DISSERTATION

FINITE ELEMENT 2-D TRANSPORT MODEL OF

GROUNDWATER RESTORATION FOR IN SITU

SOLUTION MINING OF URANIUM

Submitted by

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WE HEREBY RECOMMEND THAT THE THESIS PREPARED UNDER OUR SUPERVISION

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for In Situ Solution Mining of Uranium

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ABSTRACT

Developing technologies such as in situ solution mining of uranium represent a new, more complex solute transport problem in site restoration than traditional transport problems such as contaminant migration. The method consists of injecting through wells a lixiviant into the host aquifer containing the uranium. The uranium is preferentially dissolved and the uranium-bearing groundwater is recovered through pumping wells. The environmental advantages of solution mining over conventional mining techniques are several; however, it has the disadvantage of potentially contaminating the groundwater system. A computer model of groundwater restoration for the in situ solution mining of uranium is developed and documented. The model is based on the Galerkin-finite element method using triangular elements and linear shape functions.

The computer model calculates the dual changes in concentration of two reacting solutes subject to binary cation exchange in flowing groundwater. This cation exchange process is important in the groundwater restoration of solution mining. Both the concentration in solution and the concentration adsorbed on the solid aquifer material are calculated for both solutes at specified places and times due to the process of convective transport, hydrodynamic dispersion, mixing from fluid sources and cation exchange. No other reactions are assumed which would affect the solution concentrations. The model also has the capacity to simulate conservative solute transport. A complete documentation of the computer model and a detailed description of the numerical solution of both the groundwater flow equation and the solute-transport equations are presented.

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The model was successfully applied to an actual field problem of ammonium restoration for a pilot scale uranium solution mining operation in northeast Colorado near the town of Grover. The computer model is offered as a basic working tool that should be readily adaptable to many other field problems. The model should have wide applicability by regulating agencies, mining companies and others concerned with groundwater restoration for in situ solution mining.

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CHAPTER I

INTRODUCTION

1.1 Description of the Problem

Solute transport problems in groundwater are recognized as becoming increasingly more common and increasingly more complex. Previous evaluation of transport problems have been concerned with contaminant migration away from waste disposal sites and with determination of the fate of various chemical constituents in the groundwater. More commonly only conservative transport problems have been considered. Developing technologies such as in situ solution mining represent a new, more complex contaminant transport problem in site restoration.

In situ solution mining is a relatively new technology that is being used with increased frequency throughout the mining industry. There are numerous environmental advantages of solution mining over conventional uranium mining techniques such as open pit or underground. With solution mining there is minimal surface disturbance, essentially no tailings to dispose and no dewatering of the aquifer. However, in situ solution mining has the disadvantage of potentially contaminating the groundwater system.

In situ solution mining of uranium consists of injecting through wells a lixiviant (consisting of a leaching agent and an oxidizing agent) into the sandstone formation which contains the uranium deposits. The uranium ore is preferentially dissolved from the host rock and the uranium-bearing groundwater is recovered through pumping wells. Ammonium bicarbonate is the most commonly used leaching agent. During mining, the groundwater is contaminated with high levels of many

chemical constituents including ammonium. Much concern has been expressed on the relatively high concentration of ammonium immediately following mining.

After mining, restoration of the contaminated aquifer is required. In the normal restoration procedure the contaminated groundwater is pumped from the aquifer and replaced by groundwater entering the mined area from the surrounding unaffected aquifer; or alternatively the contaminated groundwater is pumped from the aquifer, purified and possibly fortified with eluting chemicals and then reinjected. Improper or incomplete restoration may result in contaminated groundwater being left in the aquifer. When an ammonium-bicarbonate based lixiviant is used, the ammonium is adsorbed on the clays in the aquifer during mining when it is in high concentrations in the groundwater. Later, during the restoration process when ammonium concentrations in the groundwater are lower, the ammonium is released back to the groundwater. The desorption of the ammonium occurs slowly and may result in significant residual ammonium concentrations adsorbed in the aquifer after the restoration process was thought to be completed. Few studies have been conducted to determine the extent to which solution mining does have impact on the groundwater system.

Approximately 90% of the U.S. uranium reserves occur in sandstone formations. Since these sandstone formations often have significant permeability the uranium in them is particularly amenable to solution-mining. At present, in situ mining of uranium has been tested on pilot scale operations in the states of Texas, Wyoming, Colorado, New Mexico and Utah, but only Texas has thus far had commercial scale

operations. Recently, in the State of Colorado, permission was given to begin a commercial scale operation in that state. Expectations are that in situ solution mining will become increasingly important in meeting our future uranium energy needs. If solution mining is to meet these expectations as a major mining method, then it is important to evaluate the environmental impact of the method on the groundwater system.

1.2 Objective

At present monitoring is the only method available to assess the extent of groundwater restoration. With monitoring the groundwater can only be sampled for contamination at a few selected points, namely at the monitoring wells and also at the production and recovery wells in the leach field. Other test holes could also be drilled for sampling to aid in determination of the extent of groundwater contamination, but at much additional expense. The extent of groundwater contamination beyond these few points can only be surmised. Improper or incomplete groundwater restoration could result in undetected areas of contaminated groundwater remaining in the aquifer.

There exists a need by regulating agencies, mining companies and others for a predictive tool that can be used to evaluate alternative restoration strategies for complex groundwater flow and solute transport problems. The usefulness of such a predictive tool for planning purposes would include assessment of the trade off benefits between differing levels of restoration efforts versus desired restorative objectives, restoration time requirements, total volumes of water

required for restoration, effects of varying recirculation rates, effects of varying eluting chemical concentrations, etc.

The objectives of this investigation are:

1) Develop a computer model capable of simulating the groundwater restoration for the in situ solution mining of uranium. This computer model could be used as a basic working tool and should have wide applicability by both regulating agencies and mining companies for prediction and planning purposes.

2) Demonstrate application of this computer model to an actual field problem of ammonium restoration for a pilot scale uranium solution mining operation in northeast Colorado near the town of Grover. The model should be readily adaptable to many other field problems.

1.3 Method of Investigation

This report describes a mathematical treatment of the site restoration of contaminants subject to adsorption and exchange on the porous media. The adsorption reaction is treated as an equilibrium controlled reversible binary cation exchange process. This requires that both chemical species involved in the exchange process be followed as they flow with the groundwater through the porous media. The mathematical formulation of the problem includes one equation describing groundwater flow plus two additional equations for solute transport (one equation for each of the solute species involved in the binary cation exchange). The transport equations are coupled through two additional equations which describe the cation exchange process. In a leap-frog fashion

the partial differential equation for groundwater flow is solved for
the head distribution in the aquifer and the two coupled partial differ-
ential equations for solute transport are solved simultaneously for the
dual changes in dissolved concentration for both solute species. The
adsorbed concentration for both exchanging solutes is then also
obtained.

1.4 Previous investigations

The general mathematical treatment for cation exchange used in
this dissertation was originally formulated by Rubin and James (1973)
for one-dimensional groundwater flow with constant groundwater
velocity. The method has received little attention until now because
of much simpler methods such as the Freundlich Isotherm which is
applicable in general to contaminant migration problems.

Several other studies have also taken somewhat similar approaches
to the cation exchange problem. Lai and Jurinak (1971) presented a
finite difference technique for the binary cation exchange problem with
constant anion concentration. Smith (1978) later extended this method
to allow for a changing anion concentration. Based on these previous
works, Humenick, Schechter and Turk (1978) applied the method to the
problem of ammonium migration and elution. It can be easily shown that
the above studies are a slightly more restrictive formulation of the
more general method presented by Rubin and James. In all of these
studies the problem of cation adsorption and exchange was considered
only for the case of one-dimensional groundwater flow with constant
groundwater velocity without mixing of fluid sources.

More recent studies of the cation exchange problem have attempted
to consider two-dimensional groundwater flow. An interesting approach
was used by Bommer (1979). In this study a streamline-concentration
balance was performed. In essence, the procedure consisted of genera-
ting a family of streamlines for the groundwater flow field. A mass
balance was then performed along these streamlines. A major dis-
advantage of the study was that it only considered an isotropic
homogeneous aquifer. Schwartz (1975) considered the case of cation
exchange coupled with radioactive decay. In the latter study the
method of characteristics solution was used for two-dimensional flow
in a vertical cross-section.

Very recently Charbeneau (1981) has considered adsorption and cation
exchange for the one-dimensional case without dispersion. The method
of characteristics solution was used in this study and applied to the
case of groundwater restoration for one-dimensional radial flow to a
well in a circular mining site. The method has the advantage of being
very simple. The major disadvantage of the method is that it only
provides "desk top" answers and would not probably be applicable to
complex flow and transport problems.

The method of Rubin and James is in this dissertation extended to two-
dimensions and coupled with the solution of the partial differential
equation for groundwater flow. Changes in dissolved concentration are
considered for convective transport, hydrodynamic dispersion, fluid
sources and cation exchange reactions. Only binary cation exchange is
considered but the method can be easily extended for multiple exchange
reactions (Rubin and James, 1973). The Galerkin-finite element was

used to solve the resulting partial differential equations for ground-water flow and solute transport.

Before proceeding to a detailed description of the mathematical treatment of this problem a discussion of the fundamentals of cation exchange reactions will be given. The interested reader is referred to Appendix A for a discussion of in situ solution mining of uranium.

CHAPTER II

CATION EXCHANGE

The exchange of cations adsorbed on a porous medium with cations contained in water flowing through the porous medium is generally referred to as cation exchange. This exchange process requires that a cation in solution be adsorbed on the porous medium and simultaneously an adsorbed cation be released from the porous medium into solution. This cation exchange process is important in contaminant migration because it may retard the movement of contaminants which are in solution in the groundwater. It is also a major concern in in situ solution mining because it results in contaminants being accumulated during the mining process)on the porous medium when the contaminants are in high concentrations in the groundwater. Later, during the restoration process when contaminant concentrations in the groundwater are lower, the contaminants are released back to the groundwater. This cation exchange process must be considered in the proper restoration of the groundwater.

The cation exchange process is of a particular concern in in situ solution mining when either an ammonium bicarbonate or sulfuric acid based lixiviant is used (see Appendix A). With ammonium bicarbonate, the ammonium ion (NH_4^+) is adsorbed. The ammonium ion is not particularly harmful and humans consume large amounts of ammonium daily. However, under an oxidizing environment and in the presence of certain nitrifying bacteria, the ammonium is converted to nitrate (NO_3). Large amounts of nitrate are known to be harmful to humans. The mobility of ammonium in groundwater systems is low because of this cation exchange process in which the ammonium is adsorbed onto the porous medium. However, if the

ammonium is converted to nitrate, then the mobility is increased significantly.

With sulfuric acid, the hydrogen ion (H^+) is adsorbed onto the porous medium. Later, if the groundwater is not properly restored, hydrogen is released back to the groundwater, resulting in low pH (acidic) groundwater.

2.1 Cation Exchange Capacity

The exchange capability of a porous medium is given as the cation exchange capacity (CEC), reported as milliequivalents per 100 grams (meq/100g) of sample. The cation exchange capacity is a measure of the number of exchange sites that are available. The exchange sites occur on the surface of the individual particles comprising the porous medium. The CEC varies significantly for different types of porous medium. In natural groundwater systems, the geologic materials that account for most of the CEC are the clay minerals, especially the montmorillonites and illites. The process of cation exchange in clays is very complicated and only partly understood. The two most important structural characteristics of the clay mineral that account for the very high CEC are: (1) Broken bonds located on the edges and surfaces of the clay particles, and (2) isomorphous substitution (substitution between cations of unequal valence within the clay mineral lattice, e.g. substitution of Al^{+3} for Si^{+4}). Both of these structural characteristics result in an unbalanced negative charge on the surface or between the lattices of the clay mineral which is neutralized by cations in the surrounding solution. Because this charge imbalance on the porous medium is negative, the anions in solution in the groundwater are unaffected by this exchange process.

Charges resulting from isomorphous substitution are much larger than those due to broken bonds. Therefore, clay minerals such as montmorillonite in which most of their charges are from isomorphous replacement have very large CEC and clay minerals such as Kaolinite in which most of their charges are from broken bonds have a much smaller CEC. Since the charges from isomorphous substitution are within the clay mineral lattice, physical changes in the clay mineral particle do not affect the number of isomorphous substitution exchange sites but these sites can be blocked and thus clays such as montmorillonite are subject to fixation. Broken bond charges are located on the surface of the clay particle and physical differences in the clay mineral particles, such as a decrease in grain size and a resulting increase in surface area, would in this case increase the number of broken bond exchange sites and thus the CEC of clays such as Kaolinite increase as the particle size decreases.

The total sites availabel in a given porous medium for cation exchange is constant. These cation exchange sites must always be filled. This insures electroneutrality. Thus, to remove one cation, another cation must replace it. A solution of distilled water cannot be used to remove adsorbed cations. A few would be displaced by free hydrogen ions in the water but stripping of the adsorbed cation from the clay would be completed much more rapidly if a solution containing a high concentration of replacement cations were used.

The CEC of selected clay minerals is given in Table 1. Compared to the exchange capacity of most clays the exchange capacity of other constituents in the porous medium is very low. Carroll (1959 reports

TABLE 1. -- Cation Exchange Capacity of Clay Minerals
(Source: Carroll, 1959)

Clay Mineral	Cation Exchange Capacity meq/100g
Kaolinite	3-15
Halloysite ($2H_2O$)	5-10
Halloysite ($4H_2O$)	40-50
Montmorillonite group	70-100*
"Illites" (hydrous micas)	10-40
Vermiculite	100-150
Chlorite	10-40?
Glauconite	11-20+
Palygorskite group	20-30
Allophone	≈70

*Certain members may have a much lower exchange capacity

that even for fine-grained minerals which would have a large surface area, the CEC is about 1 to 3 meq/100g. Therefore, the CEC of a porous medium is largely determined by the amount of clay contained in the porous medium.

2.2 Affinity for Cation Exchange

While the CEC of a porous medium is necessary to determine the magnitude of the cation exchange reaction, many other factors affect this process. The affinity for cation exchange varies considerably between different cations. In general, the affinity for adsorption onto the porous medium increases for a cation with an increase in the valence and in the atomic weight as shown below (Carrol, 1959 or Grim, 1968)

$$Ca^{++} > Mg^{++} > H^{+} > NH_4^{+} > K^{+} > Na^{+} \qquad (1)$$

Several important factors affect this relationship. The first factor is the ionic strength of the solution. The ionic strength of the solution has little effect on the preference for exchange when the cations are of the same valence. However, for cations of different valences, the preference for adsorption for the cation with the higher valence decreases as the ionic strength of the solution increases.

A second factor, termed fixation, is caused by a normally exchangeable cation being held in a nonremovable state by the porous medium. Fixation only occurs at interlayer exchange sites whose charges are from isomorphous substitution and occurs when cations, such as sodium, calcium, and magnesium that expand the clay mineral lattice, are

replaced by either ammonium or potassium which cause the lattice to contract. Since both potassium and ammonium have large radii, the lattice contraction is sufficient to trap them inside the clay particle. This indicates that in solution mining, if montmorillonite is present, the restoration process may be slow and incomplete, if an ammonium bicarbonate based lixiviant is used.

Another factor that affects the affinity of cations for exchange is pH. It has been shown that hydrogen ions have a preference for broken-bond sites and that the hydrogen ion is more firmly held than other monovalent ions. The potential exists that other cations may have preferences for different types of exchange sites.

The assumption is made throughout this study that the process of cation exchange is an entirely reversible process and that the CEC of a porous medium is a constant.

2.3 Adsorption Isotherm

The relative proportion of the exchange sites filled by each cation in the exchange process can be expressed using an adsorption or exchange isotherm. The adsorption isotherm is a plot of the relative concentration in solution for a given cation, expressed as a ratio of dissolved concentration C to the total solution concentration Co, versus the relative adsorbed concentration, expressed as a ratio of the adsorbed concentration $\overline{C}$ to the cation exchange capacity CEC. An example of an adsorption isotherm is shown on Figure 1. The adsorption isotherm is experimentally determined, maintaining a constant total solution concentration and composition. Different adsorption isotherms are
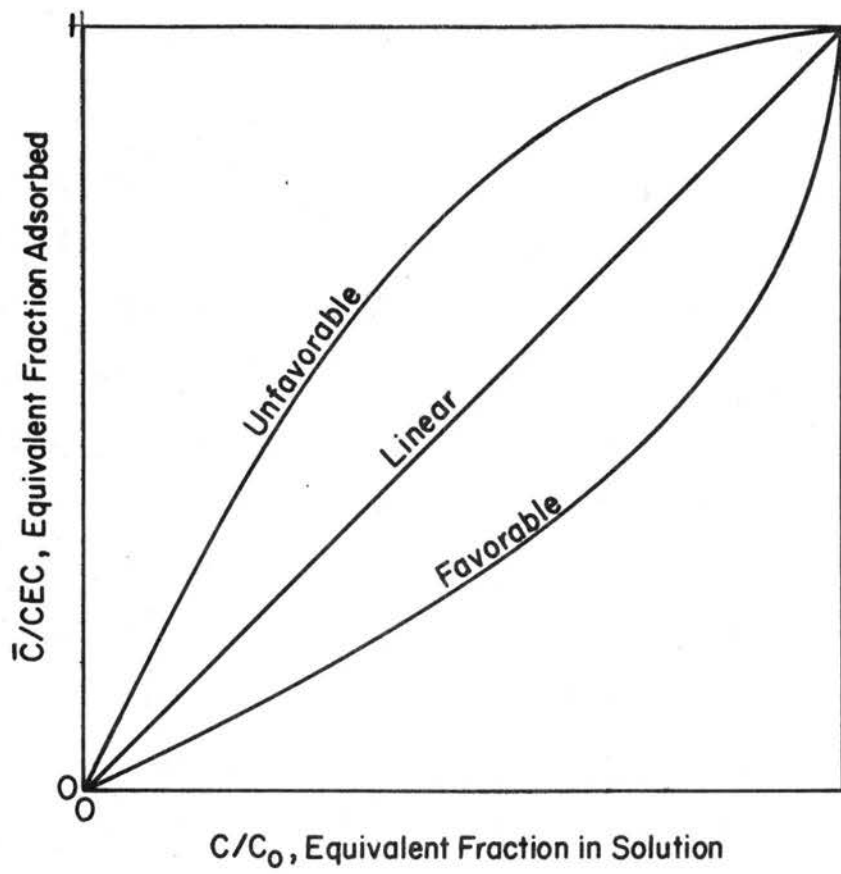
Figure 1. -- Adsorption isotherm.

obtained for each chemical species. In addition, an infinite set of adsorption isotherms are obtained depending on the nature of the porous medium, the total solution concentration and the solution composition (i.e. which competing cations are present in the solution).

Two types of isotherms often encountered in cation exchange are shown on Figure 1. The concave upward curve is called an unfavorable isotherm and the convex upward curve is called a favorable isotherm (Perry, 1963). The unfavorable isotherm describes the exchange of a preferentially adsorbed cation like calcium by a cation having less affinity for adsorption like sodium. The favorable isotherm describes the reverse exchange. Straight line isotherms comprise an intermediate class. Complex isotherms are possible that include both favorable and unfavorable parts.

Favorable and unfavorable adsorption isotherms result in different rates of movement and different concentration profiles in the transport of chemical constituents through the porous medium. All other factors being the same, the rate of movement through the porous medium for a chemical constituent described by an unfavorable adsorption isotherm is less than for a favorable adsorption isotherm. In essence, more of the chemical constituent is adsorbed for the unfavorable isotherm than for the favorable isotherm, which retards the movement of the more highly adsorbed constituent relative to the lesser adsorbed constituent.

For the favorable isotherm, higher concentrations will advance faster than lower concentrations which result in a steepening of the concentration profile at the exchange front (Reiniger and Bolt, 1972).

This steepening is called the self-sharpening tendency of the favorable isotherm. This self-sharpening tendency is normally balanced by the flattening effects of hydrodynamic dispersion. However, for the favorable isotherm, the concentration profile at the exchange front will be steeper than for an unfavorable isotherm.

2.4 Cation Exchange Equations

Numerous equations have been developed to quantitatively describe the cation exchange process. These equations have been classified by Grim (1968) as: (1) Empirical equations based on adsorption isotherms; (2) Kinetic-Theory equations; and (3) Mass-action (thermodynamic) equations. Regardless of the approach used, most of the equations assume the following two premises: (1) the CEC is a constant and represents a finite limit to the quantity that can be adsorbed and (2) the cation exchange reaction occurs very rapidly relative to the flow of water through the porous medium and local equilibrium conditions are assumed to apply.

2.4.1 Empirical Equations

The two most commonly used empirical equations are the Freundlich Isotherm and the Langmuir Isotherm.

2.4.1.1 Freundlich Isotherm

The Freundlich Isotherm was one of the earliest attempts to quantify the adsorption process (originally formulated in 1909) but is still widely used today mainly because of its mathematical simplicity. It was

originally for the adsorption of a gas by a solid but has been widely adapted to the adsorption of ions in solution by a solid as (Freeze and Cherry, 1979)

$$\overline{C} = K_d C^\alpha \qquad (2)$$

where $\overline{C}$ is the adsorbed concentration, C is the dissolved concentration, and K_d (commonly called the distribution coefficient) and α are constants which are determined from the best fit to an experimentally determined adsorption isotherm. If $\alpha = 1$, then equation (2) is called the linear adsorption isotherm. Adamson (1976) has derived the Freundlich Isotherm from theoretical considerations but basically the equation is an empirical one.

The Freundlich Isotherm has been widely criticized because it does not predict a maximum adsorption value but with appropriate constraints over a limited range of concentration it yields fairly reliable results. The Freundlich Isotherm has been used extensively in groundwater for contaminant migration problems.

2.4.1.2 Langmuir Isotherm

The Langmuir Isotherm was also originally formulated for adsorption of a gas by a solid (Langmuir, 1918) but with redefinition of the appropriate terms has been used to express the adsorption of cations in solution by a solid (Kelley, 1948)

$$\overline{C} = \frac{\overline{C}_m K C}{1 + K C} \qquad (3)$$

where $\overline{C}$ = adsorbed concentration, $\overline{C}_m$ = maximum adsorbed concentration (i.e. concentration when all of the exchange sites are filled by the chemical species under consideration), C = dissolved concentration and K = constant. The Langmuir Isotherm has theoretical justification also in that it can be derived from Kinetic considerations (Smith, 1970 or Adamson, 1976) or from statistical thermodynamical considerations (Adamson, 1976). The important assumptions of the Langmuir Isotherm are (Smith, 1970): (1) homogeneous solid surface (i.e. the solid surface has a uniform activity for adsorption, (2) no interaction between adsorbed molecules, (3) all adsorption occurs by the same mechanism and, (4) the extent of adsorption is less than one complete monomolecular layer on the surface. The Langmuir Isotherm is basically an empirical equation since no determination of the constant K is possible for the adsorption of solution cations by a solid other than from a best fit to the experimentally determined adsorption isotherm.

The Langmuir Isotherm has been used very little in the study of groundwater problems whereas the Freundlich Isotherm has been used extensively. The Langmuir Isotherm is subject to the same limitations as the Freundlich Isotherm and in general provides no better results. The Freundlich Isotherm is mathematically slightly more simple to use than the Langmuir Isotherm which accounts for its more extensive use.

Many other empirical equations could also be mentioned but in general the Freundlich and Langmuir Isotherms embody most of the characteristics of these other equations. Most of the empirical equations assume that the adsorbed concentration $\overline{C}$ is only a function of the dissolved concentration C (i.e. $\overline{C} = f(C)$), whereas in reality

the adsorbed concentration is also a function of the concentrations of all other competing cations in solution. Recall that the adsorption isotherm was determined for a constant solution concentration and solution composition. Empirial equations based on the adsorption iso-therm are not valid, in general, for varying solution concentrations and solution composition. The empirical equations have their merit in providing simple mathematical relationships for problems of adsorption of a single cation species but have little value in cation exchange problems where two or more species of cations are competing for exchange sites. The problem of groundwater restoration for in situ solution mining belongs to this latter class of problems.

2.4.2 Kinetic-Theory Equations

The Kinetic-theory equations are based on the diffuse double layer model of the cation exchange process. A structure of the double layer was first proposed by Helmholtz in 1879. The Helmholtz double layer consisted of 2 rigid electrical layers (analogous to the plates of a condenser), one layer formed by the solid particle surface and a second layer formed by the cations in solution. The theory was modified by Gouy in 1910 and again later by Stern in 1924 as the diffuse double layer model. They considered a double layer consisting of a rigid layer formed by the solid particle surface and a diffuse mobile layer of charges formed by the cations in solution. The cations in the diffuse layer are subject to two opposing forces, electrostatic forces that attract them to the charged surface and diffusion forces that force them away from the surface towards the external solution where their

concentration is smaller. There is no sharp boundary between the two layers and the concentration of the cations in the diffuse layer varies with the distance from the solid particle surface. For a more complete description of the diffuse double layer model the interested reader is referred to Van Olphen (1977).

2.4.2.1 Gapon equation

Gapon (1933) considered cation exchange in terms of the double layer exchange between a liquid and a monomolecular layer of another liquid adsorbed on a solid. Gapon assumed that the quantity of a given liquid adsorbed by a solid is proportional to the surface area occupied by that liquid. The Gapon equation may be written as

$$\frac{C_2 \cdot f_1}{C_1(f_o - f_1)} = K \tag{4}$$

where

f_o = total surface area,

f_1 = surface area occupied by liquid C_1 at equilibrium,

f_2 = surface area occupied by liquid C_2 at equilibrium, and

K = constant.

In the Gapon equation the CEC = f_o = $f_1 + f_2$.

Gapon applied this equation only to binary exchange between monovalent and divalent cations for the following equilibrium reaction which is based on a ratio of surface areas

$$(\overline{C}_{2\ \frac{1}{2}})_{Ads} + (C_1)_{Sol} \rightleftharpoons (\overline{C}_1)_{Ads} + \frac{1}{2}(C_2)_{Sol} \tag{5}$$
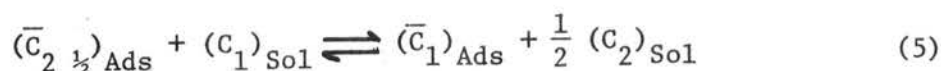
where cation 1 is the monovalent cation and cation 2 is the divalent cation. For the monovalent-divalent exchange Gapon obtained

$$\frac{(C_2)^{\frac{1}{2}} (\overline{C}_1)}{(C_1) (CEC - \overline{C}_1)} = K \tag{6}$$

where C denotes the solution concentrations and $\overline{C}$ denotes the adsorbed concentrations. Kelley (1948) applied the Gapon equation to the binary exchange between monovalent cations for the equilibrium reaction

$$(\overline{C}_2)_{Ads} + (C_1)_{Sol} \rightleftharpoons (\overline{C}_1)_{Ads} + (C_2)_{Sol} \tag{7}$$

where both cations are monovalent ions. For the monovalent-monovalent exchange the Gapon equation yields

$$\frac{(C_2) (\overline{C}_1)}{(C_1) (\overline{C}_2)} = K. \tag{8}$$

2.4.2.2 Jenny Equation

Jenny (1936) reasoned that each cation adsorbed by the solid is not at rest but is in a continuous state of thermal agitation and Brownian movement. Cation exchange occurs when a cation in solution chances to pass between the adsorbed cation and the electrical charge of the solid particle surface. The cation previously in solution becomes adsorbed and simultaneously the previously adsorbed cation is released into solution. Applying the laws of probability to this concept of cation exchange, Jenny developed the following equilibrium equation for binary exchange between cations of equal valence

$$\frac{(Z_1)\,(N_2)}{(Z_2)\,(N_1)} = \frac{V_1}{V_2} \tag{9}$$

where Z_1 and Z_2 = the number at equilibrium of adsorbed cations for

species 1 and 2 respectively,

N_1 and N_2 = the number at equilibrium of cations in free solution

for species 1 and 2 respectively, and

V_1 and V_2 = the oscillation volumes for adsorbed cations 1 and 2

respectively.

The oscillation volumes are constants for the given species in the

exchange. The Jenny equation and the Gapon equation for monovalent-

monovalent exchange (equation 8) are identical when $V_1/V_2 = K$ = constant.

On the basis of Jenny's probability oscillation volume concept,

Davis (1945a)developed the following equation for the exchange between

monovalent and divalent ions

$$\frac{(Z_1)(N_2)^{\frac{1}{2}}}{(Z_2)(N_1)} = K \tag{10}$$

where Z and N are defined as in equation (9) with the subscript 1

referring to the monovalent cation and the subscript 2 referring to the

divalent cation and K = constant. As Davis pointed out, this equation

is identical with Gapon's equation (6).

2.4.3 Mass-Action Equations

Based on thermodynamic arguments Kerr (1928) formulated the cation

exchange process in terms of the law of mass action. For the equilibrium

reaction given in equation (7) for the binary exchange between monovalent

cations the law of mass action is written as

$$\frac{C_2 \ \overline{C}_1}{C_1 \ \overline{C}_2} = K \tag{11}$$

where C and $\overline{C}$ are defined as before and K = constant called the selectivity coefficient. The selectivity coefficient K may be determined theoretically from thermodynamic considerations or from a best fit to the experimentally determined adsorption isotherm.

For the binary exchange between monovalent and divalent cations for the equilibrium reaction

$$(\overline{C}_2)_{Ads} + 2(C_1)_{Sol} \rightleftharpoons 2(\overline{C}_1)_{Ads} + (C_2)_{Sol} \tag{12}$$

where again cation 1 is a monovalent cation and cation 2 is a divalent cation, the law of mass action is written as

$$\frac{(C_2) \ (\overline{C}_1)^2}{(C_1)^2 \ (\overline{C}_2)} = K. \tag{13}$$

For monovalent-monovalent exchange the law of mass action is equivalent to the kinetic-theory equations. However, for monovalent-divalent exchange the law of mass action and the kinetic-theory equations are of similar but of different form.

Kerr expressed his mass-action formulas in terms of concentrations. Vanselow (1932) realized this was an error and that all mass-action formulas should be expressed in terms of activities. Vanselow also suggested that the use of mole fractions for the adsorbed concentrations (defined as $\overline{C}$/CEC). For monovalent-monovalent exchange the use of mole

fractions does not alter the law of mass action for this case (equation 11). However, for monovalent-divalent exchange, the use of mole fractions in equation (13) yields the following

$$\frac{(C_2)\ (\overline{C}_1)^2\ CEC}{(C_1)^2\ (\overline{C}_2)} = K \tag{14}$$

Equation (14) normally gives slightly better results than equation (13).

The law of mass action applies to all equilibrium controlled chemical reactions. A tacit assumption in considering the cation exchange process as a chemical reaction is that the adsorbed cations and the solution cations are definable as separate entities. This idea conflicts with the diffuse-double layer concept in which the cation exchange process is viewed as merely a rearrangement of cations in the double layer and not as a chemical reaction. Because of this several authors (e.g. Davis, 1945b, and Bolt, 1955) have questioned the use of the law of mass action to describe the cation exchange process.

The kinetic-theory equations have been criticized in that they neglect the finite size of the cations which accounts for the valence effect observed in the cation exchange process (Laudelout et al, 1968). The kinetic-theory equations also assume no interference due to activity between competing cations in solution which is contrary to experimental observations of the cation exchange process.

It should be noted that although the Gapon and Jenny equations are kinetically derived formulas, these equations are of a mass-action type (Bear, 1964). In fact, Gapon himself considered his equation to

be a mass-action equation. Recall that for monovalent-monovalent exchange the kinetically derived equations are the same as the law of mass action but for monovalent-divalent exchange the two types of equations are different. Kelley (1948) suggested that the difference between the Gapon equation and the law of mass action for monovalent-divalent exchange is due to the form of the equilibrium reaction used by Gapon (equation 5) with the standard form of the equilibrium reaction (equation 12). Krishnamoorthy and Overstreet (1950) compared the Gapon equation with the law of mass action to their experimental results and concluded that for monovalent-divalent exchange the law of mass action yielded better results. In a recent study, Hill and Lake (1978) also showed that for their own experimental results, the mass action law yielded somewhat more accurate results than the Gapon equation, but no conclusions as to superiority were reached.

Until recently, equations based on the diffuse double layer theory such as the Gapon equation have been in wide use. At present, equations based on thermodynamic considerations (i.e. law of mass action) appear to be most widely accepted. Such authors as Helfferich (1962), Bear (1964), Garrels and Christ (1965), Laudelout et al (1968), Gilbert and Van Bladel (1970), Stumm and Morgan (1970), Hem (1970), Helfferich and Klein (1970), and Freeze and Cherry (1979) use the law of mass action to describe the cation exchange process. However, adoption of the law of mass action has not been universal and Bolt and Bruggenwert (1976) use the Gapon equation to describe the cation exchange process. For this present study the cation exchange process will be described using the law of mass action which will be discussed in somewhat greater detail in the next section.

The preceeding discussion of the cation exchange equations has been intended only as a review of the major equations in the literature and not as an exhaustive review of the subject. No mention has been made of equations based on the Donnan equilibrium theory of the cation exchange process in which the solid particle surface is comprised of colloidal particles separated from the external solution by a membrane (impermeable to the colloidal particles but permeable to the ions in solution). For a more complete review of cation-exchange equations the interested reader is referred to Bolt (1967). Boast (1973) reviews a number of both equilibrium and nonequilibrium cation exchange equations that have been used in modeling the movement of chemicals in soils by water.

2.5 Law of Mass Action

The preference for exchange between competing cations for the equilibrium controlled cation exchange reaction

$$(z_2\bar{C}_1)_{Ads} + (z_1C_2)_{Sol} \rightleftharpoons (z_1\bar{C}_2)_{Ads} + (z_2C_1)_{Sol} \tag{15}$$
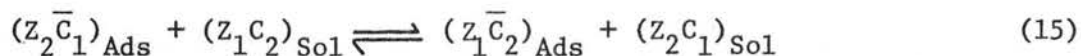
can be expressed in quantitative terms by the law of mass action given as (Helfferich, 1962)

$$K = \frac{[\bar{c}_2]^{z_1} [c_1]^{z_2}}{[\bar{c}_1]^{z_2} [c_2]^{z_1}} \tag{16}$$

where

$[c_1]$, $[c_2]$ = activity of cations 1 and 2 in solution respectively,

$[\overline{C_1}]$, $[\overline{C_2}]$ = activity of cations 1 and 2 adsorbed on the porous medium respectively,

Z_1, Z_2 = valences of cations 1 and 2 respectively, and

K = selectivity coefficient.

The ratio between activity and the actual or analytical concentration of a substance is called the activity coefficient. For an infinitely dilute solution, the activity coefficient is 1 and the activity equals the actual concentration. The activities may be expressed in concentration units of molality, m (moles per 1,000 grams of water), molarity, M (moles per liter), equivalence, C (equivalents per liter, defined as $C_i = Z_i m_i$) or equivalent ionic fractions, N (dimensionless, defined as $N_i = Z_i m_i / \sum_{\text{all } j} Z_j m_j$). For homovalent exchange (in essence monovalent-monovalent exchange or divalent-divalent exchange) the selectivity coefficient K is dimensionless. However, for hetervalent exchange (in essence monovalent-divalent exchange) the selectivity coefficient K is not dimensionless but has concentration units of molality, molarity, or equivalence. In this study, the activities for the adsorbed cations will be expressed in equivalent fractions, N (dimensionless), while the activities for the cations in solution will be expressed in molality, m (moles per 1,000g), or equivalence, C (equivalents per liter). This follows the terminology suggested by Vanselow (1932) and adopted by most present day authors on the subject.

The relationship between activities and concentrations for the adsorbed phase is given as (Garrels and Christ, 1965)

$$[\overline{C_i}] = \overline{\lambda_i} \overline{N_i} \qquad (17)$$

where

$[\overline{C_i}]$ = the activity of cation i in the adsorbed phase,

$\overline{N}_i$ = concentration of cation i in the adsorbed phase, and

$\overline{\lambda}_i$ = rational activity coefficient (dimensionless) for cation i in the adsorbed phase.

The relationship between activities and concentrations for the solution phase is given as (Garrels and Christ, 1965)

$$[c_i] = \gamma_i m_i \tag{18}$$

where

$[c_i]$ = the activity of cation i in the solution phase,

m_i = concentration of cation i in the solution phase, and

γ_i = individual ion activity coefficient (dimensionless) for cation i in the solution phase.

Substitution of equations (17) and (18) into equation (16) yields

$$K = \frac{\overline{\lambda}_2^{z_1} \overline{N}_2^{z_1} \gamma_1^{z_2} m_1^{z_2}}{\overline{\lambda}_1^{z_2} \overline{N}_1^{z_2} \gamma_2^{z_1} m_2^{z_1}} . \tag{19}$$

The activity coefficients γ_i for the solution phase have been determined and for dilute solutions may be calculated using the Debye-Huckel equation (Hem, 1961)

$$- \log \gamma_i = \frac{AZ_i^2 \sqrt{I}}{1 + Ba_i \sqrt{i}} \tag{20}$$

where

γ_i = the activity coefficient of cation i in the solution phase,

A = constant relating to the solvent (for water at 25°C it is

0.5085),

Z_i = valence of cation i,

B = constant relating to the solvent (for water at 25°C it is

0.3281×10^8),

a_i = constant relating to the effective diameter of the cation

in solution (on Figure 2, a_i for Ca^{++} is 6×10^{-8} and a_i

for NH_4^+ is 3×10^{-8}), and

I = ionic strength of the solution (defined as $I = \sum_{\text{all } i} \frac{m_i Z_i^2}{2}$).

The Debye-Huckel equation is valid for a solution with an ionic strength of about tenth. At greater ionic strengths the mean salt method (Garrels and Christ, 1965) must be used to determine the activity coefficients. Plots of the activity coefficient versus ionic strength for Ca^{++} and for NH_4^+ are shown on Figure 2. The activity coefficients for the adsorbed phase $\overline{\lambda}_i$ are unknown.

The law of mass action was used to calculate several adsorption isotherms (Figure 3) to illustrate the effects of valence and solution concentration on the cation exchange process. Recall that the adsorption isotherm is a plot of C_i/C_o versus $\overline{C}_i/CEC$ where C_o equals the solution concentration. Calculations of $\overline{C}_1/CEC$ were made using the mass action law uncorrected for activity in either the solution phase or the adsorbed phase for varying concentration levels of C_1 and C_2 such that $C_1 + C_2 = C_o$, where C_o is kept constant.
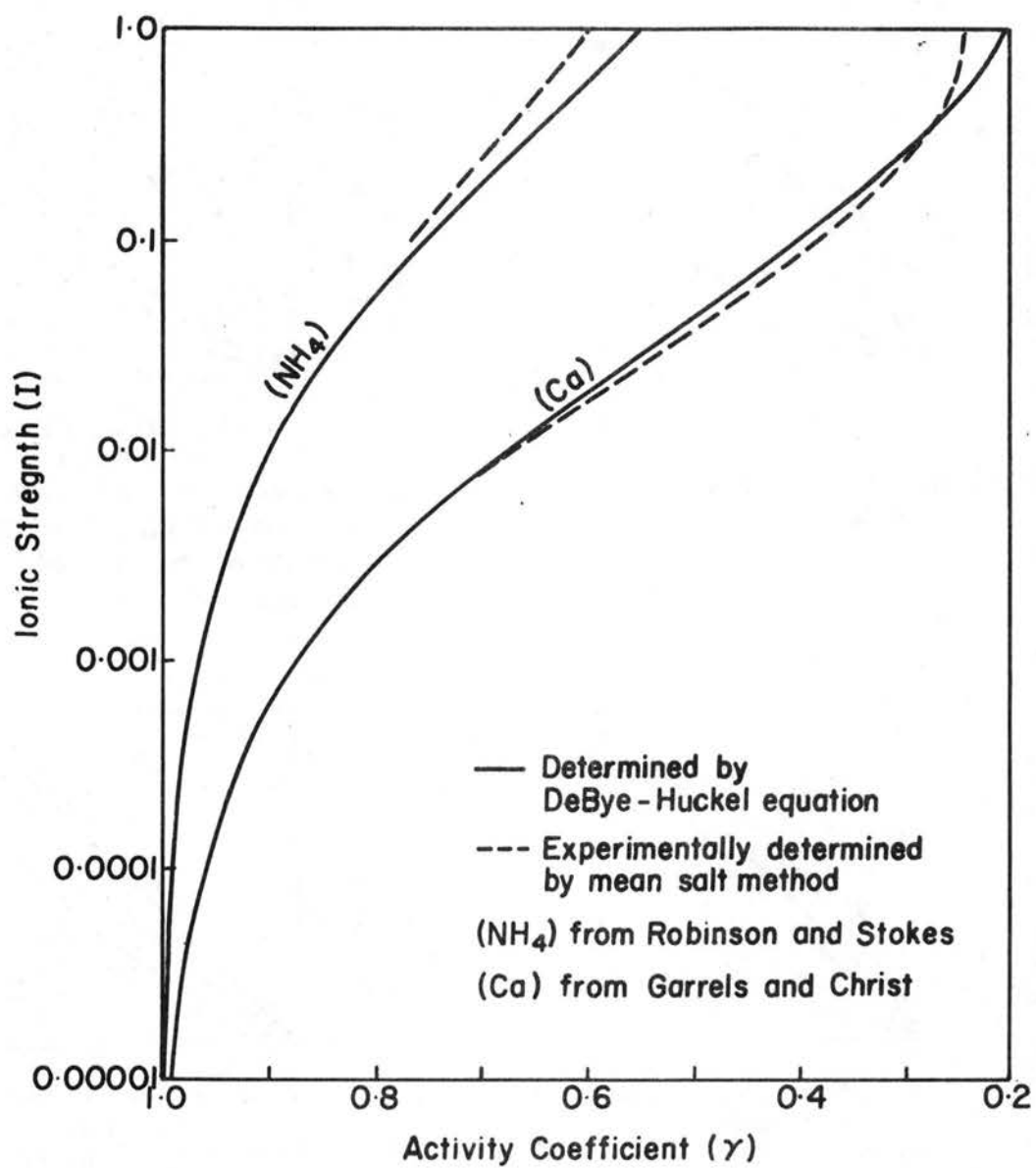
Figure 2. -- Activity coefficients in solution for Calcium and Ammonium .
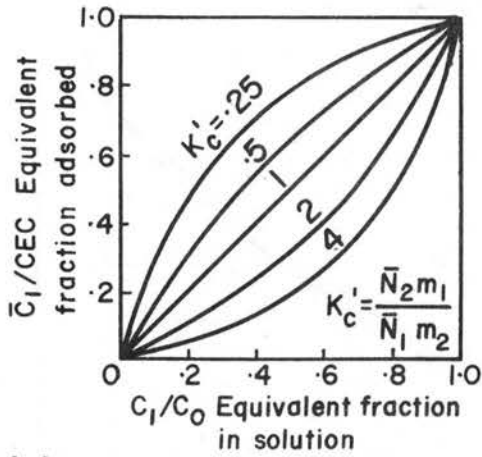
(a) Isotherm for monovalent-
monovalent cation exchange.
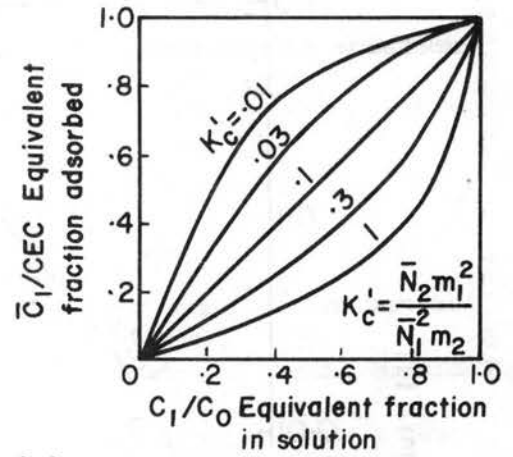
(b) Isotherm for monovalent-
divalent cation exchange for
a solution concentration of
50 meq/ℓ.
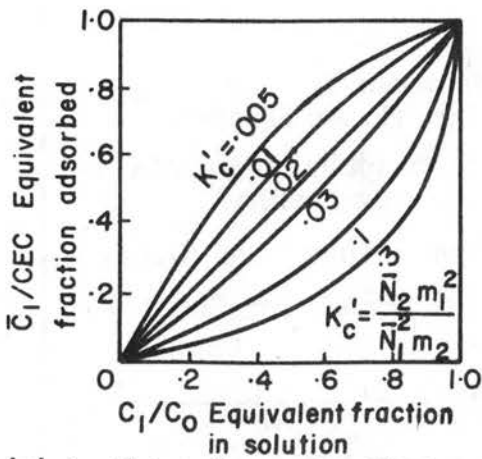
(c) Isotherm for monovalent-
divalent cation exchange for
a solution concentration of
10 meq/ℓ.
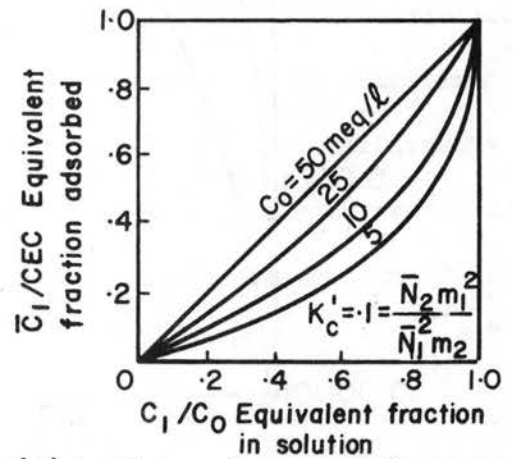
(d) Isotherm for monovalent-
divalent cation exchange for
varying solution concentration
and $K_c' = \cdot 1$.

Figure 3. -- Adsorption isotherms calculated from the law of mass
action.

On Figure 3a is shown the adsorption isotherm for a monovalent-mono-
valent cation exchange process. On this Figure, a value of the selectivity
coefficient equal to 1 represents a linear adsorption isotherm for which
the proportion of cation 1 adsorbed on the porous medium is equal to
the proportion of cation 1 in solution. A value of the selectivity
coefficient greater than 1 indicates the proportion of cation 1 adsorbed
on the porous medium is less than the proportion of cation 1 in solution.
Recall from the previous discussion of the adsorption isotherm that this
type of curve is obtained when cation 2 has a greater affinity for
adsorption than does cation 1. The reverse exchange occurs when the
selectivity coefficient has a value less than 1 which indicates that the
proportion of cation 1 adsorbed on the porous medium is greater than the
proportion of cation 1 in solution and occurs when cation 1 has a greater
affinity for adsorption than does cation 2. For the case of monovalent-
monovalent exchange, the solution concentration C_o has no affect on the
adsorption isotherm.

On Figures 3b,3c and 3d are shown adsorption isotherms for a monovalent-
divalent cation exchange process where cation 1 is a monovalent cation
and cation 2 is a divalent cation. For a monovalent-divalent cation
exchange process, an infinite set of adsorption isotherms would be
obtained for varying solution concentrations C_o. Comparison of figures
3b and 3c with 3a illustrate the preference for adsorption for the
cation with the higher valence. On both figures 3b and 3c for a given
value of the selectivity coefficient, the adsorption isotherms are
shifted from figure 3a in the direction of the unfavorable to the
favorable isotherm. This shift is more pronounced on Figure 3c

for a solution concentration of 10 meq/L than on Figure 3b for a solution concentration of 50 meq/L. The adsorption isotherm shown on Figure 3d is for constant selectivity coefficient and varying solution concentration. Figure 3d clearly shows that the preference for adsorption of the higher valence cation decreases with an increase in solution concentration.

2.6 Selectivity Coefficient

The selectivity coefficient K in the law of mass action may be determined for the particular cation exchange reaction being considered either from theoretical thermodynamic considerations or from a best fit to an experimentally determined adsorption isotherm. In general, the latter method yields better estimates of K and the procedure for this method will be presented.

The selectivity coefficient K defined by equation (19) is corrected for both activities in the solution phase and the adsorbed phase and can be considered a constant. If, however, the activity coefficients are neglected in the law of mass action then the selectivity coefficient K_c', uncorrected for activity in either the solution phase or the adsorbed phase, is defined as

$$K_c' = \frac{\bar{N}_2^{z_1} m_1^{z_2}}{\bar{N}_1^{z_2} m_2^{z_1}} \tag{21}$$

Equation (21) was used to calcaulate the adsorption isotherms shown on Figure 3. While these adsorption isotherms show constant values for K_c' for individual curves, in actuality K_c' is a variable. The selectivity

coefficient K, corrected for activity in both the solution phase and the adsorbed phase, is a constant, but the selectivity coefficient K'_c, uncorrected for activity in either the solution phase or the adsorbed phase is a variable.

The correction for activity in the solution phase is made by multiplying K'_c by the experimentally known activity coefficients γ_i for the solution phase. Recall that the solution phase activity coefficients are calculated using the Debye-Huckel equation (20). This correction for activity in the solution phase is expressed mathematically as

$$K_c = \frac{K'_c \gamma_1^{z_2}}{\gamma_2^{z_1}} = \frac{\overline{N}_2^{z_1} [m_1]^{z_2}}{\overline{N}_1^{z_2} [m_2]^{z_2}} \tag{22}$$

where

K_c = selectivity coefficient corrected for activity in the solution phase but uncorrected for activity in the adsorbed phase, and all other variables are as previously defined.

A preferable method to obtain K_c is to plot values of K'_c versus ionic strength and extrapolate to zero ionic strength. For an infinitely dilute solution, the activity coefficients γ_i are 1 and K_c equals K'_c. This method has the advantage that it helps eliminate errors from incomplete attainment of equilibrium and there is no need to calculate the solution activity coefficients γ_i. Van Bladel and Laudelout (1967) observed that the logarithm of K'_c versus the square root of twice the ionic strength plots as a straight line.

The selectivity coefficient K corrected for activity in both the solution phase and the adsorbed phase is related to K_c by

$$K = \frac{K_c \; \bar{\lambda}_2^{-Z_1}}{\bar{\lambda}_1^{-Z_2}} \tag{23}$$

The surface activity coefficients $\bar{\lambda}_i$ are not known. However, an estimate of K can be made by averaging the surface-activity coefficients over the entire range of composition of the solid material. The selectivity coefficient K can then be determined by the method of Gaines and Thomas (1953 and 1955) using the following approximation

$$\text{Ln } K \simeq (Z_1 - Z_2) + \int_0^1 \text{Ln } K_c \, d\bar{N}_1 \tag{24}$$

For the inverse formulation of the law of mass action given in equation (16) the term $(Z_1 - Z_2)$ in equation (24) is replaced with the term $(Z_2 - Z_1)$. The integration shown in equation (24) is carried out graphically.

As an example of this method, consider the binary exchange between calcium and ammonium cations. The equilibrium controlled cation exchange reaction for this case is written as

$$(2\bar{C}_{NH_4})_{Ads} + (C_{Ca})_{Sol} \rightleftharpoons (\bar{C}_{Ca})_{Ads} + (2C_{NH_4})_{Sol} \tag{25}$$
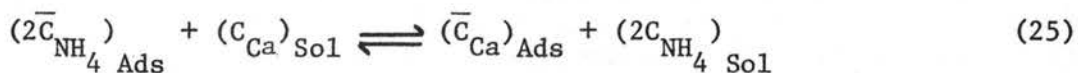
The law of mass action for this reaction is written as

$$K = \frac{\bar{\lambda}_{Ca} \; \bar{N}_{Ca} \; \gamma_{NH_4}^2 \; C_{NH_4}^2}{\bar{\lambda}_{NH_4}^2 \; \bar{N}_{NH_4}^2 \; \gamma_{Ca} \; C_{Ca}} \tag{26}$$

where

C_{Ca}, C_{NH_4} = concentration of calcium and ammonium in solution respectively in units of meq/L,

γ_{Ca}, γ_{NH_4} = activity coefficient for calcium and ammonium in solution respectively (dimensionless),

$\overline{N}_{Ca}$, $\overline{N}_{NH_4}$ = equivalent fraction of calcium and ammonium occupying the cation exchange sites respectively (dimensionless),

$\overline{\lambda}_{Ca}$, $\overline{\lambda}_{NH_4}$ = rational activity coefficient for the adsorbed calcium and ammonium cations respectively (dimensionless), and

K = selectivity coefficient corrected for activity in both the solution and the adsorbed phases in meq/L.

