEDS THIS PRODUCT;  TO AVOID OSCILLATIONS BETWEEN
C THE PRECIPITATE WANTING TO FORM OR NOT, THE SOLUBILITY PRODUCT
C IS INCLUDED ONLY WHEN IT IS EXCEEDED FOR TWO CALCULATIONS
C
      IF (NUM(5).EQ.0) GO TO 40
      DO 20 I=1,M5
      AKSOL=1.0
      M1=NUM(1)
      DO 5 J=1,M1
    5 AKSOL=AKSOL*(AC(J,N)*CM(J))**SS(J,I)
C
C IF A SOLID HAS BEEN PUT IN CONTACT WITH THE GROUNDWATER AT THE
C FIRST NODE POINT, THE SOLUBILITY PRODUCT OF THAT PRECIPITATE WILL
C ALWAYS BE INCLUDED FOR THE DISTRIBUTION OF SPECIES AT THE INNER
C BOUNDARY CONDITION.
C
      IF ((LEACH1(1).EQ.I).AND.(N.EQ.NB)) INDEX1(I)=1
```

```
      IF ((LEACH1(1).EQ.I).AND.(N.EQ.NB)) GO TO 15
      INDEX1(I)=0
      IJ=NUM(12)+NUM(4)+I
      EK=0.001*EQCONST(IJ)
      IF ((EQCONST(IJ).LT.AKSOL).OR.(CM(NTOT+I).GT.1.E-16)) ITERP(I)=
     1 ITERP(I)+1
      IF ((EQCONST(IJ).LT.AKSOL).OR.(CM(NTOT+I).GT.1.E-16)) GO TO 10
      ITERP(I)=0
   10 IF (ITERP(I).GE.2) INDEX1(I)=1
   15 IF (INDEX1(I).EQ.1) NSOL=NSOL+1
      M9=NUM(9)
      IF(ITER.GT.IN) WRITE(6,900)(CM(J),J=1,M9),AKSOL,EQCONST(IJ)
   20 CONTINUE
   40 CONTINUE
C
C  RESIDUES OF THE CONSTRAINT EQUATIONS FOR THE INITIAL AND BOUNDARY
C  CONDITIONS AND THE MASS ACTION AND SITE CONSTRAINT EQUATION ARE
C  CALCULATED IN THE SUBROUTINE RESEQ
C
      CALL RESEQ(WCONST,CM,INDEX1,INDEX2,Y,N,CTOT,MDIM,NUM,LCHRG,LNH,
     1 NSOL)
      NTOTP=NTOT+NSOL
      IF (ITER.GT.IN) WRITE (6,1000) (Y(I),I=1,NTOTP)
C
C  THE JACOBIAN FOR THE EQUILIBRIUM DISTRIBUTION OF SPECIES; I.E. FOR THE
C  EQUATIONS IN SUBROUTINE RESEQ IS CALCULATED HERE
C
      CALL JACOB2(Z,CM,WCONST,INDEX1,INDEX2,Y,NUM,N,CTOT,NSOL,LCHRG,
     1LNH,MDIM)
C
C  FROM THE JACOBIAN AND THE RESIDUES FOR THE LAST GUESS, CALCULATE THE
C  NEW GUESS FOR THE ALL THE SPECIES
C
      CALL SIMQ(Z,Y,NTOTP,MDIM)
C
      IF (ITER.GT.IN) WRITE (6,101) ITER
      DO 60 J=1,NTOT
      CC1=CM(J)
      CM(J)=CM(J)-Y(J)
      IF (ITER.GT.IN) WRITE (6,1000) CC1,CM(J),Y(J)
C
C  THE CONCENTRATION OF THE SPECIES IS NOT ALLOWED TO GO NEGATIVE OR
C  FOR THE SURFACE COMPLEXATION MODEL, THE SORBED CONCENTRATION CANNOT
C  BE GREATER THAN THE TOTAL NUMBER OF SITES
C
      IF(CM(J).LT.0.) CM(J)=CC1/10.
      IF ((J.GT.NUM(6)).AND.(J.LT.NUM(7)).AND.(CM(J).GT.SOH)) CM(J)=SOH
   60 CONTINUE
C
      INDEX=0
C
C  CALCULATE THE AMOUNT OF THE PRECIPITATES;  ONLY PRECIPITATES THAT ARE FORMING
C  ARE INCLUDED IN THIS CALCULATION
```

```
C
      IF (NUM(5).EQ.0) GO TO 66
      DO 65 I=1,M5
      IF (INDEX1(I).EQ.0) GO TO 65
      INDEX=INDEX+1
      CC1=CM(NTOT+I)
      CM(NTOT+I)=CM(NTOT+I)-Y(NTOT+INDEX)
      II=NTOT+I
      III=NTOT+INDEX
      IF (ITER.GT.IN) WRITE (6,1000) CC1,CM(II),Y(III)
      IF (CM(NTOT+I).LT.0.) ITERP(I)=0
      IF (CM(NTOT+I).LT.0.) CM(NTOT+I)=0.
   65 CONTINUE
   66 CONTINUE
C
C  CHECK CONVERGENCE;  IF WITHIN THE CRITERIA SET, THEN END THE
C  ITERATIONS, OTHERWISE CONTINUE
C
      DO 70 J=1,NTOTP
      IF (CM(J).LT.1.E-30) GO TO 70
      IF(ABS(Y(J)/CM(J)).GT.1.E-6) GO TO 2
   70 CONTINUE
      RETURN
   90 WRITE(6,100) ITER
  100 FORMAT(# NO CONVERGENCE IN EQLIB AFTER ITER =#I3)
  101 FORMAT (4X,I5,10X,*VALUES FOR THIS ITERATION*,/)
  900 FORMAT (4X,*PRECIPITATION CHECK*,9(1PE12.4))
 1000 FORMAT (/,4X,10(8(1PE12.4),/))
      STOP
      END
```