On Figure 4, an experimentally determined adsorption isotherm for a montmorillonite clay is shown for the replacement of ammonium by calcium for four solution concentrations, 50, 25, 10 and 5 meq/L. As can be seen, the preference for adsorption of the calcium cation decreases with increases in the ionic strength of the solution. From this data at values of $\overline{N}_{NH_4}$ ranging from 0.1 to 0.9, values of K'_c were calculated using equation (21) for each of the four solution concentrations.

Shown on Figure 5 are the plots of the logarithm of K'_c versus the square root of twice the ionic strength. Values of K_c were then determined by extrapolating to zero ionic strength.

Equation (24) rewritten for this case is

$$\text{Ln } K = -1 + \int_0^1 \text{Ln } K_c \, d\overline{N}_{NH_4} \tag{27}$$

The integral in equation (27) was evaluated graphically using the plot of Ln K_c versus $\overline{N}_{NH_4}$ (Figure 6). The selectivity coefficient K was then calculated to be 17.6 meq/L for this particular case.
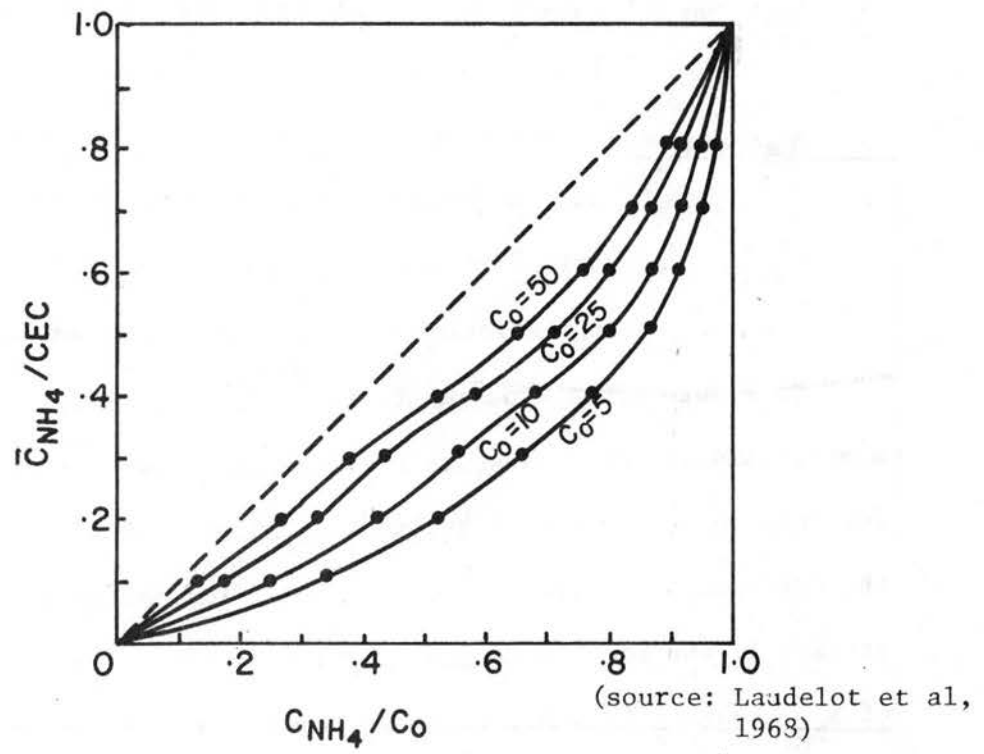
Figure 4. -- Adsorption isotherm for Calcium and Ammonium.
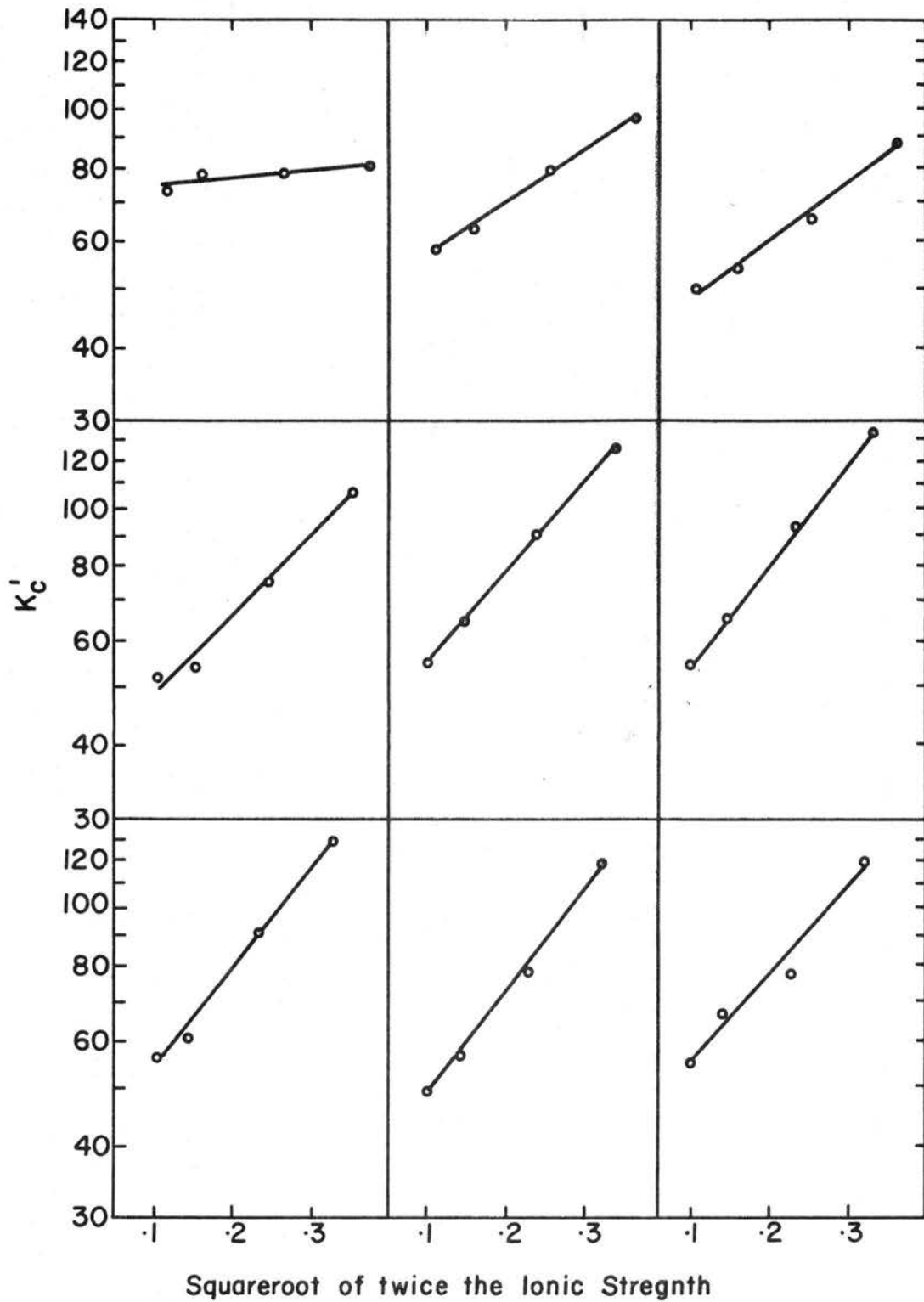
Figure 5. -- Logarithm of K'_c versus square root of twice the ionic strength.
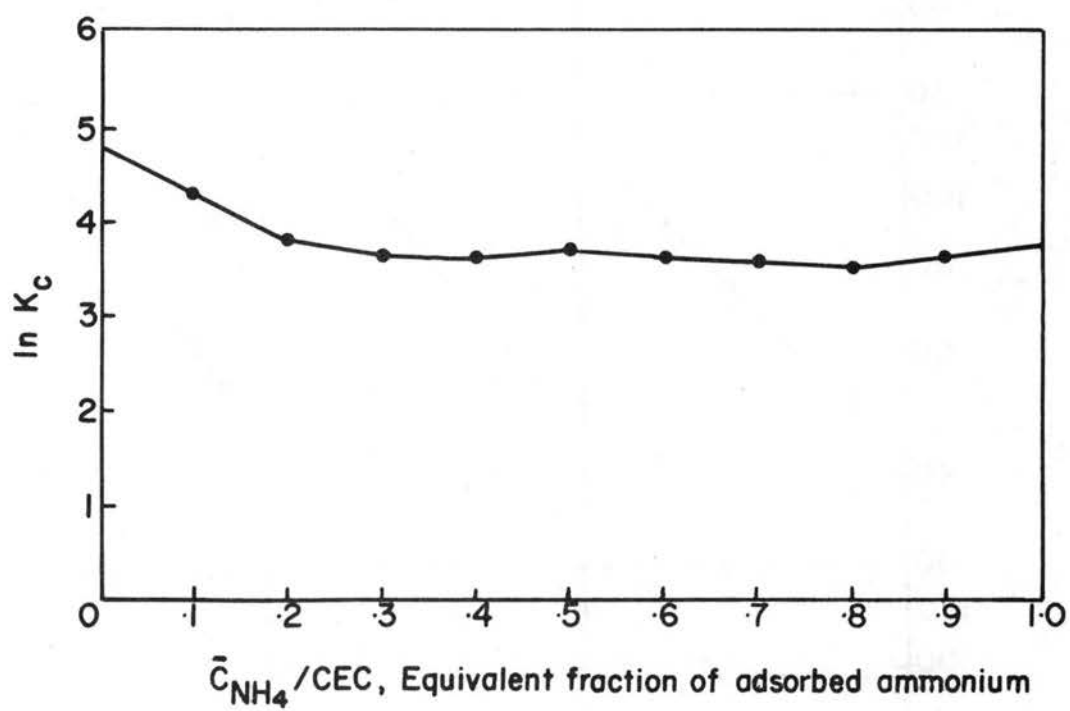
Figure 6. -- Natural logarithm of K_c versus the equivalent fraction of adsorbed ammonium.

In summary, the cation exchange process was considered as an equilibrium controlled reversible chemical reaction that could be quantitatively formulated in terms of the law of mass action. The adsorbed concentration for a given chemical species is dependent not only on its own solution concentration but also on the concentration of all other competing chemical species in solution. This requires that all chemical species involved in the cation exchange process be followed as they flow with the groundwater through the porous media. It remains then to combine the law of mass action with the partial differential equation which describes this movement by groundwater through the porous media of reacting solutes subject to cation exchange reactions.

SOLUTE TRANSPORT WITH ADSORPTION

The equation describing two-dimensional mass transport for a reacting solute subject to adsorption and desorption in flowing groundwater was derived from the principal of mass conservation in Appendix B, equation (B16). This equation is written as

$$
-\frac{\partial C}{\partial t} - \frac{\partial \overline{C}}{\partial t} = \frac{\partial}{\partial x}(CV_x) + \frac{\partial}{\partial y}(CV_y) + \frac{\partial}{\partial x}\left(-D_{xx}\frac{\partial C}{\partial x}\right)
$$

$$
+ \frac{\partial}{\partial y}\left(-D_{yy}\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial x}\left(-D_{xy}\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial y}\left(-D_{yx}\frac{\partial C}{\partial x}\right) \qquad (28)
$$

$$
+ \frac{WC'}{\varepsilon b} + \sum_{p=1}^{m}\left(\delta(x-x_p)\,\delta(y-y_p)\,\frac{Q_p C'}{\varepsilon b}\right)
$$

where

$C = C(x,y,t)$ = dissolved concentration of the solute (M/L^3),

$\overline{C} = \overline{C}(x,y,t)$ = adsorbed concentration of the solute (M/L^3),

$C' = C'(x,y,t)$ = dissolved concentration of the solute in the source
or sink fluid (M/L^3),

$V_x = V_x(x,y,t)$ = average interstitial velocity in the x-direction (L/T),

$V_y = V_y(x,y,t)$ = average interstitial velocity in the y-direction (L/T),

$(D_{xx}, D_{yy}, D_{xy}, D_{yx}) = D_{ij}(x,y,t)$ = components of the coefficient of
hydrodynamic dispersion (L^2/T),

$b = b(x,y,t)$ = saturated thickness (L),

$\varepsilon = \varepsilon(x,y,t)$ = porosity (dimensionless)

$W = W(x,y,t)$ = volumetric water flux per unit area from a distributed
source or sink (L/T),

$Q_p = Q_p(t)$ = volumetric water flux from a point source or sink at (x_p, y_p), positive sign for withdrawal and negative sign for injection, there are m such points (L^3/T),

$\delta(x-\xi)$ = Dirac delta function,

t = time (T), and

x, y = cartesian coordinates in the principal direction of hydraulic conductivity (L).

Equation (28) is referred to as the convection-dispersion equation with adsorption and incorporates the effects of: (1) convective transport in which chemical constituents are carried with the average motion of the flowing groundwater; (2) hydrodynamic dispersion, in which primarily variations in local velocity cause a spread of the chemical constituents from the average direction of groundwater flow; (3) fluid sources, in which water of a certain chemical composition is injected into water of a different chemical composition; and (4) adsorption/desorption reactions. Equation (28) contains two unknowns, C and $\overline{C}$. Thus, at least one additional equation is needed for solution.

The desirability of use of empirical equations such as the Freundlich isotherm is readily apparent in the solution of equation (28). Recall that most of the empirical equations assume that the adsorbed concentration $\overline{C}$ is only a function of the dissolved concentration C (i.e. $\overline{C} = f(C)$) which can then be differentiated with respect to time and substituted directly into equation (28) to yield an equation in terms of only the dissolved concentration C. This equation may then be solved independently of all other equations. However, as was pointed out earlier, these empirical equations are applicable only under some rather stringent criteria, namely that the total solution concentration and composition remain fairly constant.

A more general solution will now be given with particular application to site restoration of solution mining. Only the case of binary cation exchange will be considered but the method can be extended to any number of exchanging solute species (Rubin and James, 1973). Both chemical species involved in the exchange process must be followed as they flow with the groundwater through the porous media. To do this, equation (28) is written for both chemical species in terms of C_1 and C_2 as

$$
-\frac{\partial C_1}{\partial t} - \frac{\partial \overline{C}_1}{\partial t} = \frac{\partial}{\partial x}(C_1 V_x) + \frac{\partial}{\partial y}(C_1 V_y) + \frac{\partial}{\partial x}\left(-D_{xx}\frac{\partial C_1}{\partial x}\right)
$$

$$
+ \frac{\partial}{\partial y}\left(-D_{yy}\frac{\partial C_1}{\partial y}\right) + \frac{\partial}{\partial x}\left(-D_{xy}\frac{\partial C_1}{\partial y}\right) + \frac{\partial}{\partial y}\left(-D_{yx}\frac{\partial C_1}{\partial x}\right) \tag{29}
$$

$$
+ \frac{WC_1'}{\varepsilon b} + \sum_{p=1}^{m}\left(\delta(x-x_p)\,\delta(y-y_p)\frac{Q_p C_1'}{\varepsilon b}\right) \quad,
$$

and

$$
-\frac{\partial C_2}{\partial t} - \frac{\partial \overline{C}_2}{\partial t} = \frac{\partial}{\partial x}(C_2 V_x) + \frac{\partial}{\partial y}(C_2 V_y) + \frac{\partial}{\partial x}\left(-D_{xx}\frac{\partial C_2}{\partial x}\right)
$$

$$
+ \frac{\partial}{\partial y}\left(-D_{yy}\frac{\partial C_2}{\partial y}\right) + \frac{\partial}{\partial x}\left(-D_{xy}\frac{\partial C_2}{\partial y}\right) + \frac{\partial}{\partial y}\left(-D_{yx}\frac{\partial C_2}{\partial x}\right) \tag{30}
$$

$$
+ \frac{WC_2'}{\varepsilon b} + \sum_{p=1}^{m}\left(\delta(x-x_p)\,\delta(y-y_p)\frac{Q_p C_2'}{\varepsilon b}\right).
$$

Equations (29) and (30) are coupled through two additional equations which describe the cation exchange process. The first of these equations is the law of mass action which may be written as

$$K = \frac{\bar{\lambda}_2^{Z_1} \bar{N}_2^{Z_1} \gamma_2^{Z_2} C_1^{Z_2}}{\bar{\lambda}_1^{Z_2} \bar{N}_1^{Z_2} \gamma_2^{Z_1} C_2^{Z_2}} \tag{31}$$

where

C_1, C_2 = dissolved concentration of cations 1 and 2 respectively (M/L^3),

$\bar{N}_1, \bar{N}_2$ = equivalent fraction of cations 1 and 2 occupying the cation exchange sites respectively, defined as $\bar{C}_1/CEC$ and $\bar{C}_2/CEC$ respectively (dimensionless),

γ_1, γ_2 = activity coefficients for cations 1 and 2 in solution respectively (dimensionless),

$\bar{\lambda}_1, \bar{\lambda}_2$ = rational activity coefficients for the adsorbed cations 1 and 2 respectively (dimensionless), and

K = selectivity coefficient.

The second equation is obtained from requiring that all of the cation exchange sites must be filled and for binary cation exchange are filled with either $\bar{C}_1$ or $\bar{C}_2$. Also recall that the total cation exchange sites for a given porous medium is a constant and is equal to the cation exchange capacity (CEC). This is expressed mathematically as

$$\bar{C}_1 + \bar{C}_2 = CEC \tag{32}$$

Equations (29), (30), (31) and (32) define a set of 4 equations and 4 unknowns. The direct simultaneous solution of these equations could be accomplished but is not desirable since (1) the problem would be very large (with any sort of numerical method solution a value of C_1, $\bar{C}_1$, C_2 and $\bar{C}_2$ must be solved for at each of the n nodes, the

dimension of the problem would therefore be 4n x 4n), and (2) the inclusion of the law of mass action results in a nonlinear set of equations which is difficult to solve. The complexity and size of the problem is reduced using the following alternative formulations

Equation (31) is rewritten as

$$
K = \frac{\bar{\lambda}_2^{Z_1} (\bar{C}_2/CEC)^{Z_1} \gamma_1^{Z_2} c_1^{Z_2}}{\bar{\lambda}_1^{Z_2} (\bar{C}_1/CEC)^{Z_2} \gamma_2^{Z_1} c_2^{Z_1}} .
\tag{33}
$$

Substitution of equation (32) into equation (33) and expansion yields

$$
K \bar{\lambda}_1^{Z_2} (\bar{C}_1/CEC)^{Z_2} \gamma_2^{Z_1} c_2^{Z_1} - \bar{\lambda}_2^{Z_1}(1-\bar{C}_1/CEC)^{Z_1} \gamma_1^{Z_2} c_1^{Z_2} = 0.
\tag{34}
$$

Differentiation of equation (34) with respect to time yields

$$
K \bar{\lambda}_1^{Z_2} (\bar{C}_1/CEC)^{Z_2} \gamma_2^{Z_1} Z_1 c_2^{Z_1-1} \frac{\partial c_2}{\partial t}
$$

$$
+ K \bar{\lambda}_1^{Z_2} \gamma_2^{Z_1} c_2^{Z_1} Z_2 \frac{\bar{C}_1^{Z_2-1}}{CEC^{Z_2}} \frac{\partial \bar{C}_1}{\partial t}
$$

$$
- \bar{\lambda}_2^{Z_1} (1-\bar{C}_1/CEC)^{Z_1} \gamma_1^{Z_2} Z_2 c_1^{Z_2-1} \frac{\partial c_1}{\partial t}
$$

$$
+ \bar{\lambda}_2^{Z_1} \gamma_1^{Z_2} c_1^{Z_2} Z_1 \frac{(1-\bar{C}_1 CEC)^{Z_1-1}}{CEC} \frac{\partial \bar{C}_1}{\partial t} = 0 .
$$

$$
\tag{35}
$$

Now letting

$$g_1 = -\bar{\lambda}_2^{Z_1} (1-\bar{C}_1/CEC)^{Z_1} \gamma_1^{Z_2} Z_2 C_1^{Z_2-1}, \tag{36}$$

$$g_2 = -K\bar{\lambda}_1^{Z_2} (\bar{C}_1/CEC)^{Z_2} \gamma_2^{Z_1} Z_1 C_2^{Z_1-1}, \text{ and} \tag{37}$$

$$g_3 = -K\bar{\lambda}_1^{Z_2} \gamma_2^{Z_1} C_2^{Z_1} Z_2 \frac{\bar{C}_1^{Z_2-1}}{CEC^{Z_2}} - \bar{\lambda}_2^{Z_1} \gamma_1^{Z_2} C_1^{Z_2} Z_1 \frac{(1-\bar{C}_1/CEC)^{Z_1-1}}{CEC} \tag{38}$$

then equation (35) is written as

$$g_1 \frac{\partial C_1}{\partial t} - g_2 \frac{\partial C_2}{\partial t} = g_3 \frac{\partial \bar{C}_1}{\partial t} \tag{39}$$

or as

$$\frac{\partial \bar{C}_1}{\partial t} = \frac{g_1}{g_3} \frac{\partial C_1}{\partial t} - \frac{g_2}{g_3} \frac{\partial C_2}{\partial t}. \tag{40}$$

From differentiation of equation (32)

$$\frac{\partial \bar{C}_1}{\partial t} = -\frac{\partial \bar{C}_2}{\partial t}. \tag{41}$$

Substitution of equation (41) into equation (40) yields

$$\frac{\partial \bar{C}_2}{\partial t} = \frac{g_2}{g_3} \frac{\partial C_2}{\partial t} - \frac{g_1}{g_3} \frac{\partial C_1}{\partial t}. \tag{42}$$

Substitution of equation (40) into the convection-dispersion equation for cation 1 (equation 29) and substitution of equation (42) into the convection-dispersion equation for cation 2 (equation 30) yields

$$
-\left(1+\frac{g_1}{g_3}\right)\frac{\partial C_1}{\partial t} +\left(\frac{g_2}{g_3}\right)\frac{\partial C_2}{\partial t} = \frac{\partial}{\partial x}(C_1 V_x) + \frac{\partial}{\partial y}(C_1 V_y)
$$

$$
+\frac{\partial}{\partial x}\left(-D_{xx}\frac{\partial C_1}{\partial x}\right) + \frac{\partial}{\partial y}\left(-D_{yy}\frac{\partial C_1}{\partial y}\right) + \frac{\partial}{\partial x}\left(-D_{xy}\frac{\partial C_1}{\partial y}\right) \tag{43}
$$

$$
+\frac{\partial}{\partial y}\left(-D_{yx}\frac{\partial C_1}{\partial x}\right) + \frac{WC_1'}{\varepsilon b} + \sum_{p=1}^{m}\left(\delta(x-x_p)\,\delta(y-y_p)\,\frac{Q_p C_1'}{\varepsilon b}\right),
$$

and

$$
-\left(1+\frac{g_2}{g_3}\right)\frac{\partial C_2}{\partial t} + \left(\frac{g_1}{g_3}\right)\frac{\partial C_1}{\partial t} = \frac{\partial}{\partial x}(C_2 V_x) + \frac{\partial}{\partial y}(C_2 V_y)
$$

$$
+\frac{\partial}{\partial x}\left(-D_{xx}\frac{\partial C_2}{\partial x}\right) + \frac{\partial}{\partial y}\left(-D_{yy}\frac{\partial C_2}{\partial y}\right) + \frac{\partial}{\partial x}\left(-D_{xy}\frac{\partial C_2}{\partial y}\right) \tag{44}
$$

$$
+\frac{\partial}{\partial y}\left(-D_{yx}\frac{\partial C_2}{\partial x}\right) + \frac{WC_2'}{\varepsilon b} + \sum_{p=1}^{m}\left(\delta(x-x_p)\,\delta(y-y_p)\,\frac{Q_p C_2'}{\varepsilon b}\right).
$$

The unknowns $\overline{C}_1$ and $\overline{C}_2$ do not appear explicitly in either equation (43) or (44) but are embedded in the variable coefficients g_1, g_2 and g_3. This allows a leap-frog solution technique to be used wherein equations (43) and (44) are solved iteratively with the partial differential equation for groundwater flow. A schematic of the leap-frog solution is shown on Figure 7. The groundwater flow equation is first solved for the head distribution in the aquifer at the specified time from which the values of groundwater velocity V and the dispersion coefficient D are obtained. Using
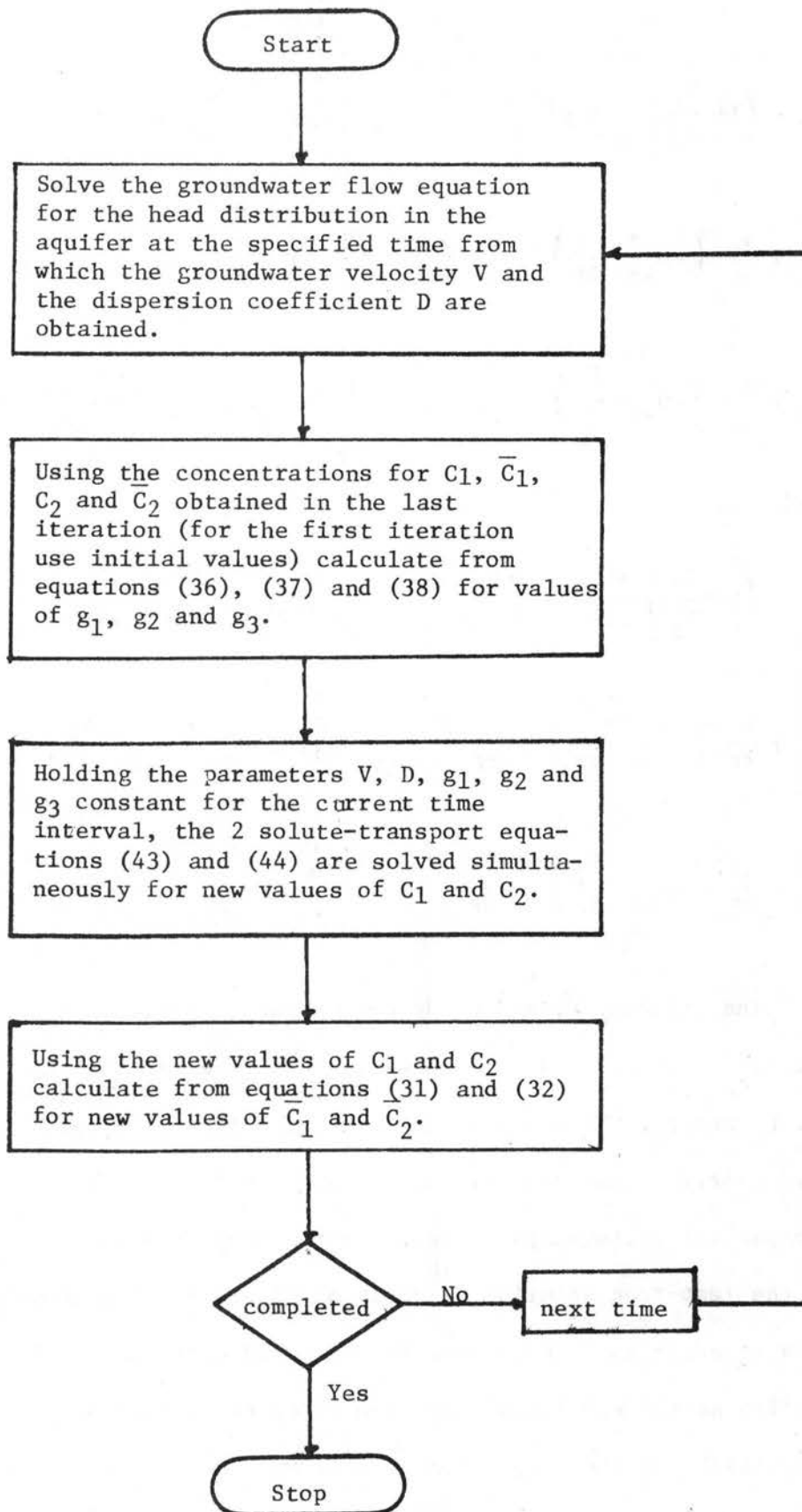
Figure 7. -- Schematic of the leap-frog solution technique

the initial concentrations for C_1, $\overline{C}_1$, C_2 and $\overline{C}_2$, initial values of g_1, g_2 and g_3 are obtained from equations (36), (37) and (38). The parameters V, D, g_1, g_2 and g_3 are then held constant over the next time interval and the two solute transport equations, (43) and (44), are solved simultaneously for new values of C_1 and C_2. These new values of C_1 and C_2 are used in equations (31) and (32) to solve for new values of $\overline{C}_1$ and $\overline{C}_2$. The groundwater flow equation is solved again for the head distribution in the aquifer at a new given time from which updated values of V and D are obtained. Using the values of C_1, $\overline{C}_1$, C_2 and $\overline{C}_2$ obtained in the last iteration, updated values of g_1, g_2 and g_3 are calculated and the leap-frog procedure is repeated as before.

The partial differential equation for groundwater flow and the two coupled partial differential equations of solute transport, equations (43) and (44) were solved subject to the appropriate boundary conditions by the Galerkin-finite element method. In the finite element method, approximating integral equations are formed to replace the original partial differential equations. The integration of these integral equations is required. Because the transport equations contain the nonlinear variable coefficients g_1, g_2 and g_3, which are dependent on concentration changes, these integrations must be repeated frequently. Triangular elements and linear shape functions were used in the solution by the Galerkin-finite element method. This allowed the use of some very powerful integration formulas which considerably reduced the computational effort and time required from that which would have otherwise been required. The details of the Galerkin-finite element method used to the solution of the problem of contaminant transport with adsorption is presented in the next section of the dissertation.

CHAPTER IV

GALERKIN-FINITE ELEMENT METHOD

4.1 Methodology

The fundamental basis of the finite element method consists of
formulating approximating integral equations to replace the original
governing differential equation. There are several methods to formula-
ting these approximate integral equations which can be grouped into
variational techniques or weighted residuals techniques. The Rayleigh-
Ritz method based on the calculus of variations has been used very
extensively in the finite element procedure. However, the method of
weighted residuals has been shown to be much more general than methods
based on variational techniques. Of the weighted residual methods, the
Galerkin method has been found best for mass-transport equations and
is the method used here.

4.1.1 Finite Elements

In the finite element method, the domain of interest is discretized
into a number of subdomains called elements (Figure 8). Triangular
elements are used here although other shapes may be used. The triangular
element can be used to represent irregular boundaries and also can be
concentrated in those regions of the domain where a rapidly varying
solution is expected. The complexity of the computation using triangular
finite elements is less than that for many other shapes. Using these
elements, a continuous function is replaced by values of the function
that are specified at a finite number of discrete points called nodes
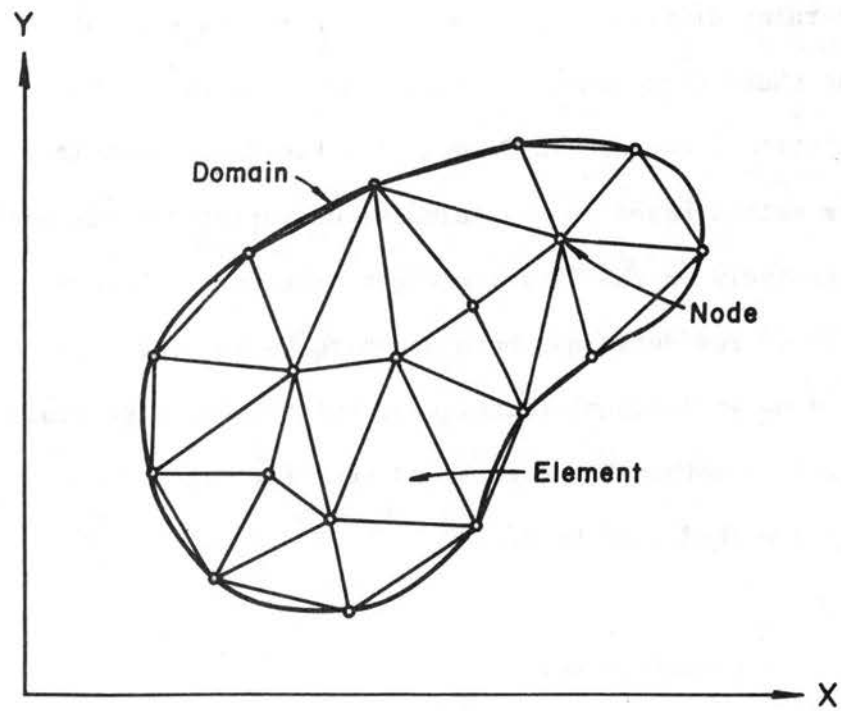
Figure 8. -- Finite element discretization.

(Figure 8). Function values between the nodes are calculated using piecewise continuous interpolating functions defined for each element. The boundary of the domain is represented by a series of piecewise continuous segments.

4.1.2 Galerkin Approximation

Consider a linear differential operator of the form

$$L(u) = 0 \qquad \text{on Domain D.} \qquad (45)$$

To solve $L(u) = 0$, assume a trial solution $\hat{u}(x,y,t)$ which is made up of a linear combination of suitable shape functions that satisfy the essential boundary conditions of the problem. The trial solution can be expressed as

$$u(x,y,t) \simeq \hat{u}(x,y,t) = \sum_{j=1}^{n} (G_j(t) \; \phi_j(x,y)). \qquad (46)$$

In equation (46) $\hat{u}$ is a series approximation to u and ϕ_j is a set of independent shape functions (also called basis, coordinate or trial functions) which are specified beforehand. The G_j are undetermined coefficients and n represents the number of nodal points. As n appoaches infinity, the trial solution $\hat{u}$ approaches the actual solution u. However, for a finite series, the trial solution is an approximation to the actual solution.

Substitution into the linear differential operator L of the trial solution $\hat{u}$ for the exact solution u will result in a residual R. This residual is defined by

$$R(x,y,t) = L(\hat{u}) = L \left[\sum_{j=1}^{n} G_j(t) \; \phi_j(x,y) \right] \qquad (47)$$

If the trial solution were the exact solution, the residual would be zero. This residual is forced to be zero, in an average sense over the entire domain D, through the selection of the undetermined coefficients G_j. The G_j are calculated by setting the weighted integral of the residual to zero. In the Galerkin method, the shape functions are used as the weighting functions and the resulting integral formed is

$$\iint_D R(x,y,t) \; \phi_i(x,y) \; dx \; dy = 0 \qquad (48)$$

$$i = 1,2,\ldots n$$

or in terms of the linear operator L is

$$\iint_D L \left[\sum_{j=1}^{n} G_j(t) \; \phi_j(x,y) \right] \; \phi_i(x,y) \; dx \; dy = 0 \qquad (49)$$

$$i = 1,2,\ldots n \; .$$

From this are obtained n linear equations which can be solved for the n values of G_j.

4.1.3 Shape Functions

The shape functions are selected to have characteristics that conform to the differential equation and also result in simplified equations for ease of computation. Two common shape functions that are used are linear and cubic polynomials. In this study, linear shape functions were used because the computational effort for the integration

is much less than with the cubic polynomials but still provided reliable results.

The computational effort required by the finite element method is greatly minimized by using local shape functions v^e. These local shape functions are defined such that v_i^e is nonzero over only element e, equal to unity at node i, and equal to zero at all other nodes. Thus, for each element e with nodes i, j, k there are only three non zero shape functions, v_i^e, v_j^e and v_k^e (Figure 9a, b and c). These linear shape functions are defined as

$$v_i^e(x,y) = a_i + b_i x + c_i y,$$

$$v_j^e(x,y) = a_j + b_j x + c_j y, \text{ and} \qquad (50)$$

$$v_k^e(x,y) = a_k + b_k x + c_k y$$

where x, y are cartesian coordinates and a, b, c are constant coefficients to be determined from the above definition. Referring to Figure 9

$$v_i^e(x_i, y_i) = 1 = a_i + b_i x_i + c_i y_i,$$

$$v_i^e(x_j, y_j) = 0 = a_i + b_i x_j + c_i y_j, \text{ and} \qquad (51)$$

$$v_i^e(x_k, y_k) = 0 = a_i + b_i x_k + c_i y_k.$$

Solution of equation (51) for a_i, b_i, and c_i yields
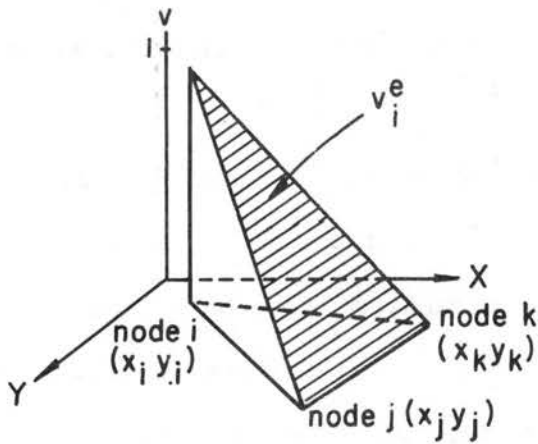
(a) $v_i^e = \dfrac{1}{2A} \left[(x_j y_k - x_k y_j) + (y_j - y_k)X + (x_k - x_j)Y \right]$
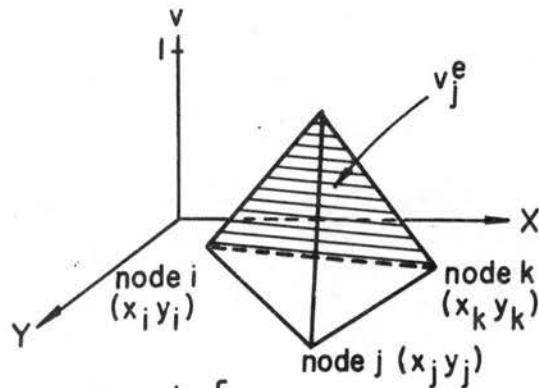
(b) $v_j^e = \dfrac{1}{2A} \left[(x_k y_i - x_i y_k) + (y_k - y_i)X + (x_i - x_k)Y \right]$
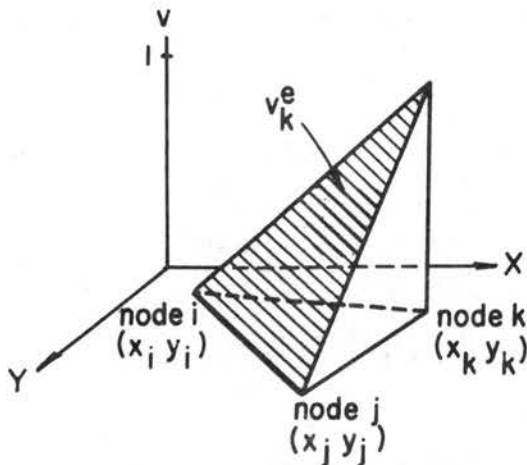
(c) $v_k^e = \dfrac{1}{2A} \left[(x_i y_j - x_j y_i) + (y_i - y_j)X + (x_j - x_i)Y \right]$

Figure 9. -- Local shape functions.

$$a_i = \frac{1}{2A\Delta} (x_j y_k - x_k y_j),$$

$$b_i = \frac{1}{2A\Delta} (y_j - y_k), \quad \text{and} \tag{52}$$

$$c_i = \frac{1}{2A\Delta} (x_k - x_j)$$

where $A\Delta$ equals the area of the triangular element bounded by nodes i,j,k and is given by Zienkiewicz (1977) as

$$A\Delta = \frac{1}{2} \begin{vmatrix} 1 & x_i & y_i \\ 1 & x_j & y_j \\ 1 & x_k & y_k \end{vmatrix}. \tag{53}$$

Substitution of the values for a_i, b_i and c_i given in equation (52) into the expression for v_i^e given in equation (50) yields

$$v_i^e(x,y) = \frac{1}{2A\Delta} \left[(x_j y_k - x_k y_j) + (y_j - y_k)x + (x_k - x_j)y \right] \tag{54}$$

for x, y in element e, otherwise $v_i^e(x,y) = 0$. In a similar manner v_j^e and v_k^e were calculated as

$$v_j^e(x,y) = \frac{1}{2A\Delta} \left[(x_k y_i - x_i y_k) + (y_k - y_i)x + (x_i - x_k)y \right] \tag{55}$$

and

$$v_k^e(x,y) = \frac{1}{2A\Delta} \left[(x_i y_j - x_j y_i) + (y_i - y_j)x + (x_j - x_i)y \right] \tag{56}$$

for x,y in element e, otherwise $v_j^e(x,y)$ and $v_k^e(x,y) = 0$. These are shown graphically on Figure 9a, b and c. Using local shape functions,

the approximating trial solution given as equation (46) is rewritten as

$$\hat{u}(x,y,t) = G_i(t)v_i^e(x,y) + G_j(t)v_j^e(x,y + G_k(t)v_k^e(x,y) \tag{57}$$

where x,y are in element e.

The global shape function ϕ_i is the union of all of the local shape functionsthat are non zero at node i. This is expressed by

$$\phi_i(x,y) = v_i^{e_1} U \quad v_i^{e_2} \quad U \ldots U \quad v_i^{e_p} \tag{58}$$

where $\left\{ v_i^{e_1}, v_i^{e_2} \ldots v_i^{e_p} \right\}$ is the set of all local shape functions that are non zero at node i. The global shape function ϕ_i is non zero only over elements which have node i as a vertice, equal to unity at node i, and equal to zero at all other nodes. The global shape function ϕ_i is shown graphically on Figure 10 for a node which has five non zero local shape functions.

From this definition of ϕ_i, the value of the approximating trial solution at node i is rewritten as

$$\hat{u}(x_i,y_i) = G_i(t)\phi_i(x_i,y_i) = G_i(t) \tag{59}$$

since $\phi_i(x_i,y_i)$ is the only non zero global shape function at node i and it has a value of unity. Thus, the undetermined coefficients, $G_i(t)$ represent the values of the function $\hat{u}$ at the nodes.

4.1.4 Integrations

In the finite element method, the integration of the approximating integral equation given in equation (49) is required. The integration
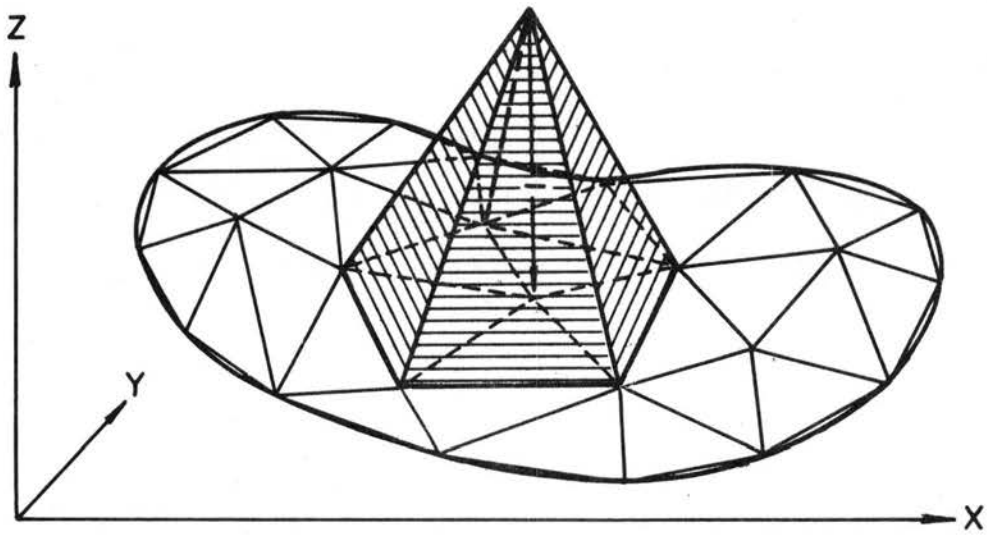
Figure 10. -- Global shape function.

is greatly simplified for linear shape function and triangular elements if an area-coordinate system ℓ is utilized as shown on Figure 11. The area coordinates of point P (Figure 11) are defined as

$$\ell_i = A\Delta_i/A\Delta$$

$$\ell_j = A\Delta_j/A\Delta, \text{ and} \tag{60}$$

$$\ell_k = A\Delta_k/A\Delta$$

Where $A\Delta_i$ is the area of the triangle bounded by nodes j, k, and the point P, $A\Delta_j$ is the area of the triangle bounded by nodes i, k, and the point P, and $A\Delta_k$ is the area of the triangle bounded by nodes i, j, and the point p. These function possess the properties that

$$\ell_i + \ell_j + \ell_k = 1,$$

$$\ell_i = 1 \text{ at node i}, \ell_i = 0 \text{ at nodes j and k},$$

$$\ell_j = 1 \text{ at node j}, \ell_j = 0 \text{ at nodes i and k, and} \tag{61}$$

$$\ell_k = 1 \text{ at node k}, \ell_k = 0 \text{ at nodes i and j}.$$

Note that these properties of ℓ are the same properties as those for the local shape functions v^e. In fact, it can be shown that the area coordinate system ℓ is identical with the local shape functions v^e.

From equations (60) and (53)

$$\ell_i = \frac{A\Delta_i}{A\Delta} = \frac{1}{2\,A\Delta} \begin{vmatrix} 1 & x & y \\ 1 & x_j & y_j \\ 1 & x_k & y_k \end{vmatrix} \tag{62}$$
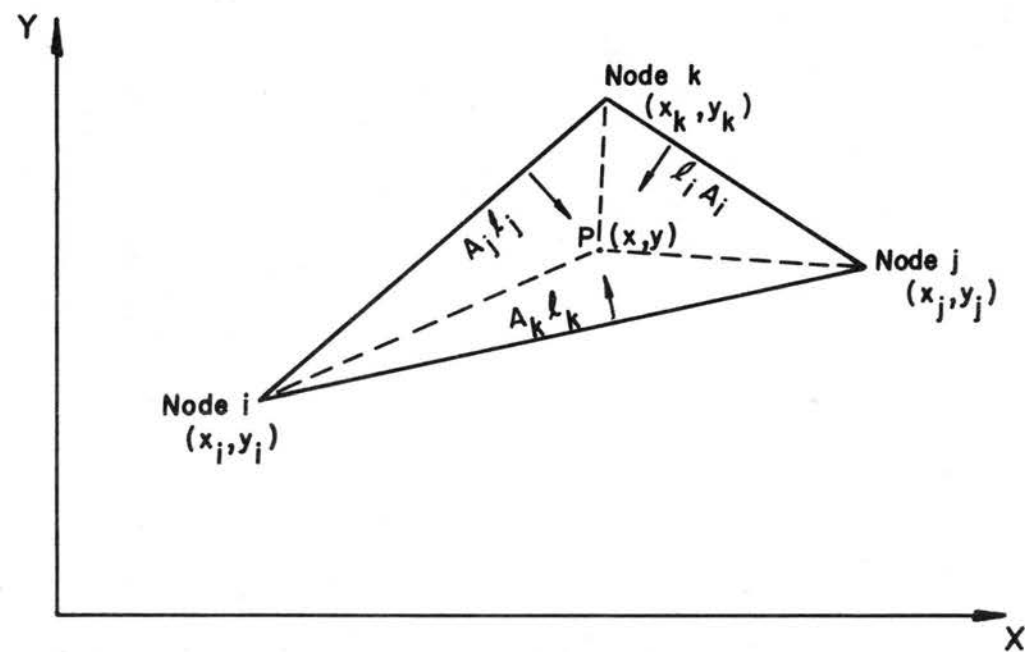
Figure 11. -- Triangular element and area-coordinate system.

Expansion of equation (62) yields

$$\ell_i = \frac{1}{2A\Delta} \quad (y_j x_k - x_k y_j) + (y_j - y_k)x + (x_k - y_j)y \tag{63}$$

which is the same as the expression for v_i^e given by equation (54). Thus

$$\ell_i = v_i^e . \tag{64}$$

Similarly, it can be shown that

$$\ell_j = v_j^e, \text{ and} \tag{65}$$

$$\ell_k = v_k^e .$$

The advantage of using the area-coordinate system is the existence of some very powerful integration formulas given by Segerlind (1976) as

$$\int_L \ell_i^a \ \ell_j^b \ d1 = \frac{a!b!}{(a+b+1)!} L \tag{66}$$

for length integrals and

$$\iint_A \ell_i^a \ \ell_j^b \ \ell_k^c \ dA = \frac{a!b!c!}{(a+b+c+2)!} \ 2A \tag{67}$$

for area integrals, where a and b are specified integers.

Substitution of $\ell_i = v_i^e$, $\ell_j = v_j^e$ and $\ell_k = v_k^e$ into equations (66) and (67) yields

$$\int_L (v_i^e)^a \ (v_j^e)^b \ d\ell = \frac{a!b!}{(a+b+1)!} L, \text{ and} \tag{68}$$

$$\int_A (v_i^e)^a \ (v_j^e)^b \ (v_k^e)^c \ dA = \frac{a!b!c!}{(a+b+c+2)!} \ 2A . \tag{69}$$

Integrals of the form of equations (68) and (69) occur frequently in the finite element method. These integration formulas will be used in the solution of the groundwater flow equation and in the mass-transport equations.

4.2 Solution of the Groundwater Flow Equation

4.2.1 Galerkin Approximation

The equation describing the transient two-dimensional areal flow of groundwater in a confined nonhomogeneous anisotropic aquifer is expressed as (Bear, 1979 or McWhorter and Sunada, 1977)

$$\frac{\partial}{\partial x}(T_x \frac{\partial h}{\partial x}) + \frac{\partial}{\partial y}(T_y \frac{\partial h}{\partial y}) = S\frac{\partial h}{\partial t} + W + \sum_{p=1}^{m} (\delta(x-x_p)\delta(y-y_p) Q_p) \qquad (70)$$

where $T_x = T_x(x,y)$ = transmissivity in the x-direction (L^2/T),

$\quad T_y = T_y(x,y)$ = transmissivity in the y-direction (L^2/T),

$\quad h = h(x,y,t)$ = potentiometric head (L),

$\quad S = S(x,y)$ = storage coefficient (dimensionless),

$\quad W = W(x,y,t)$ = distributed volumetric water flux per unit area, positive sign for discharge and negative sign for recharge (L/T),

$\quad Q_p = Q_p(t)$ = volumetric water flux at a point located at (x_p,y_p), positive sign for withdrawal and negative sign for injection, there are m such points (L^3/T),

$\quad \delta(x-\xi)$ = Dirac Delta function, defined as $\delta(x-\xi) = 0$ if $x \neq \xi$ and $\int_{\xi-\varepsilon}^{\xi+\varepsilon} \delta(x-\xi)dx = 1$

t   =   time (T), and

x,y   =   cartesian coordinates in the principal direction

                 of transmissivity (L).

The linear differential operator corresponding to equation (70)
is defined as

$$L(h) = \frac{\partial}{\partial x} (T_x \frac{\partial h}{\partial x}) + \frac{\partial}{\partial y} (T_y \frac{\partial h}{\partial y}) - S \frac{\partial h}{\partial t} - W$$

(71)

$$- \sum_{p=1}^{m} (\delta(x-x_p) \delta(y-y_p) Q_p) = 0.$$

Equation (71) is solved over the Domain D and enclosed by the Boundary B
by the Galerkin-finite element method. The boundary conditions are
given as

$$\frac{\partial h}{\partial x} = \text{constant} = \frac{\partial h}{\partial x}\Big|_B \qquad \text{on Boundary B} \qquad (72)$$

and

$$\frac{\partial h}{\partial y} = \text{constant} = \frac{\partial h}{\partial y}\Big|_B \qquad \text{on Boundary B} \qquad (73)$$

where $\frac{\partial h}{\partial x}$ and $\frac{\partial h}{\partial y}$ are the outward pointing derivatives from the boundary in
the x and y directions respectively. These boundary conditions represent
constant gradient boundaries (for a confined aquifer with constant values
of transmissivity in time, these boundary conditions also represent

constant flux boundaries). For the special case where $\frac{\partial h}{\partial x}\big|_B = 0$ and $\frac{\partial h}{\partial y}\big|_B = 0$ then the boundary conditions represent a no flow boundary.

To solve $L(h) = 0$ a trial solution given as

$$h(x,y,t) \simeq \hat{h}(x,y,t) = \sum_{j=1}^{n} (G_j(t)\phi_j(x,y)) \tag{74}$$

is used. Substitution of the trial solution given by equation (74) into the linear differential operator $L(h)$ given by equation (71) yields the residual

$$R(x,y,t) = L(\hat{h}) = \frac{\partial}{\partial x}\left[T_x \frac{\partial}{\partial x} \left(\sum_{j=1}^{n} (G_j(t)\phi_j(x,y)) \right) \right]$$

$$+ \frac{\partial}{\partial y}\left[T_y \frac{\partial}{\partial y} \left(\sum_{j=1}^{n} (G_j(t)\phi_j(x,y)) \right) \right]$$

$$- S \frac{\partial}{\partial t}\left[\sum_{j=1}^{n} (G_j(t)\phi_j(x,y)) \right] \tag{75}$$

$$- W - \sum_{p=1}^{m} (\delta(x-x_p)\delta(y-y_p) Q_p).$$

The approximating integral equation is formed by substitution of the residual given by equation (75) into equation (48) which yields

$$\iint_D \left\{ \frac{\partial}{\partial x} \left[T_x \frac{\partial}{\partial x} \left(\sum_{j=1}^{n} (G_j(t)\phi_j(x,y)) \right) \right] \right.$$

$$\left. + \frac{\partial}{\partial y}\left[T_y \frac{\partial}{\partial y} \left(\sum_{j=1}^{n} (G_j(t)\phi_j(x,y)) \right) \right] \right. \tag{76}$$

$$- S \frac{\partial}{\partial t} \left[\sum_{j=1}^{n} (G_j(t)\phi_j(x,y)) \right] - W$$

$$\left. - \sum_{p=1}^{m} (\delta(x-x_p)\delta(y-y_p) Q_p) \right\} \phi_i(x,y)dxdy = 0$$

$$i = 1,2\ldots n .$$

Expansion of equation (76) and differentiation inside the summation brackets yields

$$\iint\limits_{D} \left\{ \frac{\partial T_x}{\partial x} \phi_i(x,y) \left(\sum_{j=1}^{n} \left(G_j(t) \frac{\partial \phi_j(x,y)}{\partial x} \right) \right) \right.$$

$$+ T_x \phi_i(x,y) \left(\sum_{j=1}^{n} \left(G_j(t) \frac{\partial^2 \phi_j(x,y)}{\partial x^2} \right) \right)$$

$$+ \frac{\partial T_y}{\partial y} \phi_i(x,y) \left(\sum_{j=1}^{n} \left(G_j(t) \frac{\partial \phi_j(x,y)}{\partial y} \right) \right)$$

$$\left. + T_y \phi_i(x,y) \left(\sum_{j=1}^{n} \left(G_j(t) \frac{\partial^2 \phi_j(x,y)}{\partial y^2} \right) \right) \right\} dxdy \qquad (77)$$

$$- \iint\limits_{D} \left\{ S\phi_i(x,y) \left(\sum_{j=1}^{n} \left(\phi_j(x,y) \frac{\partial G_j(t)}{\partial t} \right) \right) \right\} dxdy$$

$$- \iint\limits_{D} \left\{ W \phi_i(x,y) \right\} dxdy$$

$$- \iint\limits_{D} \left\{ \phi_i(x,y) \left(\sum_{j=1}^{m} (\delta(x-x_p)\delta(y-y_p) Q_p) \right) \right\} dxdy = 0$$

$$i = 1,2\ldots n .$$

Substitution of the trial solution given by equation (74) into the boundary conditions given by equations (72) and (73) yields corresponding boundary conditions of the form

$$\sum_{j=1}^{n} \left(G_j(t) \frac{\partial \phi_j(x,y)}{\partial x} \right) = \text{constant} = \frac{\partial h}{\partial x}\Big|_B \text{ on Boundary B, and} \quad (78)$$

$$\sum_{j=1}^{n} \left(G_j(t) \frac{\partial \phi_j(x,y)}{\partial y} \right) = \text{constant} = \frac{\partial h}{\partial y}\Big|_B \text{ on Boundary B.} \quad (79)$$

4.2.2 Linearized Approximation

The following integral transformation is derived in Appendix C, equation (C9)

$$\iint_D \left\{ \frac{\partial \Psi_1}{\partial x} \phi_1 \frac{\partial \phi_2}{\partial x} + \Psi_1\phi_1 \frac{\partial^2 \phi_2}{\partial x^2} + \frac{\partial \Psi_2}{\partial y} \phi_1 \frac{\partial \phi_2}{\partial y} + \Psi_2\phi_1 \frac{\partial^2 \phi_2}{\partial y^2} \right\} dA$$

$$= -\iint_D \left\{ \Psi_1 \frac{\partial \phi_1}{\partial x} \frac{\partial \phi_2}{\partial x} + \Psi_2 \frac{\partial \phi_1}{\partial y} \frac{\partial \phi_2}{\partial y} \right\} dA \quad (80)$$

$$+ \oint_B \left\{ \Psi_1\phi_1 \frac{\partial \phi_2}{\partial x} \ell_x + \Psi_2\phi_2 \frac{\partial \phi_2}{\partial y} \ell_y \right\} dL$$

where $\Psi_1(x,y)$, $\Psi_2(x,y)$, $\phi_1(x,y)$ and $\phi_2(x,y)$ are scalars. Equation (80) applied to equation (77) yields

$$
- \iint\limits_{D} \left\{ T_x \frac{\partial \phi_i(x,y)}{\partial x} \left(\sum_{j=1}^{n} \left(G_j(t) \frac{\partial \phi_j(x,y)}{\partial x} \right) \right) \right.
$$

$$
\left. + T_y \frac{\partial \phi_i(x,y)}{\partial y} \left(\sum_{j=1}^{n} \left(G_j(t) \frac{\partial \phi_j(x,y)}{\partial y} \right) \right) \right\} dxdy
$$

$$
+ \oint\limits_{B} \left\{ T_x \phi_i(x,y) \left(\sum_{j=1}^{n} \left(G_j(t) \frac{\partial \phi_j(x,y)}{\partial x} \right) \right) \ell_x \right.
$$

$$
\left. + T_y \phi_i(x,y) \left(\sum_{j=1}^{n} \left(G_j(t) \frac{\partial \phi_j(x,y)}{\partial y} \right) \right) \ell_y \right\} dL \qquad (81)
$$

$$
- \iint\limits_{D} \left\{ S \, \phi_i(x,y) \left(\sum_{j=1}^{n} \left(\phi_j(x,y) \frac{G_j(t)}{t} \right) \right) \right\} dxdy
$$

$$
- \iint\limits_{D} \left\{ W \, \phi_i(x,y) \right\} dxdy
$$

$$
- \iint\limits_{D} \left\{ \phi_i(x,y) \left(\sum_{p=1}^{m} \left(\delta(x-x_p) \delta(y-y_p) \, Q_p \right) \right) \right\} dxdy = 0
$$

$$
i = 1, 2 \ldots n.
$$

From the boundary conditions given in equations (78) and (79) the $\frac{\partial h}{\partial x}$ and $\frac{\partial h}{\partial y}$ are a constant everywhere on the boundary. Substitution of the boundary conditions given by equations (78) and (79) into equation (81) yields

$$\iint\limits_{D} \left\{ T_x \frac{\partial \phi_i(x,y)}{\partial x} \left(\sum_{j=1}^{n} \left(G_j(t) \frac{\partial \phi_j(x,y)}{\partial x} \right) \right) \right.$$

$$\left. + T_y \frac{\partial \phi_i(x,y)}{\partial y} \left(\sum_{j=1}^{n} \left(G_j(t) \frac{\partial \phi_j(x,y)}{\partial y} \right) \right) \right\} dxdy$$

$$- \oint\limits_{B} \left\{ T_x \phi_i(x,y) \left(\frac{\partial h}{\partial x}\Big|_B \right) \ell_x + T_y \phi_i(x,y) \left(\frac{\partial h}{\partial y}\Big|_B \right) \ell_y \right\} dL$$

$$+ \iint\limits_{D} \left\{ S \phi_i(x,y) \left(\sum_{j=1}^{n} \left(\phi_j(x,y) \frac{\partial G_j(t)}{\partial t} \right) \right) \right\} dxdy \tag{82}$$

$$+ \iint\limits_{D} \left\{ W \phi_i(x,y) \right\} dxdy$$

$$+ \iint\limits_{D} \left\{ \phi_i(x,y) \left(\sum_{p=1}^{m} (\delta(x-x_p)\delta(y-y_p) Q_p) \right) \right\} dxdy = 0$$

$$i = 1, 2 \ldots n.$$

The n equations of equation (82) are written in matrix form as

$$[A] \ \{G\} \ + \ [B] \ \{\frac{dG}{dt}\} + \ [D] \ + \ [E] \ + \ [F] = 0 \tag{83}$$

where $[A]$ and $[B]$ are n x n dimensional matrices and $[D]$, $[E]$, $[F]$, $\{G\}$ and $\{\frac{dG}{dt}\}$ are n dimensional vectors. The elements of $[A]$, $[B]$, $[D]$, $[E]$ and $[F]$ are

$$A_{ij} = \iint_D \left\{ T_x \frac{\partial \phi_i(x,y)}{\partial x} \frac{\partial \phi_j(x,y)}{\partial x} + T_y \frac{\partial \phi_i(x,y)}{\partial y} \frac{\partial \phi_j(x,y)}{\partial y} \right\} dA, \qquad (84)$$

$$B_{ij} = \iint_D \left\{ S \phi_i(x,y) \phi_j(x,y) \right\} dA, \qquad (85)$$

$$D_i = \iint_D \left\{ W \phi_i(x,y) \right\} dA, \qquad (86)$$

$$E_i = \iint_D \left\{ \phi_i(x,y) \left(\sum_{p=1}^{m} (\delta(x-x_p)\delta(y-y_p) Q_p) \right) \right\} dA , \text{ and} \qquad (87)$$

$$F_i = -\oint_B \left\{ T_x \phi_i(x,y) \left(\frac{\partial h}{\partial x}\Big|_B \right)\ell_x + T_y \phi_i(x,y) \left(\frac{\partial h}{\partial y}\Big|_B \right)\ell_y \right\} dL \qquad (88)$$

4.2.3 Integrations

The integration of equations (84), (85), (86) and (88) is performed in a piecewise manner on an element basis. In doing so, element matrices are formed. Because there are three nodes in a triangular element, each element matrix will be of order three. The global matrix for the entire domain is formed from these element matrices by summing for a given node the

contribution to that node from each element matrix. In the element integration the local shape functions v^e replace the global shape functions ϕ. Using local shape functions, the approximating trial solution for h (equation 74) for the triangular element shown on Figure 11 with nodes i, j and k becomes

$$h(x,y,t) \simeq \hat{h}(x,y,t) = G_i(t)\, v_i^e(x,y)$$

$$+ G_j(t)\, v_j^e(x,y) + G_k(t)\, v_k^e(x,y). \tag{89}$$

The nodes i, j and k are numbered counterclockwise around the triangular element.

4.2.3.1 Integration of [A]

Consider the integration of equation (84). Assuming the values of transmissivity are known at the nodes, then in a manner analous to the trial solution for h the following approximations for transmissivity are made

$$T_x(x,y) \simeq T_{xi}\, v_i^e(x,y) + T_{xj}\, v_j^e(x,y) + T_{xk}\, v_k^e(x,y), \text{ and} \tag{90}$$

$$T_y(x,y) \simeq T_{yi}\, v_i^e(x,y) + T_{yj}\, v_j^e(x,y) + T_{yk}\, v_k^e(x,y) \tag{91}$$

where T_{xi}, T_{xj}, T_{xk}, T_{yi}, T_{yj} and T_{yk} are the known values of transmissivity at the nodes.

The element matrix [a] is

$$[a] = \iint_e (T_{xi} v_i^e + T_{xj} v_j^e + T_{xk} v_k^e) \begin{bmatrix} \dfrac{\partial v_i^e}{\partial x} \dfrac{\partial v_i^e}{\partial x} & \dfrac{\partial v_i^e}{\partial x} \dfrac{\partial v_j^e}{\partial x} & \dfrac{\partial v_i^e}{\partial x} \dfrac{\partial v_k^e}{\partial x} \\[2em] \dfrac{\partial v_j^e}{\partial x} \dfrac{\partial v_i^e}{\partial x} & \dfrac{\partial v_j^e}{\partial x} \dfrac{\partial v_j^e}{\partial x} & \dfrac{\partial v_j^e}{\partial x} \dfrac{\partial v_k^e}{\partial x} \\[2em] \dfrac{\partial v_k^e}{\partial x} \dfrac{\partial v_i^e}{\partial x} & \dfrac{\partial v_k^e}{\partial x} \dfrac{\partial v_j^e}{\partial x} & \dfrac{\partial v_k^e}{\partial x} \dfrac{\partial v_k^e}{\partial x} \end{bmatrix} dA$$

$$(92)$$

$$+ \iint_e (T_{yi} v_i^e + T_{yj} v_j^e + T_{yk} v_k^e) \begin{bmatrix} \dfrac{\partial v_i^e}{\partial y} \dfrac{\partial v_i^e}{\partial y} & \dfrac{\partial v_i^e}{\partial y} \dfrac{\partial v_j^e}{\partial y} & \dfrac{\partial v_i^e}{\partial y} \dfrac{\partial v_k^e}{\partial y} \\[2em] \dfrac{\partial v_j^e}{\partial y} \dfrac{\partial v_i^e}{\partial y} & \dfrac{\partial v_j^e}{\partial y} \dfrac{\partial v_j^e}{\partial y} & \dfrac{\partial v_j^e}{\partial y} \dfrac{\partial v_k^e}{\partial y} \\[2em] \dfrac{\partial v_k^e}{\partial y} \dfrac{\partial v_i^e}{\partial y} & \dfrac{\partial v_k^e}{\partial y} \dfrac{\partial v_j^e}{\partial y} & \dfrac{\partial v_k^e}{\partial y} \dfrac{\partial v_k^e}{\partial y} \end{bmatrix} dA$$

The partial derivatives $\dfrac{\partial v^e}{\partial x}$ and $\dfrac{\partial v^e}{\partial y}$ are obtained from differentiation of equations (54), (55), and (56) which yields

$$\frac{\partial v_i^e}{\partial x} = \frac{1}{2A\Delta} (y_j - y_k), \qquad \frac{\partial v_i^e}{\partial y} = \frac{1}{2A\Delta} (x_k - x_j), \qquad (93)$$

$$\frac{\partial v_j^e}{\partial x} = \frac{1}{2A\Delta} (y_k - y_i), \qquad \frac{\partial v_j^e}{\partial y} = \frac{1}{2A\Delta} (x_i - x_k), \text{ and} \qquad (94)$$

$$\frac{\partial v_k^e}{\partial x} = \frac{1}{2A\Delta} (y_i - y_j), \qquad \frac{\partial v_k^e}{\partial y} = \frac{1}{2A\Delta} (x_j - x_i). \qquad (95)$$

The partial derivatives $\frac{\partial v^e}{\partial x}$ and $\frac{\partial v^e}{\partial y}$ given by equations (93), (94) and (95) are constants and may be removed from under the integration sign in equation (92). This leaves the following integrations to perform

$$\iint_e (T_{xi} \, v_i^e + T_{xj} \, v_j^e + T_{xk} \, v_k^e) \, dA, \text{ and} \tag{96}$$

$$\iint_e (T_{yi} \, v_i^e + T_{yj} \, v_j^e + T_{yk} \, v_k^e) \, dA. \tag{97}$$

Recall that T_{xi}, T_{xj}, T_{xk}, T_{yi}, T_{yj} and T_{yk} are known values of transmissivity at the nodes and are constants. Integration of equations (96) and (97) are performed using the integration formula given in equation (69) from which

$$\iint_e v_r^e \, dA = \frac{A\Delta}{3} \qquad r = i,j,k \tag{98}$$

is obtained. Substitution of equations (93), (94) and (95) into equation (92) and applying equation (98) to equation (92) yields

$$[a] = \frac{(T_{xi}+T_{xj}+T_{xk})}{12A\Delta} \begin{bmatrix} (y_j-y_k)^2 & (y_j-y_k)(y_k-y_i) & (y_j-y_k)(y_i-y_j) \\ (y_k-y_i)(y_j-y_k) & (y_k-y_i)^2 & (y_k-y_i)(y_i-y_j) \\ (y_i-y_j)(y_j-y_k) & (y_i-y_j)(y_k-y_i) & (y_i-y_j)^2 \end{bmatrix} \tag{99}$$

$$+ \frac{(T_{yi}+T_{yj}+T_{yk})}{12A\Delta} \begin{bmatrix} (x_k-x_j)^2 & (x_k-x_j)(x_i-x_k) & (x_k-x_j)(x_j-x_i) \\ (x_i-x_k)(x_k-x_j) & (x_i-x_k)^2 & (x_i-x_k)(x_j-x_i) \\ (x_j-x_i)(x_k-x_j) & (x_j-x_i)(x_i-x_k) & (x_j-x_i)^2 \end{bmatrix} \text{(99 cont.)}$$

The global matrix [A] is formed by summing the element matrices [a] for all of the elements in the domain D. If nodes i and j in the local nodal system correspond to nodes p and q in the global nodal system, then a_{ij} in the element matrix is added to A_{pq} in the global matrix.

4.2.3.2 Integration of [B]

Consider the integration of equation (85). Assume the storage coefficient S is a constant over the entire domain D and, thus, also constant over the element of integration. Therefore S is removed from under the integration sign in equation (85).

The element matrix [b] is

$$[b] = S \iint_e \begin{bmatrix} v_i^e v_i^e & v_i^e v_j^e & v_i^e v_k^e \\ v_j^e v_i^e & v_j^e v_j^e & v_j^e v_k^e \\ v_k^e v_i^e & v_k^e v_j^e & v_k^e v_k^e \end{bmatrix} \tag{100}$$

The integration of equation (100), like the integration of [A] is most easily performed using the integration formula given in equation (69) from which this time

$$\iint_e v_r^e \, v_r^e \, dA = \frac{A \Delta}{6} \qquad r = i,j,k, \text{ and} \tag{101}$$

$$\iint_e v_r^e \, v_p^e \, dA = \frac{A\Delta}{12} \qquad r = i,j,k, \quad p = i,j,k, \text{ and } r \neq p \tag{102}$$

are obtained. Equations (101) and (102) applied to equation (100) yields

$$[b] = \begin{bmatrix} \dfrac{SA\Delta}{6} & \dfrac{SA\Delta}{12} & \dfrac{SA\Delta}{12} \\[3mm] \dfrac{SA\Delta}{12} & \dfrac{SA\Delta}{6} & \dfrac{SA\Delta}{12} \\[3mm] \dfrac{SA\Delta}{12} & \dfrac{SA\Delta}{12} & \dfrac{SA\Delta}{6} \end{bmatrix} . \tag{103}$$

The element matrix [b] is inserted into the global matrix [B] in an identical procedure as that used to insert [a] into [A].

4.2.3.3 Integration of [D]

Consider the integration of equation (86). In this equation W represents the volumetric water flux per unit area over the element of integration from a distributed source or sink and is a constant for the element. The element matrix [d] is

$$[d] = W \iint_e \begin{bmatrix} v_i^e \\[3mm] v_j^e \\[3mm] v_k^e \end{bmatrix} dA . \tag{104}$$

This integration was performed earlier for [a] in equation (98). Equation (98) applied to equation (104) yields

$$[d] = \begin{bmatrix} WA\Delta/3 \\ WA\Delta/3 \\ WA\Delta/3 \end{bmatrix}. \tag{105}$$

The element matrix [d] physically represents the sum of distributed source and sink terms (e.g. recharge or evapotranspiration) within the element of integration. The total volumetric water flux from a distributed source or sink for the element is $WA\Delta$. With the finite element method the source and sink terms are applied at the nodes. One-third of the total volumetric water flux from a distributed source or sink is therefore distributed to each of the three nodes comprising the vertices of the element.

If node i in the local nodal system corresponds to node p in the global nodal system then the global matrix [D] is formed by adding d_i to D_p.

2.4.3.4 Integration of [E]

Consider the integration of equation (87) which unlike the previous integrations is done globally. Equation (87) physically represents the point source and sink terms. If these point source and sink terms are applied only at the nodes then

$$E_i = \iint\limits_{D} \left\{ \sum_{p=1}^{n} (\delta(x-x_p)\delta(y-y_p) Q_p) \; \phi_i(x,y) \right\} dA \tag{106}$$

where Q_p represents the volumetric water flux at a node from a point source or sink which is a function of time only and therefore is considered as a constant in the integration and δ is the dirac delta function. A useful property of the dirac delta function is (Korn and Korn, 1968 or Pearson, 1974)

$$\int_a^b f(x)\delta(x-\xi)dx = \begin{cases} 0 & \text{if } x<a \quad \text{ or } x>b \\ f(\xi) & \text{if } a \quad <x <b \end{cases}.$$ (107)

Using equation (107), the integration of equation (106) was carried out in parts by integrating over an infinitesimally small area around each of the nodes and then over the reminder of the domain to yield

$$[E] = \begin{bmatrix} \sum\limits_{p=1}^{n} Q_p\phi_1(x_p,y_p) \\ \\ \sum\limits_{p=1}^{n} Q_p\phi_2(x_p,y_p) \\ \cdot \\ \cdot \\ \sum\limits_{p=1}^{n} Q_p\phi_n(x_p,y_p) \end{bmatrix}$$ (108)

Recall from the previous definition for the global shape functions ϕ that $\phi_i = 1$ at node i (i.e. $\phi_i(x_i,y_i) = 1$ and $\phi_i = 0$ at all other nodes (i.e. $\phi_i(x_j,y_j) = 0$, $j \neq i$). Thus, equation (108) simplifies to

$$[E] = \begin{bmatrix} Q_1 \\ Q_2 \\ \cdot \\ \cdot \\ \cdot \\ Q_n \end{bmatrix}$$ (109)

4.2.3.5 Integration of [F]

Finally, consider the integration of equation (88). The integration path for [F] is along the global boundary B. The boundary is broken into a series of piecewise continuous segments ΔL. Let nodes i and j be two nodes forming a boundary segment. The terms $\frac{\partial h}{\partial x}\big|_B$ and $\frac{\partial h}{\partial y}\big|_B$ in equation (88) are constant everywhere on the boundary and are known from the boundary conditions. The terms ℓ_x and ℓ_y are the cosines of the angles that the outward pointing normal makes with the x and y directions respectively (see Figure C1, Appendix C). These are specified along the boundary.

The matrix [f] is then

$$[f] = -\left(\frac{\partial h}{\partial x}\Big|_B\right)\ell_x \int_{\Delta L} (T_{xi}\, v_i^e + T_{xj}\, v_j^e)\begin{bmatrix} v_i^e \\ \\ v_j^e \end{bmatrix} dL$$

$$-\left(\frac{\partial h}{\partial y}\Big|_B\right)\ell_y \int_{\Delta L} (T_{yi}\, v_i^e + T_{yj}\, v_j^e)\begin{bmatrix} v_i^e \\ \\ v_i^e \end{bmatrix} dL. \tag{110}$$

The integration of equation (110) is performed using the integration formula given in equation (68) from which

$$\int_{\Delta L} v_r^e\, v_r^e\, dL = \frac{\Delta L}{3} \qquad r = i,j, \qquad \text{and} \tag{111}$$

$$\int_{\Delta L} v_r^e\, v_p^e\, dL = \frac{\Delta L}{6} \quad r = i,j, \quad p = i,j, \quad \text{and } r \neq p \tag{112}$$

are obtained. Equations (111) and (112) applied to equation (110) yields

$$[f] = -\left(\frac{\partial h}{\partial x}\Big|_B\right)\ell_x \frac{\Delta L}{6} \begin{bmatrix} 2T_{xi}+T_{xj} \\ \\ T_{xi}+2T_{xj} \end{bmatrix} - \left(\frac{\partial h}{\partial y}\Big|_B\right) \ell_y \frac{\Delta L}{6} \begin{bmatrix} 2T_{yi}+T_{yj} \\ \\ T_{yi}+2T_{yj} \end{bmatrix} \tag{113}$$

The order of [f] is two since only two nodes comprise a boundary segment. Equation (112) represents the volumetric water flux across the boundary segment. If $T_{xi} = T_{xj}$ and $T_{yi} = T_{yj}$ then one-half of the flux is assigned to node i and one-half of the flux is assigned to node j.

If node i in the local nodal system corresponds to node p in the global nodal system then the global matrix [F] is formed by adding f_i to F_p.

4.2.4 Time Derivative Approximation

Although the matrices [A] and [B] and the vectors [D], [E] and [F] have been evaluated, it is still necessary to solve the set of n ordinary differential equations given in equation (83) and repeated below

$$[A] \ \{G\} \ + [B] \ \{\frac{dG}{dt}\} \ + [D]+[E] \ + [F] = 0. \tag{114}$$

The time derivative is approximated by using a first-order correct implicit, finite-difference scheme

$$\frac{dG}{dt} = \frac{G_{t+\Delta t} - G_t}{\Delta t} \quad . \tag{115}$$

The vector $\{G\}$ is known at the time t and is to be evaluated for at the time $t + \Delta t$. Substitution of equation (115) into equation (114) and rearranging yields

$$\left([A] + \frac{1}{\Delta t} [B] \right) \{G_{t+\Delta t}\} = \frac{1}{\Delta t} [B] \{G_t\} - [D] - [E] - [F] \tag{116}$$

with all of the terms on the right hand side of the equation being known. Equation (116) was solved for using a point-iterative successive overrelaxation technique (Varga, 1962).

The partial differential equation for groundwater flow has been solved by the Galerkin finite-element method but it still remains to solve the coupled partial differential equations for solute transport (equations 43 and 44).

4.3 Solution of the Coupled Solute Transport Equations

4.3.1 Galerkin Approximation

The linear differential operators L_1 and L_2 are defined as

$$L_1(C) = \frac{\partial}{\partial x} \left(D_{xx} \frac{\partial C_1}{\partial x} \right) + \frac{\partial}{\partial y} \left(D_{yy} \frac{\partial C_1}{\partial y} \right) + \frac{\partial}{\partial x} \left(D_{xy} \frac{\partial C_1}{\partial y} \right)$$

$$+ \frac{\partial}{\partial y} \left(D_{yx} \frac{\partial C_1}{\partial x} \right) - \frac{\partial}{\partial x} (C_1 V_x) - \frac{\partial}{\partial y} (C_1 V_y)$$

(117)

$$- \left(1 + \frac{g_1}{g_3} \right) \frac{\partial C_1}{\partial t} + \left(\frac{g_2}{g_3} \right) \frac{\partial C_2}{\partial t} - \frac{WC_1'}{\varepsilon b}$$

$$- \sum_{p=1}^{m} \left(\delta(x-x_p) \delta(y-y_p) \frac{Q_p C_1'}{\varepsilon b} \right) \qquad \text{(117 cont.)}$$

for equation (43) and

$$L_2(C) = \frac{\partial}{\partial x} \left(D_{xx} \frac{\partial C_2}{\partial x} \right) + \frac{\partial}{\partial y} \left(D_{yy} \frac{\partial C_2}{\partial y} \right) + \frac{\partial}{\partial x} \left(D_{xy} \frac{\partial C_2}{\partial y} \right)$$

$$+ \frac{\partial}{\partial y} \left(D_{yx} \frac{\partial C_2}{\partial x} \right) - \frac{\partial}{\partial x} (C_2 V_x) - \frac{\partial}{\partial y} (C_2 V_y)$$

$$- \left(1 + \frac{g_2}{g_3} \right) \frac{\partial C_2}{\partial t} + \left(\frac{g_1}{g_3} \right) \frac{\partial C_1}{\partial t} - \frac{WC_2'}{\varepsilon b} \qquad \text{(118)}$$

$$- \sum_{p=1}^{m} \left(\delta(x-x_p) \delta(y-y_p) \frac{Q_p C_2'}{\varepsilon b} \right)$$

for equation (44). Equations (117) and (118) are solved on Domain D and enclosed by the boundary B by the Galerkin-finite element method. The boundary conditions are given as

$$C_1 = C_{1B}(x,y,t) = C_1 \big|_B \qquad \text{on Boundary B,} \qquad \text{(119)}$$

$$\frac{\partial C_1}{\partial x} = 0 = \frac{\partial C_1}{\partial x} \bigg|_B \qquad \text{on Boundary B,} \qquad \text{(120)}$$

$$\frac{\partial C_1}{\partial y} = 0 = \frac{\partial C_1}{\partial y}\Big|_B \qquad \text{on Boundary B,} \qquad (121)$$

$$C_2 = C_{2B}(x,y,t) = C_2\Big|_B \quad \text{on Boundary B,} \qquad (122)$$

$$\frac{\partial C_2}{\partial x} = 0 = \frac{\partial C_2}{\partial x}\Big|_B \qquad \text{on Boundary B, and} \qquad (123)$$

$$\frac{\partial C_2}{\partial y} = 0 = \frac{\partial C_2}{\partial y}\Big|_B \qquad \text{on Boundary B} \qquad (124)$$

where C_B is the prescribed concentration of C on the boundary and $\frac{\partial C}{\partial x}$ and $\frac{\partial C}{\partial y}$ are the outward pointing derivatives from the boundary in the x and y directions respectively. With these boundary conditions the concentration is prescribed everywhere on the boundary and the concentrations are constant across the boundary. The mass flux of the solute across the boundary due to hydrodynamic dispersion is zero (in essence the mass flux of the solute across the boundary is due solely to convective transport and is prescribed by the boundary conditions). The adsorbed concentrations are considered immobile.

To solve $L_1(C) = 0$ and $L_2(C) = 0$ trial solutions given as

$$C_1(x,y,t) \simeq \hat{C}_1(x,y,t) = \sum_{j=1}^{n} (G_{1j}(t)\phi_j(x,y)), \text{ and} \qquad (125)$$

$$C_2(x,y,t) \simeq \hat{C}_2(x,y,t) = \sum_{j=1}^{n} (G_{2j}(t)\phi_j(x,y)) \qquad (126)$$

are used. Only the Galerkin-finite element solution for equation (117)

is presented here. It is shown later how the simultaneous solution to both equations (117) and (118) are obtained. Substitution of the trial solutions for C_1 and C_2 given by equation (125) and (126) into the linear differential operator $L_1(C)$ given by equation (117) yields the residual

$$R_1(x,y,t) = L_1(\hat{C}) = \frac{\partial}{\partial x}\left[D_{xx} \frac{\partial}{\partial x}\left(\sum_{j=1}^{n} (G_{1j}(t)\phi_j(x,y)) \right) \right]$$

$$+ \frac{\partial}{\partial y}\left[D_{yy} \frac{\partial}{\partial y}\left(\sum_{j=1}^{n} (G_{1j}(t)\phi_j(x,y)) \right) \right]$$

$$+ \frac{\partial}{\partial x}\left[D_{xy} \frac{\partial}{\partial y}\left(\sum_{j=1}^{n} (G_{1j}(t)\phi_j(x,y)) \right) \right]$$

$$+ \frac{\partial}{\partial y}\left[D_{yx} \frac{\partial}{\partial x}\left(\sum_{j=1}^{n} (G_{1j}(t)\phi_j(x,y)) \right) \right]$$

$$- \frac{\partial}{\partial x}\left[V_x \sum_{j=1}^{n} (G_{1j}(t)\phi_j(x,y)) \right]$$

$$- \frac{\partial}{\partial y}\left[V_y \sum_{j=1}^{n} (G_{1j}(t)\phi_j(x,y)) \right]$$

$$- \left(1 + \frac{g_1}{g_3}\right)\left(\frac{\partial}{\partial t}\left[\sum_{j=1}^{n} (G_{1j}(t)\phi_j(x,y)) \right] \right)$$

(127)

(cont.next page)

$$+ \left(\frac{g_2}{g_3}\right)\left(\frac{\partial}{\partial t}\left[\sum_{j=1}^{n} (G_{2j}(t)\phi_j(x,y))\right]\right)$$

$$- \frac{WC_1'}{\varepsilon b} - \sum_{p=1}^{m} \left(\delta(x-x_p)\delta(y-y_p)\frac{Q_p C_1'}{\varepsilon b}\right).$$

The approximating integral equation is formed by substitution of the residual given by equation (127) into equation (48) which yields

$$\iint_{D} \left\{ \frac{\partial}{\partial x}\left[D_{xx}\frac{\partial}{\partial x}\left(\sum_{j=1}^{n}(G_{1j}(t)\phi_j(x,y))\right)\right] + \frac{\partial}{\partial y}\left[D_{yy}\frac{\partial}{\partial y}\left(\sum_{j=1}^{n}(G_{1j}(t)\phi_j(x,y))\right)\right]\right.$$

$$+ \frac{\partial}{\partial x}\left[D_{xy}\frac{\partial}{\partial y}\left(\sum_{j=1}^{n}(G_{1j}(t)\phi_j(x,y))\right)\right] + \frac{\partial}{\partial y}\left[D_{yx}\frac{\partial}{\partial x}\left(\sum_{j=1}^{n}(G_{1j}(t)\phi_j(x,y))\right)\right]$$

$$- \frac{\partial}{\partial x}\left[V_x\sum_{j=1}^{n}(G_{1j}(t)\phi_j(x,y))\right] - \frac{\partial}{\partial y}\left[V_y\sum_{j=1}^{n}(G_{1j}(t)\phi_j(x,y))\right] \qquad (128)$$

$$- \left(1+\frac{g_1}{g_3}\right)\left(\frac{\partial}{\partial t}\left[\sum_{j=1}^{n}(G_{1j}(t)\phi_j(x,y))\right]\right) + \left(\frac{g_2}{g_3}\right)\left(\frac{\partial}{\partial t}\left[\sum_{j=1}^{n}(G_{2j}(t)\phi_j(x,y))\right]\right)$$

$$\left. - \frac{WC_1'}{\varepsilon b} - \sum_{p=1}^{m}\left(\delta(x-x_p)\delta(y-y_p)\frac{Q_p C_1'}{\varepsilon b}\right)\right\}\phi_i(x,y)\ dxdy = 0$$

$$i = 1,2\ldots n.$$

Expansion of equation (128) and differentiation inside the summation brackets yields

$$
\iint\limits_{D} \left\{ \frac{\partial D_{xx}}{\partial x}\phi_i(x,y)\left(\sum_{j=1}^{n}\left(G_{1j}(t)\frac{\partial \phi_j(x,y)}{\partial x}\right)\right) + D_{xx}\phi_i(x,y)\left(\sum_{j=1}^{n}\left(G_{1j}(t)\frac{\partial^2 \phi_j(x,y)}{\partial x^2}\right)\right) \right.
$$

$$
\left. + \frac{\partial D_{yy}}{\partial y}\phi_i(x,y)\left(\sum_{j=1}^{n}\left(G_{1j}(t)\frac{\partial \phi_j(x,y)}{\partial y}\right)\right) + D_{yy}\phi_i(x,y)\left(\sum_{j=1}^{n}\left(G_{1j}(t)\frac{\partial^2 \phi_j(x,y)}{\partial y^2}\right)\right) \right\} dxdy
$$

$$
+ \iint\limits_{D} \left\{ \frac{\partial D_{xy}}{\partial x}\phi_i(x,y)\left(\sum_{j=1}^{n}\left(G_{1j}(t)\frac{\partial \phi_j(x,y)}{\partial y}\right)\right) + D_{xy}\phi_i(x,y)\left(\sum_{j=1}^{n} G_{1j}(t)\frac{\partial^2 \phi_j(x,y)}{\partial x\partial y}\right) \right.
$$

$$
\left. + \frac{\partial D_{yx}}{\partial y}\phi_i(x,y)\left(\sum_{j=1}^{n}\left(G_{1j}(t)\frac{\partial \phi_j(x,y)}{\partial x}\right)\right) + D_{yx}\phi_i(x,y)\left(\sum_{j=1}^{n}\left(G_{1j}(t)\frac{\partial^2 \phi_j(x,y)}{\partial x\partial y}\right)\right) \right\} dxdy
$$

$$
- \iint\limits_{D} \left\{ \frac{\partial V_x}{\partial x}\phi_i(x,y)\left(\sum_{j=1}^{n}\left(G_{1j}(t)\phi_j(x,y)\right)\right) + V_x\phi_i(x,y)\left(\sum_{j=1}^{n}\left(G_{1j}(t)\frac{\partial \phi_j(x,y)}{\partial x}\right)\right) \right.
$$

(129)

$$
\left. + \frac{\partial V_y}{\partial y}\phi_i(x,y)\left(\sum_{j=1}^{n}\left(G_{1j}(t)\phi_j(x,y)\right)\right) + V_y\phi_i(x,y)\left(\sum_{j=1}^{n}\left(G_{1j}(t)\frac{\partial \phi_j(x,y)}{\partial y}\right)\right) \right\} dxdy
$$

$$
- \iint\limits_{D} \left\{ \left(1 + \frac{g_1}{g_3}\right)\phi_i(x,y)\left(\sum_{j=1}^{n}\left(\phi_j(x,y)\frac{\partial G_{1j}(t)}{\partial t}\right)\right) \right\} dxdy
$$

$$
+ \iint\limits_{D} \left\{ \left(\frac{g_2}{g_3}\right)\phi_i(x,y)\left(\sum_{j=1}^{n}\left(\phi_j(x,y)\frac{\partial G_{2j}(t)}{\partial t}\right)\right) \right\} dxdy
$$

$$-\iint_D \left\{ \frac{WC_1'}{\varepsilon b} \phi_i(x,y) \right\} dxdy - \iint_D \left\{ \phi_i(x,y) \left(\sum_{p=1}^{m} \delta(x-x_p) \delta(y-y_p) \frac{Q_p C_1'}{\varepsilon b} \right) \right\} dxdy = 0$$

(129 cont.)

$$i = 1,2,\ldots n.$$

Substitution of the trial solution for C_1 given by equation (125) into the boundary conditions given by equations (119), (120) and (121) yields corresponding boundary conditions of the form

$$\sum_{j=1}^{n} G_{1j}(t) \phi_j(x,y) = C_{1B}(x,y,t) = C_1 \big|_B \qquad \text{on Boundary B,} \qquad (130)$$

$$\sum_{j=1}^{n} G_{1j}(t) \frac{\partial \phi_j(x,y)}{\partial x} = 0 = \frac{\partial C_1}{\partial x} \big|_B \qquad \text{on Boundary B, and} \qquad (131)$$

$$\sum_{j=1}^{n} G_{1j}(t) \frac{\partial \phi_j(x,y)}{\partial y} = 0 = \frac{\partial C_1}{\partial y} \big|_B \qquad \text{on Boundary B.} \qquad (132)$$

4.3.2 Linearized Approximation

The following integral transformations are derived in Appendix C, equations (C9), (C13) and (C17).

$$\iint_D \left\{ \frac{\partial \Psi_1}{\partial x} \phi_1 \frac{\partial \phi_2}{\partial x} + \Psi_1 \phi_1 \frac{\partial^2 \phi_2}{\partial x^2} + \frac{\partial \Psi_2}{\partial y} \phi_1 \frac{\partial \phi_2}{\partial y} + \Psi_2 \phi_1 \frac{\partial^2 \phi_2}{\partial y^2} \right\} dA$$

$$= - \iint_D \left\{ \Psi_1 \frac{\partial \phi_1}{\partial x} \frac{\partial \phi_2}{\partial x} + \Psi_2 \frac{\partial \phi_1}{\partial y} \frac{\partial \phi_2}{\partial y} \right\} dA \tag{133}$$

$$+ \oint_B \left\{ \Psi_1 \phi_1 \frac{\partial \phi_2}{\partial x} \ell_x + \Psi_2 \phi_2 \frac{\partial \phi_2}{\partial y} \ell_y \right\} dL,$$

$$\iint_D \left\{ \frac{\partial \Psi_1}{\partial x} \phi_1 \frac{\partial \phi_2}{\partial y} + \Psi_1 \phi_1 \frac{\partial^2 \phi_2}{\partial x \partial y} + \frac{\partial \Psi_2}{\partial y} \phi_1 \frac{\partial \phi_2}{\partial x} + \Psi_2 \phi_1 \frac{\partial^2 \phi_2}{\partial x \partial y} \right\} dA$$

$$= - \iint_D \left\{ \Psi_1 \frac{\partial \phi_1}{\partial x} \frac{\partial \phi_2}{\partial y} + \Psi_2 \frac{\partial \phi_1}{\partial y} \frac{\partial \phi_2}{\partial x} \right\} dA \tag{134}$$

$$+ \oint_B \left\{ \Psi_1 \phi_1 \frac{\partial \phi_2}{\partial y} \ell_x + \Psi_2 \phi_1 \frac{\partial \phi_2}{\partial x} \ell_y \right\} dL \quad , \text{ and}$$

$$\iint_D \left\{ \frac{\partial \Psi_1}{\partial x} \phi_1 \phi_2 + \Psi_1 \phi_1 \frac{\partial \phi_2}{\partial x} + \frac{\partial \Psi_2}{\partial y} \phi_1 \phi_2 + \Psi_2 \phi_1 \frac{\partial \phi_2}{\partial y} \right\} dA$$

$$= - \iint_D \left\{ \Psi_1 \frac{\partial \phi_1}{\partial x} \phi_2 + \Psi_2 \frac{\partial \phi_1}{\partial y} \phi_2 \right\} dA \tag{135}$$

$$+ \oint_B \left\{ \Psi_1 \phi_1 \phi_2 \ell_x + \Psi_2 \phi_1 \phi_2 \ell_y \right\} dL$$

where $\psi_1(x,y)$, $\psi_2(x,y)$, $\phi_1(x,y)$ and $\phi_2(x,y)$ are scalars.

Equations (133), (134) and (135) applied to equation (129) yields

$$- \iint_D \left\{ D_{xx} \frac{\partial \phi_i(x,y)}{\partial x} \left(\sum_{j=1}^{n} \left(G_{1j}(t) \frac{\partial \phi_j(x,y)}{\partial x} \right) \right) \right.$$

$$\left. + D_{yy} \frac{\partial \phi_i(x,y)}{\partial y} \left(\sum_{j=1}^{n} \left(G_{1j}(t) \frac{\partial \phi_j(x,y)}{\partial y} \right) \right) \right\} dxdy$$

$$+ \oint_B \left\{ D_{xx} \phi_i(x,y) \left(\sum_{j=1}^{n} \left(G_{1j}(t) \frac{\partial \phi_j(x,y)}{\partial x} \right) \right) \ell_x \right.$$

$$\left. + D_{yy} \phi_i(x,y) \left(\sum_{j=1}^{n} \left(G_{1j}(t) \frac{\partial \phi_j(x,y)}{\partial y} \right) \right) \ell_y \right\} dL$$

$$- \iint_D \left\{ D_{xy} \frac{\partial \phi_i(x,y)}{\partial x} \left(\sum_{j=1}^{n} \left(G_{1j}(t) \frac{\partial \phi_j(x,y)}{\partial y} \right) \right) \right.$$

(136)
(cont.next page)

$$\left. + D_{yx} \frac{\partial \phi_i(x,y)}{\partial y} \left(\sum_{j=1}^{n} \left(G_{1j}(t) \frac{\partial \phi_j(x,y)}{\partial x} \right) \right) \right\} dxdy$$

$$+ \oint_B \left\{ D_{xy} \phi_i(x,y) \left(\sum_{j=1}^{n} \left(G_{1j}(t) \frac{\partial \phi_j(x,y)}{\partial y} \right) \right) \ell_x \right.$$

$$\left. + D_{yx} \phi_i(x,y) \left(\sum_{j=1}^{n} \left(G_{1j}(t) \frac{\partial \phi_j(x,y)}{\partial x} \right) \right) \ell_y \right\} dL$$

$$+ \iint_D \left\{ V_x \frac{\partial \phi_i(x,y)}{\partial x} \left(\sum_{j=1}^n \left(G_{1j}(t) \phi_j(x,y) \right) \right) \right.$$

$$\left. + V_y \frac{\partial \phi_i(x,y)}{\partial y} \left(\sum_{j=1}^n \left(G_{1j}(t) \phi_j(x,y) \right) \right) \right\} dxdy$$

$$- \oint_B \left\{ V_x \phi_i(x,y) \left(\sum_{j=1}^n \left(G_{1j}(t) \phi_j(x,y) \right) \right) \ell_x \right.$$

$$\left. + V_y \phi_i(x,y) \left(\sum_{j=1}^n \left(G_{1j}(t) \phi_j(x,y) \right) \right) \ell_y \right\} dL$$

$$- \iint_D \left\{ \left(1 + \frac{g_1}{g_3} \right) \phi_i(x,y) \left(\sum_{j=1}^n \left(\phi_j(x,y) \frac{\partial G_{1j}(t)}{\partial t} \right) \right) \right\} dxdy$$

(136 cont.)

$$+ \iint_D \left\{ \left(\frac{g_2}{g_3} \right) \phi_i(x,y) \left(\sum_{j=1}^n \left(\phi_j(x,y) \frac{\partial G_{2j}(t)}{\partial t} \right) \right) \right\} dxdy$$

$$- \iint_D \left\{ \frac{W C_1'}{\varepsilon b} \phi_i(x,y) \right\} dxdy$$

$$- \iint_D \left\{ \phi_i(x,y) \left(\sum_{p=1}^m \delta(x-x_p) \delta(y-y_p) \frac{Q_p C_1'}{\varepsilon b} \right) \right\} dxdy = 0$$

$$i = 1, 2 \ldots n \ .$$

Recall from the boundary conditions given in equations (131) and (132) the $\partial C_1/\partial x$ and $\partial C_1/\partial y$ are zero everywhere on the boundary. Substitution of these boundary conditions into equation (136) causes the first two boundary integrals which contain these terms to vanish. From the boundary condition given in equation (130) the concentration C_1 is prescribed everywhere on the boundary and is equal to C_{1B}. Substitution of this boundary condition into the remaining boundary integral in equation (136) yields

$$
\iint_D \left\{ D_{xx} \frac{\partial \phi_i(x,y)}{\partial x} \left(\sum_{j=1}^{n} \left(G_{1j}(t) \frac{\partial \phi_j(x,y)}{\partial x} \right) \right) + D_{yy} \frac{\partial \phi_i(x,y)}{\partial y} \left(\sum_{j=1}^{n} \left(G_{1j}(t) \frac{\partial \phi_j(x,y)}{\partial y} \right) \right) \right.
$$

$$
+ D_{xy} \frac{\partial \phi_i(x,y)}{\partial x} \left(\sum_{j=1}^{n} \left(G_{1j}(t) \frac{\partial \phi_j(x,y)}{\partial y} \right) \right) + D_{yx} \frac{\partial \phi_i(x,y)}{\partial y} \left(\sum_{j=1}^{n} \left(G_{1j}(t) \frac{\partial \phi_j(x,y)}{\partial x} \right) \right)
$$

$$
\left. - V_x \frac{\partial \phi_i(x,y)}{\partial x} \left(\sum_{j=1}^{n} (G_{1j}(t) \phi_j(x,y)) \right) - V_y \frac{\partial \phi_i(x,y)}{\partial y} \left(\sum_{j=1}^{n} (G_{1j}(t) \phi_j(x,y)) \right) \right\} dxdy
$$

$$(137)$$
(cont. next page)

$$
+ \oint_B \left\{ V_x \phi_i(x,y) C_{1B}(x,y,t) \ell_x + V_y \phi_i(x,y) C_{1B}(x,y,t) \ell_y \right\} dL
$$

$$
+ \iint_D \left\{ \left(1 + \frac{g_1}{g_3} \right) \phi_i(x,y) \left(\sum_{j=1}^{n} \left(\phi_j(x,y) \frac{\partial G_{1j}(t)}{\partial t} \right) \right) \right\} dxdy
$$

$$
- \iint_D \left\{ \left(\frac{g_2}{g_3} \right) \phi_i(x,y) \left(\sum_{j=1}^{n} \left(\phi_j(x,y) \frac{\partial G_{2j}(t)}{\partial t} \right) \right) \right\} dxdy
$$

$$+ \iint_D \left| \frac{WC_1'}{\varepsilon b} \phi_i(x,y) \right| dxdy + \iint_D \left| \phi_i(x,y) \left(\sum_{p=1}^{m} \delta(x-x_p)\delta(y-y_p) \frac{Q_p C_1'}{\varepsilon b} \right) \right| dxdy = 0$$

<div align="right">(137 cont.)</div>

$$i = 1,2...n.$$

The n equations of equation (137) are written in matrix form as

$$[A]\ \{G_1\} + [B]\ \{\frac{dG_1}{dt}\} + [C]\ \{\frac{dG_2}{dt}\} + [D] + [E] + [F] = 0 \tag{138}$$

where [A], [B] and [C] are n x n dimensional matrices and [D], [E], [F], $\{G_1\}$, $\{\frac{dG_1}{dt}\}$ and $\{\frac{dG_2}{dt}\}$ are n dimensional vectors. The elements of [A], [B], [C], [D], [E] and [F] are

$$A_{ij} = \iint_D \left\{ D_{xx} \frac{\partial\phi_i(x,y)}{\partial x} \frac{\partial\phi_j(x,y)}{\partial x} + D_{yy} \frac{\partial\phi_i(x,y)}{\partial y} \frac{\partial\phi_j(x,y)}{\partial y} \right.$$

$$+ D_{xy} \frac{\partial\phi_i(x,y)}{\partial x} \frac{\partial\phi_j(x,y)}{\partial y} + D_{yx} \frac{\partial\phi_i(x,y)}{\partial y} \frac{\partial\phi_j(x,y)}{\partial x} \tag{139}$$

$$\left. - V_x \frac{\partial\phi_i(x,y)}{\partial x} \phi_j(x,y) - V_y \frac{\partial\phi_i(x,y)}{\partial y} \phi_j(x,y) \right| dA,$$

$$B_{ij} = \iint_D \left(1 + \frac{g_1}{g_3}\right) \phi_i(x,y)\phi_j(x,y)\ dA, \tag{140}$$

$$C_{ij} = -\iint_D \left(\frac{g_2}{g_3}\right) \phi_i(x,y)\phi_j(x,y) \; dA, \tag{141}$$

$$D_i = \iint_D \left| \frac{WC_1'}{\varepsilon b} \phi_i(x,y) \right| dA, \tag{142}$$

$$E_i = \iint_D \left\{ \phi_i(x,y) \left(\sum_{p=1}^{m} \delta(x-x_p)\delta(y-y_p) \frac{Q_p C_1'}{\varepsilon b} \right) \right\} dA, \text{ and} \tag{143}$$

$$F_i = \oint_B \left\{ V_x \phi_i(x,y) C_{1B}(x,y,t) \ell_x + V_y \phi_i(x,y) C_{1B}(x,y,t) \ell_y \right\} dL \tag{144}$$

4.3.3 Integrations

The integration of equations (139), (140), (141), (142) and (144) is performed in a piecewise manner on an element basis. Just as with the flow equation, element matrices are formed. The global matrix for the entire domain is formed from these element matrices by summing for a given node the contribution to that node from each element matrix. In the element integration the local shape functions v^e replace the global shape functions ϕ. Using local shape functions, the approximating trial solutions for C_1 and C_2 (equations 125 and 126) for a triangular element shown on Figure 11 with nodes i, j and k become

$$C_1(x,y,t) \simeq \hat{C}_1(x,y,t) = G_{1i}(t) \, v_i^e(x,y)$$

$$+ G_{1j}(t) \, v_j^e(x,y) + G_{1k}(t) \, v_k^e(x,y), \text{ and} \tag{145}$$

$$C_2(x,y,t) \simeq \hat{C}_2(x,y,t) = G_{2i}(t) \; v_i^e(x,y)$$

$$\text{(146)}$$

$$+ \; G_{2j}(t) \; v_j^e(x,y) + G_{2k}(t) \; v_k^e(x,y).$$

Again the nodes i,j,k are numbered counterclockwise around the triangular element.