```
      SUBROUTINE DECBT(M,N,MDIM,A,B,C,IP,IER)
C     *******************************************************************
C   THE NEXT FOUR SUBROUTINES ARE TO INVERT THE BLOCK TRI-DIAGONAL
C   MATRIX TO GET THE NEW GUESSES FOR THE CONCENTRATIONS.  THE
C   SUBROUTINES INVOLVED HERE ARE DECBT, DEC, SOL, AND SOLBT AND WERE
C   WRITTEN BY A.C. HINDMARSH OF LAWRENCE LIVERMORE LABORATORY.  THESE
C   SUBROUTINES ARE COVERED IN A SEPARATE DOCUMENT UCID-30150
C   "SOLUTION OF BLOCK-TRIDIAGONAL SYSTEMS OF LINEAR ALGEBRAIC EQUATIONS"
C     *******************************************************************
      INTEGER M,N,MDIM,IP(MDIM,N),IER
      DIMENSION A(MDIM,MDIM,N),B(MDIM,MDIM,N),C(MDIM,MDIM,N)
      REAL DP
      LEVEL 2,A,B,C
      IF (M .LT. 1 .OR. N .LT. 4) GO TO 210
      NM1 = N - 1
      NM2 = N - 2
      CALL DEC(M,MDIM,A,IP,IER)
      K = 1
      IF (IER .NE. 0) GO TO 200
      DO 10 J = 1,M
      CALL SOL(M,MDIM,A,B(1,J,1),IP)
      CALL SOL(M,MDIM,A,C(1,J,1),IP)
 10     CONTINUE
      DO 40 J = 1,M
        DO 30 I = 1,M
          DP = 0.
          DO 20 L = 1,M
 20         DP = DP + C(I,L,2)*C(L,J,1)
          B(I,J,2) = B(I,J,2) - DP
 30       CONTINUE
 40     CONTINUE
      DO 100 K = 2,NM1
        KM1 = K - 1
        DO 70 J = 1,M
          DO 60 I = 1,M
            DP = 0.
            DO 50 L = 1,M
 50           DP = DP + C(I,L,K)*B(L,J,KM1)
            A(I,J,K) = A(I,J,K) - DP
 60         CONTINUE
 70       CONTINUE
      CALL DEC(M,MDIM,A(1,1,K),IP(1,K),IER)
        IF (IER .NE. 0) GO TO 200
        DO 80 J = 1,M
 80       CALL SOL(M,MDIM,A(1,1,K),B(1,J,K),IP(1,K))
 100    CONTINUE
      DO 130 J = 1,M
        DO 120 I = 1,M
          DP = 0.
          DO 110 L = 1,M
 110        DP = DP + B(I,L,N)*B(L,J,NM2)
          C(I,J,N) = C(I,J,N) - DP
 120      CONTINUE
```

```
 130      CONTINUE
        DO 160 J = 1,M
          DO 150 I = 1,M
            DP = 0.
            DO 140 L = 1,M
 140          DP = DP + C(I,L,N)*B(L,J,NM1)
            A(I,J,N) = A(I,J,N) - DP
 150        CONTINUE
 160      CONTINUE
        CALL DEC(M,MDIM,A(1,1,N),IP(1,N),IER)
        K = N
        IF (IER .NE. 0) GO TO 200
        RETURN
 200    IER = K
        RETURN
 210    IER = -1
        RETURN
        END
C
        SUBROUTINE SOLBT(M,N,MDIM,A,B,C,Y,IP)
        DIMENSION Y(MDIM,N)
        INTEGER M,N,IP(MDIM,N),MDIM
        DIMENSION A(MDIM,MDIM,N),B(MDIM,MDIM,N),C(MDIM,MDIM,N)
        REAL DP
        LEVEL 2,A,B,C,Y
        NM1 = N - 1
        NM2 = N - 2
        CALL SOL(M,MDIM,A,Y,IP)
        DO 30 K = 2,NM1
          KM1 = K - 1
          DO 20 I = 1,M
            DP = 0.
            DO 10 J = 1,M
 10           DP = DP + C(I,J,K)*Y(J,KM1)
            Y(I,K) = Y(I,K) - DP
 20         CONTINUE
        CALL SOL(M,MDIM,A(1,1,K),Y(1,K),IP(1,K))
 30       CONTINUE
        DO 50 I = 1,M
          DP = 0.
          DO 40 J = 1,M
 40         DP = DP + C(I,J,N)*Y(J,NM1) + B(I,J,N)*Y(J,NM2)
          Y(I,N) = Y(I,N) - DP
 50       CONTINUE
        CALL SOL(M,MDIM,A(1,1,N),Y(1,N),IP(1,N))
        DO 80 KB = 1,NM1
          K = N - KB
          KP1 = K + 1
          DO 70 I = 1,M
            DP = 0.
            DO 60 J = 1,M
 60           DP = DP + B(I,J,K)*Y(J,KP1)
            Y(I,K) = Y(I,K) - DP
```

```
 70         CONTINUE
 80       CONTINUE
      DO 100 I = 1,M
        DP = 0.
        DO 90 J = 1,M
 90       DP = DP + C(I,J,1)*Y(J,3)
        Y(I,1) = Y(I,1) - DP
 100    CONTINUE
      RETURN
      END
C
      SUBROUTINE DEC (N, NDIM, A, IP, IER)
      DIMENSION  IP(N)
      DIMENSION A(NDIM,N)
      LEVEL 2,A
      IER = 0
      IP(N) = 1
      IF (N .EQ. 1) GO TO 70
      NM1 = N - 1
      DO 60 K = 1,NM1
        KP1 = K + 1
        M = K
        DO 10 I = KP1,N
 10       IF (ABS(A(I,K)) .GT. ABS(A(M,K))) M = I
        IP(K) = M
        T = A(M,K)
        IF (M .EQ. K) GO TO 20
        IP(N) = -IP(N)
        A(M,K) = A(K,K)
        A(K,K) = T
 20     IF (T .EQ. 0.) GO TO 80
        T = 1./T
        DO 30 I = KP1,N
 30       A(I,K) = -A(I,K)*T
        DO 50 J = KP1,N
          T = A(M,J)
          A(M,J) = A(K,J)
          A(K,J) = T
          IF (T .EQ. 0.) GO TO 50
          DO 40 I = KP1,N
 40         A(I,J) = A(I,J) + A(I,K)*T
 50       CONTINUE
 60     CONTINUE
 70   K = N
      IF (A(N,N) .EQ. 0.) GO TO 80
      RETURN
 80   IER = K
      IP(N) = 0
      RETURN
      END
C
      SUBROUTINE SOL (N, NDIM, A, B, IP)
      DIMENSION B(N), IP(N), A(NDIM,N)
```

```
      LEVEL 2, A,B
      IF (N .EQ. 1) GO TO 50
      NM1 = N - 1
      DO 20 K = 1,NM1
        KP1 = K + 1
        M = IP(K)
        T = B(M)
        B(M) = B(K)
        B(K) = T
        DO 10 I = KP1,N
10        B(I) = B(I) + A(I,K)*T
20      CONTINUE
      DO 40 KB = 1,NM1
        KM1 = N - KB
        K = KM1 + 1
        B(K) = B(K)/A(K,K)
        T = -B(K)
        DO 30 I = 1,KM1
30        B(I) = B(I) + A(I,K)*T
40      CONTINUE
50    B(1) = B(1)/A(1,1)
      RETURN
      END
```