4.3.3.1 Integration of [A]

Consider the integration of equation (139). Earlier in the solution of the flow equation the transmissivity T of the aquifer was assumed known at the nodes. It is further assumed that all other aquifer properties are also known at the nodes and the following approximations can therefore be made

$$V_x(x,y,t) \simeq V_{xi}(t) \; v_i^e(x,y) + v_{xj}(t) \; v_j^e(x,y) + V_{xk}(t) \; v_k^e(x,y), \quad \text{(147)}$$

$$V_y(x,y,t) \simeq V_{yi}(t) \; v_i^e(x,y) + V_{yj}(t) \; v_j^e(x,y) + v_{yk}(t) \; v_k^e(x,y), \quad \text{(148)}$$

$$D_{xx}(x,y,t) \simeq D_{xxi}(t) \; v_i^e(x,y) + D_{xxj}(t) \; v_j^e(x,y) + D_{xxk}(t) \; v_k^e(x,y), \quad \text{(149)}$$

$$D_{yy}(x,y,t) \simeq D_{yyi}(t) \; v_i^e(x,y) + D_{yyj}(t) \; v_j^e(x,y) + D_{yyk}(t) \; v_k^e(x,y), \quad \text{(150)}$$

$$D_{xy}(x,y,t) \simeq D_{xyi}(t) \; v_i^e(x,y) + D_{xyj}(t) \; v_j^e(x,y) + D_{xyk}(t) \; v_k^e(x,y), \text{ and } \text{(151)}$$

$$D_{yx}(x,y,t) \simeq D_{yxi}(t) \; v_i^e(x,y) + D_{yxj}(t) \; v_j^e(x,y) + D_{yxk}(t) \; v_k^e(x,y) \quad \text{(152)}$$

where V_{xi}, V_{xj}, V_{xk}, V_{yi}, V_{yj} and V_{yk} are known values of velocity at the nodes and D_{xxi}, D_{xxj}, D_{xxk}, D_{yyi}, D_{yyj}, D_{yyk}, D_{xyi}, D_{xyj}, D_{xyk}, D_{yxi}, D_{yxj} and D_{yxk} are known values of the dispersion coefficient at the nodes.

The element matrix [a] is

$$
[a] = \iint_e (D_{xxi} v_i^e + D_{xxj} v_j^e + D_{xxk} v_k^e)
\begin{bmatrix}
\dfrac{\partial v_i^e}{\partial x} \dfrac{\partial v_i^e}{\partial x} & \dfrac{\partial v_i^e}{\partial x} \dfrac{\partial v_j^e}{\partial x} & \dfrac{\partial v_i^e}{\partial x} \dfrac{\partial v_k^e}{\partial x} \\[2ex]
\dfrac{\partial v_j^e}{\partial x} \dfrac{\partial v_i^e}{\partial x} & \dfrac{\partial v_j^e}{\partial x} \dfrac{\partial v_j^e}{\partial x} & \dfrac{\partial v_j^e}{\partial x} \dfrac{\partial v_k^e}{\partial x} \\[2ex]
\dfrac{\partial v_k^e}{\partial x} \dfrac{\partial v_i^e}{\partial x} & \dfrac{\partial v_k^e}{\partial x} \dfrac{\partial v_j^e}{\partial x} & \dfrac{\partial v_k^e}{\partial x} \dfrac{\partial v_k^e}{\partial x}
\end{bmatrix} dA
$$

$$
+ \iint_e (D_{yyi} v_i^e + D_{yyj} v_j^e + D_{yyk} v_k^e)
\begin{bmatrix}
\dfrac{\partial v_i^e}{\partial y} \dfrac{\partial v_i^e}{\partial y} & \dfrac{\partial v_i^e}{\partial y} \dfrac{\partial v_j^e}{\partial y} & \dfrac{\partial v_i^e}{\partial y} \dfrac{\partial v_k^e}{\partial y} \\[2ex]
\dfrac{\partial v_j^e}{\partial y} \dfrac{\partial v_i^e}{\partial y} & \dfrac{\partial v_j^e}{\partial y} \dfrac{\partial v_j^e}{\partial y} & \dfrac{\partial v_j^e}{\partial y} \dfrac{\partial v_k^e}{\partial y} \\[2ex]
\dfrac{\partial v_k^e}{\partial y} \dfrac{\partial v_i^e}{\partial y} & \dfrac{\partial v_k^e}{\partial y} \dfrac{\partial v_j^e}{\partial y} & \dfrac{\partial v_k^e}{\partial y} \dfrac{\partial v_k^e}{\partial y}
\end{bmatrix} dA \quad (153)
$$

(cont. next page)

$$
+ \iint_e (D_{xyi} v_i^e + D_{xyj} v_j^e + D_{xyk} v_k^e)
\begin{bmatrix}
\dfrac{\partial v_i^e}{\partial x} \dfrac{\partial v_i^e}{\partial y} & \dfrac{\partial v_i^e}{\partial x} \dfrac{\partial v_j^e}{\partial y} & \dfrac{\partial v_i^e}{\partial x} \dfrac{\partial v_k^e}{\partial y} \\[2ex]
\dfrac{\partial v_j^e}{\partial x} \dfrac{\partial v_i^e}{\partial y} & \dfrac{\partial v_j^e}{\partial x} \dfrac{\partial v_j^e}{\partial y} & \dfrac{\partial v_j^e}{\partial x} \dfrac{\partial v_k^e}{\partial y} \\[2ex]
\dfrac{\partial v_k^e}{\partial x} \dfrac{\partial v_i^e}{\partial y} & \dfrac{\partial v_k^e}{\partial x} \dfrac{\partial v_j^e}{\partial y} & \dfrac{\partial v_k^e}{\partial x} \dfrac{\partial v_k^e}{\partial y}
\end{bmatrix} dA
$$

$$+ \iint_e (D_{yxi}v_i^e + D_{yxj}v_j^e + D_{yxk}v_k^e) \begin{bmatrix} \dfrac{\partial v_i^e}{\partial y}\dfrac{\partial v_i^e}{\partial x} & \dfrac{\partial v_i^e}{\partial y}\dfrac{\partial v_j^e}{\partial x} & \dfrac{\partial v_i^e}{\partial y}\dfrac{\partial v_k^e}{\partial x} \\[2ex] \dfrac{\partial v_j^e}{\partial y}\dfrac{\partial v_i^e}{\partial x} & \dfrac{\partial v_j^e}{\partial y}\dfrac{\partial v_j^e}{\partial x} & \dfrac{\partial v_j^e}{\partial y}\dfrac{\partial v_k^e}{\partial x} \\[2ex] \dfrac{\partial v_k^e}{\partial y}\dfrac{\partial v_i^e}{\partial x} & \dfrac{\partial v_k^e}{\partial y}\dfrac{\partial v_j^e}{\partial x} & \dfrac{\partial v_k^e}{\partial y}\dfrac{\partial v_k^e}{\partial x} \end{bmatrix} dA$$

$$- \iint_e (V_{xi}v_i^e + V_{xj}v_j^e + V_{xk}v_k^e) \begin{bmatrix} \dfrac{\partial v_i^e}{\partial x}v_i^e & \dfrac{\partial v_i^e}{\partial x}v_j^e & \dfrac{\partial v_i^e}{\partial x}v_k^e \\[2ex] \dfrac{\partial v_j^e}{\partial x}v_i^e & \dfrac{\partial v_j^e}{\partial x}v_j^e & \dfrac{\partial v_j^e}{\partial x}v_k^e \\[2ex] \dfrac{\partial v_k^e}{\partial x}v_i^e & \dfrac{\partial v_k^e}{\partial x}v_j^e & \dfrac{\partial v_k^e}{\partial x}v_k^e \end{bmatrix} dA \qquad \text{(153 cont.)}$$

$$- \iint_e (V_{yi}v_i^e + V_{yj}v_j^e + V_{yk}v_k^e) \begin{bmatrix} \dfrac{\partial v_i^e}{\partial y}v_i^e & \dfrac{\partial v_i^e}{\partial y}v_j^e & \dfrac{\partial v_i^e}{\partial y}v_k^e \\[2ex] \dfrac{\partial v_j^e}{\partial y}v_i^e & \dfrac{\partial v_j^e}{\partial y}v_j^e & \dfrac{\partial v_j^e}{\partial y}v_k^e \\[2ex] \dfrac{\partial v_k^e}{\partial y}v_i^e & \dfrac{\partial v_k^e}{\partial y}v_j^e & \dfrac{\partial v_k^e}{\partial y}v_k^e \end{bmatrix} dA$$

The partial derivatives $\dfrac{\partial v^e}{\partial x}$ and $\dfrac{\partial v^e}{\partial y}$ were obtained previously in equations (93), (94) and (95) for the solution of the flow equation. Recall that these partial derivations are constants and thus could be removed from under the integration sign. This leaves integrations of the form

$$\iint_e (D_r v_r^e) \, dA \qquad\qquad r=i,j,k, \tag{154}$$

$$\iint_e (V_r v_r^e v_r^e) \, dA \qquad r=i,j,k, \text{ and} \tag{155}$$

$$\iint_e (V_p v_p^e v_r^e) \, dA \qquad r=i,j,k, \qquad p=i,j,k, \text{ and} \quad r \neq p. \tag{156}$$

Recall that D_i, D_j, D_k, V_i, V_j and V_k are known values at the nodes which are functions of time only and as such may be considered constants in this integration. These integrations were performed earlier in the solution of the flow equation as equations (98), (101) and (102) and are repeated below as

$$\iint_e v_r^e \, dA = \frac{A\Delta}{3} \qquad\qquad r=i,j,k, \tag{157}$$

$$\iint_e v_r^e v_r^e \, dA = \frac{A\Delta}{6} \qquad\qquad r=i,j,k, \text{ and} \tag{158}$$

$$\iint_e v_p^e v_r^e \, dA = \frac{A\Delta}{12} \qquad r=i,j,k, \qquad p=i,j,k, \text{ and} \quad r \neq p. \tag{159}$$

Substitution of equations (93), (94) and (95) into equation (153) and applying equations (157), (158) and (159) to equation (153) yields

$$[a] = \left(\frac{D_{xxi}+D_{xxj}+D_{xxk}}{12A\Delta}\right)\begin{bmatrix} (y_j-y_k)^2 & (y_j-y_k)(y_k-y_i) & (y_j-y_k)(y_i-y_j) \\ (y_k-y_i)(y_j-y_k) & (y_k-y_i)^2 & (y_k-y_i)(y_i-y_j) \\ (y_i-y_j)(y_j-y_k) & (y_i-y_j)(y_k-y_i) & (y_i-y_j)^2 \end{bmatrix}$$

$$+ \left(\frac{D_{yyi}+D_{yyj}+D_{yyk}}{12A\Delta}\right)\begin{bmatrix} (x_k-x_j)^2 & (x_k-x_j)(x_i-x_k) & (x_k-x_j)(x_j-x_i) \\ (x_i-x_k)(x_k-x_j) & (x_i-y_k)^2 & (x_i-x_k)(x_j-x_i) \\ (x_j-x_i)(x_k-x_j) & (x_j-x_i)(x_i-x_k) & (x_j-x_i)^2 \end{bmatrix}$$

(160)

$$+ \left(\frac{D_{xyi}+D_{xyj}+D_{xyk}}{12A\Delta}\right)\begin{bmatrix} (y_j-y_k)(x_k-x_j) & (y_j-y_k)(x_i-x_k) & (y_j-y_k)(x_j-x_i) \\ (y_k-y_i)(x_k-x_j) & (y_k-y_i)(x_i-x_k) & (y_k-y_i)(x_j-x_i) \\ (y_i-y_j)(x_k-x_j) & (y_i-y_j)(x_i-x_k) & (y_i-y_j)(x_j-x_i) \end{bmatrix}$$

$$+ \left(\frac{D_{yxi}+D_{yxj}+D_{yxk}}{12A\Delta}\right)\begin{bmatrix} (x_k-x_j)(y_j-y_k) & (x_k-y_j)(y_k-y_i) & (x_k-x_j)(y_i-y_j) \\ (x_i-x_k)(y_j-y_k) & (x_i-y_k)(y_k-y_i) & (x_i-x_k)(y_i-y_j) \\ (x_j-x_i)(y_j-y_k) & (x_j-x_i)(y_k-y_i) & (x_j-x_i)(y_i-y_j) \end{bmatrix}$$

$$
-\frac{1}{24}
\begin{bmatrix}
(2V_{xi}+V_{xj}+V_{xk})(y_j-y_k) & (V_{xi}+2V_{xj}+V_{xk})(y_j-y_k) & (V_{xi}+V_{xj}+2V_{xk})(y_j-y_k) \\
\\
(2V_{xi}+V_{xj}+V_{xk})(y_k-y_i) & (V_{xi}+2V_{xj}+V_{xk})(y_k-y_i) & (V_{xi}+V_{xj}+2V_{xk})(y_k-y_i) \\
\\
(2V_{xi}+V_{xj}+V_{xk})(y_i-y_j) & (V_{xi}+2V_{xj}+V_{xk})(y_i-y_j) & (V_{xi}+V_{xj}+2V_{xk})(y_i-y_j)
\end{bmatrix}
$$

(160 cont.)

$$
-\frac{1}{24}
\begin{bmatrix}
(2V_{yi}+V_{yj}+V_{yk})(x_k-x_j) & (V_{yi}+2V_{yj}+V_{yk})(x_k-x_j) & (V_{yi}+V_{yj}+2V_{yk})(x_k-x_j) \\
\\
(2V_{yi}+V_{yj}+V_{yk})(x_i-x_k) & (V_{yi}+2V_{yj}+V_{yk})(x_i-x_k) & (V_{yi}+V_{yj}+2V_{yk})(x_i-x_k) \\
\\
(2V_{yi}+V_{yj}+V_{yk})(x_j-x_i) & (V_{yi}+2V_{yj}+V_{yk})(x_j-x_i) & (V_{yi}+V_{yj}+2V_{yk})(x_j-x_i)
\end{bmatrix}
$$

The element matrix [a] is inserted into the global matrix [A] as follows. If nodes i and j in the nodal system correspond to nodes p and q in the global system, then a_{ij} in the element matrix is added to A_{pq} in the global matrix.

4.3.3.2 Integration of [B] and [C]

Consider the integration of equations (140) and (141). Recall that the parameters g_1, g_2 and g_3 in these equations were defined by equations (36), (37) and (38) and are dependent on the dissolved concentration C, the adsorbed concentration $\overline{C}$ and the CEC of the porous media (all of which are either calculated or assumed known at the nodes). Similar to the approximations made for transmissivity T, velocity V, and coefficient of dispersion D, the following approximations are made

$$\frac{g_1(x,y,t)}{g_3(x,y,t)} \simeq \frac{g_{1i}(t)}{g_{3i}(t)} \ v_i^e(x,y) + \frac{g_{1j}(t)}{g_{3j}(t)} \ v_j^e(x,y) + \frac{g_{1k}(t)}{g_{3k}(t)} \ v_k^e(x,y), \text{ and} \quad (161)$$

$$\frac{g_2(x,y,t)}{g_3(x,y,t)} \simeq \frac{g_{2i}(t)}{g_{3i}(t)} \ v_i^e(x,y) + \frac{g_{2j}(t)}{g_{3j}(t)} \ v_j^e(x,y) + \frac{g_{2k}(t)}{g_{3k}(t)} \ v_k^e(x,y) \quad (162)$$

where g_{1i}, g_{1j}, g_{1k}, g_{2i}, g_{2j}, g_{2k}, g_{3i}, g_{3j} and g_{3k} are known values of the parameters at the nodes.

The element matrices [b] and [c] are

$$[b] = \iint\limits_{e} \left(1 + \frac{g_{1i}}{g_{3i}} v_i^e + \frac{g_{1j}}{g_{3j}} v_j^e + \frac{g_{1k}}{g_{3k}} v_k^e\right) \begin{bmatrix} v_i^e v_i^e & v_i^e v_j^e & v_i^e v_k^e \\ v_j^e v_i^e & v_j^e v_j^e & v_j^e v_k^e \\ v_k^e v_i^e & v_k^e v_j^e & v_k^e v_k^e \end{bmatrix} dA \quad (163)$$

, and

$$[c] = -\iint\limits_{e} \left(\frac{g_{2i}}{g_{3i}} v_i^e + \frac{g_{2j}}{g_{3j}} v_j^e + \frac{g_{2k}}{g_{3k}} v_k^e\right) \begin{bmatrix} v_i^e v_i^e & v_i^e v_j^e & v_i^e v_k^e \\ v_j^e v_i^e & v_j^e v_j^e & v_j^e v_k^e \\ v_k^e v_i^e & v_k^e v_j^e & v_k^e v_k^e \end{bmatrix} dA \quad (164)$$

The integration of equations (163) and (164) is performed using integration formulas developed from equation (69) from which

$$\iint\limits_{e} v_r^e v_r^e \ dA = \frac{A\Delta}{6} \qquad r=i,j,k, \tag{165}$$

$$\iint\limits_{e} v_r^e v_p^e \ dA = \frac{A\Delta}{12} \qquad r=i,j,k, \quad p=i,j,k, \quad \text{and } r \neq p, \tag{166}$$

$$\iint\limits_{e} v_r^e v_r^e v_r^e \ dA = \frac{A\Delta}{10} \qquad r=i,j,k, \tag{167}$$

$$\iint\limits_{e} v_r^e v_r^e v_p^e \ dA = \frac{A\Delta}{30} \qquad r=i,j,k, \quad p=i,j,k, \quad \text{and } r \neq p, \text{ and} \tag{168}$$

$$\iint\limits_{e} v_r^e v_p^e v_q^e \ dA = \frac{A\Delta}{60} \qquad r=i,j,k, \quad p=i,j,k, \quad q=i,j,k,$$

$$\text{and } r \neq p \neq q, \tag{169}$$

are obtained. Equations (165) - (169) applied to equations (163) and (164) yields

$$[b] = \frac{A\Delta}{60} \begin{bmatrix} 10+6g_{13i}+2g_{13j}+2g_{13k} & 5+2g_{13i}+2g_{13j}+g_{13k} & 5+2g_{13i}+g_{13j}+2g_{13k} \\ 5+2g_{13i}+2g_{13j}+g_{13k} & 10+2g_{13i}+6g_{13j}+2g_{13k} & 5+g_{13i}+2g_{13j}+2g_{13k} \\ 5+2g_{13i}+g_{13j}+2g_{13k} & 5+g_{13i}+2g_{13j}+2g_{13k} & 10+2g_{13i}+2g_{13j}+6g_{13k} \end{bmatrix} \quad (170)$$

where $g_{13} = g_1/g_3$ and

$$[c] = -\frac{A\Delta}{60} \begin{bmatrix} 6g_{23i}+2g_{23j}+2g_{23k} & 2g_{23i}+2g_{23j}+g_{23k} & 2g_{23i}+g_{23j}+2g_{23k} \\ 2g_{23i}+2g_{23j}+g_{23k} & 2g_{23i}+6g_{23j}+2g_{23k} & g_{23i}+2g_{23j}+2g_{23k} \\ 2g_{23i}+g_{23j}+2g_{23k} & g_{23i}+2g_{23j}+2g_{23k} & 2g_{23i}+2g_{23j}+6g_{23k} \end{bmatrix} \quad (171)$$

where $g_{23} = g_2/g_3$.

The element matrices [b] and [c] are inserted into the global matrices [B] and [C] respectively, in an identical procedure as that used to insert [a] into [A].

4.3.3.3 Integration of [D]

Consider the integration of equation (142). In this equation, W represents the volumetric flux per unit area over the element of integration from a distributed source or sink and C_1' is the concentration of W. Both are constants for the element. The porosity ε is assumed a constant over the entire Domain D and thus

also constant over the element of integration. Recall that all aquifer properties are assumed known at the nodes. Similar to the previous approximations, the following approximation is made

$$\frac{1}{b(x,y,t)} = \frac{1}{b_i(t)} v_i^e + \frac{1}{b_j(t)} v_j^e + \frac{1}{b_k(t)} v_k^e \tag{172}$$

where b_i, b_j and b_k are the known saturated thicknesses of the aquifer at the nodes.

The element matrix [d] is

$$[d] = \frac{C_1'W}{\varepsilon} \iint_e \left(\frac{1}{b_i} v_i^e + \frac{1}{b_j} v_j^e + \frac{1}{b_k} v_k^e \right) \begin{bmatrix} v_i^e \\ v_j^e \\ v_k^e \end{bmatrix} dA \tag{173}$$

This integration has been performed several times before in equations (101) and (102), (158) and (159), or (165) and (166). Integration of equation (173) yields

$$[d] = \frac{C_1'WA\,\Delta}{\varepsilon 6} \begin{bmatrix} \dfrac{1}{b_i} + \dfrac{1}{2b_j} + \dfrac{1}{2b_k} \\[2ex] \dfrac{1}{2b_i} + \dfrac{1}{b_j} + \dfrac{1}{2b_k} \\[2ex] \dfrac{1}{2b_i} + \dfrac{1}{2b_j} + \dfrac{1}{b_k} \end{bmatrix} \tag{174}$$

The element matrix [d] physically represents the sum of the mass flux from distributed sources or sinks within the element of integration. With the finite element method a source or sink is applied at the

nodes. If $b_i = b_j = b_k$ then the total mass flux for the element from distributed sources or sinks per unit volume of solution per unit thickness of the aquifer is $\dfrac{C_1^{'}WA\Delta}{\epsilon b}$ of which one-third is distributed to each of the three nodes comprising the veritices of the element.

If node i in the local nodal system corresponds to node p in the global nodal system then the global matrix [D] is formed by adding d_i to D_p.

4.3.3.4   Integration of [E]

Consider the integration of equation (144) which, unlike most of the previous integrations, is done globally. Equation (143) physically represents the mass flux from a point source or sink. If these point sources or sinks are applied only at the nodes then

$$E_i = \iint\limits_{D} \left\{ \sum_{p=1}^{n} \delta(x-x_p)\delta(y-y_p) \frac{Q_p C_{1p}^{'}}{\epsilon b_p} \phi_i(x,y) \right\} dA \tag{175}$$

where Q_p represents the volumetric flux from a point source or sink at the node and $C_{1p}^{'}$ is the concentration of C_1 in Q_p. Both of these are functions of time only and therefore are considered as constants in the space integration. The porosity ϵ is assumed constant everywhere in the Domain D. Recall that δ is the dirac delta function. The integration of equation (175) is done in an identical manner as the integration of equation (106) for a point source or sink in the solution of the groundwater flow equation. Using the property of the dirac delta function given in equation (107) that

$$\int_a^b f(x)\delta(x-\xi)dx = \left\{ \begin{array}{l} 0 \text{ if } x<a \text{ or } x>b \\ f(\xi) \text{ if } a<x<b \end{array} \right\} \tag{176}$$

then the integration of (175) was carried out in parts by integrating over an infinitismally small area around each of the nodes and then over the remainder of the domain to yield

$$[E] = \begin{bmatrix} \sum_{p=1}^{n} \frac{Q_p C'_{1p}}{\varepsilon b_p} \phi_1(x_p, y_p) \\ \\ \sum_{p=1}^{n} \frac{Q_p C'_{1p}}{\varepsilon b_p} \phi_2(x_p, y_p) \\ \vdots \\ \sum_{p=1}^{n} \frac{Q_p C'_{1p}}{\varepsilon b_p} \phi_n(x_p, y_p) \end{bmatrix} \cdot \tag{177}$$

The aquifer thickness b is known at the nodes and thus could be treated as a constant in the infinitesimally small area about each node. Recall from the previous definition for the global shape functions ϕ that $\phi_i = 1$ at node i (i.e. $\phi_i(x_i, y_i) = 1$) and $\phi_i = 0$ at all other nodes (i.e. $\phi_i(x_j, y_j) = 0$, $j \neq i$). Thus equation (177) simplifies to

$$[E] = \begin{bmatrix} \dfrac{Q_1 C'_{11}}{\varepsilon b_1} \\ \\ \dfrac{Q_2 C'_{12}}{\varepsilon b_2} \\ \vdots \\ \dfrac{Q_n C'_{1n}}{\varepsilon b_n} \end{bmatrix} \tag{178}$$

4.3.3.5 Integration of [F]

Finally, consider the integration of equation (144). The integration path for [F] is along the global boundary B. The boundary is broken into a series of piecewise continuous segments ΔL. Let nodes i and j be two nodes forming a boundary segment. The boundary concentration C_{1B} in equation (144) is known from the boundary conditions and is specified along the boundary segment ΔL as

$$C_{1B}(x,y,t) \simeq C_{1Bi}(t)\, v_i^e(x,y) + C_{1Bj}(t)\, v_j^e(x,y) \tag{179}$$

where C_{1Bi} and C_{1Bj} are known values of the concentration of C_1 at the boundary nodes. The terms ℓ_x and ℓ_y are the cosines of the angles that the outward pointing normal makes with the x and y directions respectively (see Figure C1, Appendix C).These are specified along the boundary.

The element matrix [f] is then

$$[f] = \ell_x \int_{\Delta L} (V_{xi}\, v_i^e + V_{xj}\, v_j^e)(C_{1Bi}\, v_i^e + C_{1Bj}\, v_j^e) \begin{bmatrix} v_i^e \\ \\ v_j^e \end{bmatrix} dL$$

$$+ \ell_y \int_{\Delta L} (V_{yi}\, v_i^e + V_{yj}\, v_j^e)(C_{1Bi}\, v_i^e + C_{1Bj}\, v_j^e) \begin{bmatrix} v_i^e \\ \\ v_j^e \end{bmatrix} dL \tag{180}$$

The integration of equation (180) is performed using the integration formula given in equation (68)   from which

$$\int_{\Delta L} v_r^e \, v_r^e \, v_r^e \, dL = \frac{\Delta L}{4} \qquad\qquad r=i,j, \text{ and} \qquad\qquad (181)$$

$$\int_{\Delta L} v_r^e \, v_r^e \, v_p^e \, dL = \frac{\Delta L}{12} \qquad r=i,j, \quad p=i,j, \text{ and } \quad r \ne p \qquad (182)$$

are obtained. Equations (181) and (182) applied to equation (180) yields

$$[f] = \ell_x \frac{\Delta L}{12} \begin{bmatrix} 3V_{xi} \, C_{1Bi} + V_{xi} \, C_{1Bj} + V_{xj} \, C_{1Bi} + V_{xj} \, C_{1Bj} \\ \\ V_{xi} \, C_{1Bi} + V_{xi} \, C_{1Bj} + V_{xj} \, C_{1Bi} + 3V_{xj} \, C_{1Bj} \end{bmatrix}$$

$$(183)$$

$$+ \ell_y \frac{\Delta L}{12} \begin{bmatrix} 3V_{yi} \, C_{1Bi} + V_{yi} \, C_{1Bj} + V_{yj} \, C_{1Bi} + V_{yj} \, C_{1Bj} \\ \\ V_{yi} \, C_{1Bi} + V_{yi} \, C_{1Bj} + V_{yj} \, C_{1Bi} + 3V_{yj} \, C_{1Bj} \end{bmatrix}$$

The order of [f] is two since only two nodes comprise a boundary segment. Equation (183) represents the mass flux of the solute across the boundary due to convective transport. Recall from the boundary conditions that the mass flux of the solute across the boundary due to hydrodynamic dispersion is zero.

If node i in the local nodal system corresponds to node p in the global nodal system then the global matrix [F] is formed by adding f_i to F_p.

4.3.4 Time-Derivative Approximation

Although the matrices [A], [B], and [C] and the vectors [D], [E], and [F] have been evaluated, it is still necessary to solve the set of n ordinary differential equations given in equation (138) and repeated below

$$[A] \ \{G_1\} + [B] \ \{\frac{dG_1}{dt}\} + [C] \ \{\frac{dG_2}{dt}\} + [D] + [E] + [F] = 0 \tag{184}$$

As was done with the flow equation, the time derivative is approximated by using a first-order correct implicit, finite-difference scheme

$$\frac{dG}{dt} = \frac{G_{t+\Delta t} - G_t}{\Delta t} \tag{185}$$

The vector $\{G\}$ is known at the time t and is to be evaluated for at the time $t + \Delta t$. Substitution of equation (185) into equation (184) and rearranging yields

$$([A] + \frac{1}{\Delta t} \ [B]) \ \{G_{1 \ t+\Delta t}\} + \frac{1}{\Delta t} \ [C] \ \{G_{2 \ t+\Delta t}\}$$

$$\tag{186}$$

$$= \frac{1}{\Delta t} \ [B] \ \{G_{1t}\} + \frac{1}{\Delta t} \ [C] \ \{G_{2t}\} - [D] - [E] - [F]$$

with all of the terms on the right hand side of the equation being known.

Recall that there were two equations to be solved $L_1(C) = 0$ (equation 117) and $L_2(C) = 0$ (equation 118) and thus far only the solution of $L_1(C) = 0$ has been considered. It remains then to solve $L_2(C) = 0$. The simultaneous solution of $L_1(C) = 0$ and $L_2(C) = 0$ is

obtained by assembling a coupled matrix equation similar in form to equation (186).

4.3.5 Assembly of the Coupled Solutions

The solution of $L_2(C) = 0$ proceeds in an identical manner as the previous solution to $L_1(C) = 0$. Let the subscript 1 denote matrices relating to solution of $L_1(C) = 0$ and the subscript 2 denote matrices relating to solution of $L_2(C) = 0$. It is then easy to show that the element matrices are related as

$$[a_2] = [a_1] \qquad \text{(see equation 160),} \qquad (187)$$

$$[b_2] = [b_1] \qquad \text{with the value } g_{13} \text{ in } b_1 \text{ replaced by } g_{23}$$
$$\text{in } b_2 \text{ (see equation 170)} \qquad (188)$$

$$[c_2] = [c_1] \qquad \text{with the value } g_{23} \text{ in } c_1 \text{ replaced by } g_{13}$$
$$\text{in } c_2 \text{ (see equation 171)} \qquad (189)$$

$$[d_2] = [d_1] \qquad \text{with the value } C_1' \text{ in } d_1 \text{ replaced by } C_2' \text{ in}$$
$$d_2 \text{ (see equation 174)} \qquad (190)$$

$$[E_2] = [E_1] \qquad \text{with the value } C_1' \text{ in } E_1 \text{ replaced by } C_2' \text{ in}$$
$$E_2 \text{ (see equation 178)} \qquad (191)$$

$$[f_2] = [f_1] \qquad \text{with the value } C_{1B} \text{ in } f_1 \text{ replaced by } C_{2B}$$
$$\text{in } f_2 \text{ (see equation 183)} \qquad (192)$$

Using this notation then equation (186) is rewritten as

$$([A_1] + \frac{1}{\Delta t} [B_1] \quad \{G_{1 \ t+\Delta t}\} + \frac{1}{\Delta t} [C_1] \{G_{2 \ t+\Delta t}\}$$

$$(193.)$$

$$= \frac{1}{\Delta t} [B_1] \{G_{1t}\} + \frac{1}{\Delta t} [C_1] \{G_{2t}\} - [D_1] - [E_1] - [F_1].$$

The parallel equation is

$$([A_2] + \frac{1}{\Delta t} [B_2]) \{G_{2 \ t+\Delta t}\} + \frac{1}{\Delta t} [C_2] \{G_{1 \ t+\Delta t}\}$$

$$(194)$$

$$= \frac{1}{\Delta t} [B_2] \{G_{2t}\} + \frac{1}{\Delta t} [C_2] \{G_{1t}\} - [D_2] - [E_2] - [F_2].$$

The simultaneous solution of equations (193) and (194) for $\{G_{1 \ t+\Delta t}\}$ and $\{G_{2 \ t+\Delta t}\}$ is obtained by assembling the matrix equation

$$([A'] + \frac{1}{\Delta t} [B']) \{G'_{t+\Delta t}\} = \frac{1}{\Delta t} [B'] \{G'_t\} - [D'] - [E'] - [F'] \quad (195)$$

where

$$[A'] = \begin{bmatrix} A_1 & \vdots & 0 \\ - & - \vdots - & - \\ 0 & \vdots & A_2 \end{bmatrix} \quad ,$$

$$[B'] = \begin{bmatrix} B_1 & \vdots & C_1 \\ - & - \vdots - & - \\ C_2 & \vdots & B_2 \end{bmatrix} \quad ,$$

$$[D'] = \begin{bmatrix} D_1 \\ - & - \\ D_2 \end{bmatrix} \quad ,$$

$$[E^\prime] = \begin{bmatrix} E_1 \\ -- \\ E_2 \end{bmatrix},$$

$$[F^\prime] = \begin{bmatrix} F_1 \\ -- \\ F_2 \end{bmatrix},$$

$$\{G_t^\prime\} = \begin{Bmatrix} G_{1t} \\ --- \\ G_{2t} \end{Bmatrix} \text{ and }$$

$$\{G_{t+\Delta t}^\prime\} = \begin{Bmatrix} G_{1\ t+\Delta t} \\ ---- \\ G_{2\ t+\Delta t} \end{Bmatrix}$$

Equation (195) was solved using a block-iterative Gaussian elimination procedure for $\{G_{t+\Delta t}\}$ from which $\{G_{1\ t+\Delta t}\}$ and $\{G_{2\ t+\Delta t}\}$ are obtained.

Based on the previous mathematical derivations, a computer program was written which calculates the dual changes in concentration of two reacting solutes subject to binary cation exchange in flowing groundwater. The computer program calculates both solution concentration and adsorbed concentration at any specified place and time due to the process of convective transport, hydrodynamic dispersion, mixing from fluid sources and cation exchange processes. The program allows specification of any number of injection or withdrawal wells and of spatially varying distributed recharge or discharge, leakage, saturated

thickness, transmissivity, cation exchange capacity, boundary conditions and initial heads and concentrations. The program can simulate either transient flow - transient transport or steady state flow - transient transport. A complete documentation of the program is contained in the following section of the report.

CHAPTER V

COMPUTER PROGRAM

The purpose of this section of the report is to describe the
computer program which was written from the previously developed theory.
A listing of the computer program is presented in Appendix D.   The
computer program is segmented into a main program and twelve subroutines.
It contains about 2,500 lines and is written in Fortran IV. The definition
of selected variables in the program is presented in Appendix E.   This
should help the reader relate the program variables to their corresponding
mathematical terms.   Also presented is a complete set of data deck
instructions for the program (Appendix F), a listing of a sample data
deck (Appendix G) and a sample output from a model simulation (Appendix H).

5.1 Simplified Flow-Chart

The major steps in the program are summarized in the simplified
flow-chart shown on Figure 12.   The flow chart illustrates that at a
given time step the groundwater flow equation is solved sequentially
with the simultaneous solution of the two coupled convection-dispersion
equations in a leap-frog solution technique (this was discussed earlier
in Chapter 3 and diagramatically shown on Figure 7).   The groundwater
flow equation is solved first for the head distribution in the aquifer
and then the two coupled transport equations are solved for both the
dissolved and adsorbed concentrations.

An implicit finite difference approximation (which is stable for any
size time step) is made to the time derivatives in both the groundwater
flow equation and the transport equations.   The user must specify the
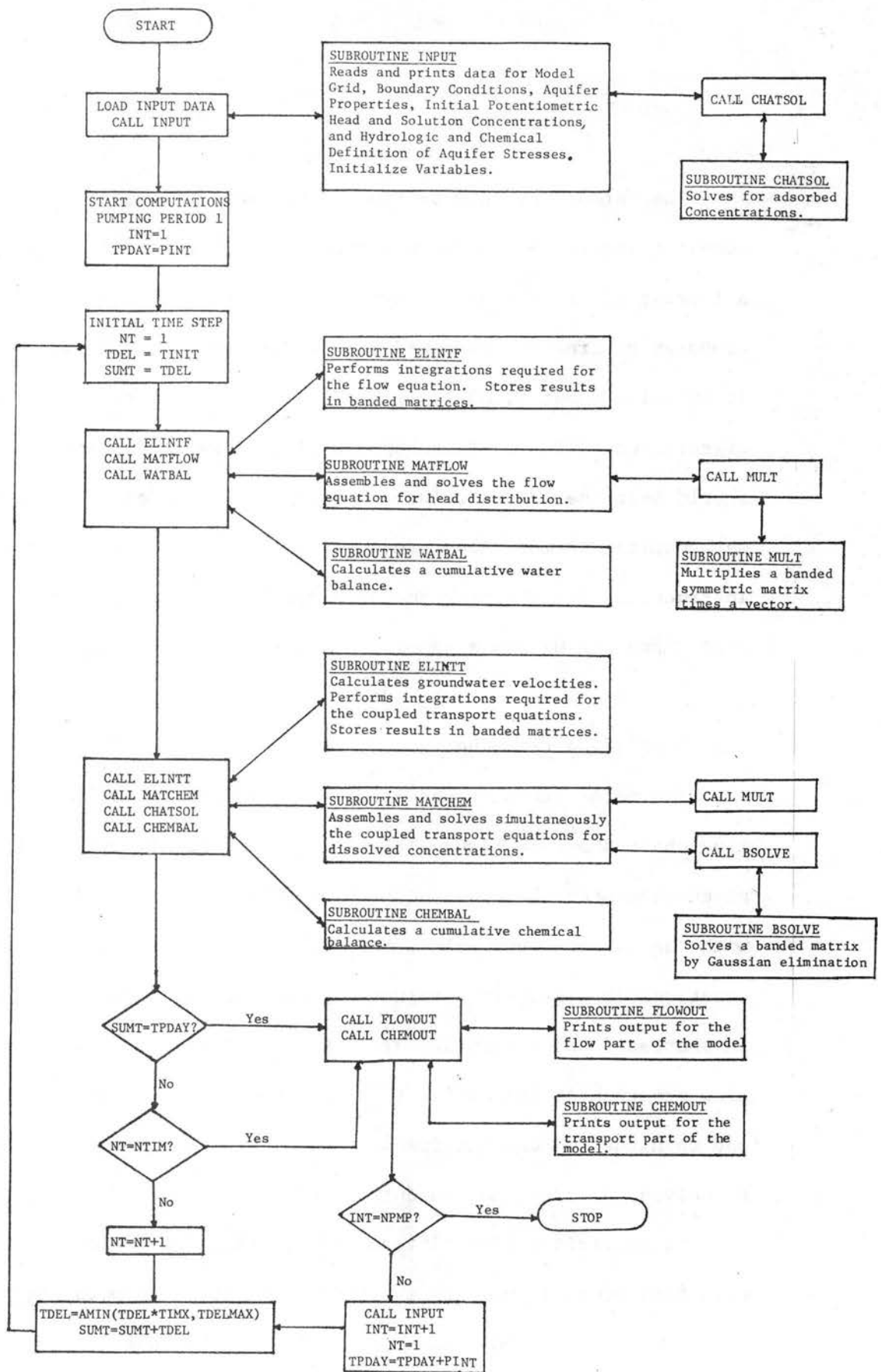
FIGURE 12. -- Simplified Flow Chart

initial time step (TINIT), time increment multiplier (TIMX) and maximum time step (TDELMAX) in the model. All subsequent time steps are automatically determined by the model. A maximum time step is required since the transport equations contain variable parameters g_1, g_2 and g_3 which are dependent on concentration changes and thus from experience unreliable results are obtained if too large of a time step is used. The program printouts are at the end of each pumping period (NPMP) which are of length (PINT). The model assumes that stresses are constant with time during each pumping period. However, these stresses may be changed for successive pumping periods.

The general program presented in Appendix D is dimensioned for 35 nodes and 50 elements. The user should redimension the program arrays to the appropriate size for the problem being solved. These arrays are contained in COMMON statements, BLOCKA, BLOCKD, BLOCKE, BLOCKG, BLOCKH and BLOCKI and in the DIMENSION statements in subroutines MULT and BSOLVE.

5.2 Program Segments

5.2.1 Main Program

The primary purpose of the main program is to control the overall execution sequence of the program. Subroutines for input, output, integration of coefficient matrices, assembly and solution of the flow and transport equations, and mass balance are called from the main program. The main program also calsulates the time steps.

5.2.2 Subroutine Input

All of the input data are read through subroutine INPUT. These
data define the model grid, the boundary conditions, time-step factors,
aquifer properties, initial potentiometric head, initial solution
concentrations, hydrologic and chemical definition of stresses on the
groundwater, and other hydrologic and chemical parameters. The values
of many program variables are also initialized in subroutine INPUT.
The initial adsorbed concentrations are calculated in this subroutine by
a call to subroutine CHATSOL assuming that equilibrium conditions hold.
Some other preliminary calculations are also performed such as calculation
of element areas and calculation of initial mass stored in the aquifer.
A printout is provided of all input data. Subroutine INPUT is also
used to selectively update model input data at the end of each pumping
period.

The program includes an element identification array (IDELEM) and
a node identification array (NODEID) which allows certain elements or
nodes to be identified by a unique code number. Each code number is
equated with a specified flux, source concentration, aquifer property
and/or boundary condition. These identification arrays are used to
specify the aquifer stresses, aquifer properties and/or boundary conditions
for elements or nodes with the same code number. The identification array
feature can save much time and effort in the preparation of input data
for the model.

5.2.3 Subroutine ELINTF

The purpose of subroutine ELINTF is to perform the integrations
required for the flow equation. These integrations are carried out in

a piecewise manner on an element basis. Global matrices are then formed by summing for a given node the contribution to that node from each element. These global matrices for the flow equation are banded and symmetric. To reduce computer storage requirements, these matrices are stored as half bandwidth column matrices.

5.2.4 Subroutine MATFLOW

Subroutine MATFLOW assembles and solves the flow equation. Solution is by the point successive over-relaxation technique (Varga, 1962). The technique consists of the following iterative procedure: (1) Assign an initial value of head h for each unknown in the set of equations to be solved. (2) Starting with the first equation solve for the first unknown using the initial values as estimates for the other unknowns. A new estimate of the first unknown is then made as

new estimate = old estimate + w (new value calculated − old estimate) (196)

where

        w   = relaxation factor.

(3) Proceed to the second equation and solve it for the second unknown using the new estimate of the first unknown and the initial values for the remaining unknowns. A new estimate of the second unknown is then made in an identical procedure as was done for the first unknown. (4) Proceed with the remaining equations, solving for the next unknown and always using the latest estimates for the other unknowns in the equation. When the final equation has been solved, yielding a value for the last unknown, then 1 iteration is said to have been completed.

(5) Continue iterating until the value of each unknown determined in a particular iteration differs from its previous value obtained in a preceeding iteration by less than some arbitrarily specified tolerance.

For a relaxation factor $w > 1$ the method is called over-relaxation and for $0 < w < 1$ is called under-relaxation. The rate of convergence of the method is strongly dependent on the value of the relaxation factor chosen. A typical value of the relaxation factor for over-relaxation is 1.7. For a relaxation factor $w = 1$ the method is equivalent to the Gauss-Seidel method (Varga, 1962). The method absolutely converges for a diagonally dominant matrix and the program contains a convergence test. Fortunately in most groundwater flow problems the matrices are diagonally dominant. The values of the relaxation factor, tolerance and the maximum allowable number of iterations are specified internally within the program and may require redefinition for efficient application to other problems.

5.2.5 Subroutine ELINTT

The purpose of subroutine ELINTT is to perform the integrations required for the transport equations. These integrations are carried out in a piecewise manner on an element basis. Global matrices are then formed by summing for a given node the contribution to that node from each element. These global matrices for the transport equation are banded and to reduce computer storage requirements are stored as column matrices. If the global matrix is also symmetric then it is stored as a half bandwidth matrix.

To perform the integrations required for the transport equations, the groundwater velocity V and the coefficient of hydrodynamic dispersion D must be evaluated. The groundwater velocities V are calculated from Darcy's law as

$$V_x = - K_x \frac{\partial h}{\partial x} \tag{197}$$

and

$$V_y = - K_y \frac{\partial h}{\partial y} \tag{198}$$

where K_x and K_y are the hydraulic conductivity of the aquifer in the x and y directions respectively (the hydraulic conductivity K equals the transmissivity T divided by the saturated thickness b of the aquifer). The partial derivatives $\partial h/\partial x$ and $\partial h/\partial y$ are obtained from differentiation of the trial solution for h (equation 89) with the coefficients G replaced with the known values of h at the nodes (determined from the solution of the flow equation), which yields

$$\frac{\partial h}{\partial x} \simeq \frac{\partial \hat{h}}{\partial x} = h_i(t) \frac{\partial v_i^e(x,y)}{\partial x} + h_j(t) \frac{\partial v_j^e(x,y)}{\partial x} + h_k(t) \frac{\partial v_k^e(x,y)}{\partial x} \tag{199}$$

and

$$\frac{\partial h}{\partial y} \simeq \frac{\partial \hat{n}}{\partial y} = h_i(t) \frac{\partial v_i^e(x,y)}{\partial y} + h_j(t) \frac{\partial v_j^e(x,y)}{\partial y} + h_k(t) \frac{\partial v_k^e(x,y)}{\partial y} \tag{200}$$

The partial derivatives $\frac{\partial v^e}{\partial x}$ and $\frac{\partial v^e}{\partial y}$ were calculated in equations (93), (94) and (95). Substitution of equations (93), (94), (95), (199) and (200) into equations (197) and (198) yields

$$V_x = - \frac{K_x}{2A\Delta}[h_i(t)(y_j - y_k) + h_j(t)(y_k - y_i) + h_k(t)(y_i - y_j)] \tag{201}$$

and

$$V_y = - \frac{K_y}{2A\Delta} [h_i(t) (x_k-x_j) + h_j(t) (x_i-x_k) + h_k(t) (x_j-x_i)] \qquad (202)$$

Equations (201) and (202) are used in the model and hold only for the interior of domain D.

The groundwater velocity along the boundary B is known from the boundary conditions for the flow equation. Recall that the $\frac{\partial h}{\partial x}$ and $\frac{\partial h}{\partial y}$ are specified constants on the boundary (equations 72 and 73) and thus from Darcy's law

$$V_x = - K_x (\frac{\partial h}{\partial x}\big|_B) \text{ on Boundary B, and} \qquad (203)$$

$$V_y = - K_y (\frac{\partial h}{\partial y}\big|_B) \text{ on Boundary B} \qquad (204)$$

are obtained.

The dispersion coefficients D are obtained in the model from the velocity of the groundwater and the dispersivity of the aquifer as (Bear, 1979)

$$D_{xx} = \alpha_L \frac{V_x^2}{|V|} + \alpha_T \frac{V_y^2}{|V|} - \frac{V_x^2 \Delta t}{2}, \qquad (205)$$

$$D_{yy} = \alpha_T \frac{V_x^2}{|V|} + \alpha_L \frac{V_y^2}{|V|} - \frac{V_y^2 \Delta t}{2}, \text{ and} \qquad (206)$$

$$D_{xy} = D_{yx} = (\alpha_L - \alpha_T) \frac{V_x V_y}{|V|} - \frac{V_x V_y \Delta t}{2} \qquad (207)$$

where

α_L = longitudinal dispersivity of the porous medium (L),

α_T = transverse dispersivity of the porous medium (L), and

$|V|$ = magnitude of the groundwater velocity (L/T).

Numerical dispersion is introduced in the solution of the transport equations from the implicit finite-difference approximation to the time derivative (Lantz, 1971). This numerical dispersion is of magnitude $\frac{V^2 \Delta t}{2}$. The dispersion coefficients D given in equations (205), (206) and (207) are defined to compensate for this numerical dispersion. A minimum dispersivity α is required in either finite-element or finite-difference solutions to the convection-dispersion equation otherwise stability problems will result. The dispersivity of the aquifer is rarely known from field measurements (dispersivity is a fourth order tensor with 81 components). The dispersivity is normally estimated either from stability considerations or from a trial and error calibration procedure to obtain a best fit between model-calculated concentrations and observed concentrations.

5.2.6 Subroutine MATCHEM

Subroutine MATCHEM assembles and solves simultaneously the two coupled convection-dispersion equations. The solution is by a block iterative-Gaussian elimination technique. The technique consists of the following iterative procedure: (1) Assign an initial value of concentration C_1 and C_2 for each unknown in the set of equations to be solved (equation (193) for $L_1(C) = 0$ and equation (194) for $L_2(C) = 0$ are to be solved simultaneously). (2) Starting with equation (193) for $L_1(C) = 0$, solve

it by Gaussian elimination for new values of C_1 using the initial values as estimates for C_2. (3) Proceed to equation (194) for $L_2(C) = 0$ and solve it also by Gaussian elimination for new values of C_2 using as estimates for C_1 the values obtained in step 2. This completes 1 iteration. (4) Continue iterating. Solve equation (193) for new values of C_1 using as estimates for C_2 the values obtained in step 3 of the previous iteration. Then solve equation (194) for new values of C_2 using as estimates for C_1 the values obtained in step 2 of the current iteration. (5) Iterating continues until the value of each unknown determined in a particular iteration differs from its previous value obtained in a preceeding iteration by less than some arbitrarily specified tolerance.

This iteration procedure has the advantage that it requires a minimum of computer storage. It has the disadvantage that it is probably slower than many other solution techniques and may also possibly not converge for some problems. The rate of convergence of this iteration procedure may possibly be increased using a relaxation technique as is done in the solution of the flow equation (see subroutine MATFLOW). The values of tolerance and the maximum number of iterations are specified internally within the program and may require redefinition for efficient application to other problems.

5.2.7 Subroutine CHATSOL

Subroutine CHATSOL solves the law of mass action (equation 31) and the electroneutrality balance (equation 32) for the adsorbed concentrations. For homovalent exchange (in essence $Z_1 = Z_2$ or for all practical purposes either monovalent-monovalent exchange or divalent-divalent exchange) the following equations are easily obtained

$$\overline{C}_1 = \frac{K'\,CEC}{1 + K'} \tag{208}$$

where

$$K' = \frac{C_1\,\gamma_1}{K_c^{-Z_1}\,C_2\gamma_2} \quad ,$$

and

$$\overline{C}_2 = CEC - \overline{C}_1 \cdot \tag{209}$$

For heterovalent exchange (in essence $Z_1 \neq Z_2$ or for all practical purposes monovalent-divalent exchange) the following equations are easily obtained

$$\overline{C}_1 = \left(\frac{-K' + \sqrt{K'^2 + 4K'}}{2} \right) CEC \tag{210}$$

where

$$K' = \frac{C_1^{\,2}\,\gamma_1^{\,2}}{K_c\,C_2\,\gamma_2} \quad ,$$

and $\tag{211}$

$$\overline{C}_2 = CEC - \overline{C}_1 \; .$$

Equation (210) was derived for $Z_2 = 2$ and $Z_1 = 1$. The values of C_1 and C_2 in equations (208) and (210) are obtained from subroutine MATCHEM for the solution of the two coupled convection-dispersion equations. Recall that the solution activity coefficients γ are obtained from the Debye-Huckel equation (equation 20).

5.2.8 Subroutine BSOLVE

This subroutine solves a banded matrix by the Gaussian elimination procedure. It is called from subroutine MATCHEM and is used in the

iterative procedure used to simultaneously solve the two coupled transport equations.

5.2.9 Subroutine MULT

This subroutine multiplies a banded symmetric matrix times a vector and returns the resulting vector to the calling program. It is called from subroutines MATFLOW and MATCHEM and is used in the assembly of the flow equation and the transport equations.

5.2.10 Subroutine WATBAL

This subroutine calculates a water balance. The volumetric water flux from distributed and point recharge and discharge sources, volumetric water flux due to vertical leakage, volumetric water flux across model boundaries and change in volume of groundwater stored in the aquifer are calculated. These quantities are printed out by subroutine FLOWOUT.

5.2.11 Subroutine CHEMBAL

This subroutine calculates a chemical balance. The mass flux from distributed and point recharge and discharge sources, mass flux due to vertical leakage, mass flux across model boundaries and change in mass stored in the aquifer for both dissolved and adsorbed chemical constituents are calculated. These quantities are printed out by subroutine CHEMOUT.

5.2.12 Subroutine FLOWOUT

This subroutine prints the results of the flow model calculations. This subroutine prints (1) the current potentiometric head matrix,

(2) a current drawdown map, (3) a cumulative water balance, and (4) the inflow and outflow fluxes by node identification and by constant head nodes. From the water balance the subroutine calculates a mass balance error which is used to estimate the accuracy of the flow model calculations.