```
      SUBROUTINE IGUESS(CM,CBASIS,NUM,LNH)
C ***********************************************************************
C THIS SUBROUTINE CALCULATES THE FIRST GUESS OF THE VALUES OF THE
C BASIS SPECIES, COMPLEXES, SORBED COMPONENTS AND PRECIPITATES
C FOR AN EQUILIBRIUM DISTRIBUTION OF SPECIES CALCULATION. IT ASSUMES
C THAT THE CONCENTRATION OF THE BASIS SPECIES IS EQUAL TO VALUE SET
C FOR THE INITIAL CONDITION FOR THAT SPECIES, I.E. IT IS SET EQUAL TO
C BI(J); THE CONCENTRATIONS OF THE COMPLEXES AND THE SORBED COMPONENTS
C ARE THEN CALCULATED FROM THE MASS ACTION EQUATIONS ASSUMING THESE
C BASIS SPECIES CONCENTRATIONS.  THE CONCENTRATION OF THE PRECIPITATES IS
C SET EQUAL TO 0 FOR THE FIRST GUESS. THE SUBROUTINE DOES NOT NECESSARILY
C MAKE THE BEST GUESS.  THE USER CAN READ IN GUESSES INSTEAD OF CALLING
C THIS ROUTINE.  SET IG=1 IF YOU WANT TO CALL THIS ROUTINE, OTHERWISE SET
C IT EQUAL TO 0.
C ***********************************************************************
      DIMENSION CM(1),NUM(1),CBASIS(25)
      COMMON/AB/VJ(75),AC(75,100),EQCONST(100),S(25,25),SS(25,25)
     1,AH(25),ILBLI(25),ILBLE(25)
      COMMON/EDL/C1,C2,AREA,SOH
      COMMON/AD/X(200),DELT,DOA,DOB,VO,CEC,H2OK
      M5=NUM(5)
      NSPECM=NUM(1)
      IF (LNH.GT.0) NSPECM=NUM(1)-1
C
C SET THE CONCENTRATION OF THE BASIS SPECIES EQUAL TO THE CONCENTRATION
C READ IN FOR THAT BASIS SPECIES EVEN THOUGH THAT VALUE MAY BE FOR
C THE TOTAL AQUEOUS PHASE CONCENTRATION OF THAT SPECIES.
C
      DO 10 J=1,NSPECM
   10 CM(J)=CBASIS(J)
      IF (LNH.GT.0) CM(NUM(1))=H2OK/CM(NUM(LNH))
C
C CALCULATE THE SORBED CONCENTRATIONS FROM THE MASS ACTION EQUATIONS
C
      IF (NUM(2).EQ.0) GO TO 100
      CM(NUM(1)+1)=CEC
      AMTOTAL=0
      J1=ILBLI(1)
      M2=NUM(2)
      DO 20 J=2,M2
      JJ=ILBLI(J)
      CM(NUM(1)+J)=(EQCONST(J)/EQCONST(1))**(1./V(J1))*CM(NUM(1)+1)
     1**(VJ(JJ)/VJ(J1))/(CM(J1)**(VJ(JJ)/VJ(J1)))
      CM(NUM(1)+J)=CM(JJ)*CM(NUM(1)+J)
   20 CONTINUE
  100 IF (NUM(3).EQ.0) GO TO 200
      IJ1=NUM(2)+1
      IJ2=NUM(2)+2
      CM(NUM(6)+3)=SOH
      KK=NUM(6)
      CM(KK+2)=CM(LNH)*SOH*0.1/EQCONST(NUM(2)+1)
      CM(KK+1)=EQCONST(NUM(2)+2)*CM(KK+3)/CM(LNH)
      IF (NUM(3).LT.4) GO TO 200
```

```
      DO 120 I=4,M3
      JJ=ILBLE(I)
      IJ=NUM(2)+I
      CM(KK+I)=EQCONST(IJ)*CM(JJ)*CM(KK+3)/(CM(LNH))**AH(I))
  120 CONTINUE
  200 CONTINUE
C
C  CALCULATE THE CONCENTRATION OF THE COMPLEXES
C  USING THE MASS ACTION EQUATIONS
C
      IF (NUM(4).EQ.0) GO TO 300
      M4=NUM(4)
      DO 250 I=1,M4
      CCM=EQCONST(NUM(12)+I)
      M1=NUM(1)
      DO 220 J=1,M1
      IF (S(J,I).EQ.0.) GO TO 220
      CCM=CCM*CM(J)**S(J,I)
  220 CONTINUE
      CM(NUM(7)+I)=CCM
  250 CONTINUE
C
C  SET THE FIRST GUESS FOR THE PRECIPITATES TO BE 0
C
  300 IF (NUM(5).EQ.0) GO TO 400
      DO 350 J=1,M5
  350 CM(NUM(8)+J)=0.0
  400 RETURN
      END
```

```
      SUBROUTINE JACOB2(Z,CM,WCONST,INDEX1,INDEX2,RE,NUM,N,CTOT,NSOL,
     1LCHRG,LNH,MDIM)
C ********************************************************************
C CALCULATION OF THE JACOBIAN  DONE FOR THE CALCULATION OF THE
C EQUILIBRIUM CONDITIONS; IT IS CALLED FROM THE SUBROUTINE EQLIB ONLY
C ********************************************************************
      DIMENSION RE(1),REN(25),CM(1),WCONST(1),INDEX1(1),
     1Z(25,25),INDEX2(1),NUM(1)
      COMMON/CONST/REL,ABSV
      M5=NUM(5)
      NTOT=NUM(8)
      NTOTP=NTOT+NSOL
      DO 15 J=1,NTOT
      COLD=CM(J)
      CM(J)=CM(J)*(1.+REL)+ABSV
      CALL RESEQ(WCONST,CM,INDEX1,INDEX2,REN,N,CTOT,MDIM,
     1 NUM,LCHRG,LNH,NSOL)
      DO 20 I=1,NTOTP
   20 Z(I,J)=(REN(I)-RE(I))/(CM(J)-COLD)
      CM(J)=COLD
   15 CONTINUE
      INDEX=0
C
C THE SOLUBILITY PRODUCT FOR A PRECIPITATE IS ONLY
C INCLUDED IF THAT SPECIES IS GOING TO PRECIPITATE
      IF (M5.EQ.0) GO TO 26
      DO 25 J=1,M5
      IF (INDEX1(J).EQ.0) GO TO 25
      INDEX=INDEX+1
      COLD=CM(NTOT+J)
      CM(NTOT+J)=CM(NTOT+J)*(1.+REL)+ABSV
      CALL RESEQ (WCONST,CM,INDEX1,INDEX2,REN,N,CTOT,MDIM,
     1 NUM,LCHRG,LNH,NSOL)
      DO 30 I=1,NTOTP
   30 Z(I,INDEX+NTOT)=(REN(I)-RE(I))/(CM(NTOT+J)-COLD)
      CM(NTOT+J)=COLD
   25 CONTINUE
   26 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE JACOBI(A,B,C,CO,CN,BC,BC2,NUM,RO,MDIM,LNH,IBND,ITYPE)
C   **********************************************************************
C   CALCULATION OF THE JACOBIAN WHICH IS THE CHANGE IN THE RESIDUES
C   OF THE TRANSPORT EQUATIONS, SITE CONSTRAINT EQUATION AND THE
C   MASS ACTION EQUATIONS FOR A CHANGE IN THE CONCENTRATIONS.  THIS SUBROUTINE
C   CONSIDERS THE RESIDUES FOR THE TIME DEPENDENT EQUATIONS
C   IT IS CALLED FROM THE MAIN PROGRAM CHEMTRN ONLY
C   **********************************************************************
      DIMENSION RO(MDIM,1),CN(1),CO(1),CNO(100),BC(1),NUM(1),IBND(1)
      DIMENSION A(MDIM,MDIM,1),B(MDIM,MDIM,1),C(MDIM,MDIM,1),BC2(1)
      COMMON/CONST/REL,ABSV
      COMMON/LCM3/RN(25,100)
      LEVEL 2,A,B,C,RN,RO
      NTOT=NUM(9)
      NMAX=NUM(14)
      DO 50 K=1,3
      DO 50 J=1,NTOT
      DO 30 N=K,NMAX,3
      CNO(N)=CN((N-1)*NTOT+J)
   30 CN((N-1)*NTOT+J)=CN((N-1)*NTOT+J)*(1.+REL)+ABSV
      CALL RES(CN,CO,BC,BC2,RN,NUM,MDIM,LNH,IBND,ITYPE)
      DO 45 N=K,NMAX,3
      DO 40 I=1,NTOT
      KK=(N-1)*NTOT+J
      IF (N.EQ.1) C(I,J,1)=0.
      IF (N.LT.2) GO TO 35
      B(I,J,N-1)=(RN(I,N-1)-RO(I,N-1))/(CN((N-1)*NTOT+J)-
     1CNO(N))
   35 A(I,J,N)=(RN(I,N)-RO(I,N))/(CN((N-1)*NTOT+J)-
     1CNO(N))
      IF (N.EQ.NMAX) B(I,J,N)=0.
      IF (N.EQ.NMAX) GO TO  40
      C(I,J,N+1)=(RN(I,N+1)-RO(I,N+1))/(CN((N-1)*NTOT+J)-CNO(N))
   40 CONTINUE
      CN((N-1)*NTOT+J)=CNO(N)
   45 CONTINUE
   50 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE REDL(CONC,RESIDUE,NP,ELCONC,LNH,NUM)
C ******************************************************************
C CALCULATES THE RESIDUES FOR THE MASS ACTION EQUATIONS, AND A SITE
C CONSTRAINT EQUATION FOR THE SURFACE COMPLEXATION MODEL FOR SORPTION;
C THE ACTUAL SURFACE COMPLEXATION MODEL IS DESCRIBED IN
C DETAIL IN THE PAPER BY J.A. DAVIS, R.O. JAMES, AND J.O. LECKIE
C IN J. COLLOID AND INTERFACE SCIENCE, VOL 63, NO. 3, MARCH, 1978
C ******************************************************************
      DIMENSION CONC(1),RESIDUE(1),NUM(1)
      COMMON/AB/VJ(75),AC(75,100),EQCONST(100),
     1S(25,25),SS(25,25),AH(25),ILBLI(25),ILBLE(25)
      COMMON/EDL/C1,C2,AREA,SOH
      COMMON/EDL2/SIGO,SIGB,SIGD,PSIO,PSIBETA,PSID
      DATA ELEC/1.602E-19/, AVOGAD/6.025E23/, BOLTZ/1.38E-23/
      DATA DIELEC/78.84/
      DATA TEMP/298.15/,FARADAY/9.6487E4/,EPSIL/8.85E-12/
      ARCSINH(X)=ALOG(X+SQRT(X*X+1))
      KK=NUM(6)
      M3=NUM(3)
C
C CALCULATE THE CHARGE DEVELOPED AT THE SURFACE (SIGO) AND
C THE BETA PLANE (SIGB) FOR THE GIVEN CONCENTRATION OF SORBED
C SPECIES
C
      SIGO=CONC(KK+2+NP)-CONC(KK+1+NP)
      SIGB=0.
      IF (NUM(3).EQ.3) GO TO 115
      DO 110 I=4,M3
      JJ=ILBLE(I)
      IF (JJ.GT.NUM(1)) JJ=JJ-NUM(12)
      SIGO=SIGO - AH(I)*CONC(KK+I+NP)
      SIGB=SIGB+VJ(JJ)*CONC(KK+I+NP)
  110 CONTINUE
  115 CONTINUE
 1000 FORMAT (4X,5(1PE12.4))
      SIGO=SIGO*1.E6*FARADAY/AREA
      SIGB=SIGB*1.E6*FARADAY/AREA
      SIGD=-SIGO-SIGB
      A1=ARCSINH(ABS(SIGD)/(8.*AVOGAD*EPSIL*BOLTZ*
     1DIELEC*TEMP*1.E7*ELCONC)**0.5)
C
C CALCULATE THE POTENTIALS DEVELOPED BETWEEN THE SURFACE PLANE, BETA
C PLANE, DIFFUSE PLANE, AND THE BULK SOLUTION
C
      PSID=-(SIGD/ABS(SIGD))*(2.*BOLTZ*TEMP/ELEC)*A1
      PSIBETA=PSID-SIGD/C2
      PSIO=PSIBETA+SIGO/C1
      ACONST=ELEC/(BOLTZ*TEMP)
      SURPLN=EXP(-ACONST*PSIO)
      BETAPLN=EXP(-ACONST*PSIBETA)
C
C SITE CONSTRAINT EQUATION FOR ALL THE SITES (SOH, SOH-, SOH2+)
C
```