5.2.13 Subroutine CHEMOUT

This subroutine prints the results of the transport model calculations. This subroutine prints for both chemical species 1 and 2, (1) the current dissolved concentration, (2) the current adsorbed concentration, and (3) a cumulative chemical balance. From the chemical balance the subroutine calculates a mass balance error which is used to estimate the accuracy of the transport model calculations.

5.3 Test Problems - Comparison with Analytical Solutions

The accuracy of the numerical solution to the groundwater flow equation and to the convection-dispersion equation can be evaluated in part by analyzing relatively simple problems for which analytical solutions are available and then comparing the model calculations with the analytical solution. The computer program consists of two linked models, a groundwater flow model and a solute transport model. The groundwater flow model was tested separately from the solute-transport model.

5.3.1 Radial Flow to a Well

To test the groundwater flow model, a comparison was made between numerical and analytical solutions for the problem of transient radial

flow to a pumping well (Figure 13). The analytical solution for this test problem is given by the Theis equation (Todd, 1980). In this test problem an infinite aquifer was simulated with a transmissivity of 5000 ft^2/day, a storage coefficient of .3 and a pumping rate of 250 gallons per minute. To take advantage of symmetry, a quadrant of the flow was analyzed in the model rather than the entire flow field. In the model, nodes were placed a radial distance from the well of 1, 2, 4, 6, 8, 10, 25, 50, 75, 100, 200, 300, 400, 500, 750, and 1000 feet. A constant head boundary was specified perpendicular to the flow at a radial distance of 1000 feet from the well. The model boundaries parallel to flow were considered as no flow boundaries.

As shown on Figure 13, comparisons between the analytical and numerical solutions were made at two different times (t = 1 day and 5 days). A fairly close agreement between numerical and analytical solutions was obtained at both times. The greatest difference between the two solutions occurs close to the pumping well where the potentiometric surface is highly nonlinear. Recall that in the numerical solutions a linear approximation to the potentiometric surface is made. At a distance of 1 foot from the well the error between the two solutions was 5.4 percent for t = 1 day and 4.6 percent for t = 5 days. At farther distances from the well, nearly exact agreement is obtained. The mass balance error calculated by the model was .005 percent. The results of this test problem indicate that the numerical model is capable of calculating the shape and position of the potentiometric surface in the aquifer.
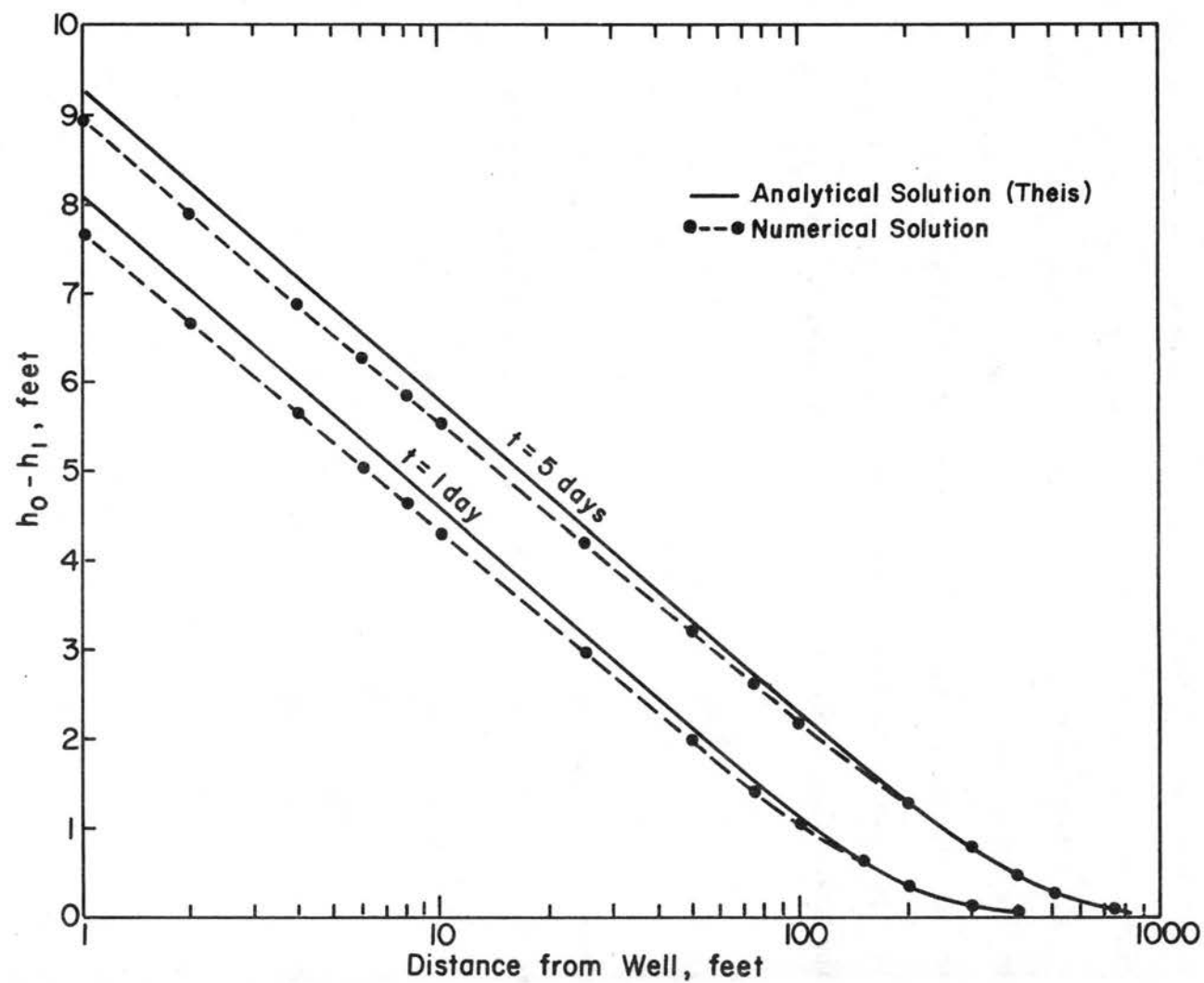
Figure 13. -- Comparison between analytical and numerical solutions for radial flow to a well.

5.3.2 1-dimensional Conservative Transport in an Infinite Column

Unfortunately, no analytical solution is available to test the numerical solution of the transport equations subject to cation exchange reactions. However, the general computer model can also simulate conservative transport and analytical solutions are available for some simple conservative transport problems which can serve as a useful test on the transport model. As a test a comparison was made between numerical and analytical solutions for the problem of 1-dimensional conservative transport in an infinite column with steady-state flow (Figures 14 and 15). The analytical solution for this test problem is given by Bear (1979).

$$C(x,t) = \frac{C_o}{2} \, \text{erfc}\left(\frac{x-vt}{\sqrt{4D_L t}}\right) \tag{212}$$

where erfc = complimentary error function.

Equation (212) is subject to the following initial conditions

$$t \leq 0, \quad -\infty < x < 0, \quad C = C_o$$
$$0 \leq x \leq +\infty, \quad C = 0$$

and to the following boundary conditions

$$t > 0, \quad x = \pm\infty, \quad \partial C/\partial x = 0$$
$$x = +\infty, \quad C = 0$$
$$x = -\infty, \quad C = C_o$$

In equation (212) the coefficient of hydrodynamic dispersion is defined as $D_L = \alpha_L V$.
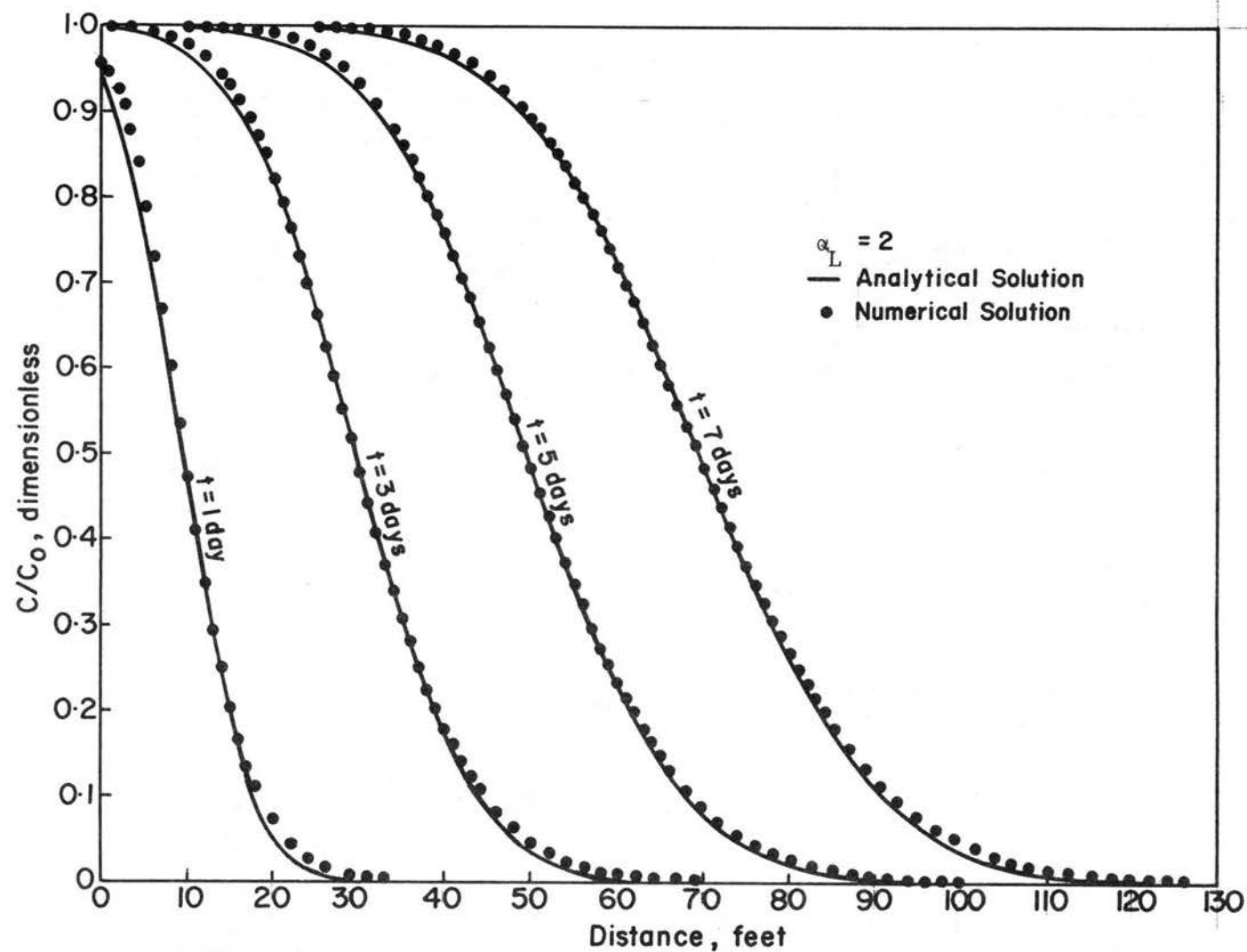
Figure 14. -- Comparison between analytical and numerical solutions for 1-dimensional conservative transport in an infinite column, $\alpha_L = 2$.
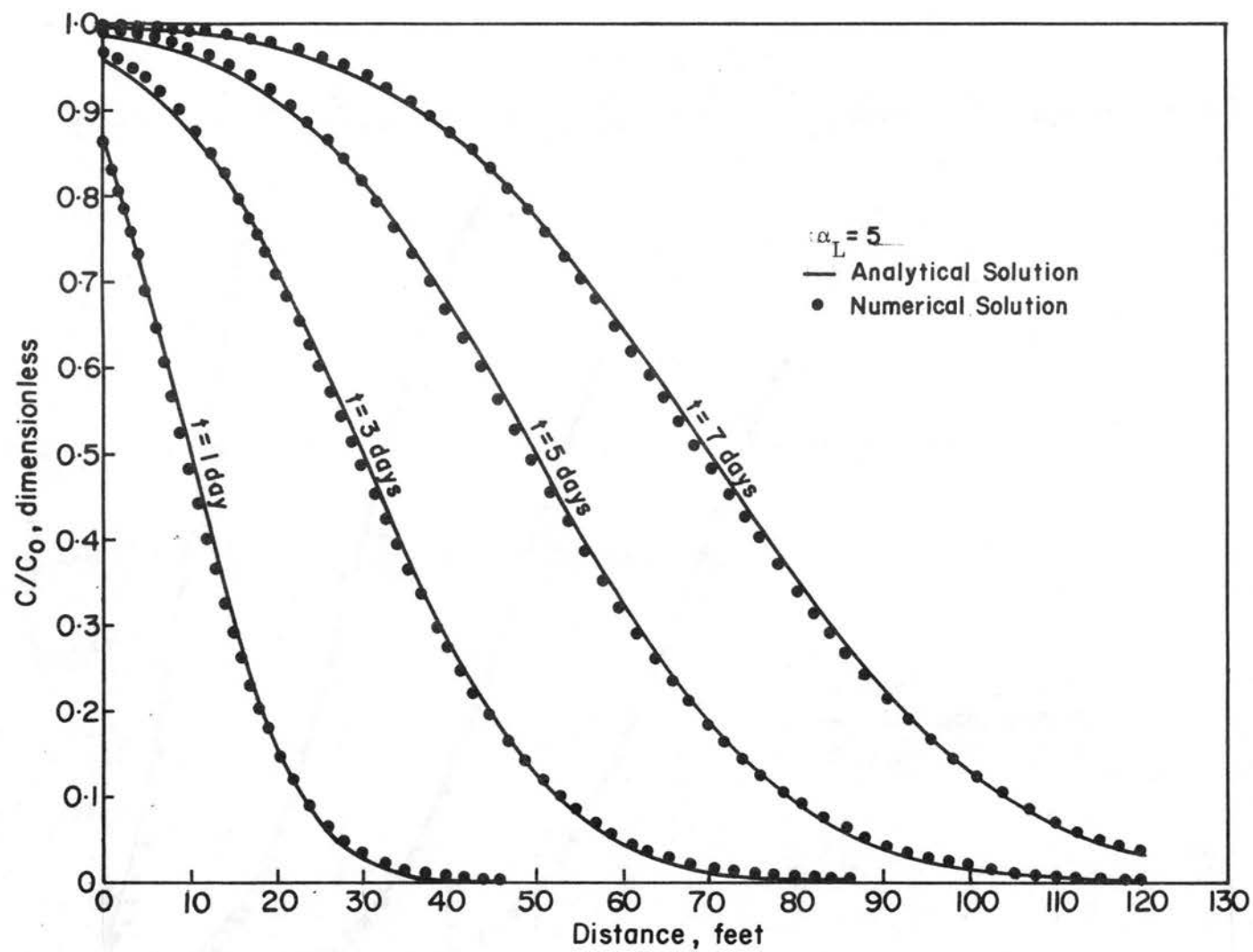
Figure 15. -- Comparison between analytical and numerical solutions for 1-dimensional conservative transport in an infinite column, $\alpha_L = 5$.

In the test problem a source concentration C_o of 100 mg/L and an interstitial velocity V of 10 ft/day was used in equation (212). In the model the aquifer properties used were a transmissivity of 1750 ft^2/day, a storage coefficient of zero, an effective porosity of .35, a saturated thickness of 50 ft, and a groundwater gradient of .1 (these aquifer properties are equivalent to steady-state groundwater flow with a constant interstitial velocity of 10 ft/day). In the model the coefficient of hydrodynamic dispersion is defined as $D = \alpha_L V - \frac{V^2 \Delta t}{2}$. Recall that the latter term in the model definition for D compensates for the numerical dispersion introduced because of the implicit finite-difference approximation to the time derivative. In the model, nodes were placed at 2 foot intervals between -50 to -20 ft, at 1 foot intervals between -20 to 100 ft, and again at 2 foot intervals between 100 to 150 ft. The initial concentration of the nodes were 100 mg/L between -50 to 0 ft and zero between 1 to 150 ft. The model boundaries parallel to the flow were specified as no flow boundaries and the upstream and downstream boundaries were specified as constant head boundaries.

As shown on Figures 14 and 15, comparisons between the analytical and numerical solutions were made at 4 times (t = 1, 3, 5 and 7 days) and for two different values of dispersivity (α_L = 2 and 5 ft). A very close agreement between numerical and analytical solutions was obtained at all times and for both values of dispersivity. The greatest difference between the two solutions occurs in the vicinity of the highly nonlinear region of the concentration fronts where the linear approximations used for concentrations by the model would have the greatest error. The results of this test problem indicate that the numerical model is capable of calculating the shape and position of the concentration profile.

5.4 <u>Example Problem</u> - <u>Solute Transport with Cation Exchange Reactions</u>

To illustrate the significance that cation exchange reactions can have in solute transport problems the following example problem is presented which considers the binary exchange between ammonium and calcium. The example problem described here is for a single injection well in a homogeneous and isotropic aquifer with the aquifer properties given in Table 2. The model grid and the nodal numbering system for this example problem is shown on Figure 16. A constant head was specified along all boundaries. The injection well is located at the center node (node 18) and had a pumping rate of 5 gpm. The concentration of the injection fluid and the initial dissolved concentration of the groundwater was varied and is given in Table 3 for each model simulation. A selectivity coefficient K_c of 38 meq/L determined as an average from Figure 6 was used in the model. Recall that K_c is the selectivity coefficient corrected for activity in the solution phase but uncorrected for activity in the adsorbed phase and is a variable. The selectivity coefficient K corrected for activity in both the solution and adsorbed phases is a constant but cannot be used in the model since the surface activity coefficients $\bar{\lambda}$ are unknown. The relationship between K_c and K is given by equation (23). For purposes of this simulation K_c was held constant and represents the value of K_c that would be obtained using average values for the surface activity coefficients in equation (23). All model simulations were for a total time period of 360 days.

All model simulation results are given in Table 4 and are graphically depicted 3-dimensionally on Figures 17-22. The model simulation shown on Figure 17 is for the injection and adsorption of ammonium. In this simulation an ammonium solution is injected into a groundwater essentially containing only calcium. Initially, all of the cation exchange sites are

TABLE 2. -- Aquifer Properties for Example Problem

Aquifer Properties		
T	=	100. ft^2/day
b	=	50. ft
s	=	3×10^{-5}
ε	=	.35
dh/dx	=	.025
α_L	=	20. ft
α_T/α_L	=	.3
CEC	=	400 meq/L

also filled essentially only with calcium. The injection of the ammonium alters the established chemical equilibrium. Some of the injected ammonium is adsorbed on the solid aquifer material and simultaneously some of the previously adsorbed calcium is released into solution and a new chemical equilibrium is established. This adsorption of the ammonium severely retards its movement from the point of injection.

EXPLANATION

O^2 Nodal point and number

O^{18} Injection well
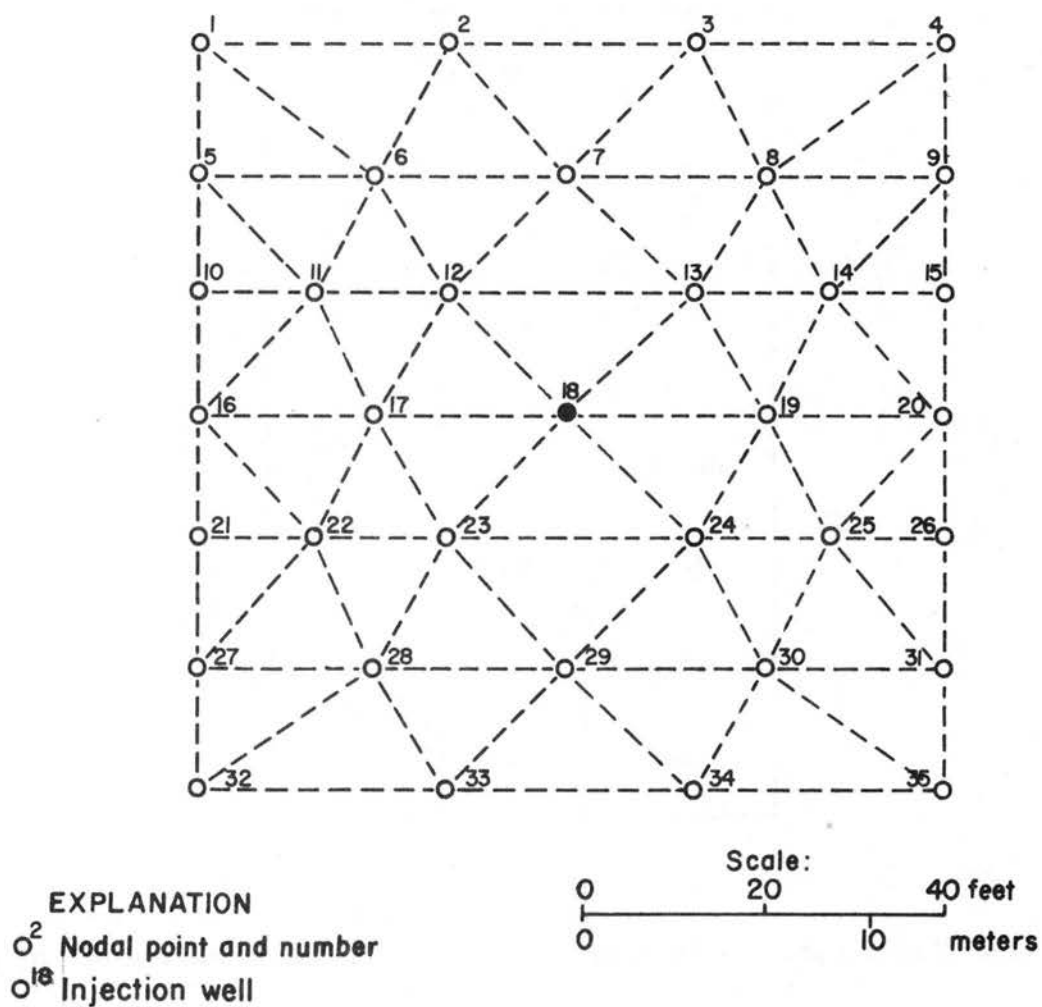
Figure 16. -- Model grid and nodal numbering system for example
problem.

TABLE 3. -- Input Concentrations for Example Problem

Simulation	Injection and Adsorption of Ca	Dilution and Desorption of NH_4	Injection and Adsorption of NH_4	Dilution and Desorption of Ca	Injection of Conservative Tracer	Dilution of Conservative Tracer
Injection Fluid Concentration (mg/L)	$C_{Ca} = 500$ $C_{NH_4} = 0$		$C_{Ca} = 0$ $C_{NH_4} = 500$		$C = 500$	$C = 0$
Initial Dissolved Concentration of Groundwater (mg/L)	$C_{Ca} = .001$ $C_{NH_4} = 200$		$C_{Ca} = 200$ $C_{NH_4} = .001$		$C = .001$	$C = 200$

TABLE 4. -- Model Results for Example Problem

Simu-lation	Injection and Adsorption of Ammonium (mg/L)						Injection and Adsorption of Calcium (mg/L)					
Node	60 Days	120 Days	180 Days	240 Days	300 Days	360 Days	60 Days	120 Days	180 Days	240 Days	300 Days	360 Days
1	0	0	0	0	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0	0	0	0	0	0
7	0	0	0	0	0	0	0	0	0	0	0	0
8	0	0	0	0	0	0	0	0	0	0	0	0
9	0	0	0	0	0	0	0	0	0	0	0	0
10	0	0	0	0	0	0	0	0	0	0	0	0
11	0	0	0	0	0	0	0	0	0	0	0	0
12	0	13	37	64	91	115	0	0	9	26	46	67
13	0	13	37	64	91	115	0	0	9	26	46	67
14	0	0	0	0	0	0	0	0	0	0	0	0
15	0	0	0	0	0	0	0	0	0	0	0	0
16	0	0	0	0	0	0	0	0	0	0	0	0
17	0	5	22	43	65	86	0	0	4	15	30	47
18	220	317	358	380	394	404	135	254	320	355	374	387
19	0	5	22	43	65	86	0	0	4	15	30	47
20	0	0	0	0	0	0	0	0	0	0	0	0
21	0	0	0	0	0	0	0	0	0	0	0	0
22	0	0	0	0	8	18	0	0	0	0	0	0
23	3	35	75	112	143	170	0	7	32	64	96	125
24	3	35	75	112	143	170	0	7	32	64	96	125
25	0	0	0	0	8	18	0	0	0	0	0	0
26	0	0	0	0	0	0	0	0	0	0	0	0
27	0	0	0	0	0	0	0	0	0	0	0	0
28	0	0	0	7	15	24	0	0	0	1	4	9
29	0	0	0	4	14	27	0	0	0	0	1	6
30	0	0	0	7	15	24	0	0	0	1	4	9
31	0	0	0	0	0	0	0	0	0	0	0	0
32	0	0	0	0	0	0	0	0	0	0	0	0
33	0	0	0	0	0	0	0	0	0	0	0	0
34	0	0	0	0	0	0	0	0	0	0	0	0
35	0	0	0	0	0	0	0	0	0	0	0	0

TABLE 4. -- Model Results for Example Problem (cont.)

Simulation Node	Injection of Conservative Tracer (mg/L)						Dilution and Desorption of Ammonium (mg/L)					
	60 Days	120 Days	180 Days	240 Days	300 Days	360 Days	60 Days	120 Days	180 Days	240 Days	300 Days	360 Days
1	0	0	0	0	0	0	200	200	200	200	200	200
2	0	0	7	33	74	121	200	200	200	200	214	234
3	0	0	7	33	74	121	200	200	200	200	214	234
4	0	0	0	0	0	0	200	200	200	200	200	200
5	0	4	37	70	98	121	200	200	200	202	210	217
6	26	101	174	236	288	331	208	244	279	308	331	350
7	9	83	160	223	272	311	200	231	272	307	334	355
8	26	101	174	236	288	331	208	244	279	308	331	350
9	0	4	37	70	98	121	200	200	200	202	210	217
10	21	93	163	217	258	288	206	241	272	293	308	319
11	71	190	274	333	376	407	230	288	330	360	381	396
12	250	349	397	426	446	459	326	373	387	386	376	363
13	250	349	397	426	446	459	326	373	387	386	376	363
14	71	190	274	333	376	407	230	288	330	360	381	396
15	21	93	163	217	258	288	206	241	272	293	308	319
16	30	156	254	321	366	398	210	272	318	350	372	388
17	223	338	396	430	451	465	313	370	392	398	393	384
18	445	471	482	488	492	494	301	205	151	123	107	97
19	223	338	396	430	451	465	313	370	392	398	393	384
20	30	156	254	321	366	398	210	272	318	350	372	388
21	47	176	278	347	392	422	220	288	335	365	385	399
22	125	259	343	396	430	452	258	324	366	394	410	418
23	290	380	425	452	468	479	346	383	381	364	342	321
24	290	380	425	452	468	479	346	383	381	364	342	321
25	125	259	343	396	430	452	258	324	366	394	410	418
26	47	176	278	347	392	422	220	288	335	365	385	399
27	10	120	238	324	382	420	200	259	317	358	386	405
28	121	254	341	397	432	455	259	326	369	395	408	414
29	154	296	374	420	448	466	273	344	386	407	418	422
30	121	254	341	397	432	455	259	326	369	395	408	414
31	10	120	238	324	382	420	200	259	317	358	386	405
32	5	105	266	318	380	420	200	251	312	358	387	406
33	79	227	325	388	427	452	238	312	359	388	406	419
34	79	227	325	388	427	452	238	312	359	388	406	419
35	5	105	266	318	380	420	200	251	312	358	387	406

TABLE 4. -- Model Results for Example Problem (cont.)

Simu-lation	Dilution and Desorption of Calcium (mg/L)						Dilution of Conservative Tracer (mg/L)					
Node	60 Days	120 Days	180 Days	240 Days	300 Days	360 Days	60 Days	120 Days	180 Days	240 Days	300 Days	360 Days
1	200	200	200	200	200	200	200	200	200	200	200	200
2	200	200	200	200	219	250	200	200	200	200	189	172
3	200	200	200	200	219	250	200	200	200	200	189	172
4	200	200	200	200	200	200	200	200	200	200	200	200
5	200	200	200	200	213	225	200	200	200	199	192	186
6	213	265	316	359	395	424	194	166	138	114	95	79
7	200	250	316	367	405	434	200	173	140	113	93	77
8	213	265	316	359	395	424	194	166	138	114	95	79
9	200	200	200	200	213	225	200	200	200	199	192	186
10	210	257	300	334	360	381	196	169	143	124	110	99
11	244	331	396	440	470	490	175	127	92	68	51	39
12	382	436	443	434	420	404	103	62	42	30	22	17
13	382	436	443	434	420	404	103	62	42	30	22	17
14	244	331	396	440	470	490	175	127	92	68	51	39
15	210	257	300	334	360	381	196	169	143	124	110	99
16	216	305	378	429	462	485	192	141	101	74	56	44
17	364	437	460	461	453	440	114	66	43	29	20	14
18	273	184	146	127	115	106	23	12	7	5	3	2
19	364	437	460	461	453	440	114	66	43	29	20	14
20	216	305	378	429	462	485	192	141	101	74	56	44
21	231	323	394	444	479	502	186	132	91	63	45	33
22	285	385	447	483	501	508	153	99	64	42	29	20
23	405	434	422	400	378	357	86	49	31	20	13	9
24	405	434	422	400	378	357	86	49	31	20	13	9
25	285	385	447	483	501	508	153	99	64	42	29	20
26	231	323	394	444	479	502	186	132	91	63	45	33
27	201	283	368	432	476	505	200	155	107	72	48	33
28	285	382	443	477	495	502	154	100	65	42	28	18
29	306	414	470	498	508	507	141	83	51	33	21	14
30	285	382	443	477	495	502	154	100	65	42	28	18
31	201	283	368	432	476	505	200	155	107	72	48	33
32	200	274	362	429	474	504	200	161	112	74	49	33
33	255	360	431	477	507	526	171	111	71	46	30	20
34	255	360	431	477	507	526	171	111	71	46	30	20
35	200	274	362	429	474	504	200	161	112	74	49	33
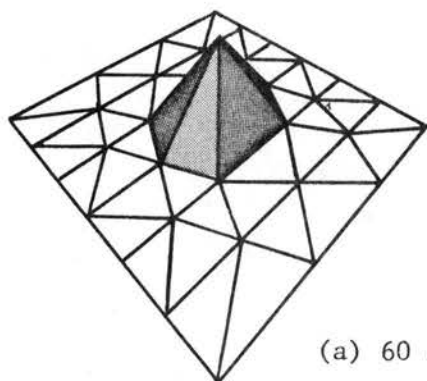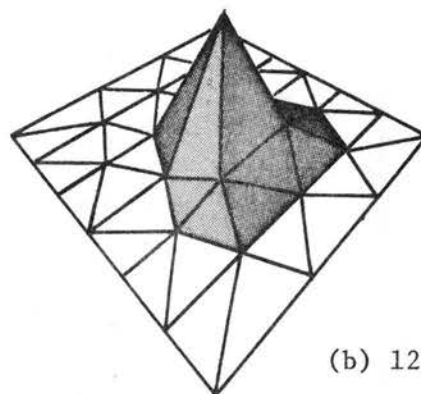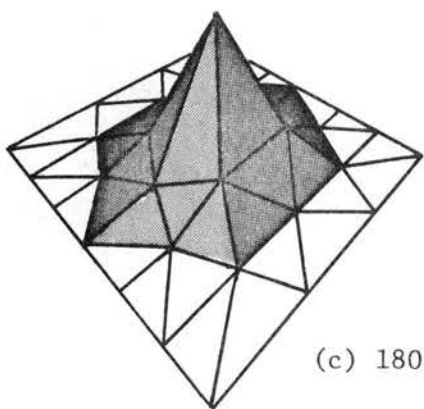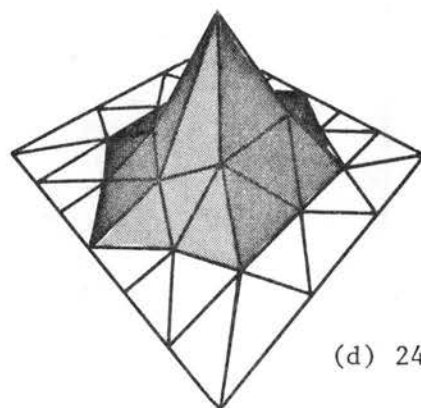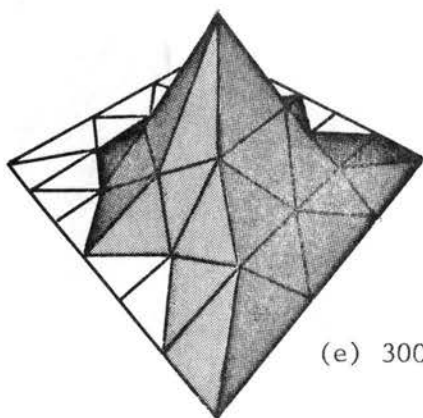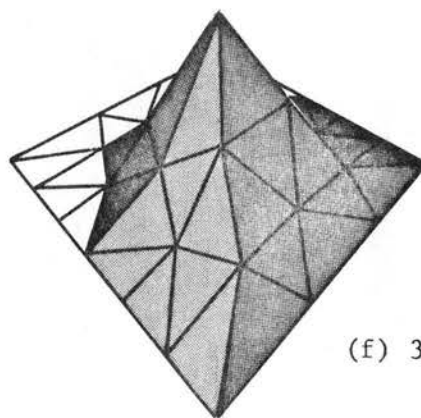
Figure 17. -- 3-dimensional graph for injection and adsorption of Ammonium - example problem.
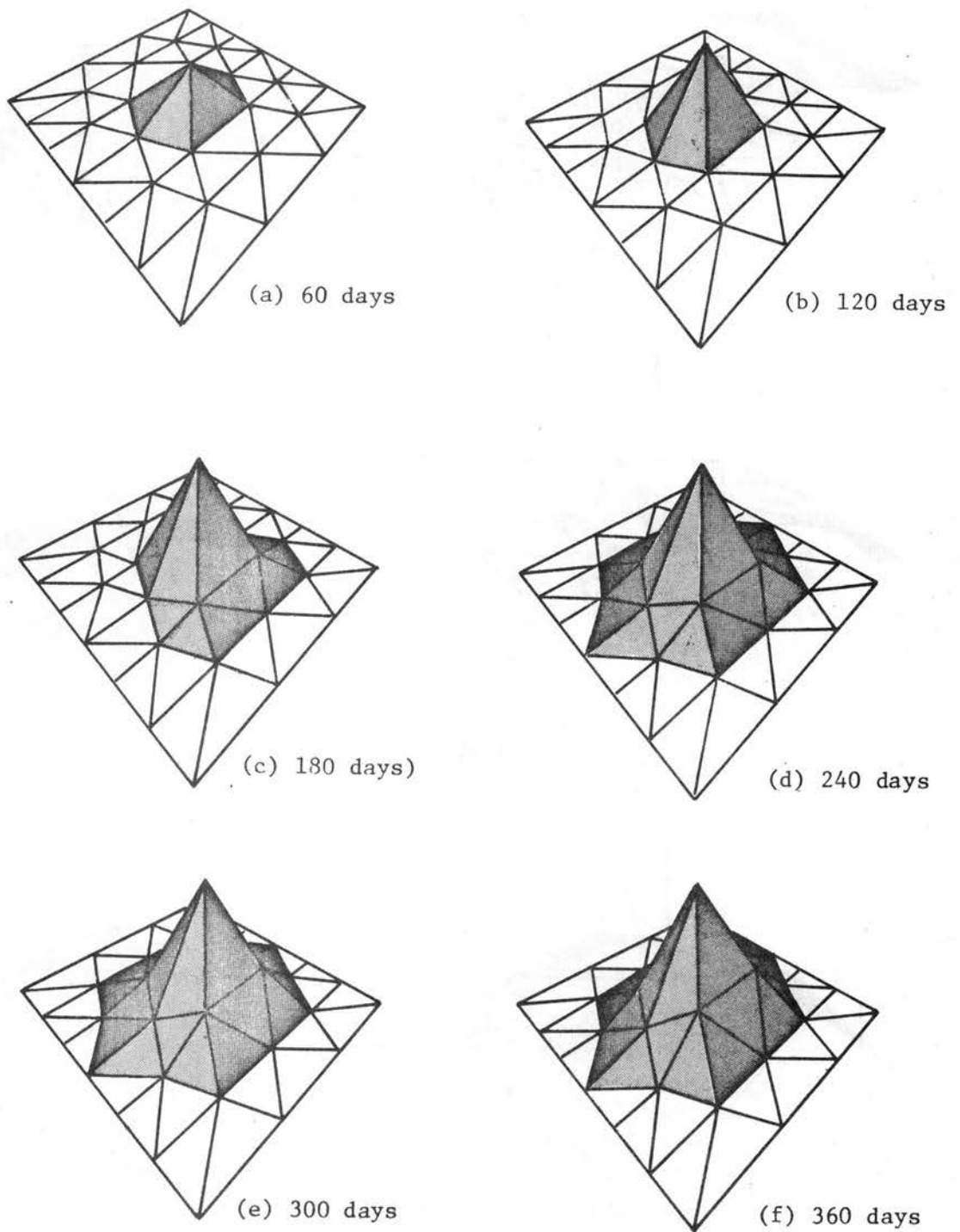
Figure 18. -- 3-dimensional graph for injection and adsorption of Calcium - example problem.
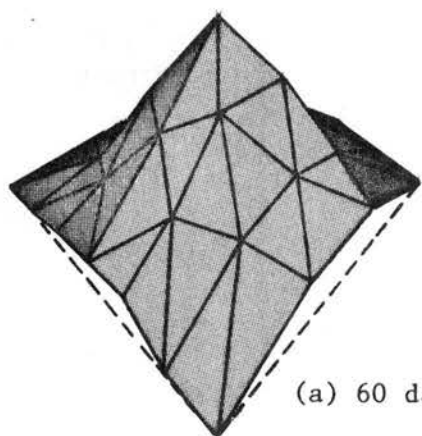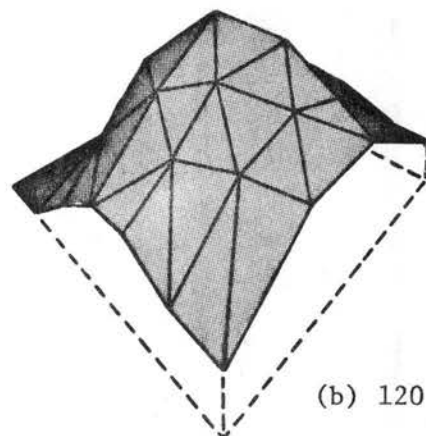
(a) 60 days

(b) 120 days
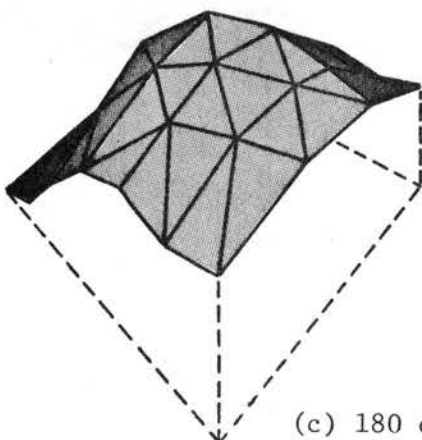
(c) 180 days
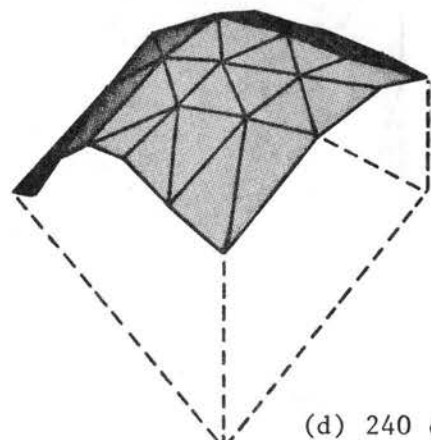
(d) 240 days
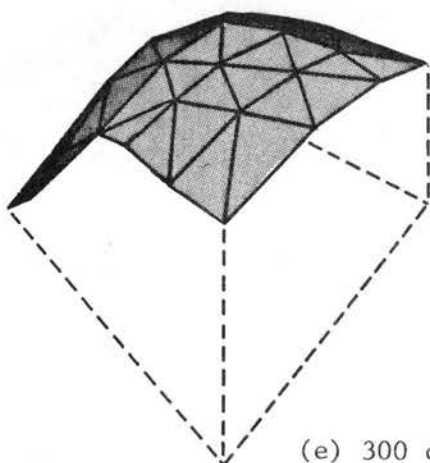
(e) 300 days
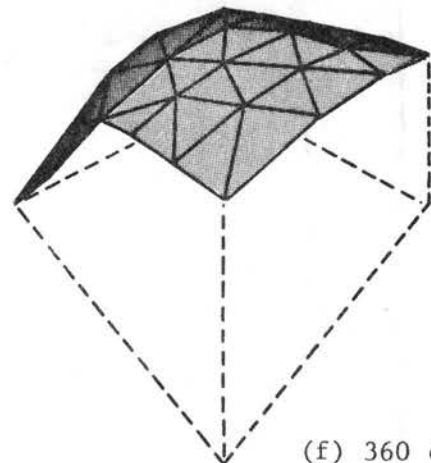
(f) 360 days

Figure 19. -- 3-dimensional graph for injection of conservative tracer - example problem.
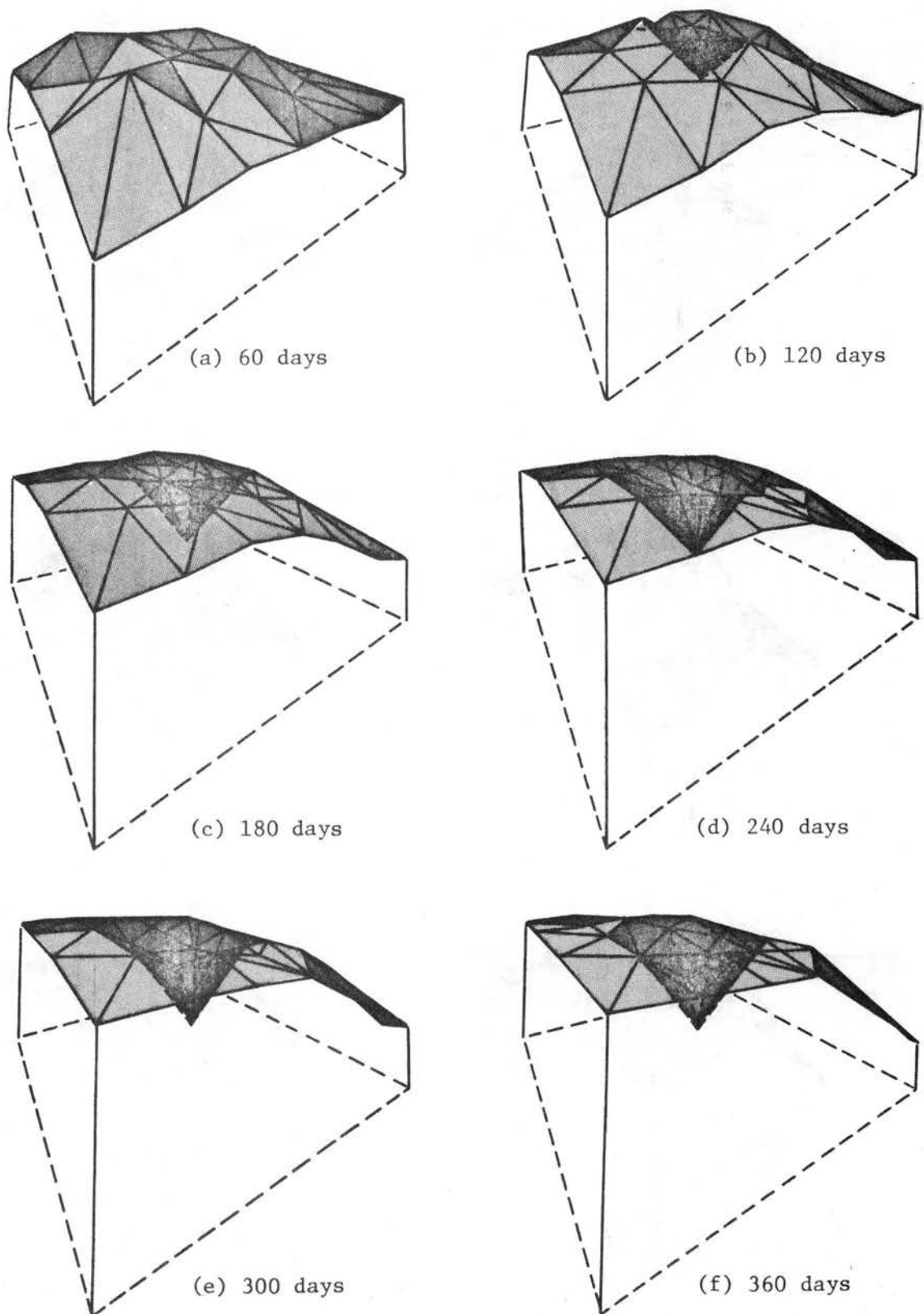
Figure 20. -- 3-dimensional graph for dilution and desorption of Ammonium - example problem.

(a) 60 days

(b) 120 days

(c) 180 days

(d) 240 days

(e) 300 days

(f) 360 days
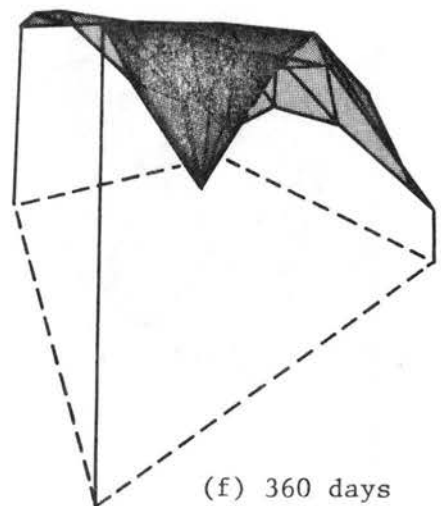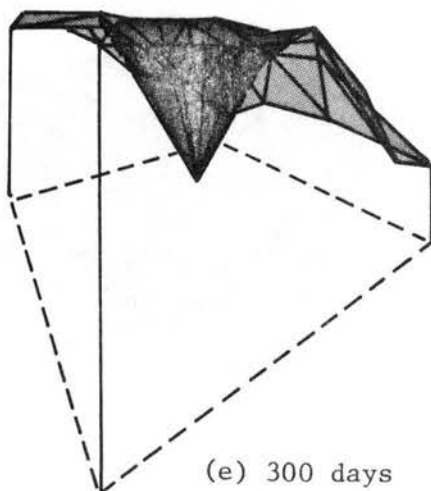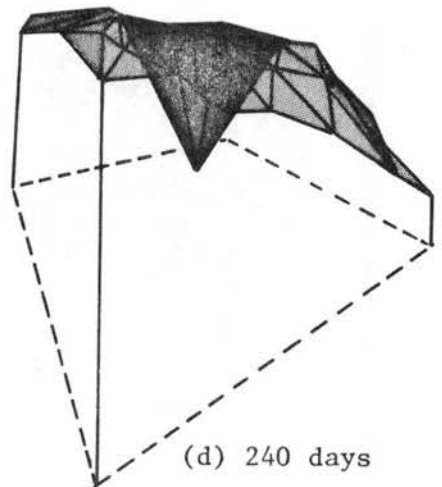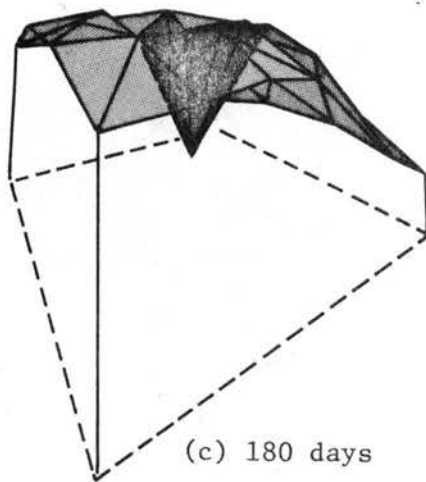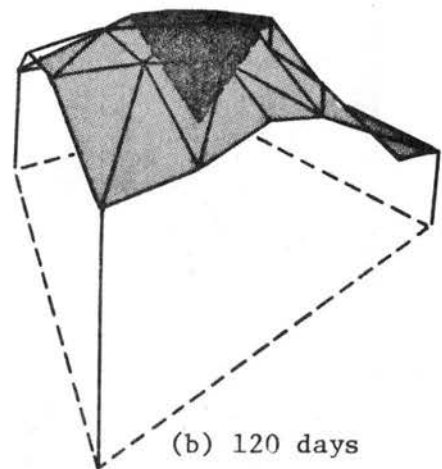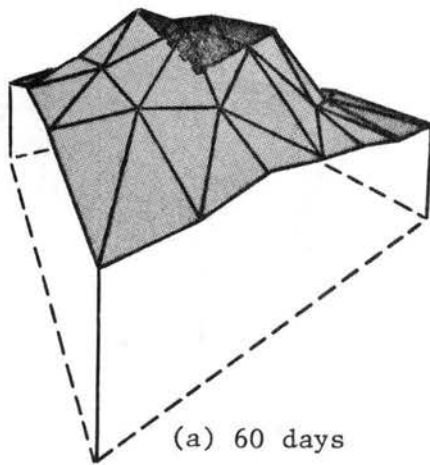
Figure 21. -- 3-dimensional graph for dilution and desorption of Calcium - example problem.
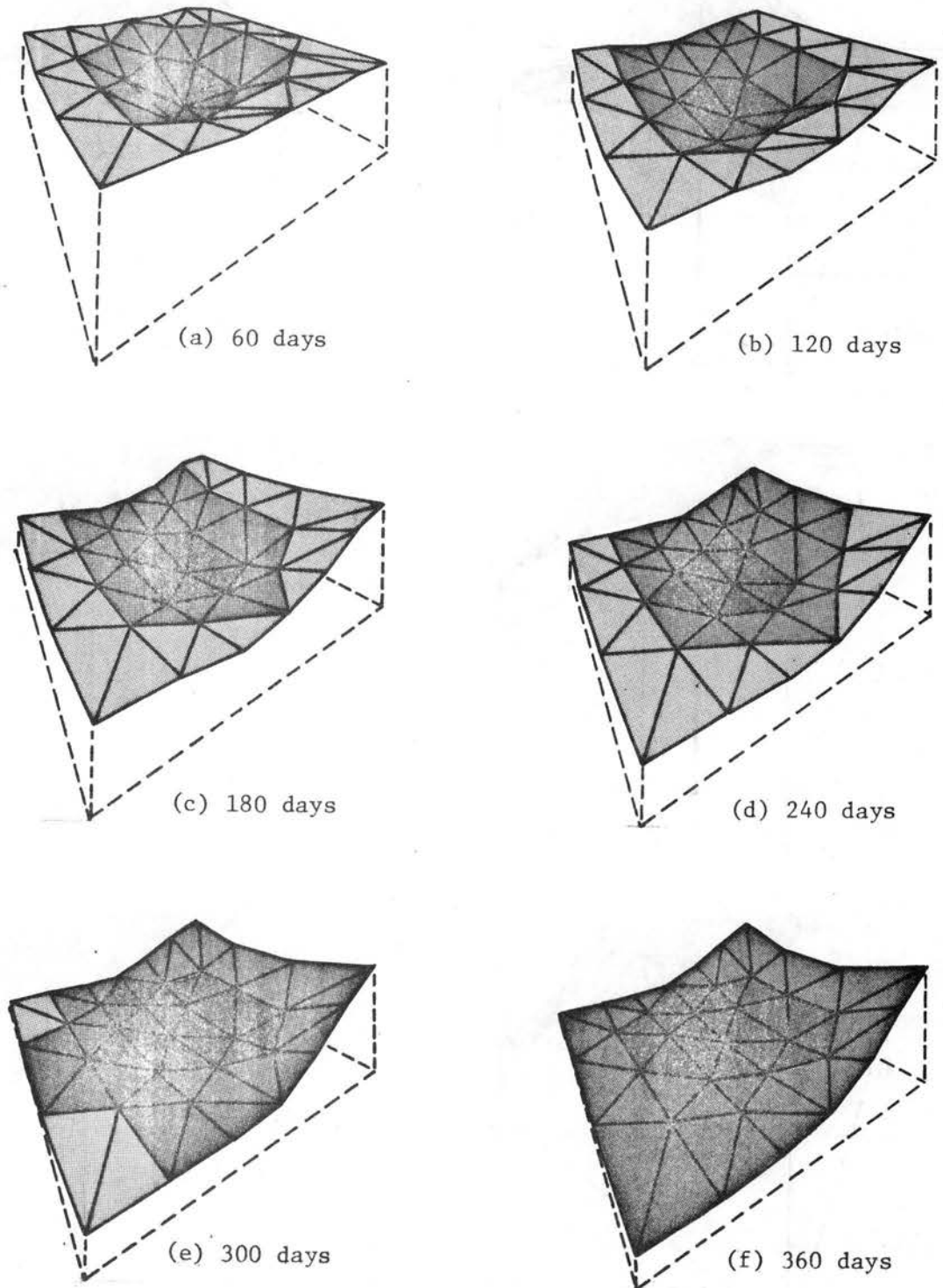
Figure 22. -- 3-dimensional graph for dilution of conservative tracer - example problem.

Shown on Figure 18 is the model results for the injection and adsorption of calcium for analogous conditions to that previously discussed for the injection and adsorption of ammonium. As with the ammonium the movement of the calcium is severely retarded by adsorption. However, calcium has an even greater affinity for adsorption than does ammonium (see equation 1) and comparison of Figures 17 and 18 indicates the mobility of calcium is slightly less than that of ammonium.

For comparison, shown on Figure 19 is the model simulation results for the injection of a conservative tracer not subject to adsorption on the porous medium. As can be easily seen by comparison of Figures 17, 18 and 19 the mobility of the conservative tracer is much greater than that of either calcium or ammonium. After 60 days the conservative tracer has moved farther than either calcium or ammonium has after 360 days.

The model simulation shown on Figure 20 is for the dilution and desorption of ammonium. In this simulation ammonium is flushed from the aquifer by the injection of a calcium solution. The initial ground-water concentration contains only ammonium and initially all of the cation exchange sites are filled with ammonium. Two processes are at work that affect dissolved ammonium concentrations in the groundwater in this model simulation. The first is dilution which acts to lower the dissolved ammonium concentration in the groundwater by the addition of the injection fluid containing only calcium. The second is the desorption of previously adsorbed ammonium which is released into solution by the exchange with the injected calcium. The desorption process acts to increase the dissolved ammonium concentration in the groundwater.

The model simulation results (see Table 4) indicate that for early times the desorption process was in general greater than the dilution affects and the dissolved ammonium concentration increased in the groundwater. At time equal to 30 days (results not shown) the dissolved ammonium concentration increased from initial concentrations of 200 mg/L to about 350 mg/L at the injection node (node 18). The surrounding nodes also had similar but smaller concentration increases. At time equal to 60 days at the injection node the dilution effect is now already greater than the desorption process and the dissolved ammonium concentration at this node decreases to about 300 mg/L. However, the surrounding nodes continue to have a concentration increase with a maximum concentration of about 346 mg/L.

At time equal to 120 days this trend continues as the dissolved ammonium concentration at the injection node continues to decrease to about 205 mg/L and at the surrounding nodes continues to increase to a maximum concentration at nodes 23 and 24 of 383 mg/L (nodes 23 and 24 are the nearest downstream nodes to the injection node). A maximum dissolved ammonium concentration of 385 mg/L occurs at nodes 23 and 24 at 150 days after which the dissolved ammonium concentration decreases at all later times at these nodes. This pattern is repeated at other surrounding nodes in which at early times the desorption process is larger than the dilution affects and the dissolved ammonium concentration at first increases and then at later times begins to decrease as the dilution effects become greater than the desorption process. At the end of the simulation period at 360 days the dissolved ammonium concentration at the injection well has decreased to about 97 mg/L. At all other

nodes the net change in the dissolved ammonium concentration has increased over the simulation time period with ending concentrations at some nodes of over 400 mg/L.

Shown on Figure 21 is the model results for the dilution and desorption of calcium for analogous conditions to that previously discussed for the dilution and desorption of ammonium. Comparison of Figures 20 and 21 indicate similar results were obtained between the two simulations. Shown on Figure 22 is the model simulation results for dilution of a conservative tracer not subject to exchange on the porous medium. As can easily be seen by comparison of Figures 20, 21 and 22 the flushing of the conservative tracer by dilution is much more extensive than for either the calcium or ammonium. Since the conservative tracer is not subject to desorption the only process that affects dissolved concentrations is dilution. After 10 days (results not shown) the concentration of the conservative tracer has been lowered at the injection node to about 69 mg/L which is lower than either the dissolved calcium or ammonium concentration at the injection node after 360 days.

This example problem demonstrates that significantly different results can be obtained by the use of the law of mass action description of the cation exchange reaction than would be obtained using the common empirical formulas such as the Freundlich isotherm. The law of mass action takes into account the competitive nature of the cation exchange process which the empirical formulas fail to do. The concentration increases calculated by the model for the dilution and desorption of either ammonium or calcium would have not been predicted using these empirical formulas. The law of mass action requires additional effort in that two coupled transport equations must be solved instead of the usual single

transport equation. However, as this example problem demonstrates this additional effort may be needed to obtain reliable results for complex transport problems involving cation exchange reactions such as groundwater restoration for the in situ solution mining of uranium.

The computer model developed in this study was applied to an actual field problem of groundwater restoration involving ammonium for a pilot scale in situ solution mining of uranium operation in northeast Colorado near the town of Grover. This represented the first application of a 2-dimensional transport model incorporating cation exchange reactions to a complex contaminant transport problem of site restoration for actual field data. The details of this study are presented in the following section.

CHAPTER VI

GROVER TEST SITE

6.1 History

The Grover uranium deposit was discovered in 1970 (Reade, 1976 and
1978) and is located in northeast Colorado near the town of Grover
(Figure 23).The major uranium mineralization occurs at a depth of about
200 - 250 feet below land surface in the Grover sandstone member of the
Laramie Formation.   In May 1976 an application was made to the Colorado
Water Quality Control Commission, Department of Health by Wyoming
Minerals Corporation to operate a pilot scale in situ uranium solution
mine at a site about 36 miles northeast of Greeley in Weld County in
Section 24, T.10 N. and R.62 W.   Wyoming Minerals was a partner in a joint
venture with Power Resources and Aquarius.   The purpose of the test was
to determine the economical and environmental feasibility of mining the
Grover uranium deposit using in situ solution mining technology.
In September 1976, Wyoming Minerals received permission to proceed with
the test.

In June 1977 solution mining was initiated at the Grover test site
using a triple 5-spot pattern with a well spacing of 40 feet (Leach
Field 1, Figure 24).An ammonium bicarbonate-hydrogen peroxide solution
was used as the lixiviant.   In September 1977 mining was terminated at
this leach field.   In October 1977 mining was recommenced in a second
leach field (a dual 5-spot pattern, Figure 24) again using ammonium
bicarbonate-hydrogen peroxide as the lixiviant.   Mining at leach field
2 was stopped in December 1977.   A changeover was made from the ammonium
bicarbonate-hydrogen peroxide lixiviant to a calcium bicarbonate-hydro-
gen peroxide lixiviant and mining was restarted in leach field 2 in
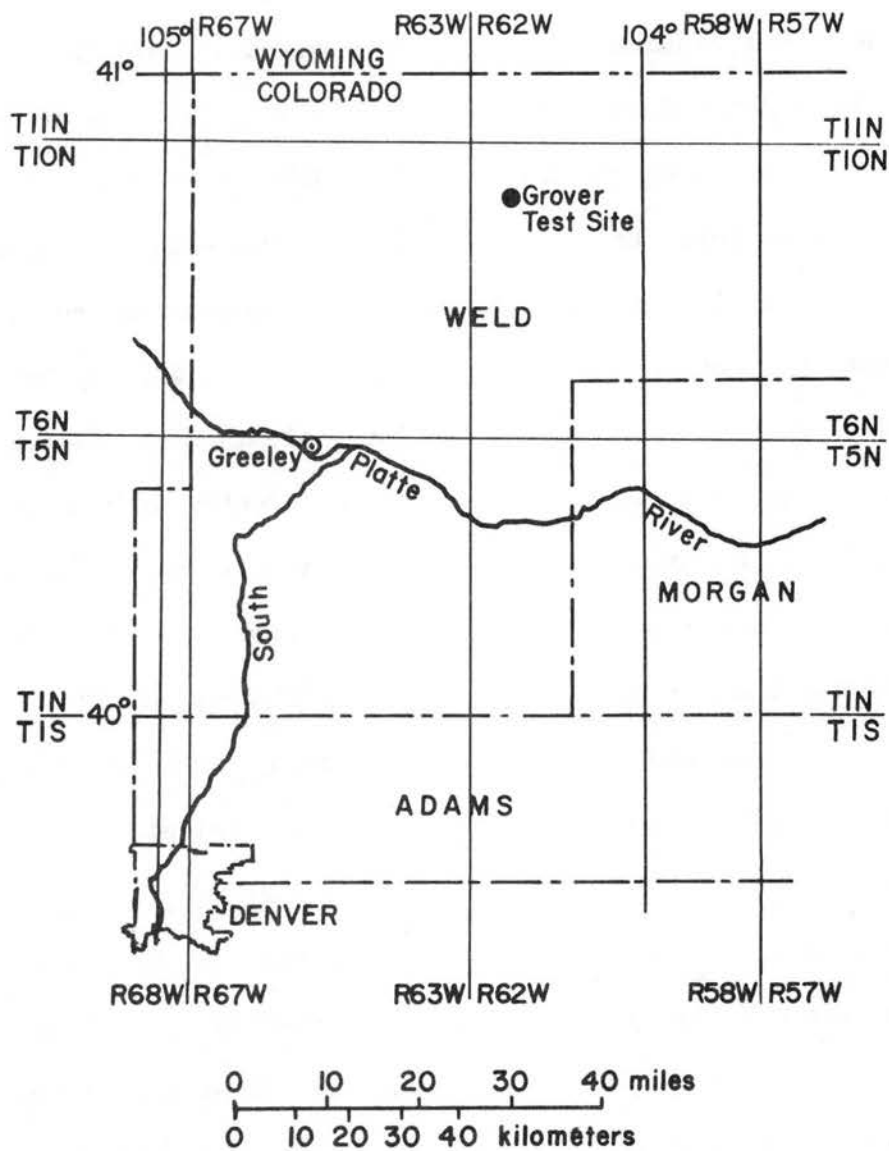
Figure 23. -- Location of the Grover test site.

EXPLANATION

- Control Points for Geologic Cross-section
- ▲GM5 Monitoring Well and Number
- A——A' Line of Section A-A'
- B——B' Line of Section B-B'
- Production Injection Wells

N

Test Site Boundary

CROW CREEK

B'

▲GM4

Leach Field I

▲GM5

GM8

Evaporation Ponds

▲GM3

Leach Field 2

A

A'

Plant Building

PM2

FM2

22C

▲4C

GM2

GM6

Model Boundary

▲PMI SW

B

GMI

GM7

FMI

Scale:

0	100	200	300	400 feet
0		50		100 meters
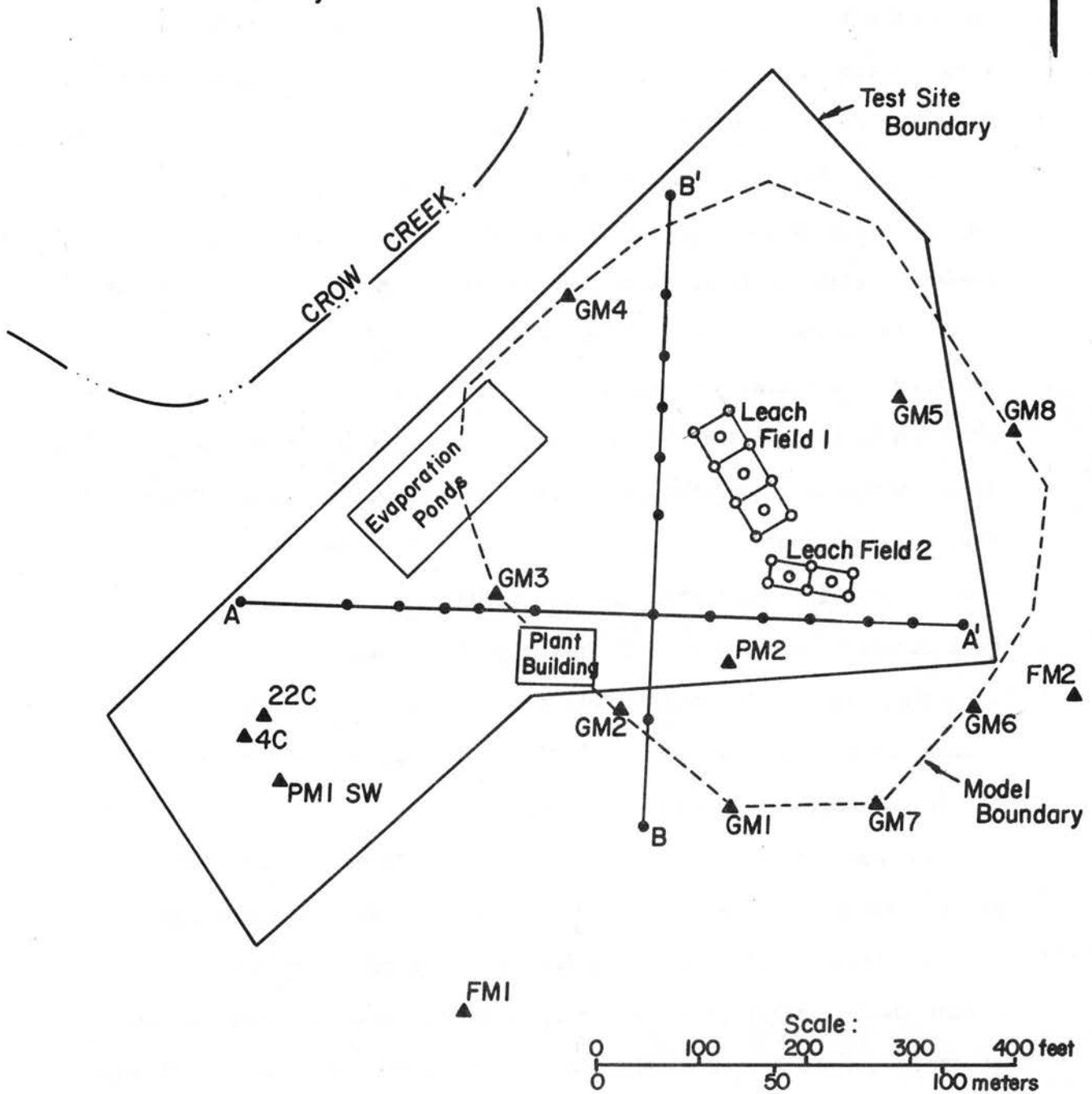
Figure 24. -- Layout of the Grover test site.

February 1978. All in situ solution mining tests were terminated in April 1978.

On May 13, 1978, restoration of leach field 1 was initiated. The restoration of leach field 1 was conducted in three separate phases. Between start up and July 5, clean water recycling was used (see Appendix A) using a reverse osmosis purification system. The ammonium concentrations in the recovery water dropped at the end of this restoration phase from post mining levels of about 490 mg/L to about 85 mg/L. To increase the rate at which the adsorbed ammonium was removed from the aquifer calcium chloride was injected during phase 2. In this second restoration phase the calcium concentration in the injection solution was increased gradually in increments of 250 mg/L to a level of about 1,000 mg/L. The ammonium in solution was removed using an air stripping technique. The addition of the calcium chloride in the injection water caused an increase in the ammonium concentration in the recovery water. During phase 2 the peak ammonium concentration in the recovery water was about 163 mg/L and the ending concentration was about 108 mg/L. This chemical treatment technique continued until September 7 at which time clean water recycling was reimplemented. This third phase of the restoration procedure lasted until February 28, 1979. The ending ammonium concentration in the recovery water was about 13 mg/L.

The restoration of leach field 2 was initiated in June 1978. The first phase of restoration for this leach field was to remove the ammonium from solution by air stripping. This continued until mid-August when chemical treatment using a calcium chloride additive was started. In mid-September the restoration of the two leach fields were coupled and clean water recycling was implemented. The restoration was terminated on February 28, 1979.

Following restoration, a ninety-day stabilization period was initiated. Groundwater samples were collected from seven wells (five wells in leach field 1 and two wells in leach field 2) at 1, 45 and 90 day intervals. Ammonium levels were less than 5 mg/L for all but one well which had an ammonium concentration of between 11 - 15 mg/L during this stabilization period. A limit of 50 mg/L for post restoration dissolved ammonium concentrations was set by the Colorado Department of Health.

Fourteen monitoring wells were installed to detect any escape of the contaminated groundwater from the mine site (Figure 24). To detect vertical excursions, two of the monitoring wells (wells PMI and PM2) were located in the sandstone unit immediately above the mined zone and two of the monitoring wells (wells FM1 and FM2) were located in the sandstone unit immediately below the mined zone. The remaining ten monitoring wells (wells GM1-8, 22C, and 4C) were used to detect any lateral excursion of contaminated groundwater from the mine site. The nearest monitoring well located in the Grover sandstone was about 230 feet downgradient from the production field.

In August 1979 Wyoming Mineral Corporation made application for abandonment of the Grover test site. The request for abandonment was denied by the Water Quality Control Commission which required Wyoming Mineral Corporation to conduct an additional year of sampling. In October 1980 the commission granted permission to Wyoming Mineral Corporation to abandon the site after no further desorption of ammonium was observed.

The computer model previously discussed in this dissertation was applied to the restoration of leach field 1. Restoration of leach field 2 was not considered since the mining history for this leach field included

use of both the ammonium bicarbonate and the calcium carbonate
lixiviants.

6.2 Geohydrology

Only that geology necessary to the understanding of the hydrology
of the study site is presented in this dissertation. For a fairly
complete description of the regional geohydrologic conditions, the
interested reader is referred to Kirkham, O'Leary, and Warner (1980).
Important geologic formations at the study site are in ascending order;
the Pierre Shale, the Fox Hills Sandstone, the Laramie Formation, and
the White River Formation.

The Pierre Shale consists of Upper Cretaceous marine shales,
claystone, and siltstone, with occasional thick sections of sandstone,
silty sandstone, and siltstone. It ranges in thickness in the general
vicinity of the mine site from about 3,000 to 8,000 feet. The Pierre
shale is transitional with the overlying Fox Hills Sandstone.

The Fox Hills Standstone of upper Cretaceous age consists of at
least 3 to 7 upward-coarsening sandstone beds overlain by as many as 5
massive sandstones that are separated by relatively thin shales. The
sequence of upward-coarsening sands constitute the lower member of the
Fox Hills Sandstone and the overlying massive sands comprise the upper
member (Ethridge, Tyler and Thompson, 1979). The Fox Hills Sandstone
ranges in thickness in the general vicinity of the mine site from about
200 to 450 feet. Extensive uranium mineralization occurs in the Fox Hills
Sandstone. A commerical scale solution mine has been approved near Keoto
which is about 10 miles southeast of Grover. Mining at this site will be
from the upper member of the Fox Hills Sandstone. The Fox Hills Sandstone

is the most dependable groundwater source in the area. Wells tapping the upper Fox Hills commonly yield 20 to 100 gpm and occasionally yield over 200 gpm. The lower Fox Hills contains fewer high permeability sands and well yields are typically low.

The Upper Cretaceous Laramie Formation overlies the Fox Hills Sandstone. It consists of interbedded sandstone, shale, claystone, and coal, and ranges up to 1600 feet thick. Numerous 10 to 125-feet sandstone beds occur throughout the Laramie. Most sandstone members of the Laramie generally are lenticular channel sandstones. An individual, locally thick sandstone may irregularly split into several thinner sandstone units. The Laramie provides a significant amount of the total groundwater currently utilized in the area primarily because it underlies much of the basin at shallow depths. The upper Laramie Formation supplies two wells for the town of Grover with yields of 35 and 55 gpm. Solution mining at the Grover test site was from a sandstone unit in the lower Laramie Formation called the "Grover Standstone".

The White River Formation of Tertiary age is exposed at the surface at the test site. It consists largely of poorly permeable, ashy siltstone and claystone, but highly permeable, fluvial channels of sandstone and conglomerate occur occasionally in the formation. Some wells recover minor amounts of water from the ashy siltstone, and claystone, but production is generally very low. The fluvial channels provide moderate to high quantities of groundwater. The tuffaceous beds of the White River Formation are postulated as the source of uranium in the sandstones of the underlying Laramie and Fox Hills Formations.

6.3 Model Input Data

The data used in the model concerning the mining and restoration events at the Grover test site are part of the public information supplied by Wyoming Minerals Corporation to the Colorado Department of Health. This data represents the best available reconstruction of the mining and restoration events at the Grover test site. Some of the data may be poorly defined or contain inaccuracies because (1) records kept may be sketchy with regards to details; (2) not all of the collected data may have been released by Wyoming Minerals Corporation because of the proprietary nature of the information; or (3) inadequate data may have been collected.

6.3.1 Grid

The model area included the leach field and extended to the perimeter of the containment zone, defined in Appendix A as the line connecting the monitoring wells surrounding the leach field (Figure 24). The model grid is shown on Figure 25. The model area encompasses about 250,000 ft^2 (about 5.7 acres, or .01 mi^2) and was divided into 204 elements which required 122 nodes (nodal numbering system shown on Figure 26). This grid enabled aquifer conditions to be simulated in detail at the Grover test site.

6.3.2 Boundary Conditions

Only the Grover Sandstone in the vicinity of the test site was modeled. Adjacent parts of the Grover Sandstone completely encircle the model area. Groundwater flow occurs across this model boundary. Along the boundary a constant-head condition was specified.

(see figure 24 for location)
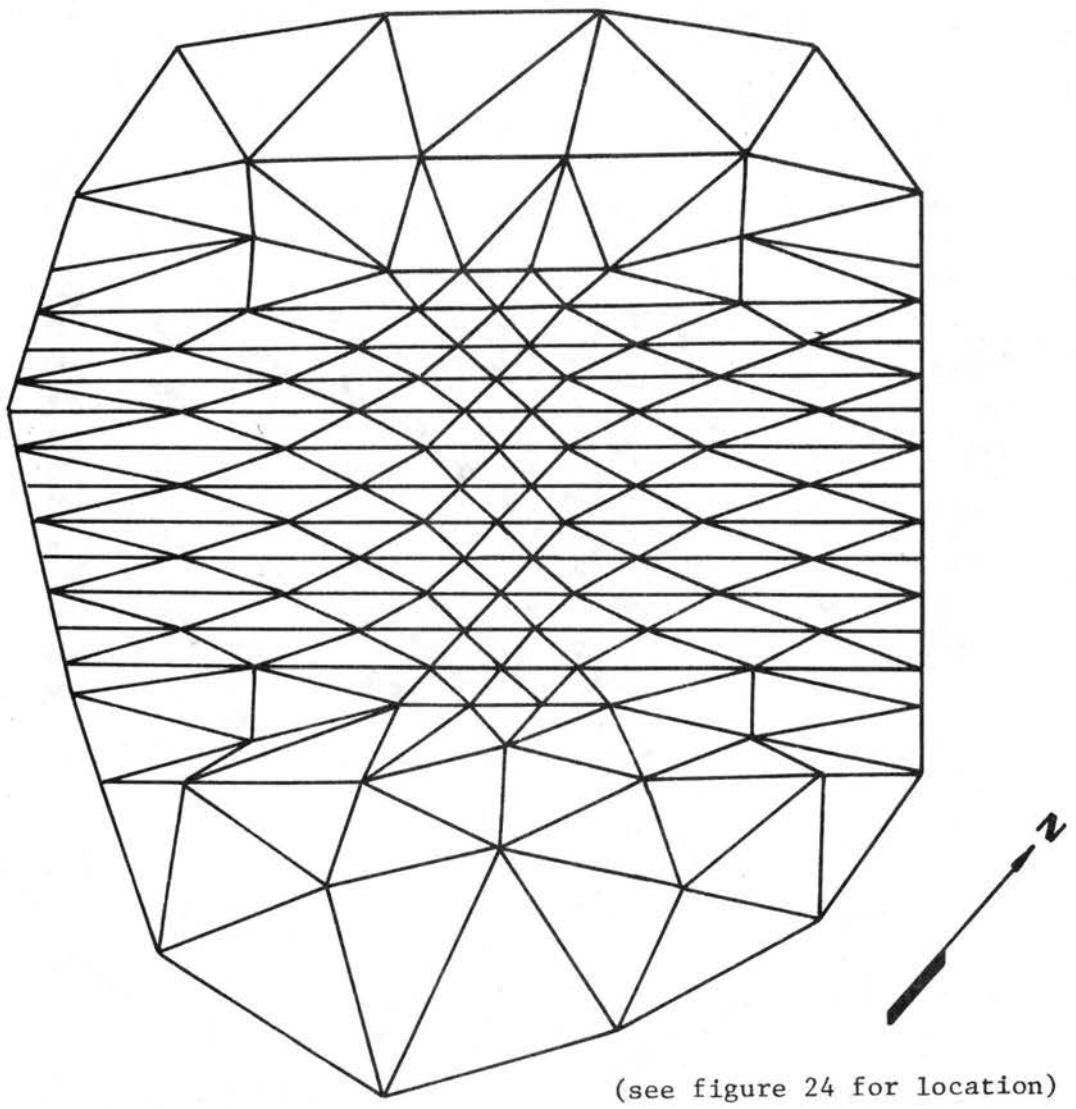
Figure 25. -- Model grid.
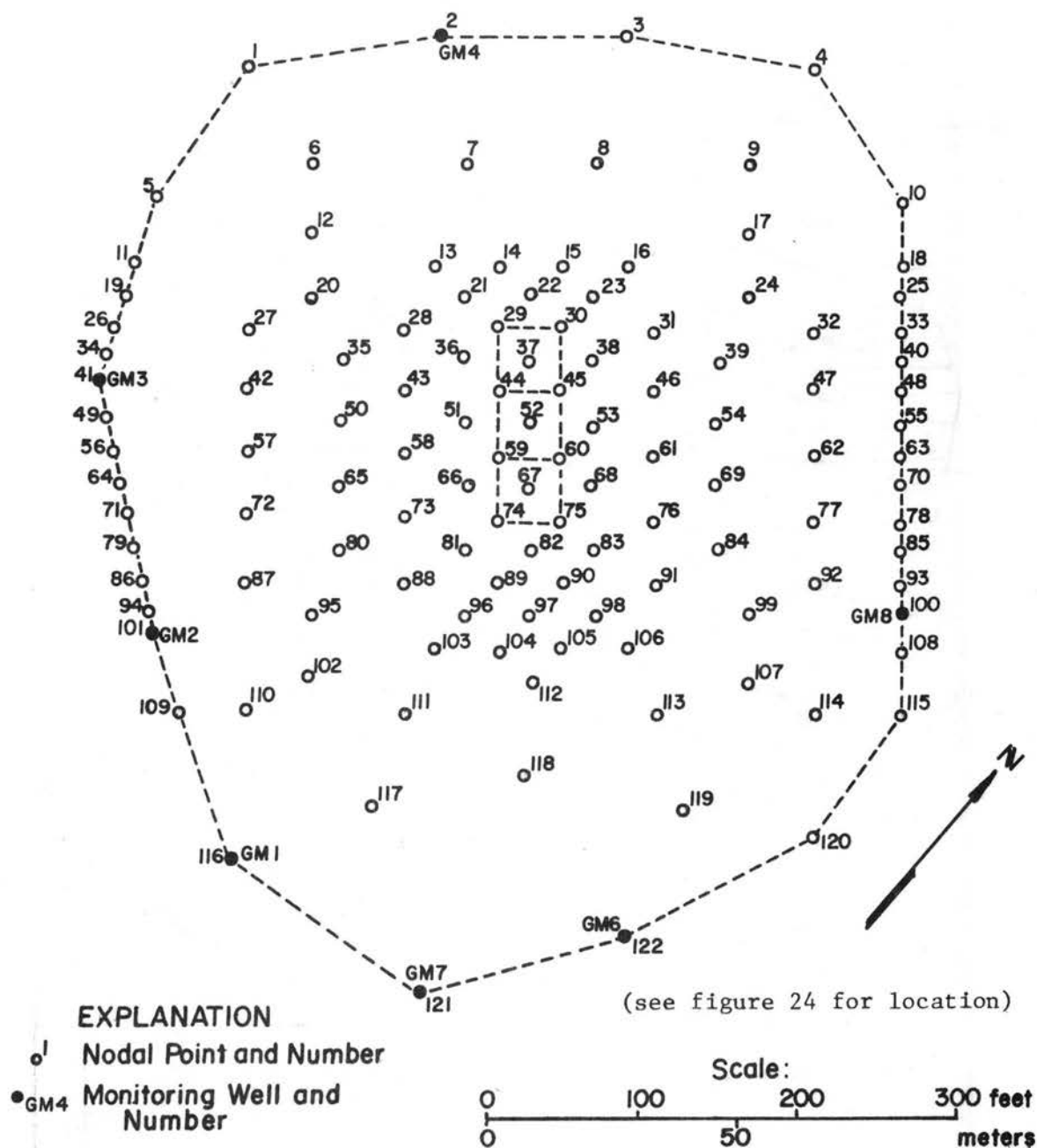
Figure 26. -- Nodal numbering system.

With a constant-head boundary, the potentiometric surface at the model boundary is not allowed to change with time, however, the rate of ground-water flow across the model boundary is allowed to vary with time.

During both the mining and restoration phases of operation, pumping rates slightly exceeded injection rates. This was done to maintain a slight groundwater gradient towards the leach field and thus prevent any migration of contaminated groundwater from the test site. Between June 1977 and January 1979 periodic water level measurements were made on the monitoring wells. Until October 1978 only slight variations in water levels were measured. However, between October 1978 and January 1979, water levels declined sharply in the monitoring wells with a maximum measured decline of about 17 feet. This decline was measured in all of the monitoring wells including well 4C which had a decline in water level of about 15 feet and which is considerably further from the leach field than the other monitoring wells. This would indicate that the water level decline measured in the monitoring wells was probably due to a regional decline in the altitude of the potentiometric surface in the Grover Sandstone and most likely related to natural varia-tions. The slight overpumping of the aquifer during mining and restora-tion was thought to have not resulted in any detectable decline in the water level in the monitoring wells.

6.3.3 Potentiometric Surface

Using water levels measured in the monitoring wells a potentio-metric surface map (Figure 27) was constructed for the model area for June 1977. The natural direction of groundwater movement within the model area is southeastward. The average drop in water level altitude
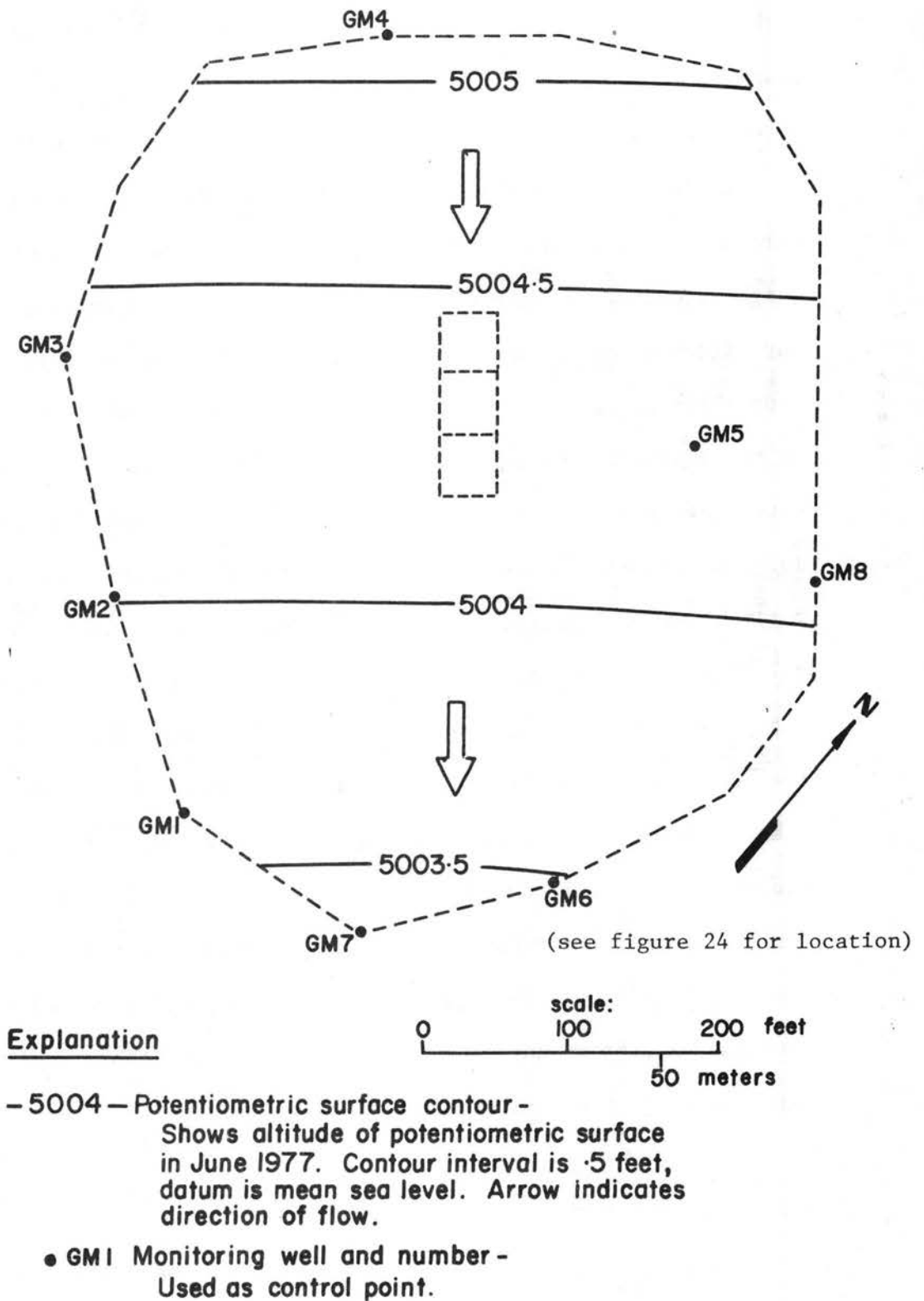
Figure 27. -- Potentiometric surface for the Grover sandstone.

between wells GM4 and GM7 was determined to be 1.7 feet. This converts
into an average groundwater gradient of 15.1 ft/mi. In comparison
Thompson, Wade and Ethridge (1980) determined the average groundwater
gradient at the Grover test site to be 26.9 ft/mi southwards. The
regional direction of groundwater movement is to the southeast towards
the South Platte River (Kirkham, O'Leary and Warner, 1980; and Reade,
1976 and 1978).

6.3.4 Saturated Thickness

Two geologic cross sections (Figures 28 and 29) were constructed
to determine the approximate thickness of the Grover Sandstone at the
test site. Within the model area the Grover Sandstone varies in thick-
ness from about 65 ft to 75 ft. The average thickness of the Grover
Sandstone within the model area is 70 ft. The regional geology indicates
that the Grover Sandstone dips to the north at a small angle (Reade,
1976) but for all practical purposes the Grover Sandstone is horizontal
within the model area.

6.3.5 Transmissivity and Storage Coefficient

Other geohydrologic data needed to construct the model include
transmissivity and storage coefficient of the aquifer. To determine
these parameters, an aquifer test was performed by personnel of
Wyoming Minerals Corporation. Analysis of the data from this aquifer
test yielded a transmissivity of 103 ft^2/day and a storage coefficient
of $.3x10^{-4}$ for the Grover Sandstone. Anisotropy was indicated with the
direction of greatest hydraulic conductivity approximately to the
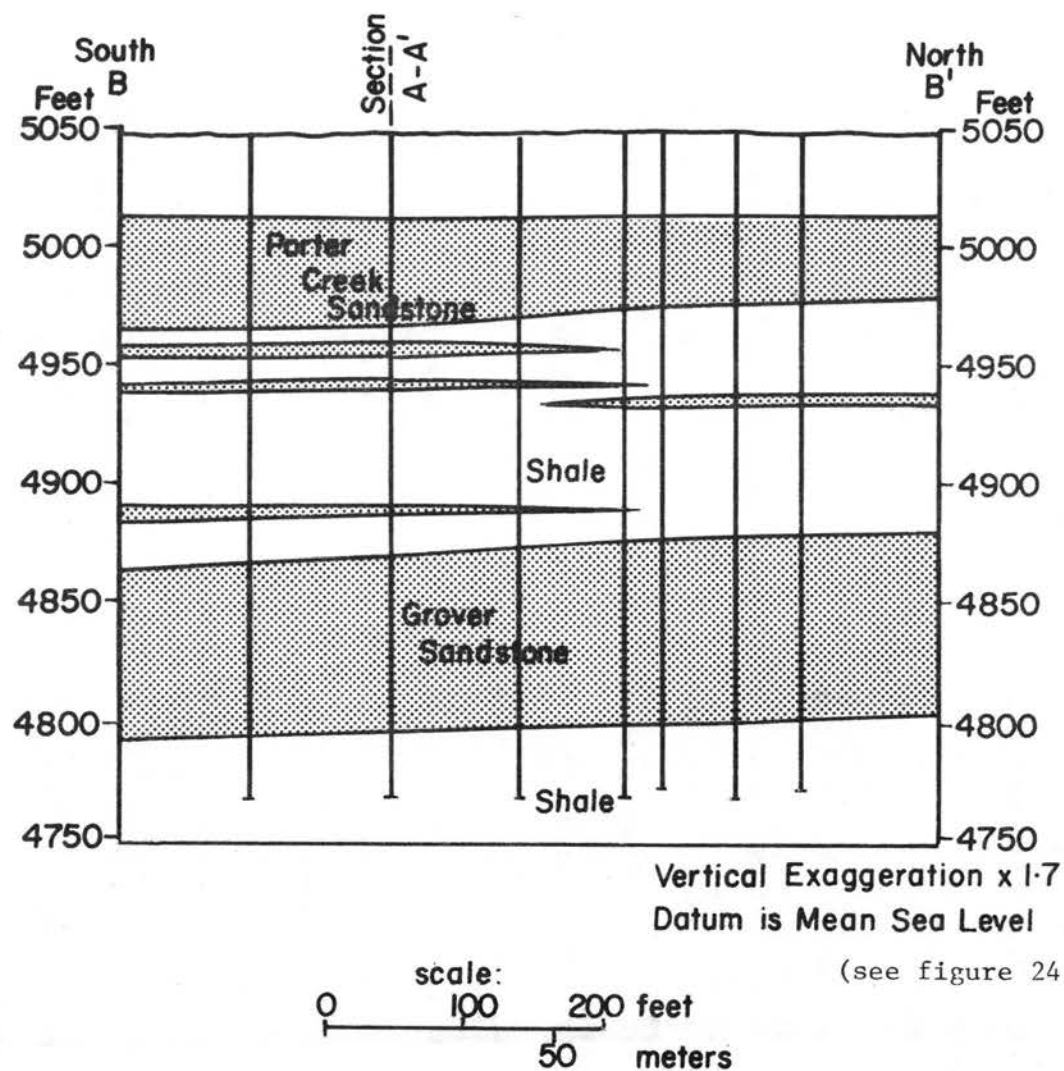
Figure 28. -- North-South geologic cross-section of the Grover test site.
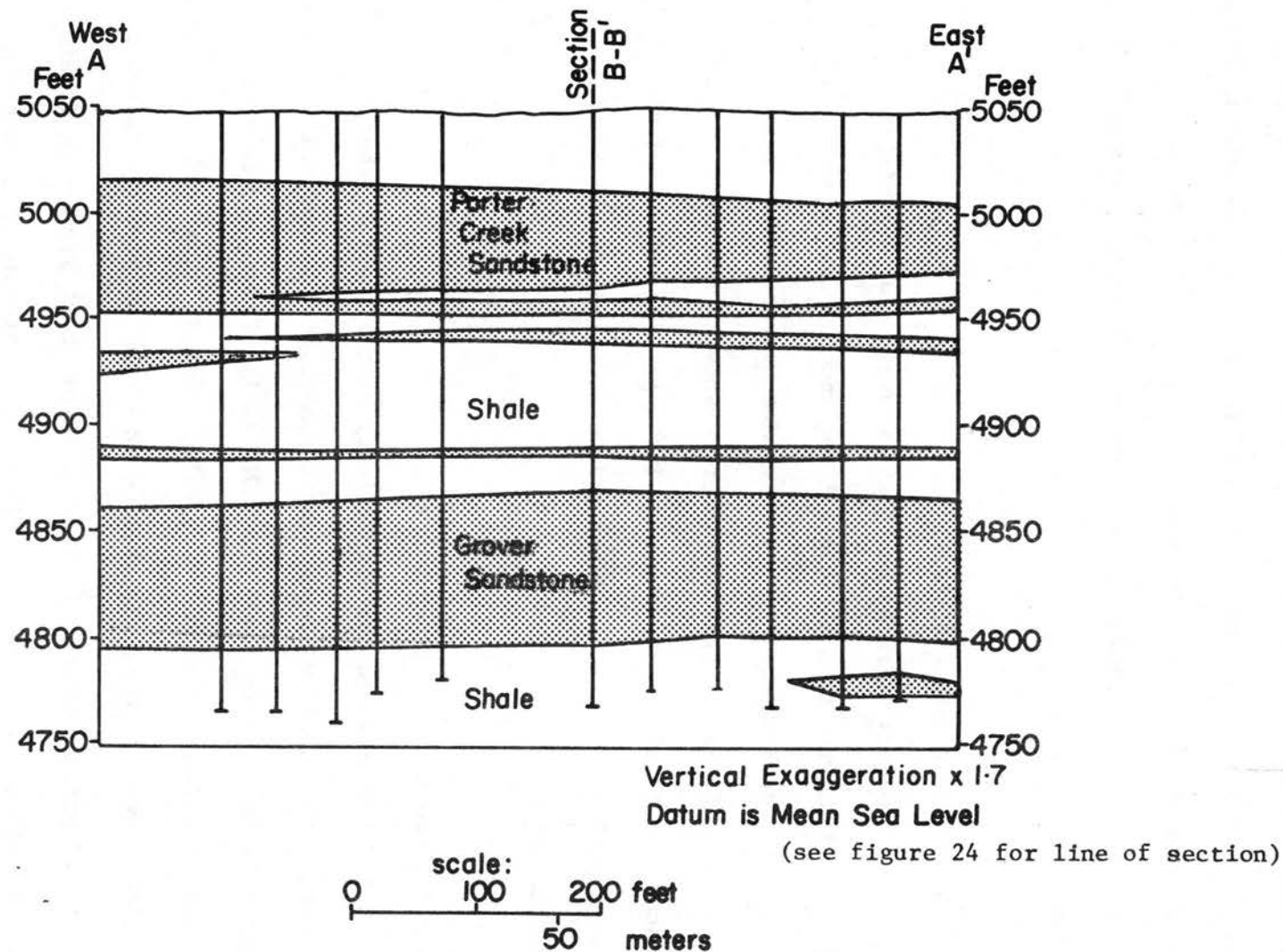
Figure 29. -- East-West geologic cross-section of the Grover test site.

northeast-southwest. Analysis of the data also indicated either the possible existence of leaky confining layers or a reduction in the pumping rate towards the end of the test. The aquifer test was of too short a duration (4 hours pumping and 4 hours recovery) with inadequate control to be conclusive.

6.3.6 Recharge Rate and Leakage

Any groundwater recharge to the Grover Sandstone within the model area from infiltration of rainfall and snowmelt was thought to be negligible and was ignored in the model. The Grover Sandstone at the test site is confined by upper and lower relatively thick shale layers. Though the aquifer test data were inconclusive, these confining layers were considered not to be leaky and were treated in the model as impermeable layers.

6.3.7 Porosity and Dispersivity

The porosity and the dispersivity of the aquifer material are also needed. The porosity of the Grover Sandstone was measured by Wyoming Minerals Corporation (1976 and 1978) to be 38 percent (an average value based on 14 samples from 1 core hole). This is supported by Thompson, Wade and Ethridge (1980) who in their work found the porosity to range from about 30 to 40 percent with an average value of about 36 percent (their value was based on 7 samples). In this study a porosity of 37 percent was used in the model. This value was assumed constant throughout the model area.

No field data were available on dispersivity. A constant value of 20 feet for longitudinal dispersivity was used in the model. This value was

sufficiently large to ensure numerical stability. A ratio of longitudinal to transverse dispersivity of .3 was used in the model.

6.3.8 Cation Exchange Capacity

The cation exchange capacity (CEC) of the Grover Sandstone was determined from 12 samples taken from 4 core holes at the Grover test site (Table 5). The CEC ranged for these samples from 4.4 to 21.0 meq/100g of solid sample with an average value of 9.4 meq/100g of solid sample. These values of the CEC are relatively low and is characteristic of samples that are primarily sandstone. The CEC is usually reported in units of meq/100g of solid sample. The model requires the CEC in units of meq/liter of solution. The conversion for this is

$$\text{CEC(meq/liter of solution)} = \left(\frac{\rho_s (1-\phi)(10)}{\phi}\right) \text{CEC(meq/100g of solid sample)} \quad (213)$$

where

ϕ = porosity, and

ρ_s = particle mass density (g/cm^3).

In equation (213) a density of water of 1000g/liter is assumed. Note the term $\rho_s(1-\phi)$ is simply the bulk mass density ρ_B. Values of particle mass density are given in Lambe and Whitman (1969) as ρ_s = 2.65 g/cm^3 for quartz, ρ_s = 2.61 g/cm^3 for kaolinite, ρ_s = 2.84 g/cm^3 for illite and ρ_s = 2.74 g/cm^3 for montmorillonite.

Using values of ϕ = .37 and ρ_s = 2.65 g/cm^3 in equation (213) the CEC of the Grover Sandstone ranged for the 12 samples from 198.5 to 947.6 meq/liter of solution with an average value of 423 meq/liter of solution. Expressed in constituent concentrations the CEC ranged from

TABLE 5.--Cation Exchange Capacity for the Grover Sandstone

Location Node (see Figure 26)	Depth (feet)	Cation Exchange Capacity (meq/100g)*
53	215	10.0
	220	4.4
	221	7.3
51	210	21.0
	223	7.0
37	217	12.0
	222	5.3
	231	9.1
	233	4.5
52	223	6.5
	235	5.4
	238	20.0

*of solid sample

3,600 to 17,100 mg/L of ammonium or from 4,000 to 19,000 mg/L of calcium.
For even the relatively low CEC of the Grover Sandstone, the cation
exchange process is significant. The net effect of the cation exchange
process is to potentially concentrate contaminants such as ammonium in
much greater concentrations in the adsorbed phase than are found in
solution.

The cation exchange capacity of the aquifer was chosen within the
limits of the field data to achieve the "best fit" during the calibration
of the model. The CEC was assumed constant throughout the model area.

6.3.9 Selectivity Coefficient

Recall that the selectivity coefficient K, corrected for activity
in both the solution phase and the adsorbed phase, was given for the
exchange between calcium and ammonium as (equation 26)

$$K = \frac{\overline{\lambda}_{Ca}\ \overline{N}_{Ca}\ \gamma_{NH_4}^{2}\ C_{NH_4}^{2}}{\overline{\lambda}_{NH_4}^{2}\ \overline{N}_{NH_4}^{2}\ \gamma_{Ca}\ C_{Ca}} \qquad (214)$$

where

C_{Ca}, C_{NH_4} = concentration of calcium and ammonium in solution
respectively in units of meq/L,

γ_{Ca}, γ_{NH_4} = activity coefficient for calcium and ammonium in
solution respectively (dimensionless),

$\overline{N}_{Ca}$, $\overline{N}_{NH_4}$ = equivalent fraction of calcium and ammonium occupying
the cation exchange sites respectively (dimensionless),

$\overline{\lambda}_{Ca}$, $\overline{\lambda}_{NH_4}$ = rational activity coefficient for the adsorbed calcium
and ammonium cations respectively (dimensionless), and

K = selectivity coefficient corrected for activity in both the solution and the adsorbed phases in meq/L.

In this equation the selectivity coefficient K is a constant.

The activity coefficients γ for the solution phase can be easily calculated using the Debye-Huckel equation (equation 20). Unfortunately, the rational activity coefficients $\overline{\lambda}$ for the adsorbed phase are unknown. Therefore, the selectivity coefficient K_c corrected for activity in the solution phase, but not in the adsorbed phase, was used in the model. The two selectivity coefficients are related by equation (23) as

$$K_c = \frac{K \, \overline{\lambda}^2_{NH_4}}{\overline{\lambda}_{Ca}} \tag{215}$$

Recall that though the selectivity coefficient K is a constant, the selectivity coefficient K_c is a variable. Values of K_c determined from Figure 5 are plotted for adsorption levels between .1 and .9 (Figure 30). A cubic polynomial was fitted to this data to obtain

$$K_c = 97.1 - 329 \, (\overline{N}_{NH_4}) + 552 \, (\overline{N}_{NH_4})^2 - 292 \, (\overline{N}_{NH_4})^3 \tag{216}$$

6.3.10 Initial Concentrations

Initial constituent concentration values for the groundwater are also required for model input. Premining and postmining water quality data at the Grover test site is shown in Table 6. The model has the capacity to simulate binary cation exchange (exchange between 2 cations). Multi cation exchange cannot be simulated. In this model application
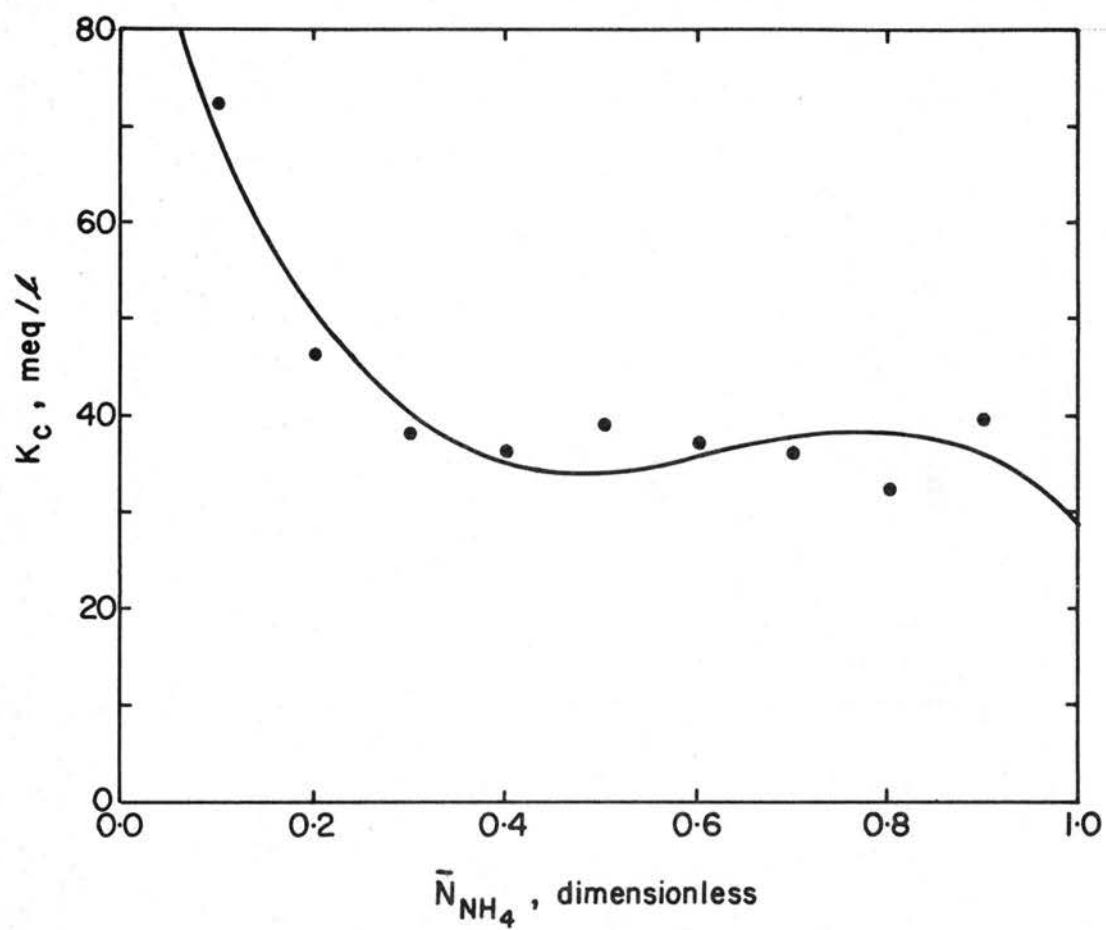
Figure 30. -- K_c versus $\overline{N}_{NH_4}$.