```
      RESIDUE(1)=SOH-CONC(KK+1+NP)-CONC(KK+2+NP)-CONC(KK+3+NP)
      IF (NUM(3).LT.4) GO TO 120
      DO 125 I=4,M3
      RESIDUE(1)=RESIDUE(1)-CONC(KK+I+NP)
  125 CONTINUE
  120 CONTINUE
C
C  MASS ACTION EQUATION DESCRIBING THE DISSOCIATION OF SOH2+ SITE
C
      RESIDUE(2)=EQCONST(NUM(2)+1)*CONC(KK+2+NP)/SURPLN-CONC(KK+3+NP)*
     1CONC(LNH+NP)
C
C  MASS ACTION EQUATION DESCRIBING THE DISSOCIATION OF THE SOH SITE
C
      RESIDUE(3)=EQCONST(NUM(2)+2)*CONC(KK+3+NP)/SURPLN-CONC(KK+1+NP)*
     1CONC(LNH+NP)
      IF (NUM(3).LT.4) GO TO 126
C
C  MASS ACTION EQUATIONS FOR THE FORMATION OF SITES (SO-SPECIES) OR
C  (SOH2+ -SPECIES)
C
      DO 127 I=4,M3
      JJ=ILBLE(I)
      J2=JJ
      IF (JJ.GT.NUM(1)) J2=JJ-NUM(12)
      QUAN=CONC(KK+I+NP)*(CONC(LNH+NP)*SURPLN)**AH(I)
      DENOM=CONC(JJ+NP)*CONC(KK+3+NP)*BETAPLN**VJ(J2)
      RESIDUE(I)=(DENOM)-QUAN/EQCONST(NUM(2)+I)
  127 CONTINUE
  126 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE RES(CN,CO,BC,BC2,R,NUM,MDIM,LNH,IBND,ITYPE)
C  ************************************************************************
C  CALCULATES THE RESIDUES OF THE TRANSPORT EQUATIONS, THE SITE
C  CONSTRAINT EQUATION, THE MASS ACTION EQUATIONS, AND THE BOUNDARY
C  CONDITIONS. THE BOUNDARY CONDITIONS ARE STORED IN THE ARRAYS BC
C  AND BC2.  IF BOUNDARY CONDITIONS OTHER THAN THE CONCENTRATION AND
C  FLUX CONDITIONS ARE OF INTEREST, THE USER WOULD HAVE TO SUPPLY HOW
C  THE VALUES OF BC AND BC2 WOULD CHANGE.  FOR THE CONCENTRATION BOUNDARY
C  CONDITION AT THE INNER NODE, BC STORES THE TOTAL CONCENTRATION OF A
C  SPECIES IN THE AQUEOUS PHASE AND IN THE FORM OF A PRECIPITATE.  FOR THE
C  FLUX CONDITION AT THIS BOUNDARY, BC STORES THE FLUID VELOCITY TIMES
C  THE TOTAL AQUEOUS PHASE CONCENTRATION OF EACH SPECIES.  FOR THE OUTER
C  BOUNDARY, FOR THE CONCENTRATION CONDITION, BC2 STORES THE BASIS
C  SPECIES CONCENTRATION OF THE INITIAL CONDITIONS, AND FOR THE NO FLUX
C  CONDITION IT IS NOT USED.
C  THE SUBROUTINE IS CALLED FROM BOTH THE MAIN PROGRAM AND THE SUBROUTINE
C  JACOBI.
C  ************************************************************************
      DIMENSION CN(1),CO(1),BC(1),R(MDIM,1),NUM(1),IBND(1),BC2(1)
      LEVEL2,R
      COMMON/AB/VJ(75),AC(75,100),EQCONST(100)
     1,S(25,25),SS(25,25),AH(25),ILBLI(25),ILBLE(25)
      COMMON/NJ/ISORPI(30),ISORPE(30),IION,IEION
      COMMON/AD/X(200),DELT,DOA,DOB,VO,CECNS,H2OK
      COMMON/AC/ELCONC(100)
      NMAX=NUM(14)
      NMAXM=NMAX-1
      M1=NUM(1)
      M2=NUM(2)
      M3=NUM(3)
      M4=NUM(4)
      M5=NUM(5)
      NTOT=NUM(9)
C
C  CALCULATE THE ACTIVITIES OF THE AQUEOUS PHASE SPECIES
C
      CALL ACTIVE(NUM,CN,VJ,AC,ELCONC,75,1,NUM(14))
C
C  ********************************************************
C   INNER BOUNDARY CONDITION SET HERE
C ********************************************************
      N=1
      N1=2
      IF (IBND(1).EQ.1) GO TO 40
C
C  FOR THE CONCENTRATION BOUNDARY CONDITIONS, THE RESIDUES
C  ARE CALCULATED HERE;  ACTUALLY THE RESIDUES WILL
C  ALWAYS BE CLOSE TO ZERO HERE UNLESS BC IS CHANGED BY THE USER;
C  AT A LATER TIME, THIS CALCULATION COULD BE USED TO HAVE A PRECIPITATE
C  DISSOLVE INTO THE GROUNDWATER AS A FUNCTION OF TIME.
C
      DO 35 J=1,M1
      R(J,1)=BC(J)-CN(J)
```

```
      IF (NUM(4).EQ.0) GO TO 15
      DO 10 I=1,M4
   10 R(J,1)=R(J,1)- S(J,I)*CN(NUM(7)+I)
   15 IF (NUM(5).EQ.0) GO TO 25
      DO 20 I=1,M5
      R(J,1)=R(J,1)-SS(J,I)*CN(NUM(8)+I)
   20 CONTINUE
   25 CONTINUE
   35 CONTINUE
      GO TO 45
   40 N1=1
   45 CONTINUE
C
C  CALCULATE THE RESIDUES FOR THE MASS ACTION EQUATIONS
C
      CALL ALGEBRC(NUM,CN,R,1,1,MDIM,ELCONC,LNH,0)
C
C *************************************************************
C  CALCULATION OF CHANGES IN THE POROUS MEDIUM
C **************************************************************
      DO 170 N=N1,NMAXM
      NEVEN=(N-1)*NTOT
      NPLUS=NEVEN+NTOT
      NMINUS=NEVEN-NTOT
      II=0
      IE=3
      DO 140 J=1,M1
      DD=DOA*VO+DOB
      VV=VO
      XNM=X(N-1)
C
C  FOR A FLUX CONDITION AT THE INNER BOUNDARY AND FOR
C  RADIAL FLOW, THE DISPERSION COEFFICIENT AND THE FLUID VELOCITY
C  FOR THE FIRST GRID ARE CALCULATED HERE
C
      IF (N.EQ.1) XNM=-X(1)
      IF (ITYPE.EQ.1) DD=(DOA*VO+DOB)/X(N)
      IF (ITYPE.EQ.1) VV=VO/X(N)
      IF (N.EQ.1) GO TO 50
C
C  CALCULATE THE RESIDUES OF THE TRANSPORT EQUATIONS FOR NODES
C  2 THROUGH NMAX-1 INCLUDING THE CHANGES IN THE BASIS SPECIES
C
      R(J,N)=(CN(NEVEN+J)-CO(NEVEN+J))/DELT-DD*((CN(NPLUS+J)-
     1CN(NEVEN+J))/(X(N+1)-X(N))-(CN(NEVEN+J)-CN(NMINUS+J))
     2/(X(N)-X(N-1)))/(0.5*(X(N+1)-X(N-1)))+VV*(CO(NEVEN+J)-
     3CO(NMINUS+J))/(X(N)-X(N-1))
      GO TO 55
C
C  FOR THE FLUX BOUNDARY CONDITION AT THE FIRST NODE POINT,
C  CALCULATE THE CHANGES IN THE FIRST NODE POINT FOR THE
C  BASIS SPECIES
C
```