TABLE 6. -- Water Quality Data at the Grover Test Site (Data from Wyoming Mineral Corp., 1979)

Constituent	Premining[1] MG/L	Premining[1] MEQ/L	Postmining[2] MG/L	Postmining[2] MEQ/L
Calcium (CA^{+2})	9.1	.4541	75.8	3.7824
Magnesium (Mg^{+2})	1.1	.0905	22.4	1.8426
Sodium (Na^{+1})	85.2	3.7062	237.5	10.3313
Potassium (K^{+1})	4.4	.1133	13.1	.3350
Ammonium (NH_4^{+1})	.25	.0139	304	16.8538
		4.378		33.1451
Bicarbonate (HCO^{-1})	220.1	3.6074	1127.3	18.4765
Carbonate (CO_3^{-2})	4.3	.1437	11.6	.3866
Sulfate (SO_4^{-2})	38.3	.7974	311.0	6.4750
Chloride (Cl^{-1})	7.0	.1975	75.5	2.1300
Nitrate (NO_3^{-1})	1.4	.0226	5.2	.0839
Flouride (F^{-1})	.7	.0369	.1	.0053
		4.806		27.5573

[1]Premining Water Quality Data represents the average of 4 samples from each of 3 wells taken during June 1977 prior to the initiation of mining.

[2]Postmining Water Quality Data represents the average of 1 sample from each of 6 wells.

only the exchange between calcium and ammonium is considered. A necessary simplifying assumption was therefore to lump all cations except ammonium (in essence calcium, magnesium, sodium and potassium) into an equivalent concentration of calcium. The resulting premining equivalent concentration of calcium was 92 mg/L. The premining concentration of ammonium was 0.25 mg/L. The resulting postmining equivalent concentration of calcium was 327 mg/L and the postmining concentration of ammonium was 304 mg/L. Between the end of the mining phase and the beginning of the restoration phase, a bleed off of the adsorbed ammonium occurred and ammonium concentrations in solution in the contaminated zone increased from post mining levels of about 304 mg/L to prerestoration levels of about 490 mg/L.

No migration of contaminated groundwater was detected in the monitoring wells, during either the mining or restoration phases of operation. After the mining phase, core holes were drilled to determine the areal extent of groundwater contamination outside the leach field. It was determined that the ammonium contamination of the groundwater extended less than one cell distance (approximately 40 feet) from the leach field.

The wells in the leach field were perforated only in the zone of uranium mineralization within the Grover Sandstone. This was done to concentrate the flow of the lixiviant during the mining phase within the mineralized zone. The average well screen interval was 5 feet. Horizontal flow is simulated in the model, but in actuality the streamlines diverge vertically away from the injection wells and converge vertically approaching pumping wells as illustrated on Figure A4. Core hole

drilling after the mining indicated that an approximate 12 foot thickness of the Grover Sandstone had been contaminated by the adsorption of ammonium.

The adsorbed concentrations of calcium and ammonium were calculated in the model assuming that equilibrium conditions hold. For the initial premining condition, essentially all of the cation exchange sites on the solid aquifer material are filled by the calcium and none by the ammonium. For the initial prerestoration condition, the model calculated that approximately 54 percent of the cation exchange sites were filled by the ammonium and approximately 46 percent of the sites were filled by the calcium.

6.3.11 Pumpage and Injection Rates

The pumpage and injection rates for each phase of the restoration are shown on Figure 31. During each phase of the restoration a different pumpage and injection pattern was used in order to assure a fairly complete sweeping of the contaminated groundwater from the leach field.

During phase 1, a total of about 2.25 million gallons were recovered. The pumpage rate was approximately 40,000 gpd (the limit of the primary reverse osmosis unit). The injection rate was approximately 34,200 gpd. The net pumpage rate over the injection rate was therefore about 4 gpm. This excess was disposed of in evaporation ponds.

During phase 2, a total of about 2.5 million gallons were recovered. The rate of pumpage was maintained at 40,000 gpd. However, injection rates were increased so that there was a balance between pumpage and injection rates due to the high level of water in the evaporation

(a) Phase 1   (b) Phase 2   (c) Phase 3
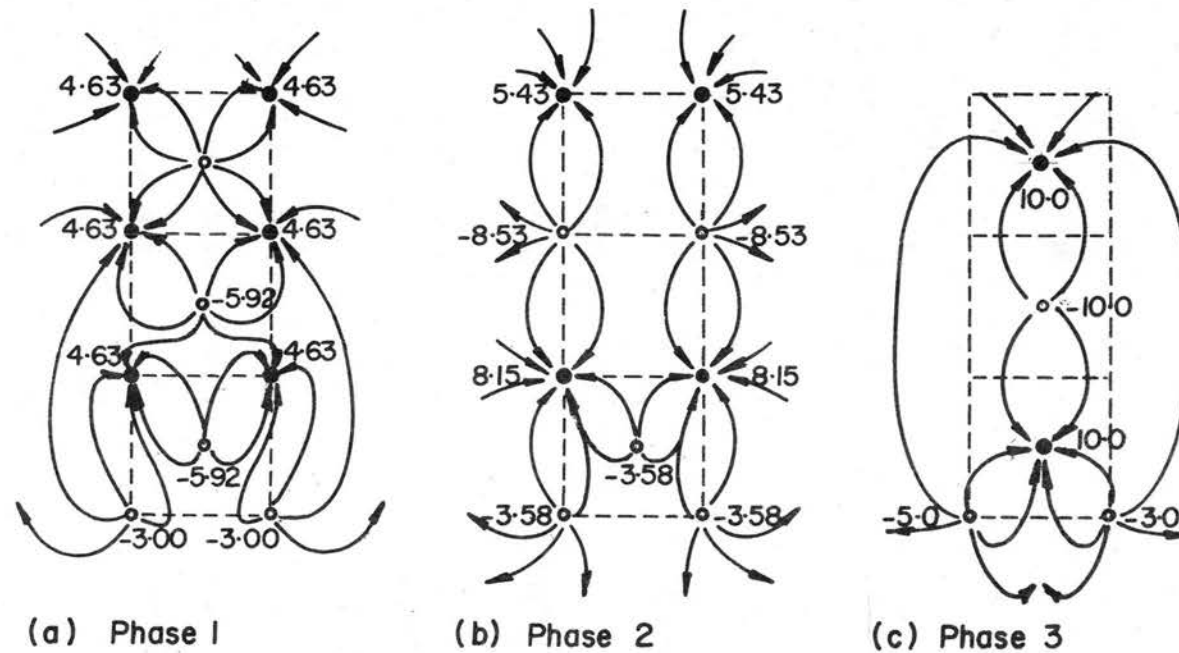
Explanation

● Pumping well

◆ Injection well

Number adjacent to well is pumpage rate in GPM

Negative number indicates injection

Figure 31. -- Pumpage and injection rates.

ponds. During the last two weeks of phase 2, a return was made to the phase 1 pumpage and injection pattern.

During phase 3, a total of about 5.3 million gallons were recovered. The pumping rate was reduced to about 29,000 gpd. The injection rate was approximately 26,000 gpd. The net pumpage rate over the injection rate was therefore about 2 gpm. For a short time period during the phase 3 restoration heavy overpumping of the aquifer was done to cause an influx of groundwater to the leach field from the surrounding uncontaminated aquifer. The overpumping had no significant benefit and was terminated by Wyoming Minerals. In the model, this short-term overpumping of the aquifer was not included.

A total of approximately 9.8 million gallons were pumped from leach field 1 during the restoration. This represents somewhere between 25 - 50 pore volumes of contaminated groundwater being removed before restoration was completed.

6.4 Model Calibration

Calibration of the transport model consisted of a comparison between observed ammonium concentrations and model-calculated ammonium concentrations. A plot of ammonium concentration versus cumulative water recovered during restoration is shown on Figure 32 for both measured and model-calculated values. There were some erratic fluctuations in the measured ammonium concentrations indicating noise in the data, probably due to either analytical measurement errors or unknown variations in aquifer properties. The plot was visually smoothed to eliminate this noise. For comparison, a plot of model-calculated concentration values assuming conservative transport is also shown on Figure 32. The model
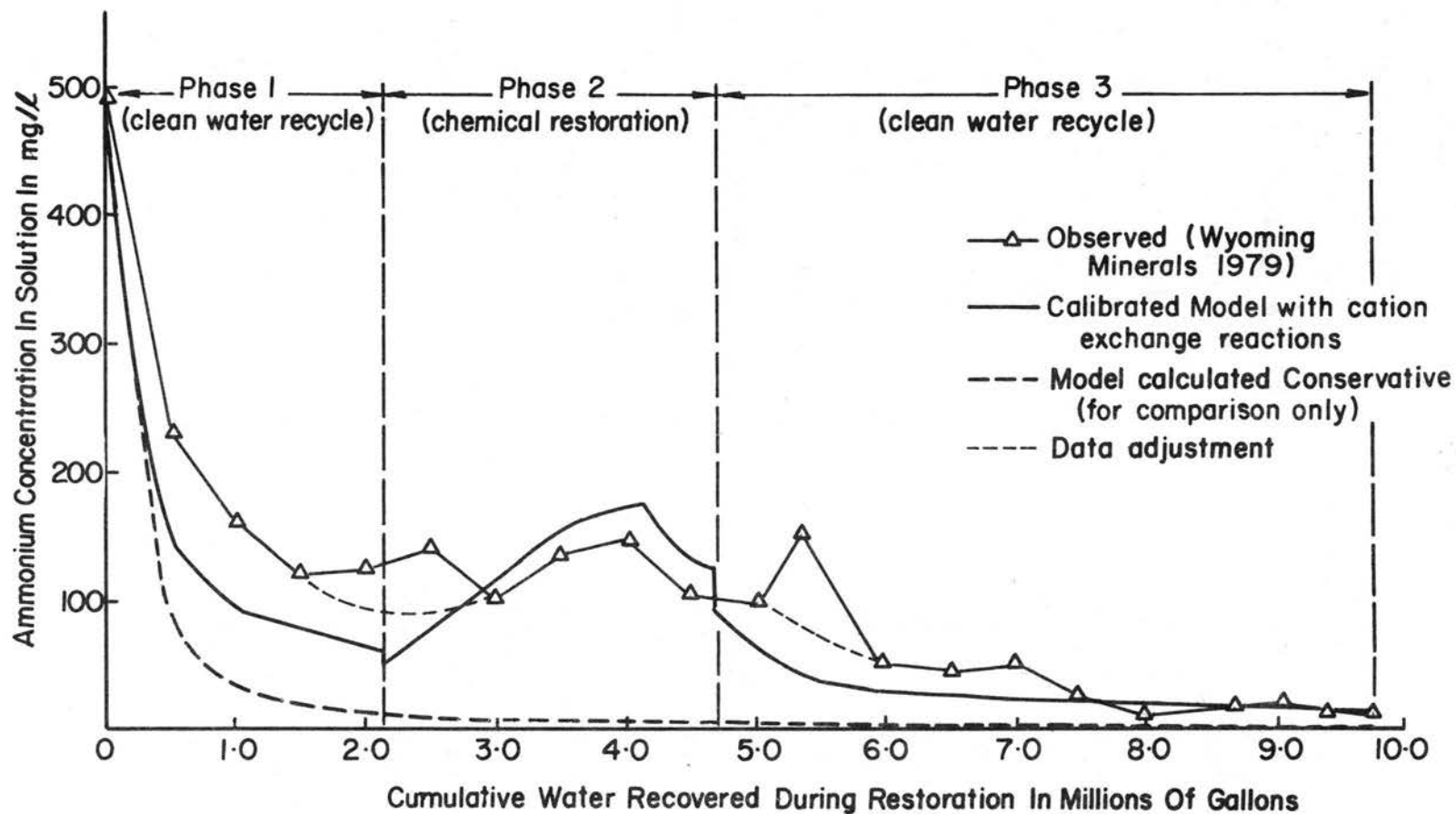
Figure 32. -- Ammonium concentration versus cumulative water recovered during restoration.

was calibrated to reduce the difference between the measured and the model-calculated total ammonium removed during restoration.

During phase 1 clean water recycling was used and the measured ammonium concentration dropped in the recovery water from an initial level of about 490 mg/L to an estimated 85 mg/L (Figure 32). The model calculated a similar but somewhat larger drop to about 61 mg/L (Figure 32). Most of the error between the observed and model-calculated ammonium concentrations is introduced during the initial .5 million gallons of water recovered. After that, the model-calculations roughly parallel observed concentrations during the phase 1 restoration. The difference may be due to many factors such as poorly defined initial concentration of ammonium in the model or poor initial efficiency of the reverse osmosis unit used to purify the contaminated water removed from the aquifer. During phase 1 of the restoration the contaminated recovery water was processed through a single reverse osmosis unit. During later restoration phases secondary and tertiary reverse osmosis units were also used. In the model an average efficiency rate of removal of 95 percent for ammonium and 97.5 percent for calcium was used.

During phase 2 a calcium chloride solution was injected to increase the rate at which the adsorbed ammonium was flushed from the aquifer. The calcium chloride was added in increments of 250 mg/L up to 1000 mg/L. This resulted in measured ammonium concentrations in the recovery water increasing from post phase 1 restoration levels of an estimated 85 mg/L to a peak of 163 mg/L. No measurable increase in calcium concentrations in the recovery water occurred during phase 2 until shortly before the peak in ammonium concentration was reached (roughly at about the 4 million gallon point in Figure 32). This breakthrough of the calcium in the recovery

water prompted Wyoming Mineral Corporation to modify the pumping pattern in order to assure a complete contact of the entire field with the calcium solution. During the final two weeks of phase 2 restoration, a return was made to the phase 1 pumping and injection pattern and the ammonium concentrations in the recovery water decreased to about 108 mg/L.

The model-calculated ammonium concentrations agreed remarkably well with the measured concentrations during phase 2. The model-calculated ammonium concentration increased from post phase 1 restoration levels of about 61 mg/L to a peak of 172 mg/L. The model-calculated peak occurred at nearly the same time as did the peak in ammonium concentration measured in the field (Figure 32). The model-calculated ending phase 2 ammonium concentration was 124 mg/L compared to 108 mg/L measured in the field.

Note that at the beginning of phase 2 restoration there was a slight drop in the model-calculated ammonium concentration in the recovery water from the ending phase 1 concentration. This results from the change in pumping patterns between phase 1 and phase 2. Different pumpage and injection wells were used and thus the slight change in the ammonium concentration of the recovery water.

The model calculated that during phase 2 the addition of the calcium chloride solution would have a greater effect of eluting adsorbed ammonium than was actually observed in the field. This difference may be caused by possibly too large of a CEC in the model. The CEC used in the model was 300 meq/L of solution. This was determined in the model by a trial and error procedure to obtain the overall best fit between model-calculated and observed ammonium concentrations for the given set of input data (in essence for the given pumpage and injection rates, initial concentration conditions, etc.). Errors in this input data

would be incorporated into the model determined CEC. The CEC of 300 meq/L used in the model is less than the average CEC of 423 meq/L measured in the field. The justification for this is that not all of the cation exchange sites may be available for the calcium-ammonium exchange due possibly to fixation of the ammonium. A second reason for the difference is the possibility of channelizing of the flow within the aquifer in the field. Permeability changes within the aquifer during restoration may have prevented a complete sweeping of the contaminated aquifer. These permeability changes could result from a detrimental reaction between the calcium-chloride solution and unreacted ammonium-bicarbonate lixiviant forming calcium carbonate, which because of its relatively low solubility in water may have been precipitated from solution and thus reduced the permeability of the aquifer along the reaction front. Ortiz, Ferentchak, Ethridge, Granger and Sunada (1980) have demonstrated similar permeability changes in the laboratory.

During phase 3 clean water recycling was repeated and the measured ammonium concentration dropped in the recovery water from about 108 mg/L to about 13 mg/L. The model-calculated ammonium concentrations dropped from 124 mg/L to ending concentrations of about 16 mg/L. Note the drop in model-calculated ammonium concentrations at the beginning of phase 3. This drop is again caused by the changing of the pumping patterns. No reason is known why similar drops were not measured in the field data by Wyoming Minerals Corporation.

In general, the agreement is fairly close between the observed and model-calculated ammonium concentrations in the recovery water shown on Figure 32. Differences are attributed to five primary factors: (1) errors in the model input data, (2) channelizing of the flow within

the aquifer in the field caused as previously discussed by permeability

changes within the aquifer during restoration from detrimental chemical

reactions, (3) insufficient number of nodes used in the model, particu-

larly in the vicinity of the leach field to provide a more detailed

definition of model-calculated ammonium concentrations in the recovery

water,(4) error in the selectivity coefficient used in the model, and

(5) assumptions such as 2-dimensional groundwater flow and binary cation

exchange upon which the model was developed may contributed also to the

difference. Errors in the model input data include unknown variations

in aquifer properties (permeability, effective porosity, CEC, etc.),

poorly defined initial concentrations of ammonium, and errors in the

reconstruction of the restoration processes used by Wyoming Minerals

Corporation (errors in pumpage and injection rates, errors in efficiency

of reverse osmosis process used to purify the recovered contaminated

groundwater, etc.). The selectivity coefficient is valid only for a

particular cation exchange reaction and for a given porous medium. The

value of the selectivity coefficient used in the model was computed from

laboratory data for the binary exchange between calcium and ammonium

for a montmorillonite clay. Analysis of the error introduced into the

selectivity coefficient because field conditions differed from the

above conditions was beyond the scope of this study.

Comparison of the plot of model-calculated ammonium concentration

assuming conservative transport in Figure 32 with the observed field

data and with the model-calculated concentrations incorporating cation

exchange reactions clearly indicate the importance of considering the

cation-exchange process in groundwater restoration for ammonium. For

chemical solutes not subject to the cation exchange process the clean up

of the contaminated aquifer occurs at a much faster rate.

The calibration of the model was performed on a "macro" level. That is no comparison was made of measured ammonium concentrations at the wells sampled (recall that there were 5 such wells in leach field 1) with model-calculated ammonium concentrations for the corresponding nodes. During the calibration of the model it was observed that ammonium concentrations at the nodes in the leach field were very sensitive to changes in the pumpage and injection patterns. Slight changes in the pumpage and injection pattern used in the model often caused considerable changes in the concentration at the nodes in the leach field. However, the overall calibration of the model was fairly insensitive to this type of error in the model input data. Even though the ammonium concentration at a specific node might change considerably depending on the pumpage and injection history for that node, the total amount of contaminated groundwater removed from the aquifer during restoration was a constant (approximately 9.7 million gallons) and the change in the total amount of ammonium recovered during restoration was small and thus on a "macro" level did not affect the extent of aquifer restoration accomplished by Wyoming Mineral Corporation. With this in mind, the following results on the groundwater restoration at the Grover test site are presented.

6.5 Results

In the field, groundwater was sampled during restoration for ammonium contamination at only a few selected points. The extent of groundwater contamination beyond these points could only be surmised. One of the major advantages of computer modeling is the capability to simulate conditions in the aquifer at essentially any place and time. The calibrated model was used to calculate the dissolved post restoration

ammonium concentrations at all 122 nodes in the model (Figure 33). The
model results indicate that at all but 2 of the nodes the dissolved
ammonium concentration is less than the 50 mg/L limit agreed to between
Wyoming Minerals Corporation and the Colorado Department of Health for
post restoration ammonium levels. Thus considering the uncertainties
in the model data, the model results do not contradict and in general
support that Wyoming Minerals Corporation has successfully restored
dissolved ammonium concentrations in the groundwater at the Grover test
site to within the agreed limit of 50 mg/L.

In general, the restoration of the aquifer was more complete within
the leach field than for the immediate surrounding area. Of the 11
nodes in the leach field, the model-calculated ammonium concentrations
were less than 10 mg/L at 5 of the nodes, between 10 to 20 mg/L at 3 of
the nodes and between 20 to 35 mg/L at 3 of the nodes.

Through the processes of hydrodynamic dispersion and convective
transport the ammonium was spread to the immediate area surrounding the
leach field. Even though overpumping in both the mining and restoration
phases was done to maintain groundwater gradients toward the leach field,
some of the groundwater follows a path initially away from the leach
field, but ultimately returns (see Figure A6). This is caused by outer
wells in the leach field being used for injection which results in local
groundwater gradients near these wells opposite to the regional ground-
water gradient. In the immediate area surrounding the leach field the
model-calculated ammonium concentrations were greater than 50 mg/L at 2
nodes, between 35 to 50 mg/L at 3 nodes, between 20 to 35 mg/L at 14
nodes and between 10 to 20 mg/L at 8 nodes. In the remaining 84 nodes in
the model the model-calculated dissolved ammonium concentrations were
less than 10 mg/L.
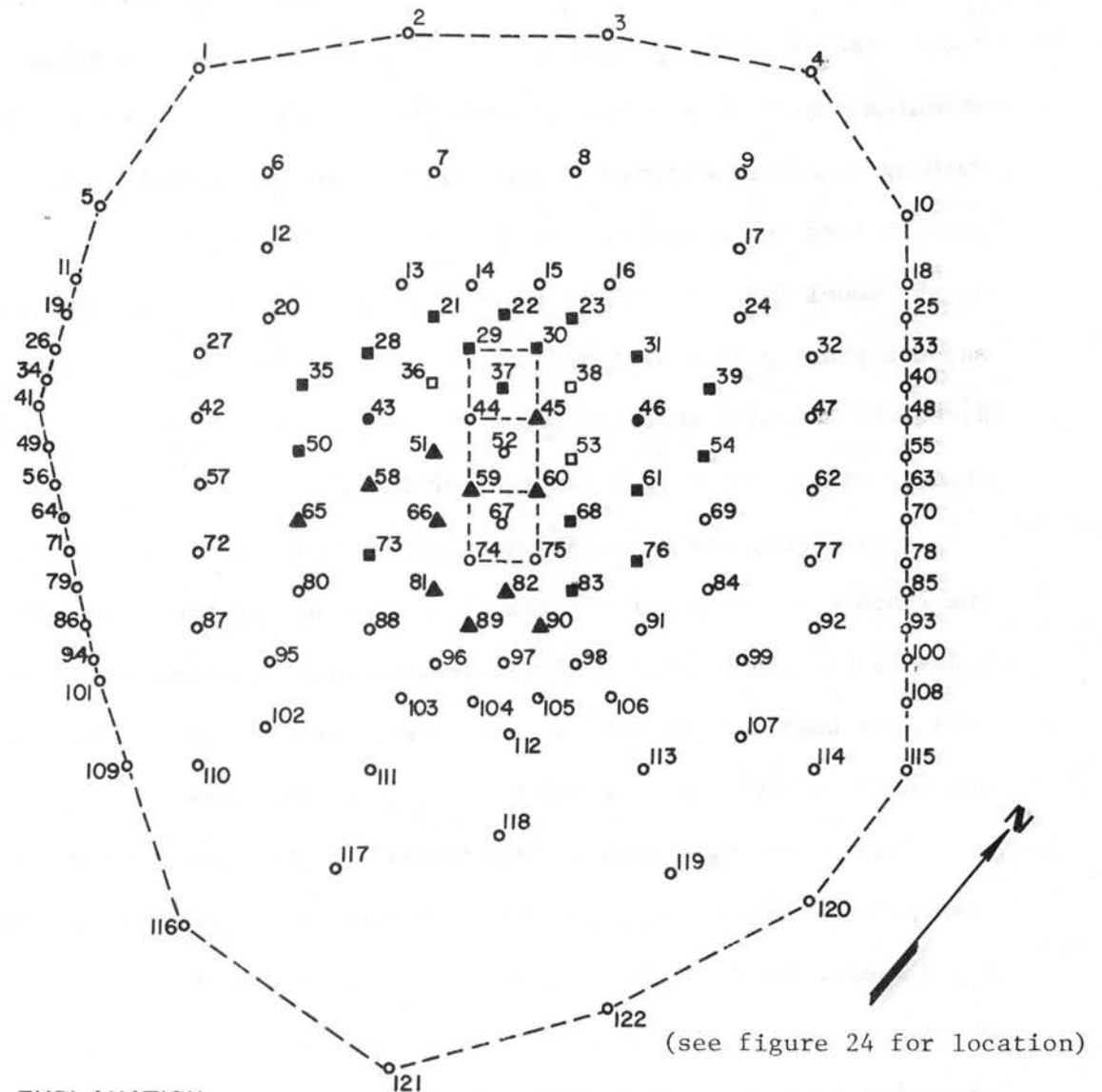
Figure 33. -- Model-calculated post restoration dissolved Ammonium concentrations.

EXPLANATION

Model-calculated dissolved ammonium concentrations in milligrams per liter:

- ● greater than 50
- ▫ between 35 and 50
- ■ between 20 and 35
- ▲ between 10 and 20
- ○ less than 10

Number adjacent to symbol is nodal numbering system (see Figure

Scale:

(see figure 24 for location)

Nodes 44 and 45 (Figure 33) had the greatest model-calculated ammonium concentrations. During the second phase of restoration, injection occurred at these nodes and high concentrations of ammonium were forced into the surrounding aquifer. The model results indicate that this ammonium remained more or less in place during later restoration efforts.

The calibrated model was also used to calculate the adsorbed post restoration ammonium concentrations at all of the nodes in the model (Figure 34). The model results indicate that potentially large quantities of adsorbed ammonium remain in the aquifer at the Grover test site. The maximum adsorbed ammonium concentration calculated by the model was greater than 1000 mg/L. At a total of 30 of the nodes in the model the adsorbed ammonium concentration was calculated to be greater than 250 mg/L and at 47 of the nodes to be greater than 50 mg/L. Eventually, all of this adsorbed ammonium will be desorbed by the exchange with other cations in the groundwater. The mobility of ammonium in groundwater is low and the process of cation exchange by itself would not probably result in high future dissolved ammonium concentrations in the groundwater.

However, the conversion of ammonium to nitrate would increase its mobility substantially and coupled with the process of cation exchange could possibly result in future high nitrate concentrations in the groundwater. The potential to convert ammonium in groundwater is not known, but thought to be reasonably possible. An oxidizing environment and certain nitrifying bacteria are required. During the solution mining phase an oxidizing environment was established. The natural occurrence of nitrifying bacteria in groundwater systems is not known. The

EXPLANATION

Model-calculated adsorbed
ammonium concentrations in
milligrams per liter :

- ● greater than 1000
- ▫ between 750 and 1000
- ■ between 500 and 750
- ▲ between 250 and 500
- △ between 50 and 250
- ○ less than 50

Number adjacent to symbol is nodal
numbering system (see Figure

(see figure 24 for location)
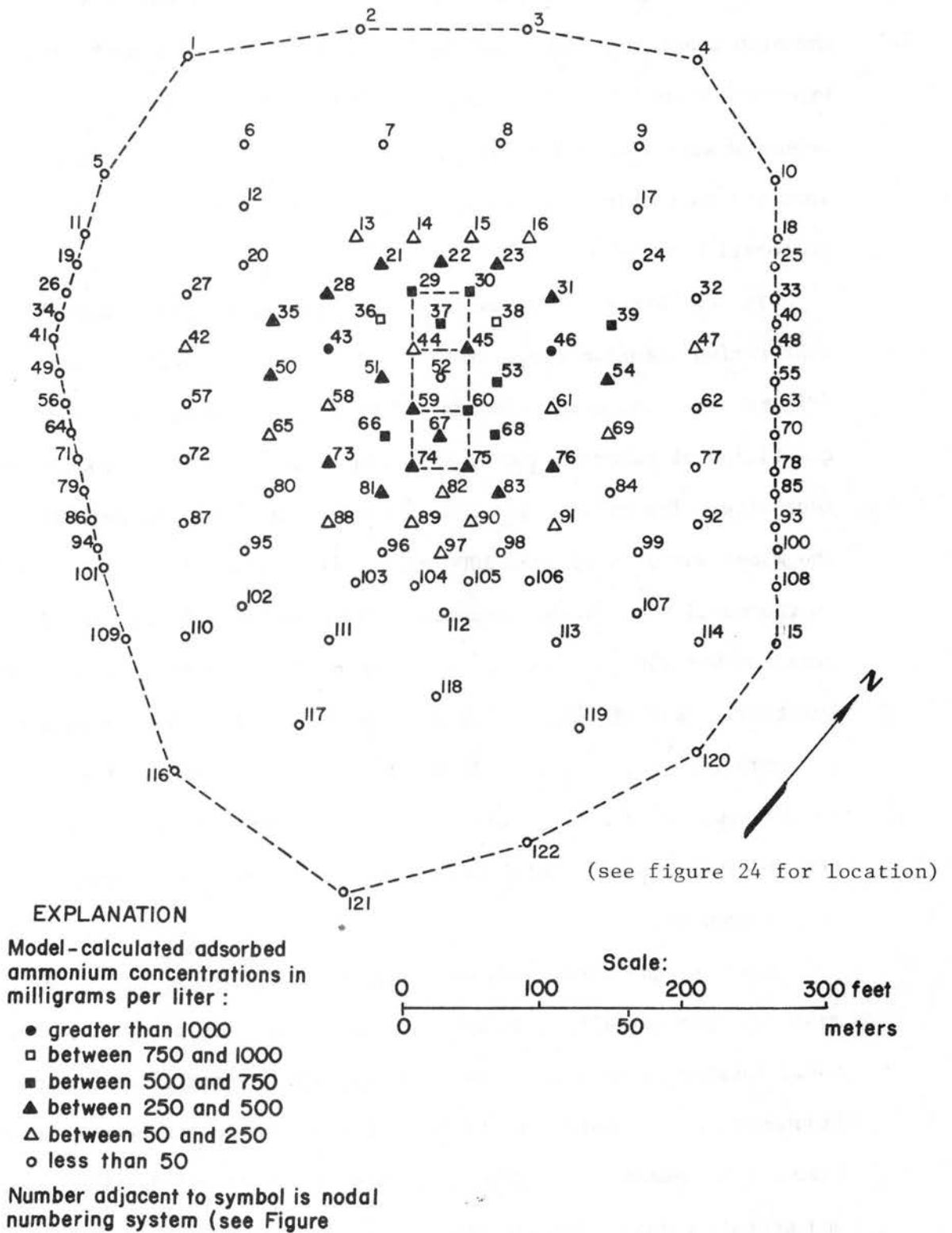
Figure 34. -- Model-calculated post restoration adsorbed Ammonium
concentrations.

possibility exists that nitrifying bacteria may have been introduced into the groundwater during solution mining.

The significance of the residual adsorbed ammonium is best left to the environmental engineer and others involved in the regulation of solution mining. However, it is the responsibility of the groundwater hydrologist to provide the best possible data to aid them in their decision making process. The model developed in this study is intended to provide this information.

CHAPTER VII

SUMMARY AND CONCLUSIONS

In situ solution mining represents a new, more complex contaminant
transport problem in site restoration than traditional contaminant
transport problems. This dissertation describes a mathematical treatment
of the site restoration of contaminants subject to adsorption and ex-
change on the porous media. The adsorption reaction is treated as an
equilibrium controlled reversible binary cation exchange process. This
requires that both chemical species involved in the exchange process be
followed as they flow with the groundwater through the porous media.
The mathematical formulation of the problem includes one equation
describing groundwater flow plus two additional equations for solute
transport (one equation for each of the chemical species involved in
the binary cation exchange). The transport equations are coupled through
two additional equations which describe the cation exchange process.
In a leap-frog fashion the groundwater flow equation is solved for the
head distribution in the aquifer and the two coupled transport equations
are solved simultaneously for the dual changes in dissolved and adsorbed
concentration for both chemical species.

A discussion of the fundamentals of the cation exchange process is
presented in the dissertation along with a review of the major cation
exchange equations. The assumption is made that the process of cation
exchange is an entirely reversible process, that the cation exchange capa-
city of the porous medium is constant and that the cation exchange sites
are always filled (the latter assumption ensures electroneutrality). The
law of mass action is the most widely used equation to quantitatively
describe the cation exchange process and is used in this study.

The groundwater flow equation and the two coupled solute transport equations were solved by the Galerkin-finite element method. In the finite element method, approximating integral equations were formed to replace the original governing partial differential equations for groundwater flow and solute transport. The integration of these integral equations were performed using triangular elements and linear shape functions. The coupled transport equations contain non-linear variable coefficients that are dependent on concentration changes and which require the integrations to be repeated frequently. The use of triangular elements and linear shape functions in the finite element solution allowed some very powerful integration formulas to be applied which considerably reduced the computational effort and time required to make these integrations than would have otherwise been required.

A computer program was written which calculates the dual changes in concentration of two reacting solutes subject to binary cation exchange in flowing groundwater. The computer program calculates both dissolved and adsorbed concentrations at any specified place and time due to the process of convective transport, hydrodynamic dispersion, mixing from fluid sources and cation exchange reactions. The program allows specification of any number of injection or withdrawal wells and of spatially varying distributed recharge or discharge, transmissivity, saturated thickness, cation exchange capacity, boundary conditions and initial heads and concentrations. The program can simulate either transient flow-transient transport or steady state flow-transient transport.

A complete documentation of the program is contained in the report.

The accuracy of the numerical solution used in the computer program to the groundwater flow equation and to the coupled convection-dispersion equations was evaluated by analyzing some relatively simple problems for which analytical solutions were available and then comparing the model calculations with the analytical solutions. In these test problems good agreement between the model and analytical results were obtained. An example problem was also presented for solute transport with cation exchange reactions. The computer program as written is general and flexible in that it can be readily and directly applied to a wide range of types of problems. However, some program modifications may be required for efficient application to specialized problems or conditions not included in the general model.

The model has specific application to groundwater restoration for the in situ solution mining of uranium. Basically in situ solution mining of uranium consists of injecting through wells a lixiviant (consisting of a leaching agent and an oxidizing agent) into the sandstone formation which contains the uranium deposits. The uranium ore is preferentially dissolved from the host rock and the uranium-bearing groundwater is recovered through pumping wells. Ammonium bicarbonate is the most commonly used leaching agent and during mining the ammonium is adsorbed on the porous media when it is in relatively high concentrations in the groundwater. Later during the restoration process when ammonium concentrations in the groundwater are lower, the ammonium is released back to the groundwater. The desorption of the ammonium occurs slowly and may result in significant residual ammonium concentrations adsorbed in the aquifer after the restoration process was thought to be completed.

The model was applied to an actual field problem of groundwater restoration involving ammonium for a pilot scale in situ solution mining of uranium operation. This represented the first application of a 2-dimensional transport model incorporating cation exchange reactions to a complex contaminant transport problem of site restoration for actual field data. The model developed in this study was demonstrated to be capable of simulating the adsorption and exchange of contaminants on the porous media. The model should be readily adaptable to many other field problems.

The model is presented as a basic working tool to be used by regulating agencies, mining companies and others concerned with groundwater restoration for in situ solution mining. The model can be used to assess the extent of groundwater restoration from either past or current restoration efforts or as a predictive tool to evaluate alternative restoration strategies. The usefulness of such a predictive tool for planning purposes would include assessment of the trade-off benefits between differing levels of restoration efforts versus desired restoration objectives, restoration time requirements, total volumes of water required for restoration, effects of varying pumpage and injection rates and patterns, effects of varying eluting concentrations, etc.

CHAPTER VIII

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APPENDIX A

IN SITU SOLUTION MINING

A.1 Uranium Geochemistry

Uranium deposits in Tertiary age sandstone formations probably
contain the largest uranium reserves in the United States. Because
these sandstones often are fairly good aquifers with significant
permeability, the uranium ore in them is particularly amenable to
solution mining techniques. To understand how solution mining works,
a description of uranium mineralogy and of the depositional process of
uranium is presented.

Uranium has many valence states (+2, +3, +4, +5 and +6), but only
the +4 and +6 states are of mining interest. In the lowest two valence
states (+2, and +3) uranium is such a powerful reducing agent that it
can free hydrogen from water. Uranium in the +5 valence, in the presence
of water, is unstable with respect to the +4 and +6 valence states.
Uranium in the +4 valence state is called tetravalent uranium and in
the +6 valence state is called hexavalent uranium.

The mineralogy and geochemistry of tetravalent and hexavalent
uranium are dissimilar. Tetravalent uranium is stable only under
reducing conditions. It oxidizes readily into hexavalent uranium.
In general, tetravalent uranium compounds are much less soluble than
the hexavalent uranium compounds. This is a very important property
related to both the deposition and the solution mining of uranium.

The method by which uranium was deposited has been extensively
studied by many researchers. Despite this, there is considerable amount
of dispute over the exact origin of the sandstone type uranium deposits.

However, most of the researchers agree that uranium in the earths'
crust was introduced hydrothermally or magmatically in alkalic granites,
arkoses or volcanic-ash tuffs. In many areas the alkalic granites
have an unusually high uranium content. Subsequent erosion of the
granites occurred and the uranium was deposited contemporaneously with
the deposition of the sandstone. The uranium was then mobilized by
oxidizing groundwater · flowing through the sandstones. The uranium was
transported in a dissolved state along with the groundwater.

As long as the groundwater conditions were such that the uranium
was kept in a hexavalent state, no precipitation occurred. When ground-
water conditions changed from an oxidizing to a reducing environment,
the uranium was changed from the hexavalent state to the tetravalent
state which is less soluble in water. The uranium was then precipi-
tated along the oxidation-reduction front (Redox front) in several
configurations, such as the classic crescent shape or more commonly as
tabular, dish-shaped, or irregular deposits (Figure A1.) Uranium deposited
in this manner is referred to as roll front uranium deposits. Roll
front uranium deposits make up the bulk of the uranium deposits in
the Western United States. Solution mining strives to reverse this
process by causing a strongly oxidizing condition to exist in which the
tetravalent uranium compounds are transformed into hexavalent uranium
compounds. The hexavalent uranium compounds are more soluble and can,
therefore, be more readily mobilized.

In nature, uranium has been found in over 104 known uranium mineral
compounds. Most of these are very rare. The most commonly found uranium
compound is an uranium oxide called uraninite. Ideally, the composition
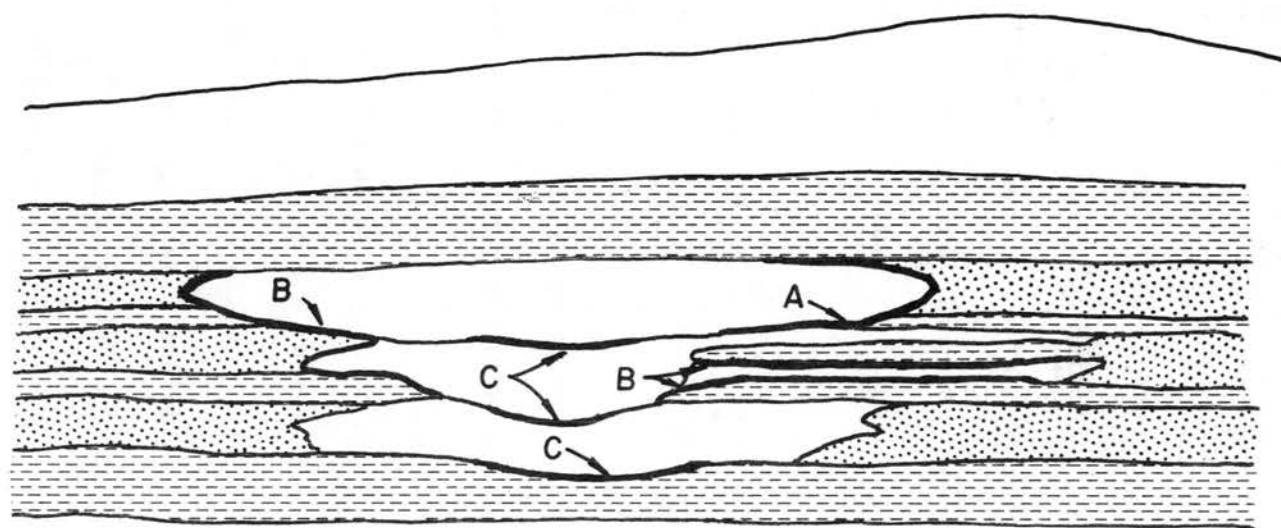
Explanation

■ Uraninum Ore

A— Classic cresent shape

B— Tabular deposits along permeability changes

C— Dish shaped deposits

▦ Shale or siltstone

▨ Reduced sandstone

☐ Oxidized sandstone

Figure A1. -- Configuration of Uranium deposits in sandstones.

of uraninite is $(UO_2)^{+2}$. Uraninite occurs as extremely fine-grained particles scattered within the sandstone matrix or as a black coating on individual sand grains. Uraninite has been identified as the dominant uranium mineral in the uranium deposits found in the Western United States.

Another uranium compound commonly found is a uranium silicate called coffenite. The composition of coffenite is $U(SiO_4)_{1-x}(OH)_{4x}$. Coffenite is frequently found together with uraninite and is usually indistinguishable by visual inspection from uraninite. Coffenite also has been identified as a minor uranium mineral in these ore deposits.

A.2 Lixiviant-Sorption Circuit

The in situ solution process can be broken down into two main circuits (1) a lixiviant-sorption circuit, and (2) an elution-precipitation circuit. The relationships between the circuits are shown in Figure A2. For purposes of this study, we are only interested in the lixiviant-sorption circuit.

The lixiviant-sorption circuit consists of the sandstone aquifer containing the uranium ore body and the uranium extraction column. A lixiviant is injected by means of injection wells into the sandstone aquifer containing the ore body. The lixiviant flows through the permeable sandstone and contacts the uranium oxides (uraninite) and uranium silicates (coffenite). The lixiviant contains an oxidizing agent that oxidizes the uranium from the tetravalent state to the hexavalent state. The lixiviant also contains a leaching agent that mobilizes the uranium as a soluble uranium-ion complex, normally as
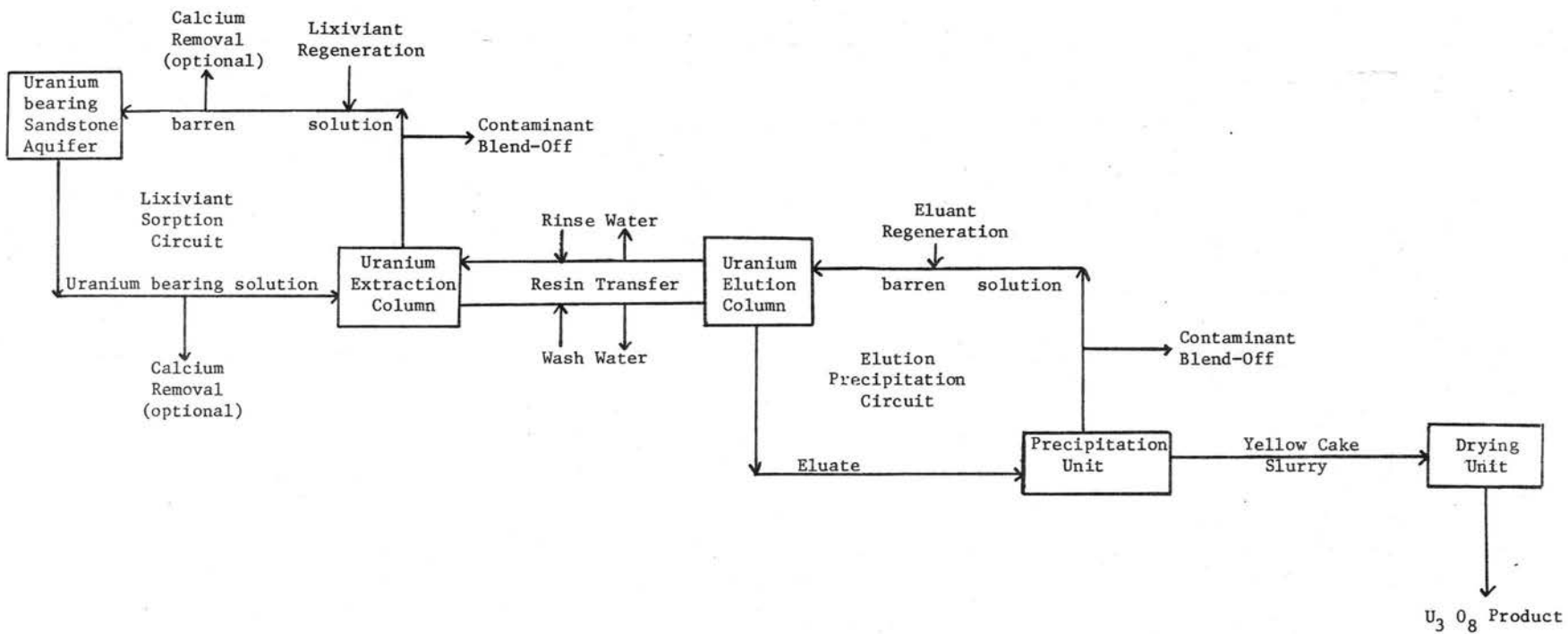
FIGURE A2. -- Schematic of the Solution Mining Process

either an uranium-carbonate complex or as an uranium-sulfate complex depending on the chemical makeup of the lixiviant. The uranium bearing groundwater is then recovered by production (recovery) wells. This solution contains the soluble uranium complexes, undesirable mobilized reaction byproducts and unreacted reagents in the lixiviant.

The well field (referred to hereafter as the leach field) provides the means by which the lixiviant is circulated through the sandstone aquifer to extract the uranium. The leach field design determines the efficiency of the uranium extraction. It also can have severe environmental effects by allowing contaminated groundwater to escape from the mine site. Several types of injection-recovery leach field patterns are used. The most common is the five-spot pattern (Figure A3A). Another pattern used is the seven-spot pattern (Figure A3B). The total number of wells and the well spacing used is determined by the hydrologic characteristics of the sandstone aquifer. The flow pattern through a vertical section of a single cell in a leach field is shown on Figure A4.

After recovery, the uranium bearing groundwater is passed through an uranium-sorption column which consists of a solid ion-exchange resin. The solution leaving the resin column is essentially barren of uranium, but does contain residual lixiviant chemicals and other undesirable contaminants. The barren solution is then regenerated with additional lixiviant chemicals and recycled to the leach field for reinjection. In some cases, a part of the barren solution is bled from the system. This net discharge lowers the groundwater levels in the localized area of the leach field causing outside groundwater to flow towards the mined zone. This reduces the possibility of escape of the lixiviant from the localized leach field area.

A – multiple 5-spot pattern   B – multiple 7-spot pattern
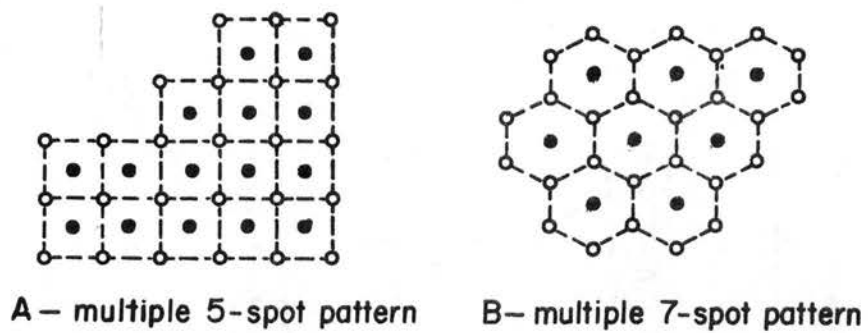
Explanation

- o Injection well
- • Recovery well

Figure A3. -- Leach field patterns.
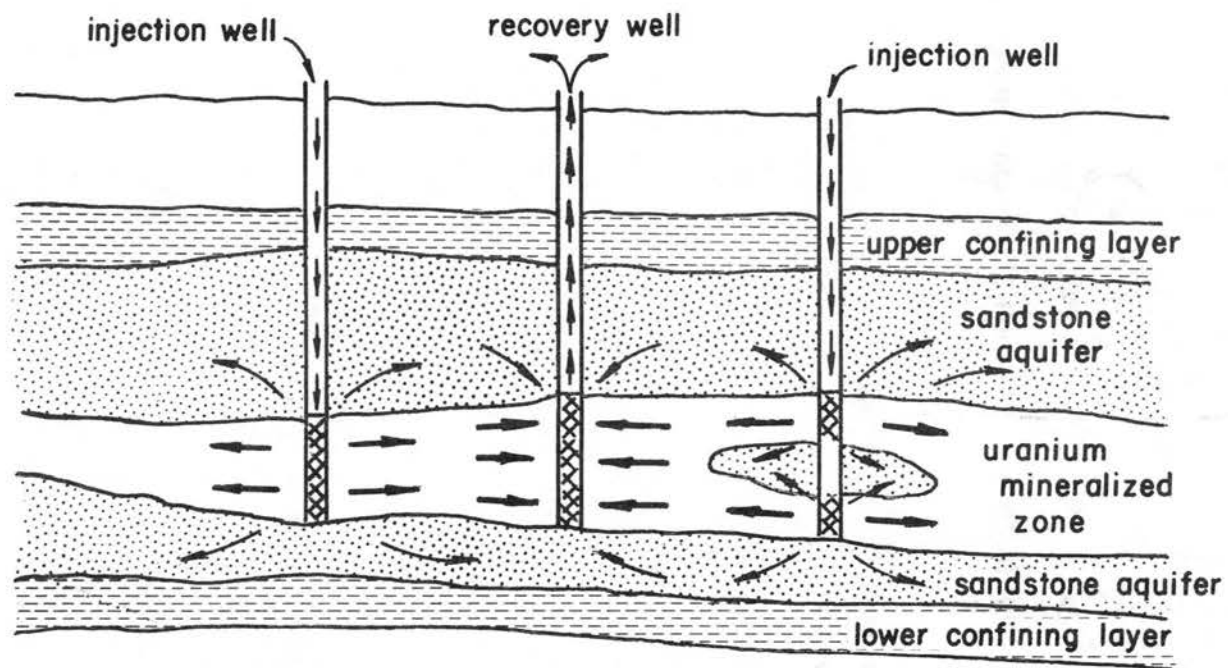
Figure A4. -- Flow pattern through a vertical section of a single cell in a leach field.

A.3 Lixiviants

The lixiviant consists of an oxidizing agent used to put the uranium into solution and a leaching agent used to mobilize the uranium by forming soluble uranium complexes. The most common oxidizing agent is hydrogen peroxide (H_2O_2). Dissolved oxygen added by aerating the solution also is used. The criteria is that the oxidizing agent must be capable of oxidizing the uranium from the tetravalent state (+4 valence) to the hexavalent state (+6 valence). The concentration of hydrogen perixide is usually between 0.25 to 1 gram per liter (g/L) in the lixiviant.

There are two major considerations in selecting a leaching agent for solution mining of uranium. First, the leaching agent must be capable of forming a soluble uranium complex which can be mobilized. Second, detrimental lixiviant reactions with other minerals present in the sandstone aquifer besides the uranium ore, such as calcite, clays, feldspars, zeolites, pyrites, and carbonaceous materials, should be minimized. These detrimental lixiviant-host rock reactions may (1) cause a decrease/increase in the permeability of the sandstone aquifer which may hinder the recovery of the uranium or allow escape of the contaminated groundwater from the mine site; (2) cause the leaching agent to be consumed and, thus, reduce the economic efficiency of the solution mining process; (3) cause other trace minerals to be dissolved along with the uranium that may interfere with chemical and ion exchange reactions in the solution mining process or cause further contamination of the groundwater; and (4) cause adsorption of the lixiviant onto the solid aquifer material which hinder the restoration of the groundwater upon completion of the mining.