```
   50 R(J,1)=(CN(NEVEN+J)-CO(NEVEN+J))/DELT
      R(J,1)=R(J,1)-DD*(CN(NPLUS+J)-CN(NEVEN+J))/((X(2)-X(1))*
     1 0.5*(X(2)-XNM))
       R(J,1)=R(J,1)+(VV*CO(NEVEN+J)-BC(J))/(X(1)-XNM)
   55  CONTINUE
C
C  INCLUDE THE CHANGE IN THE SORPTION OF THE BASIS SPECIES
C  FOR  NODES 2 THRU NMAX-1 OR 1 THRU NMAX-1 DEPENDING ON THE
C  BOUNDARY CONDITIONS; FIRST IS FOR SORPTION VIA ION EXCHANGE
C  NEXT IS FOR ANY SORPTION VIA SURFACE COMPLEXATION
C
      IF (NUM(2).EQ.0) GO TO 60
      IF (ISORPI(J).EQ.0) GO TO 60
      II=II+1
      IP=NUM(1)+II
      R(J,N)=R(J,N)+(CN(NEVEN+IP)-CO(NEVEN+IP))/DELT
   60 CONTINUE
      IF (NUM(3).EQ.0) GO TO 80
      IF (ISORPE(J).EQ.0) GO TO 80
      IF (J.EQ.LNH) GO TO 70
      IE=IE+1
      IP=NUM(6)+IE
      R(J,N)=R(J,N)+(CN(NEVEN+IP)-CO(NEVEN+IP))/DELT
      GO TO 80
   70 IP=NUM(6)
C
C  FOR SORPTION VIA SURFACE COMPLEXATION, NEED TO CONSIDER THE
C  CHANGES IN THE SOH AND SOH2+ SITES
C
      R(J,N)=R(J,N)+2*(CN(NEVEN+IP+2)-CO(NEVEN+IP+2))/DELT
     1   +(CN(NEVEN+IP+3)-CO(NEVEN+IP+3))/DELT
C
C  NEXT INCLUDE CHANGES IN THE COMPLEXES AT THE NODE POINTS;
C  TIME CHANGES, ADVECTION AND DISPERSION
C
   80 IF (NUM(4).EQ.0) GO TO 120
      DO 110 I=1,M4
      IP=NUM(7)+I
       IF (N.EQ.1) GO TO 90
      R(J,N)=R(J,N)+S(J,I)*(CN(NEVEN+IP)-CO(NEVEN+IP))/DELT-S(J,I)*
     1DD*((CN(NPLUS+IP)-CN(NEVEN+IP))/(X(N+1)-X(N))-(CN(NEVEN
     2 +IP)-CN(NMINUS+IP))/(X(N)-X(N-1)))/(0.5*(X(N+1)-X(N-1)))+
     3S(J,I)*VV*(CO(NEVEN+IP)-CO(NMINUS+IP))/(X(N)-X(N-1))
      GO TO 100
   90  CONTINUE
C
C  SPECIAL CASE FOR CONSIDERING THESE LAST CHANGES AT THE FIRST
C  NODE POINT IF FLUX BOUNDARY CONDITION AT THE INNER BOUNDARY
C
       R(J,1)=R(J,1)+S(J,I)*(CN(NEVEN+IP)-CO(NEVEN+IP))/DELT
       R(J,1)=R(J,1)-S(J,I)*DD*(CN(NPLUS+IP)-CN(NEVEN+IP))/((X(2)-X(1))
     1 *0.5*(X(2)-XNM))
        R(J,1)=R(J,1)+S(J,I)*VV*CO(NEVEN+IP)/(X(1)-XNM)
```

```
  100 CONTINUE
C
C  NEED TO ALSO INCLUDE THE CHANGES IN THE SORPTION OF THE COMPLEXES
C  WHETHER VIA ION EXCHANGE OR SURFACE COMPLEXATION
C
      IF (NUM(2).LE.IION) GO TO 105
      IF (ISORPI(J+NUM(1)).EQ.0) GO TO 105
      II=II+1
      IP=NUM(1)+II
      R(J,N)=R(J,N)+S(J,I)*(CN(NEVEN+IP)-CO(NEVEN+IP))/DELT
  105 CONTINUE
      IF (NUM(3).LE.IEION) GO TO 110
      IF (ISORPE(NUM(1)+J).EQ.0) GO TO 110
      IE=IE+1
      IP=NUM(6)+IE
      R(J,N)=R(J,N)+S(J,I)*(CN(NEVEN+IP)-CO(NEVEN+IP))/DELT
  110 CONTINUE
  120 CONTINUE
C
C  INCLUDE THE CHANGES IN THE PRECIPITATES AT A NODE POINT
C
      IF (NUM(5).EQ.0) GO TO 140
      DO 130 I=1,M5
      IP=NUM(8)+I
      R(J,N)=R(J,N)+SS(J,I)*(CN(NEVEN+IP)-CO(NEVEN+IP))/DELT
  130 CONTINUE
  140 CONTINUE
C
C  WHEN WATER DISSOCIATION IS INCLUDED, NEED TO ACTUALLY CALCULATE
C  THE CHANGES FOR THE DUMMY VARIABLE WHICH IS THE CONCENTRATION OF
C  THE H+ ION MINUS THE CONCENTRATION OF THE OH- ION
C
      IF (LNH.NE.0) R(LNH,N)=R(LNH,N)-R(NUM(1),N)
      IF (LNH.NE.0) R(NUM(1),N)=H2OK-AC(LNH,N)*CN(NEVEN+LNH)*
     1AC(NUM(1),N)*CN(NEVEN+NUM(1))
C
C  CALCULATE THE CHANGES IN THE SITE CONSTRAINT, THE MASS ACTION,
C  AND THE SOLUBILITY PRODUCTS AT THE NODE POINTS
C
  170 CONTINUE
c
C
      CALL ALGEBRC(NUM,CN,R,N1,NMAXM,MDIM,ELCONC,LNH,0)
C
C  CALCULATION OF THE CONDITIONS AT THE LAST NODE POINT
C
      N=NMAX
      NEVEN=(N-1)*NTOT
      NMINUS=(N-2)*NTOT
      IF (IBND(2).EQ.0) GO TO 210
C
C  NO FLUX CONDITION
C
```

```
      DO 200 J=1,M1
      R(J,N)=(CN(NEVEN+J)-CN(NMINUS+J))/(X(NMAX)-X(NMAX-1))
  200 CONTINUE
      GO TO 220
  210 DO 215 J=1,M1
C
C  CONCENTRATION BOUNDARY CONDITION
C
  215 R(J,N)=CN(NEVEN+J)-BC2(J)
  220 CONTINUE
      IF (LNH.NE.0) R(LNH,N)=R(LNH,N)-R(NUM(1),N)
      IF (LNH.NE.0) R(NUM(1),N)=H2OK-AC(LNH,N)*CN(NEVEN+LNH)*
     1AC(NUM(1),N)*CN(NEVEN+NUM(1))
C
C  CALCULATE THE RESIDUES FOR THE ALGEBRIC EQUATIONS FOR THE
C  CONDITIONS AT THE LAST NODE POINT
C
      CALL ALGEBRC(NUM,CN,R,NMAX,NMAX,MDIM,ELCONC,LNH,0)
      RETURN
      END
```

```
      SUBROUTINE RESEQ(WCONST,CM,INDEX1,INDEX2,RE,N,CTOT,MDIM,
     1 NUM,LCHRG,LNH,NSOL)
C     *******************************************************
C     RESIDUES OF THE EQUILIBRIUM EQUATIONS; IT IS CALLED FROM
C     THE SUBROUTINES EQLIB AND JACOB2
C    ********************************************************
      DIMENSION WCONST(1),CM(1),INDEX1(1),INDEX2(1),RE(1),NUM(1)
      COMMON/AC/ELCONC(100)
      COMMON/LCM1/R(25,100)
      LEVEL2,R
      COMMON/AB/VJ(75),AC(75,100),EQCONST(100),
     1S(25,25),SS(25,25),AH(25),ILBLI(25),ILBLE(25)
      COMMON/NJ/ISORPI(30),ISORPE(30),IION,IEION
      COMMON/AD/X(200),DELT,DOA,DOB,VO,CECNS,H2OK
      COMMON/SPEC/LEACH1(5),NB,PINI(5)
      NTOT=NUM(8)
      II=0
      IE=3
      M1=NUM(1)
      M4=NUM(4)
      M5=NUM(5)
      M2=NUM(2)
      M3=NUM(3)
C
C  CALCULATE THE ACTIVITES OF THE SPECIES IN THE AQUEOUS PHASE
C
      CALL ACTIVE(NUM,CM,V,AC,ELCONC,75,N,N)
C
C  THE FIRST SET OF EQUATIONS ARE SETTING THE CONDITIONS TO WHAT
C  WERE SPECIFIED FOR EACH SPECIES;
C
      DO 60 J=1,M1
      R(J,N)=WCONST(J)-CM(J)
      IF (ISORPI(J).EQ.0) GO TO 30
      II=II+1
C
C  IF INDEX2 .NE. 0 THEN THE AMOUNT OF THE SPECIES WHICH IS SORBED
C  ONTO THE SOLID MATRIX IS NOT INCLUDED IN THE SPECIFIED AMOUNT OF
C  THIS SPECIES
C
      IF (INDEX2(J).NE.0) GO TO 30
      R(J,N)=R(J,N)-CM(NUM(1)+II)
   30 CONTINUE
      IF (ISORPE(J).EQ.0) GO TO 35
      IE=IE+1
      IEJ=IE
      IF (J.EQ.LNH) IEJ=3
      IF (J.EQ.LNH) IE=IE-1
      IF (INDEX2(J).NE.0) GO TO 35
      R(J,N)=R(J,N)-CM(NUM(6)+IEJ)
      IF (J.EQ.LNH) R(J,N)=R(J,N)-2*CM(NUM(6)+2)
   35 CONTINUE
      IF (NUM(4).EQ.0) GO TO 41
```

```
      ICMPLX=IION
      IECMPLX=IEION
C
C  IF INDEX2 = 1 THEN ONLY THE CONCENTRATION OF THE BASIS SPECIES
C  ITSELF IS BEING GIVEN FOR THIS SPECIES
C
      IF (INDEX2(J).EQ.1) GO TO 41
      DO 40 I=1,M4
      KK=I+NUM(1)
      IF (ISORPI(KK).EQ.0) GO TO 37
      ICMPLX=ICMPLX+1
      IF (INDEX2(J).NE.0) GO TO 37
      R(J,N)=R(J,N)-S(J,I)*CM(NUM(1)+ICMPLX)
   37 CONTINUE
      IF (ISORPE(KK).EQ.0) GO TO 38
      IECMPLX=IECMPLX+1
      IF (INDEX2(J).NE.0) GO TO 38
      R(J,N)=R(J,N)-S(J,I)*CM(NUM(6)+IECMPLX)
   38 CONTINUE
   40 R(J,N)=R(J,N)-S(J,I)*CM(NUM(7)+I)
   41 IF (NUM(5).EQ.0) GO TO 60
C
C  INDEX2 MUST = 3 FOR THE CONCENTRATION OF THE PRECIPITATE
C  TO BE INCLUDED IN THE SPECIFICATION OF THAT SPECIES;  HOWEVER
C  IF THE SPECIES MAY FORM IN A PRECIPITATE, THAN INDEX2 =3 INSTEAD
C  OF INDEX2 = 2 SHOULD BE USED BECAUSE OF THE WAY THE EQUATIONS ARE
C  SET UP AT PRESENT
C
      IF ((INDEX2(J).EQ.1).OR.(INDEX2(J).EQ.2)) GO TO 60
      DO 50 I=1,M5
   50 R(J,N)=R(J,N)-INDEX1(I)*SS(J,I)*CM(NUM(8)+I)
 1000 FORMAT (10X,I5,10X,10(4(1PE12.4),/))
   60 CONTINUE
      IF (LNH.EQ.0) GO TO 72
C
C  THE DISSOCIATION OF WATER IS INCLUDED IF IT HAS BEEN SPECIFIED
C
      R(NUM(1),N)=H2OK-CM(LNH)*AC(LNH,N)*CM(NUM(1))*AC(NUM(1),N)
   72 CONTINUE
C
C  IT IS POSSIBLE TO USE A CHARGE BALANCE TO SPECIFY ONE OF THE
C  CONCENTRATIONS
C
      IF (LCHRG.EQ.0) GO TO 77
      R(LCHRG,N)=CTOT
      DO 75 J=1,M1
   75 R(LCHRG,N)=R(LCHRG,N)-CM(J)*VJ(J)
      IF (NUM(4).EQ.0) GO TO 77
      DO 76 I=1,M4
   76 R(LCHRG,N)=R(LCHRG,N)-CM(NUM(7)+I)*VJ(NUM(1)+I)
C
C  THIS IS FOR A SPECIAL CONDITION OF LEACHING OF A SOLID SO THAT
C  THE INCREASE IN THE AMOUNT OF THE SPECIES IN THE AQUEOUS PHASE
```

```
C  MAKING UP THE SOLID IS IN EQUAL AMOUNTS; OCCURS WHERE A SOLID HAS
C  BEEN PLACED IN CONTACT WITH THE GROUNDWATER.  IT CAN ONLY OCCUR
C  AT THE FIRST NODE AT PRESENT
C
   77 IF ((N.NE.NB).OR.(LEACH1(1).EQ.0)) GO TO 80
      R(LEACH1(2),N)=WCONST(LEACH1(2))-CM(NUM(8)+LEACH1(1))
      INDEX1(LEACH1(1))=1
      ILEACH=3
      J1=LEACH1(2)+1
      DO 78 J=J1,M1
      IF (J.NE.LEACH1(ILEACH)) GO TO 78
      R(LEACH1(ILEACH),N)=WCONST(LEACH1(ILEACH))-R(LEACH1(ILEACH),N)-
     1 PINI(ILEACH-1)-(WCONST(LEACH1(2))-R(LEACH1(2),N)-
     2 PINI(1))
      ILEACH=ILEACH+1
   78 CONTINUE
   80 CONTINUE
C
C  CALCULATION OF THE RESIDUES OF THE SITE CONSTRAINT, AND THE
C  MASS ACTION EQUATIONS FOR SORPTION AND FORMATION OF COMPLEXES
C  IN THE AQUEOUS PHASE
C
      CALL ALGEBRC(NUM,CM,R,N,N,25,ELCONC,LNH,1)
C
      IF (NUM(5).EQ.0) GO TO 90
C
C  FOR ANY PRECIPITATES, INCLUDE THE RESIDUES FOR THE SOLUBILITY PRODUCT
C  EQUATIONS
C
      CALL RESSOL(INDEX1,CM,NUM,NTOT,R,N,MDIM)
   90 NNN=NTOT+NSOL
      DO 100 I=1,nnn
  100 RE(I)= R(I,N)
      RETURN
      END
```

```
      SUBROUTINE RESSOL(INDEX1,CM,NUM,NTOT,R,N,MDIM)
C ************************************************************
C RESIDUES FOR THE SOLUBILITY CONSTRAINT EQUATIONS; IT IS
C ONLY USED FOR THE INITIAL EQUILIBRIUM DISTRIBUION OF SPECIES
C CALCULATION; THE SUBROUTINE RES ALSO HAS THE SOLUBILITY
C PRODUCT EQUATIONS FOR THE TIME CHANGES AT THE NODES AFTER
C A PRECIPITATE HAS FORMED
C ************************************************************
      DIMENSION CM(1),INDEX1(1),R(MDIM,1),NUM(12)
      LEVEL2,R
      COMMON/AB/VJ(75),AC(75,100),EQCONST(100),
     1S(25,25),SS(25,25),AH(25)
     2,ILBLI(25),ILBLE(25)
      INDEX=0
      M5=NUM(5)
      M1=NUM(1)
      DO 10 I=1,M5
      AKSOL=1.
      IF (INDEX1(I).EQ.0) GO TO 10
      INDEX=INDEX+1
      DO 20 J=1,M1
      IF (SS(J,I).LT.1.E-15) GO TO 20
      AKSOL=AKSOL*(AC(J,N)*CM(J))**SS(J,I)
   20 CONTINUE
      R(NTOT+INDEX,N)=AKSOL-EQCONST(NUM(12)+NUM(4)+I)
   10 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE SETUP(XMAX,DNO,AK,NMAX,ITYPE,IBND,RW)
C ******************************************************************
C CALCULATES THE GRID BASED ON AN EXPONENTIAL LAW; IF DNO IS SET
C EQUAL TO 0, A UNIFORM GRID IS CALCULATED. AT THE INNER BOUNDARY,
C A CONSTANT CONCENTRATION OR A CONSTANT FLUX CAN BE IMPOSED AT
C AT X=0 FOR THE ONE-DIMENSIONAL CASE. FOR THE RADIAL CASE, THE
C THE CONCENTRATION BOUNDARY IS IMPOSED AT R=0 AND THE FLUX BOUNDARY
C IS IMPOSED AT RW.  AT THE OUTER BOUNDARY, THE CONCENTRATION BOUNDARY
C IS IMPOSED AT THE LAST GRID POINT, OR A NO-FLUX CAN BE IMPOSED
C HALF WAY BETWEEN THE LAST AND THE NEXT TO LAST GRID POINT.  THE
C DISTANCE OF THE LAST GRID POINT FROM THE FIRST GRID POINT IS NOT
C EXACTLY XMAX FOR THE FLUX BOUNDARY CONDITION AT THE INNER BOUNDARY.
C ******************************************************************
      DIMENSION IBND(1)
      COMMON/AD/X(200),DELT,DOA,DOB,VO,CECNS,H2OK
C
      DN=1./(NMAX-1)
      X(1)=0.
      I1=2
      IF ((ITYPE.EQ.0).AND.(IBND(1).EQ.1)) I1=1
      IF ((ITYPE.EQ.1).AND.(IBND(1).EQ.1)) X(1)=2.*RW
      DO 10 I=I1,NMAX
      IP=I-1
      IF ((ITYPE.EQ.0).AND.(IBND(1).EQ.1)) IP=I
C
C CALCULATION FOR UNIFORM GRID
C
      IF (DNO.LT.1.E-16) X(I)=XMAX*DN*IP
      IF (DNO.LT.1.E-16) GO TO 10
C
C CALCULATION FOR VARIABLE GRID
C
      X(I) = XMAX*(AK**((IP)*DN/DNO)-1.)/(AK**(1./DNO)-1.)
     1 +X(1)
   10 CONTINUE
      IF ((IBND(1).EQ.0).OR.(ITYPE.EQ.1)) GO TO 20
C
C FOR FLUX BOUNDARY CONDITION AT INNER BOUNDARY MOVE GRID
C SO THAT IT IS IMPOSED AT X=0 AND NOT AT THE GIRD POINT ITSELF
C
      DX1=X(1)/2.
      DO 15 I=1,NMAX
   15 X(I)=X(I)-DX1
   20 WRITE(6,190) (X(N),N=1,NMAX)
  190 FORMAT(/55X# ** SPATIAL GRID **#/,/,(# #10G13.4))
      RETURN
      END
```

```
      SUBROUTINE SIMQ(Z,Y,N,MDIM)
C    ****************************************************
C    INVERSION OF A MATRIX; IT IS USED IN CALCULATING
C    AN EQUILIBRIUM DISTRIBUTION OF SPECIES SUCH AS
C    IN THE INITIAL CONDITIONS AND THE BOUNDARY CONDITIONS.
C    THE JACOBIAN IS STORED IN Z WHILE THE RESIDUES ARE IN
C    Y.  THIS  SUBROUTINE SOLVES THE EQUATION ZX=Y FOR X
C    ****************************************************
      DIMENSION Z(MDIM,1),Y(1)
C     PROVISION FOR N=1
      IF(N.NE.1) GO TO 50
      Y(1)=Y(1)/Z(1,1)
      RETURN
   50 CONTINUE
C     ELEMENT OF ELIMINATION
      N1=N-1
      DO 10 M=1,N1
      ZMAX=0.
      IMAX=0
C     FIND MAX OF COLUMN
      DO 20 I=M,N
      IF(ABS(Z(I,M)).LE.ZMAX) GO TO 20
      IMAX=I
      ZMAX=ABS(Z(I,M))
   20 CONTINUE
C     ERROR RETURN
      IF(IMAX.NE.0) GO TO 30
      WRITE(6,1000)
      WRITE(6,900) I,M
      WRITE (6,990) (Z(I,M),I=1,N)
   30 CONTINUE
C     ROW INTERCHANGE
      IF(IMAX.EQ.M) GO TO 35
      V=Y(M)
      Y(M)=Y(IMAX)
      Y(IMAX)=V
      DO 40 J=M,N
      V=Z(M,J)
      Z(M,J)=Z(IMAX,J)
      Z(IMAX,J)=V
   40 CONTINUE
   35 CONTINUE
C     DIAGONALIZE
      M1=M+1
      DO 70 I=M1,N
      V=Z(I,M)/Z(M,M)
      Y(I)=Y(I)-V*Y(M)
      DO 70 J=M,N
      Z(I,J)=Z(I,J)-V*Z(M,J)
   70 CONTINUE
   10 CONTINUE
C     BACK SUBSTITUTE
      Y(N)=Y(N)/Z(N,N)
```

```
      N1=N-1
      DO 100 K=1,N1
      I=N-K
      I1=I+1
      DO 90 J=I1,N
   90 Y(I)=Y(I)-Y(J)*Z(I,J)
  100 Y(I)=Y(I)/Z(I,I)
      RETURN
  900 FORMAT (4X,2I10)
  990 FORMAT (4X,5(19E12.4))
 1000 FORMAT(# SINGULAR JACOBIAN MATRIX#)
      END
```

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