There are four major leaching agents applicable to the solution mining of uranium. These are: (1) ammonium bicarbonate, (2) sodium bicarbonate, (3) alkaline-earth bicarbonates, and (4) sulfuric acid. The choice of the lixiviant to be used is determined by field testing during pilot-scale operations. The decision as to the best lixiviant to use depends on the composition of the uranium ore and the presence or lack of other minerals in the aquifer that may cause detrimental reactions to occur. A brief discussion of each of the four major lixiviants follows.

Ammonium bicarbonate (NH_4HCO_3) is the most commonly used leaching agent in the solution mining of uranium. The concentration of the ammonium bicarbonate is usually between 1 and 10 g/L in the lixiviant. The pH of the lixiviant is typically maintained at about 8. The uranium-carbonate complex formed in the reaction of the ammonium bicarbonate and the uranium ore is stable over a wide pH range of about 6 to 10. In general, trace minerals which occur together with the uranium are not subject to attack by the carbonate ion. However, the ammonium ion (NH_4^+) has a strong potential for adsorption onto the solid aquifer material.

The sodium bicarbonate lixiviant is identical to the ammonium bicarbonate lixiviant except for the substitution of the sodium ion (NA^+) for the ammonium ion (NH_4^+). The concentration of the sodium bicarbonate lixiviant is about the same as the ammonium bicarbonate lixiviant; usually about 1 to 10 g/L. The sodium bicarbonate lixiviant is only in limited use in the solution mining of uranium. The major disadvantage of sodium bicarbonate is that if there is any appreciable

amounts of clay contained in the aquifer, then the sodium causes swelling of the clay which reduces the permeability of the aquifer and thus reduces the efficiency of the uranium extraction and also may increase the potential for escape of contaminated groundwater from the mine site. Another disadvantage is that additional processing of the uranium is required to convert the sodium diurinate to the more commercially acceptable ammonium diurinate (yellowcake). In general, the sodium bicarbonate lixiviant does not readily mobilize contaminant trace minerals found with the uranium. The sodium cation does not exhibit as strong a potential for adsorption onto the aquifer material as does the ammonium cation.

The alkaline-earth bicarbonates that can be used as lixiviants are calcium carbonate and magnesium carbonate. These lixiviants have been tested on small pilot-scale operations, but have not been used, as yet, on a commercial scale operation. The difficulty with the alkaline-earth bicarbonates are their low solubility in water. Calcium compounds often precipitate out of solution and clog the injection and production wells or interfere with the ion-exchange process. Quite often calcium removal units are utilized in solution mining to remove these unwanted calcium compounds.

Sulfuric acid (H_2SO_4) is used as a lixiviant when the uranium ore resists extraction using the bicarbonate lixiviants and where already high sulfate concentrations occur in the groundwater. One of the major difficulties with sulfuric acid is that it is not very selective. It will mobilize the uranium as well as many of the other trace contaminants associated with the uranium. This increases the groundwater

contamination problem and makes restoration more difficult. Another
difficulty with sulfuric acid is that the hydrogen ion (H^+) is adsorbed
onto the aquifer material. If not properly restored the hydrogen ion
is later released back to the groundwater after restoration resulting
in a low pH acidic groundwater.

A.4 Chemical Reactions

The chemical reactions that take place during the mining depend
on the structure of the uranium ore, the lixiviant used, and on the
pH of the groundwater-aquifer system. If the uranium ore is uranite
$(UO_2)^{+2}$ and the lixiviant is ammonium bicarbonate-hydrogen perioxide,
then the following reactions hold (Larson, 1978).

$$\text{Oxidation} = UO_2 + H_2O_2 \rightleftharpoons UO_3 + H_2O$$

$$\text{Leaching} = UO_3 + H_2O + 3(NH_4)_2CO_3 \rightleftharpoons (NH_4)_4UO_2(CO_3)_3$$

$$+ 2NH_4OH; \quad pH > 10.3$$

$$= UO_3 + 2NH_4HCO_3 + (NH_4)_2CO_3 \rightleftharpoons (NH_4)_4UO_2(CO_3)_3$$

$$+ H_2O; \quad 10.3 > pH > 8.35$$

and

$$= UO_3 + 2NH_4HCO_3 \rightleftharpoons (NH_4)_2UO_2(CO_3)_2 + H_2O; \quad 8.35 > pH > \approx 5$$
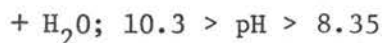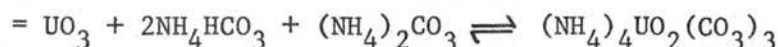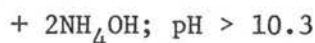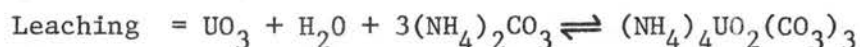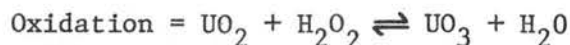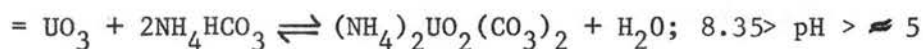
At a pH > 10.3, the dominant form of the carbonate species is the
carbonate ion $(CO_3^{=})$ (Figure A5). Between a pH of 10.3 and 6.4
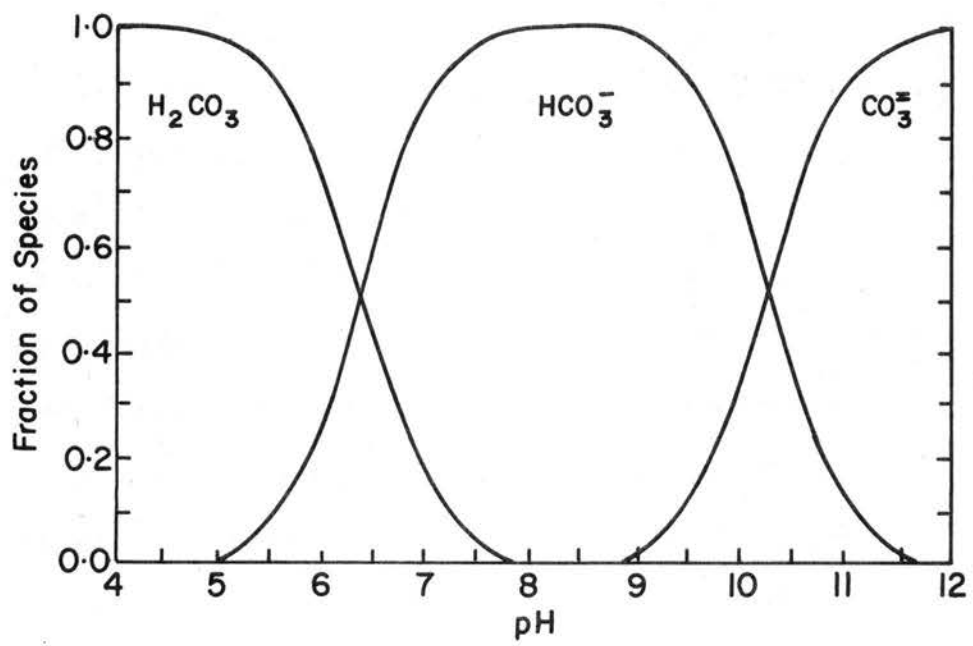
(source: Freeze and Cherry, 1979)

Figure A5. -- Carbonate species versus pH.

the dominant form of the carbonate species is the bicarbonate ion (HCO_3) (Figure A5). At a pH below 6.4, H_2CO_3 is the dominant carbonate species (Figure A5). The net product of the reaction is always an ammonium-carbonate uranyl complex which is relatively soluble in solution and fairly stable in the range of pH between 6 and 10, thus resisting reprecipitation.

A.5 Groundwater Contamination

Undoubtedly, the greatest environmental impact from solution mining is the potential contamination of the groundwater. For purposes of discussion, three groundwater quality zones are defined at a solution mine. (1) mining zone, (2) containment zone, and (3) undisturbed groundwater zone. The mining zone (Figure A6) includes the leach field and extends approximately one-well spacing or about 40 feet beyond the outermost injection wells. An areal view of the flow pattern for a 4-cell leach field is shown on Figure A6. Most of the flow occurs within the leach field in a nearly straight line between the injection wells and the production wells. However, some of the groundwater follows a path which initially leads away from the leach field but ultimately returns. The mining zone represents approximately the area contaminated under normal operating conditions.

The containment zone extends from the perimeter of the mining zone to the perimeter defined by the line connecting the monitor wells surrounding the leach field (Figure A6). Parts of this zone may become degraded during normal solution-mining operations and it may be desirable
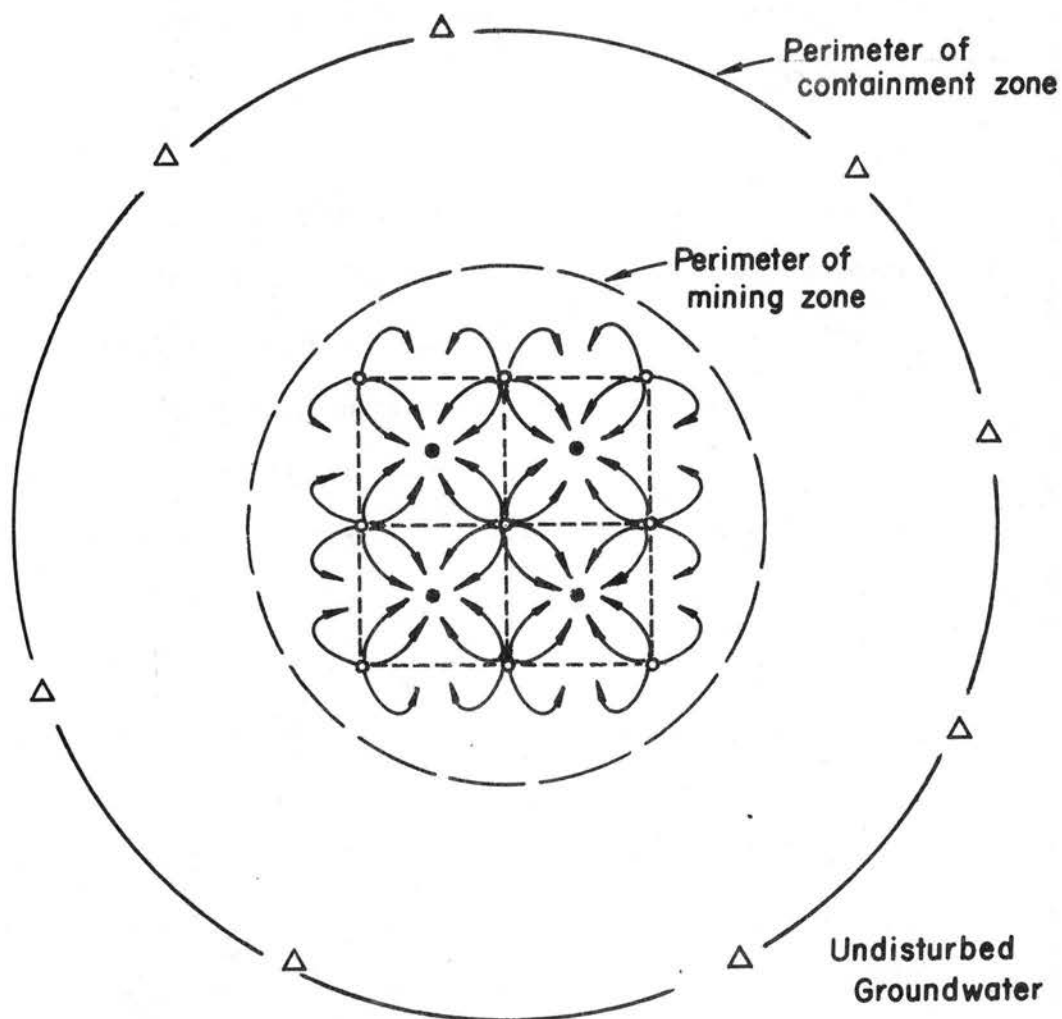
Figure A6. -- Water quality zones at a solution mine and an areal view of the flow pattern for a 4 cell leach field.

to place trend wells within this zone. The undisturbed zone is the area outside the perimeter of the containment zone (Figure A6).

Groundwater contamination can occur from (1) lateral excursions, (2) vertical excursions, and (3) improper or incomplete restoration.

A.5.1 Lateral Excursion

A lateral excursion is an uncontrolled migration of contaminated groundwater within the ore-bearing aquifer away from the mine site past the perimeter of the containment zone and technically occurs when contaminated groundwater is detected in the monitoring wells surrounding the leach field. A lateral excursion may result from undetected natural variations in aquifer permeabilities, too large of a well spacing, incorrect injection or recovery rates, or from detrimental lixiviant host rock reactions which alter the porosity or permeability of the aquifer. Of these, well spacing is probably the most important. A major cost of solution mining is the drilling and completion of the wells and, therefore, there is a tendency to increase the spacing of the wells to minimize the total number of wells required. The greater the well spacing, the less the control over the fluid flow and the more likely excursions are to occur.

To reduce the possibility of lateral excursions, pumpage rates from the leach field should exceed injection rates in order to maintain groundwater gradients toward the mine site. For minor lateral excursions, the primary remedial action taken is normally to increase the overpumping of the leach field in order to increase groundwater gradients toward the mine site and attempt to draw the contaminated

groundwater back towards the leach field. For more major excursions it may be necessary to cease all well injections and begin pumping the entire leach field in order to halt the migration of the contaminated groundwater. For the most severe excursions it may be necessary to install either an injection or a pumpage barrier downgradient to intercept the contaminated groundwater. In some cases it may be necessary to begin restoration of the aquifer.

A.5.2 Vertical Excursion

A vertical excursion is the leakage of contaminated groundwater into an overlying and/or underlying aquifer. This leakage can occur through unplugged exploration holes, through the production and recovery wells within the leach field, or through a leaky confining layer. Monitoring wells are placed within the leach field in both the underlying and overlying aquifers to detect vertical excursions. Vertical excursions can be very serious and can potentially endanger an adjacent important aquifer. Corrective actions for vertical excursions are difficult and normally require restoring the over or underlying aquifer that has been contaminated.

A.5.3 Incomplete Restoration

During solution mining, the groundwater is contaminated by the dissolved-uranium compounds, the residual lixiviant chemicals, and associated trace contaminants, such as vanadium, selenium, radium-226, cadium, arsenic, chromium, molybdenum, as well as hosts of others. After mining, restoration of the contaminated groundwater is required.

It is difficult to remove many of the trace contaminants from the groundwater system and even when left in minor amounts may result in a serious contamination problem. There is generally a substantial increase in the residual gross alpha and beta radioactivity counts in the groundwater even after restoration procedures have been implemented.

Another problem is the adsorption of certain contaminants onto the clays in the aquifer. During mining the contaminant is adsorbed on clay particles in the aquifer when it is in high concentrations in the groundwater. Later during restoration when the contaminant is in lower concentrations in the groundwater, the contaminant is released back into solution. This desorption process occurs slowly and can result in significant residual quantities of the contaminant adsorbed in the aquifer after the restoration process was thought to be completed. The restoration of contaminants subject to adsorption and desorption on the solid aquifer material is treated in detail in other sections of this dissertation.

The groundwater can only be sampled for contamination at a few selected points, namely at the monitoring wells and also at the production and recovery wells in the leach field. The extent of groundwater contamination beyond these few points can only be surmised. Improper or incomplete groundwater restoration could result in areas of contaminated groundwater remaining in the aquifer.

A.6 Groundwater Restoration Methods

Restoration is the returning of the contaminated groundwater to a condition consistent with the premining use or potential use. Establishment of restoration criteria is the initial step in any restoration

program. An often mentioned criteria is that the groundwater after mining should be returned to within 10 to 20 percent of the premining concentrations for each individual constituent in the groundwater.

The responsibility for in situ solution mining of uranium falls under the jurisdiction of both federal and state agencies. The licensing of in situ uranium solution mining falls under the jurisdiction of the U.S. Nuclear Regulatory Commission in non-agreement states and under the jurisdiction of the states in agreement states. All western states except Utah, Wyoming, Montana, South Dakota and Oklahoma are agreement states. The enforcement of groundwater protection falls to the U.S. Environmental Protection Agency (EPA). In several states, prima y for groundwater protection has been given by the EPA to various state regulatory agencies. For a discussion of the appropriate federal and state regulations governing solution mining the interested reader is referred to Riding and Rosswog (1979).

In general, groundwater restoration techniques for in situ solution mining may be grouped into three methodologies: (1) Ground-water sweeping, (2) clean-water recycling, and (3) chemical-treatment.

A.6.1 Groundwater Sweeping

Groundwater sweeping involves removing the contaminated ground-water from the mined aquifer by pumping, thereby inducing an influx of native groundwater from the surrounding undisturbed aquifer into the mine site. The contaminated groundwater and associated residual impurities are gradually displaced or swept away by the uncontaminated groundwater entering the mine site and, ideally, all contaminated

groundwater will be replaced by uncontaminated groundwater. This method is schematically shown in Figure A7a. Of the restoration methods, ground water sweeping has been tried the most, mainly because of the simplicity of operation and low cost. The method has only been partially successful in restoring the groundwater. Removal of certain contaminants which were adsorbed onto the clays during mining is very slow with groundwater sweeping. The method results in contamination of a large quantity of previously uncontaminated sweep water. Groundwater sweeping is used most extensively in Texas where deep well disposal of contaminated water is allowed.

A.6.2 Clean-Water Recyling

With clean-water recycling the contaminated groundwater is removed from the mined aquifer, purified (usually by reverse osmosis) and reinjected into the mined aquifer. The method is schematically shown in Figure A7b. Clean-water recycling has the advantage that there is very little consumptive use of groundwater compared with groundwater sweeping. A small amount of brine is generated from the reverse osmosis process which may be disposed of in evaporation ponds. Additionally, a small amount of bleedoff of the purified water before reinjection may be needed to ensure that groundwater gradients are toward the mined site.

The effectiveness of reverse osmosis in removing various ions in the water (TABLE A1) increases with increasing valence and with increasing molecular weight. Of special interest, the reduction rate by reverse osmosis for ammonium and for calcium is about 95 and 97.5
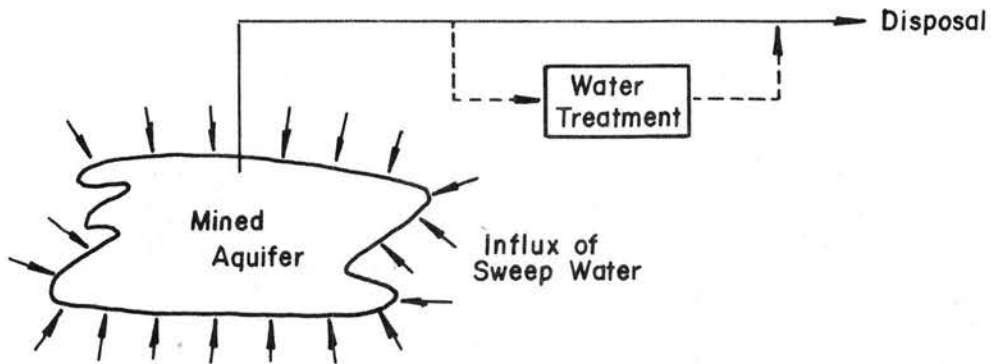
(a) Groundwater Sweep Method
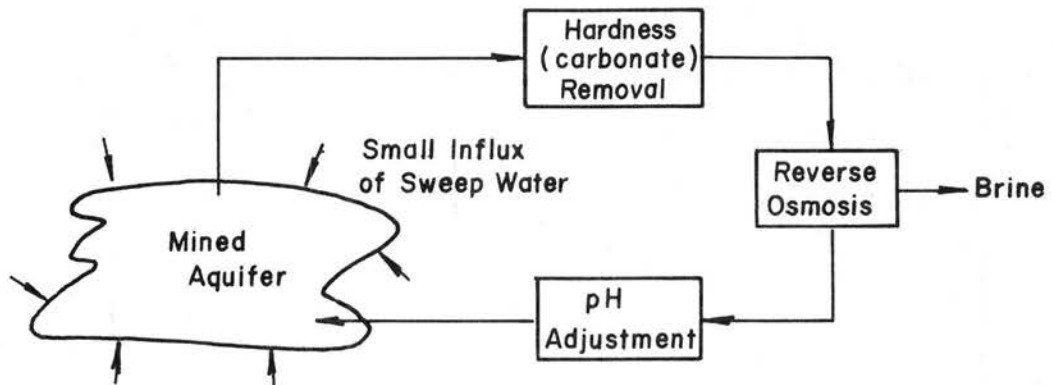
(b) Clean Water Recycle Method
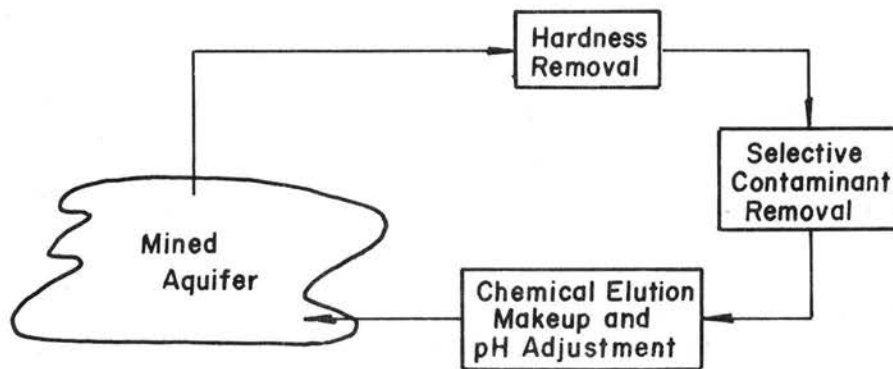
(c) Chemical Treatment Method

Figure A7. -- Groundwater restoration methods.

TABLE A1. -- Effectiveness of Reverse Osmosis

(Source: Trace Metal Data Institute, 1979)

Constituent	Percent reduction
Monovalent ions	94-98
Divalent ions	98-99.5
Trivalent ions	99-99.9
Non-electrolytes	92-95
Total dissolved solids	96-97
Radionuclides--gross alpha	85-96
Radionuclides--gross beta	95-99
Molecular weight greater than 180	98-100

percent, respectively (Thompson and others, 1978). The clean-water recycling method is used when the main purpose is reducing the residual total dissolved solids of the groundwater. The major disadvantage of this method is that it does very little to remove contaminants that have been adsorbed on the clays.

A.6.3 Chemical-Treatment

The chemical-treatment method in conjunction with recirculation is shown schematically in Figure A7c. In this method, restoration is accomplished by injecting chemicals into the mined aquifer. During mining, many contaminants were mobilized along with the uranium. One purpose of the chemical-treatment method can be to reprecipitate these contaminants by a suitable choice of the chemical, thereby reestablishing the chemical equilibrium that was present before the mining took place. Another purpose of the chemical-treatment method can be the eluting of adsorbed contaminants from the clays. For example, adsorbed ammonium can be removed from the clays by injecting a highly concentrated calcium solution. The ammonium is then selectively removed by increasing the pH of the solution which is then passed through a stripping tower through which a large volume air stream also is passed. The high pH of the solution converts the ammonium ion (NH_4^+) to the dissolved ammonia gas (NH_3) which is removed from the water by the flowing air stream.

Groundwater restoration technology is still in a developmental stage. Other methods besides sweeping and recirculation have been proposed such as bacterial precipitation (Riding and Rosswog, 1979)

but these other methods are still in the laboratory stage. Groundwater restoration by sweeping, clean-water recycling and/or chemical treatment have been demonstrated on small-scale test sites (less than 5 acres) but have never been attempted on a large-scale basis (Kasper et al., 1979). The unanswered questions remaining on groundwater restoration, effects of varying eluting chemical concentrations, effects of varying recirculation rates, restoration time requirements, etc.

APPENDIX B

Derivation of the Solute Transport Equation with Adsorption

An equation describing the two-dimensional mass transport for a reacting solute subject to adsorption in flowing groundwater is derived from the principal of conservation of mass. The derivation presented here is based on the development of Reddell and Sunada (1970).

The conservation of mass for the volume element with dimensions $\Delta x, \Delta y$ and Δz shown on Figure B1 is

(rate of mass inflow) - (rate of mass outflow)   (B1)

$\pm$ (rate of mass transfer through a source or sink)

$\pm$ (rate of mass depletion/production by adsorption/ desorption)

= (rate of change of solute mass in solution within the volume element).

The rate of mass inflow is equal to the mass flux of the solute in the x-direction across the face ABCD of the volume element (represented as M_{ox}) plus the mass flux of the solute in the y-direction across the face DCGH of the volume element (represented as M_{oy}). The rate of mass outflow is equal to the mass flux of the solute in the x-direction across the face EFGH of the volume element (represented as $M_{\Delta x}$) plus the mass flux of the solute and the y-direction across the face ABFE of the volume element (represented as $M_{\Delta y}$).
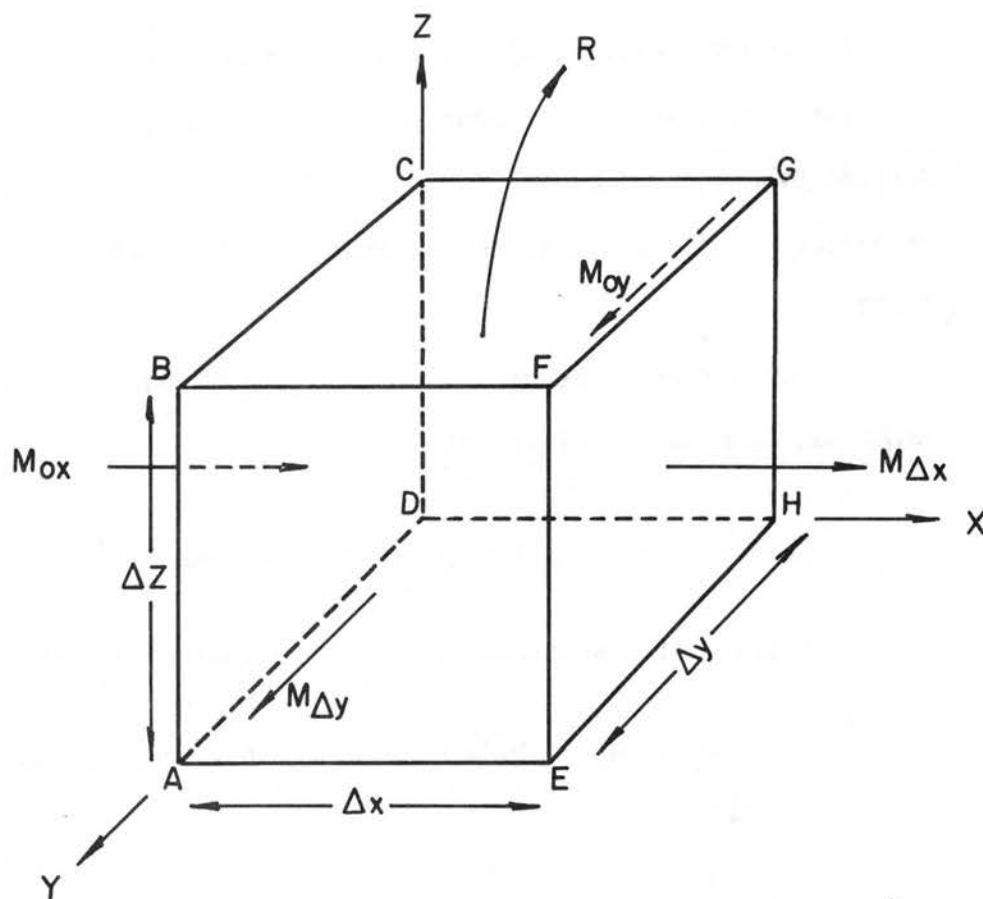
Figure B1. -- Representative volume element of a porous medium for mass balance calculation.

Expansion of $M_{\Delta x}$ and $M_{\Delta y}$ in a Taylor Series expansion about the origin yields

$$M_{\Delta x} = M_{ox} + \frac{\partial}{\partial x} (M_x) \Delta x + \text{higher order terms, and} \tag{B2}$$

$$M_{\Delta y} = M_{oy} + \frac{\partial}{\partial y} (M_y) \Delta y + \text{higher order terms.} \tag{B3}$$

Neglecting higher order terms the net mass flux in the x-direction is

$$(\text{Net Mass Flux})_x = M_{ox} - M_{\Delta x} = - \frac{\partial}{\partial x} (M_x) \Delta x \tag{B4}$$

and similarly in the y-direction is

$$(\text{Net Mass Flux})_y = M_{oy} - M_{\Delta y} = - \frac{\partial}{\partial y} (M_y) \Delta y. \tag{B5}$$

The instantaneous mass flux in the x-direction is given as

$$M_x = CV_x^* \varepsilon \Delta y \Delta z \tag{B6}$$

where

C = concentration of the solute (M/L^3),

V_x^* = instantaneous interstitial velocity of the groundwater in the x-direction (L/T), and

ε = porosity (dimensionless).

Note that the term $(\varepsilon \Delta y \Delta z)$ is simply the effective cross-sectional area. The instantaneous mass flux in the y-direction is given as

$$M_y = CV_y^* \quad \varepsilon \Delta x \Delta z \tag{B7}$$

where

V_y^* = instantaneous interstitial velocity of the groundwater

in the y-direction (L/T).

Solute enters or leaves the volume element as a flux through sources or sinks. This is expressed as

$$(\text{Source/Sink Mass Flux}) = - C'R^*\Delta x \Delta y \Delta z \tag{B8}$$

where

C' = concentration of the solute in the source or sink fluid (M/L^3), and

R^* = volume flux per unit bulk volume $(L^3/T/L^3)$.

Note that the term $(\Delta x \Delta y \Delta z)$ is simply the bulk volume of the volume element. The negative sign indicates that if a sink (withdrawal) is considered positive in sign and a source (recharge or injection) is considered negative in sign, then when all other fluxes balance, the solute mass in solution within the volume element will decrease for a sink and increase for a source.

Solute is removed from or added to solution within the volume element by the effects of adsorption or desorption. This is expressed as

$$(\text{Mass flux by Adsorption/Desorption}) = - \frac{\partial}{\partial t}(\overline{C}\varepsilon \Delta x \Delta y \Delta z) \tag{B9}$$

where $\overline{C}$ is the concentration adsorbed on the solid aquifer material per volume of solution (M/L^3). Note that the term $(\varepsilon \Delta x \Delta y \Delta z)$ is simply

the volume of the solution in the volume element. The negative sign indicates that if the adsorbed concentration increases with time, then when all other fluxes balance the solute mass in solution within the volume element will decrease.

The change of solute mass in solution within the volume element is expressed as

(Rate of change of solute mass in solution within the volume element)

$$= \frac{\partial}{\partial t} \ (C \varepsilon \Delta x \Delta y \Delta z). \tag{B10}$$

Substitution of equations (B2) − (B10) into the mass balance equation (B1) yields

$$\frac{\partial}{\partial t}(C \varepsilon \Delta x \Delta y \Delta z) = - \frac{\partial}{\partial x} \ (CV_x^* \varepsilon \Delta y \Delta z) \Delta x - \frac{\partial}{\partial y} \ (CV_y^* \varepsilon \Delta x \Delta y) \Delta y$$

$$\tag{B11}$$

$$- \frac{\partial}{\partial t} \ (\overline{C} \varepsilon \Delta x \Delta y \Delta z \ - \ C'R^* \Delta x \Delta y \Delta z \ .$$

Assuming that changes over time in the porosity ε of the aquifer are not significant, that no deformation of the volume element occurs (in essence Δx, Δy and Δz are constant), and letting x_1 represent the x-direction and x_2 represent the y-direction then equation (B11) is rewritten as

$$- \frac{\partial C}{\partial t} - \frac{\partial \overline{C}}{\partial t} = \frac{\partial}{\partial x_i} \ (CV_i^*) + \frac{C'R^*}{\varepsilon} \qquad i = 1,2. \tag{B12}$$

The instantaneous mass flux of the solute is represented by the term CV_i^* in equation (B12). This flux can be separated into a convective flux, a dispersive flux, and a diffusive flux. The convective flux represents the mass flux of the solute transported by the average fluid

motion of the groundwater through the volume element and is expressed as

$$(\text{convective flux}) = CV_i \tag{B13}$$

where

V_i = average interstitial velocity of the groundwater in the ith direction (L/T).

The dispersive and diffusive fluxes represent collectively hydrodynamic dispersion. The dispersive flux results from velocity fluctuations from the average interstitial velocity of the fluid. Bear (1979) gives the dispersive flux as

$$(\text{dispersive flux}) = - D_{ij} \frac{\partial C}{\partial x_j} \tag{B14}$$

where D is the coefficient of hydrodynamic dispersion (a second-order tensor, L^2/T). The dispersive flux is directly proportional to the concentration gradient and occurs in the direction from higher concentrations towards lower concentrations. The diffusive flux results from molecular and ionic diffusion. In flowing groundwater, diffusive fluxes are assumed negligible in comparison to dispersive fluxes.

The sources and sinks are represented by the term $\frac{C'R^*}{\varepsilon}$ in equation (B12). These sources and sinks may be either distributed sources or sinks (for example evapotranspiration and recharge) or may be point sources and sinks (for example injection or withdrawal wells). Accordingly from Bear (1979) the volumetric flux can be broken into distributive flux terms and point flux terms as

$$R^* = \frac{W}{b} + \sum_{p=1}^{m} (\delta(x-x_p)\delta(y-y_p)\frac{Q_p}{b}) \tag{B15}$$

where

W = distributive net inflow per unit area over the element $(L^3/T/L^2)$,

Q_p = net inflow at a point located at (x_p, y_p) (L^3/T),

there are m such points within the element,

δ = dirac delta function, and

b = saturated thickness.

Substitution of equations (B13) and (B14) for convective and dispersive fluxes and equation (B15) for R* into equation (B12) yields

$$-\frac{\partial C}{\partial t} - \frac{\partial \overline{C}}{\partial t} = \frac{\partial}{\partial x_i}(CV_i - D_{ij}\frac{\partial C}{\partial x_j}) + \frac{WC'}{\varepsilon b}$$

$$+ \sum_{p=1}^{m} (\delta(x-x_p)\delta(y-y_p)\frac{Q_p C'}{\varepsilon b}) \tag{B16}$$

which is the general partial differential equation for computing the concentration of a single dissolved chemical species in flowing groundwater with adsorption.

APPENDIX C

Integral Transformations

    Several integral transformations used in the solution of the groundwater flow equation and of the solute transport equations are developed from the Gauss-Divergence theorem which can be written in three dimensions for a close bounded region in space V whose surface is S as (Kreyzig, 1979 or Wylie, 1966)

$$\iiint_V \nabla \cdot \underline{f} \, d\tau = \oiint_S \underline{n} \cdot \underline{f} \, d\sigma. \tag{C1}$$

Equation (C1) is written in two dimensions as

$$\iint_D \nabla \cdot \underline{f} \, dA = \oint_B \underline{n} \cdot \underline{f} \, dL \tag{C2}$$

where D is a close bounded domain with boundary B and where $\underline{f}$ (x,y) is a vector function and $\underline{n}$ is the outward pointing unit normal on B. The symbol $\oint$ indicates that the integration is over the entire closed boundary. If $\underline{f}$ and $\underline{n}$ are written in terms of components then

$$\underline{f} = f_x \underline{i} + f_y \underline{j} \tag{C3}$$

where f_x and f_y are the components of vector $\underline{f}$ in the x and y directions, respectively, and $\underline{i}$ and $\underline{j}$ are unit vectors in the x and y directions, respectively, and

$$\underline{n} = \ell_x \, \underline{i} + \ell_y \, \underline{j} \tag{C4}$$

where $\ell_x = \cos\alpha$ and $\ell_y = \cos\beta$ as shown on Figure C1.

The divergence of the vector $\underline{f}$ is a scalar and is defined as

$$\nabla \cdot \underline{f} = (\frac{\partial}{\partial x}\,\underline{i} + \frac{\partial}{\partial y}\,\underline{j}) \cdot (f_x\,\underline{i} + f_y\underline{j}) = \frac{\partial f_x}{\partial x} + \frac{\partial f_y}{\partial y} \quad . \tag{C5}$$

A useful transformation is obtained by letting

$$\underline{f} = \psi_1\phi_1\,\frac{\partial\phi_2}{\partial x}\,\underline{i} + \psi_2\phi_1\,\frac{\partial\phi_2}{\partial y}\,\underline{j} \tag{C6}$$

where $\psi_1(x,y)$, $\psi_2(x,y)$, $\phi_1(x,y)$ and $\phi_2(x,y)$ are scalars.
Then

$$\nabla\cdot\underline{f} = (\frac{\partial}{\partial x}\,\underline{i} + \frac{\partial}{\partial y}\,\underline{j}) \cdot (\psi_1\phi_1\,\frac{\partial\phi_2}{\partial x}\,\underline{i} + \psi_2\phi_1\,\frac{\partial\phi_2}{\partial y}\,\underline{j})$$

$$= \frac{\partial}{\partial x}\,(\psi_1\phi_1\,\frac{\partial\phi_2}{\partial x}) + \frac{\partial}{\partial y}\,(\psi_2\phi_1\,\frac{\partial\phi_2}{\partial y})$$

$$\tag{C7}$$

$$= \frac{\partial\psi_1}{\partial x}\,\phi_1\,\frac{\partial\phi_2}{\partial x} + \psi_1\,\frac{\partial\phi_1}{\partial x}\,\frac{\partial\phi_2}{\partial x} + \psi_1\phi_1\,\frac{\partial^2\phi_2}{\partial x^2}$$

$$+ \frac{\partial\psi_2}{\partial y}\,\phi_1\,\frac{\partial\phi_2}{\partial y} + \psi_2\,\frac{\partial\phi_1}{\partial y}\,\frac{\partial\phi_2}{\partial y} + \psi_2\phi_1\,\frac{\partial^2\phi_2}{\partial y^2}$$

and

$$\underline{n}\cdot\underline{f} = (\ell_x\,\underline{i} + \ell_y\,\underline{j}) \cdot (\psi_1\phi_1\,\frac{\partial\phi_2}{\partial x}\,\underline{i} + \psi_2\phi_1\,\frac{\partial\phi_2}{\partial y}\,\underline{j})$$

$$\tag{C8}$$

$$= \psi_1\phi_1\frac{\partial\phi_2}{\partial x}\,\ell_x + \psi_2\phi_2\,\frac{\partial\phi_2}{\partial y}\,\ell_y.$$
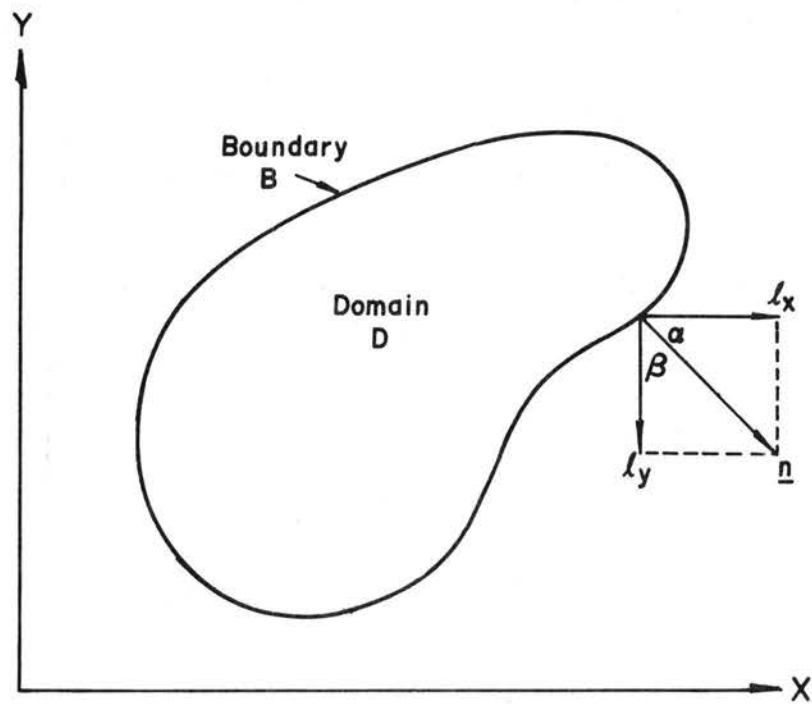
Figure C1. -- Directional cosines and the outward pointing normal to the surface.

Substitution of equations (C7) and (C8) into equation (C2) and rearranging yields

$$\iint_D \left\{ \frac{\partial \psi_1}{\partial x} \phi_1 \frac{\partial \phi_2}{\partial x} + \psi_1 \phi_1 \frac{\partial^2 \phi_2}{\partial x^2} + \frac{\partial \psi_2}{\partial y} \phi_1 \frac{\partial \psi_2}{\partial y} + \psi_2 \phi_1 \frac{\partial^2 \phi_2}{\partial y^2} \right\} \, dA$$

$$= - \iint_D \left\{ \psi_1 \frac{\partial \phi_1}{\partial x} \frac{\partial \phi_2}{\partial x} + \psi_2 \frac{\partial \phi_1}{\partial y} \frac{\partial \phi_2}{\partial y} \right\} \, dA \tag{C9}$$

$$+ \oint_B \left\{ \psi_1 \phi_1 \frac{\partial \phi_2}{\partial x} \ell_x + \psi_2 \phi_2 \frac{\partial \phi_2}{\partial y} \ell_y \right\} \, dL \, .$$

A second useful integral transformation is obtained by letting

$$\underline{f} = \psi_1 \phi_1 \frac{\partial \phi_2}{\partial y} \underline{i} + \psi_2 \phi_1 \frac{\partial \phi_2}{\partial x} \underline{j} \tag{C10}$$

where $\psi_1(x,y)$, $\psi_2(x,y)$, $\phi_1(x,y)$ and $\phi_2(x,y)$ are scalars. Then

$$\nabla \cdot \underline{f} = \left(\frac{\partial}{\partial x} \underline{i} + \frac{\partial}{\partial y} \underline{j} \right) \cdot \left(\psi_1 \phi_1 \frac{\partial \phi_2}{\partial y} \underline{i} + \psi_2 \phi_1 \frac{\partial \phi_2}{\partial x} \underline{j} \right)$$

$$= \frac{\partial}{\partial x} \left(\psi_1 \phi_1 \frac{\partial \phi_2}{\partial y} \right) + \frac{\partial}{\partial y} \left(\psi_2 \phi_1 \frac{\partial \phi_2}{\partial x} \right) \tag{C11}$$

$$= \frac{\partial \psi_1}{\partial x} \phi_1 \frac{\partial \phi_2}{\partial y} + \psi_1 \frac{\partial \phi_1}{\partial x} \frac{\partial \phi_2}{\partial y} + \psi_1 \phi_1 \frac{\partial^2 \phi_2}{\partial x \partial y}$$

$$+ \frac{\partial \psi_2}{\partial y} \phi_1 \frac{\partial \phi_2}{\partial x} + \psi_2 \frac{\partial \phi_1}{\partial y} \frac{\partial \phi_2}{\partial x} + \psi_2 \phi_1 \frac{\partial^2 \phi_2}{\partial x \partial y}$$

and

$$\underline{n} \cdot \underline{f} = (\ell_x \underline{i} + \ell_y \underline{j}) \cdot (\psi_1 \phi_1 \frac{\partial \phi_2}{\partial y} \underline{i} + \psi_2 \phi_1 \frac{\partial \phi_2}{\partial x} \underline{j})$$

$$= \psi_1 \phi_1 \frac{\partial \phi_2}{\partial y} \ell_x + \psi_2 \phi_1 \frac{\partial \phi_2}{\partial x} \ell_y.$$

(C12)

Substitution of equations (C11) and (C12) into equation (C2) and rearranging yields

$$\iint_D \left\{ \frac{\partial \psi_1}{\partial x} \phi_1 \frac{\partial \phi_2}{\partial y} + \Psi_1 \phi_1 \frac{\partial^2 \phi_2}{\partial x \partial y} + \frac{\partial \psi_2}{\partial y} \phi_1 \frac{\partial \phi_2}{\partial x} + \psi_2 \phi_1 \frac{\partial^2 \phi_2}{\partial x \partial y} \right\} dA$$

$$= - \iint_D \left\{ \psi_1 \frac{\partial \phi_1}{\partial x} \frac{\partial \phi_2}{\partial y} + \psi_2 \frac{\partial \phi_1}{\partial y} \frac{\partial \phi_2}{\partial x} \right\} dA$$

(C13)

$$+ \oint_B \left\{ \psi_1 \phi_1 \frac{\partial \phi_2}{\partial y} \ell_x + \psi_2 \phi_1 \frac{\partial \phi_2}{\partial x} \ell_y \right\} dL$$

A third useful integral transformation is obtained by letting

$$\underline{f} = \psi_1 \phi_1 \phi_2 \underline{i} + \psi_2 \phi_1 \phi_2 \underline{j}$$

(C14)

where $\psi_1(x,y)$, $\psi_2(x,y)$, $\phi_1(x,y)$ and $\phi_2(x,y)$ are scalars. Then

$$\nabla \cdot \underline{f} = (\frac{\partial}{\partial x} \underline{i} + \frac{\partial}{\partial y} \underline{j}) \cdot (\psi_1 \phi_1 \phi_2 \underline{i} + \psi_2 \phi_1 \phi_2 \underline{j})$$

$$= \frac{\partial}{\partial x} (\psi_1 \phi_1 \phi_2) + \frac{\partial}{\partial y} (\psi_2 \phi_1 \phi_2)$$

(C15)

$$= \frac{\partial \psi_1}{\partial x} \phi_1 \phi_2 + \psi_1 \frac{\partial \phi_1}{\partial x} \phi_2 + \psi_1 \phi_1 \frac{\partial \phi_2}{\partial x}$$

$$+ \frac{\partial \psi_2}{\partial y} \phi_1 \phi_2 + \psi_2 \frac{\partial \phi_1}{\partial y} \phi_2 + \psi_2 \phi_1 \frac{\partial \phi_2}{\partial y} \qquad \text{(C15 cont.)}$$

and

$$\underline{n} \cdot \underline{f} = (\ell_x \, \underline{i} + \ell_y \underline{j}) \cdot (\psi_1 \phi_1 \phi_2 \, \underline{i} + \psi_2 \phi_1 \phi_2 \, \underline{j})$$

$$\text{(C16)}$$

$$= \psi_1 \phi_1 \phi_2 \ell_x + \psi_2 \phi_1 \phi_2 \ell_y$$

Substitution of equations (C15) and (C16) into equation (C2) and rearranging yields

$$\iint\limits_{D} \left\{ \frac{\partial \psi_1}{\partial x} \phi_1 \phi_2 + \psi_1 \phi_1 \frac{\partial \phi_2}{\partial x} + \frac{\partial \psi_2}{\partial y} \phi_1 \phi_2 + \psi_2 \phi_1 \frac{\partial \phi_2}{\partial y} \right\} dA$$

$$= - \iint\limits_{D} \left\{ \psi_1 \frac{\partial \phi_1}{\partial x} \phi_2 + \psi_2 \frac{\partial \phi_1}{\partial y} \phi_2 \right\} dA \qquad \text{(C17)}$$

$$+ \oint\limits_{B} \left\{ \psi_1 \phi_1 \phi_2 \ell_x + \psi_2 \phi_1 \phi_2 \, \ell_y \right\} dL$$

COMPUTER PROGRAM
AND RELATED DATA.

APPENDIX D. -- Program Listing

COMPUTER PROGRAM LISTING

```
      PROGRAM RESTOR (INPUT,OUTPUT,TAPE6,TAPE5=INPUT,TAPE9=OUTPUT)       A 0010
C     *************************************************************      A 0020
C     *                                                           *      A 0030
C     *     2-DIMENSIONAL MASS TRANSPORT  IN FLOWING GROUNDWATER   *      A 0040
C     *     FOR 2 REACTING SOLUTES SUBJECT TO BINARY CATION EXCHANGE.  * A 0050
C     *     NUMERICAL SOLUTION BY THE GALERKIN FINITE ELEMENT METHOD    * A 0060
C     *     USING TRIANGULAR ELEMENTS AND LINEAR SHAPE FUNCTIONS.  *      A 0070
C     *     WRITTEN AND PROGRAMMED BY JAMES WARNER, 1981.          *      A 0080
C     *                                                           *      A 0090
C     *************************************************************      A 0100
      COMMON /BLOCKA/ NUMNP,X(35),Y(35),NUMEL,NI(50),NJ(50),            A 0110
     1NK(50),NUMBS,NBNDYI(18),NBNDYJ(18),COSX(18),COSY(18),            A 0120
     2DHDX(18),DHDY(18),TITLE(20),IBAND,ICT                            A 0130
      COMMON /BLOCKB/ NTIM,NPMP,PINT,TIMX,TINIT,TPDAY,SUMT,TDEL,INT,TIMY A 0140
     1,TDELMAX                                                         A 0150
      COMMON /BLOCKC/ S,POROS,BETA,DLTRAT,Z1,Z2,ATOMWT1,ATOMWT2,DBYHUK1, A 0160
     1DBYHUK2,SK                                                       A 0170
      COMMON /BLOCKD/ NCODNP,NODEID(35),TRANS(35),HYDK(35),THCK(35),    A 0180
     1REC(35),C1REC(35),C2REC(35)                                      A 0190
      COMMON /BLOCKE/ IDELEM(50),RECH(50),C1RECH(50),C2RECH(50),        A 0200
     1VPRM(50),AREA(50)                                                A 0210
      COMMON /BLOCKF/ HEAD(35),HDI(35),C1(35),C2(35),C1HAT(35),         A 0220
     1C2HAT(35),CEC(35)                                                A 0230
      COMMON /BLOCKG/ AF(35,7),BF(35,7),DF(35)                          A 0240
      COMMON /BLOCKH/ AT(35,13),BT1(35,7),BT2(35,7),                    A 0250
     1CT1(35,7),CT2(35,7),DT1(35),DT2(35)                              A 0260
      COMMON /BLOCKI/ CM(35,13),RHS(35),RHSU(35),RHSL(35)               A 0270
      COMMON /BLOCKJ/QINRCH,QOUTRCH,QINREC,QOUTREC,QINCHN,QOUTCHN,      A 0280
     1QINLEK,QOUTLEK,QINBDY,QOUTBDY,QSTOR                              A 0290
      COMMON /BLOCKK/ C1INRCH,C2INRCH,C1OTRCH,C2OTRCH,C1INREC,C2INREC,  A 0300
     1C1OTREC,C2OTREC,C1INCHN,C2INCHN,C1OTCHN,C2OTCHN,C1INLEK,C2INLEK,  A 0310
     2C1OTLEK,C2OTLEK,C1ISTOR,C2ISTOR,C1STOR,C2STOR,C1INBDY,C2INBDY,    A 0320
     3C1OTBDY,C2OTBDY                                                  A 0330
C     *************************************************************      A 0340
C     LOAD DATA                                                         A 0350
      CALL INPUT (1)                                                    A 0360
C     *************************************************************      A 0370
C     START COMPUTATIONS                                                A 0380
      NCALL = 1                                                         A 0390
C     CALCULATE TIME STEP                                               A 0400
      SUMT = 0.                                                         A 0410
      TPDAY = 0.                                                        A 0420
      DO 130 INT = 1,NPMP                                               A 0430
         TIM = TINIT/86400.                                            A 0440
         TPDAY = TPDAY + PINT                                          A 0450
         DO 110 NT = 1,NTIM                                            A 0460
            TINT = TPDAY - SUMT                                        A 0470
            TDEL = AMIN1(TIM,TINT)                                     A 0480
            TDEL = AMIN1(TDEL,TDELMAX)                                 A 0490
            SUMT = SUMT + TDEL                                         A 0500
            TIMY = SUMT/365.25                                         A 0510
            TIM = TIM * TIMX                                           A 0520
            IF (S.EQ.0.0.AND.NT.GT.1) GO TO 100                        A 0530
            CALL ELINTF (NCALL)                                        A 0540
            CALL MATFLOW                                               A 0550
  100       CALL WATBAL                                                A 0560
            CALL ELINTT                                                A 0570
            CALL MATCHEM                                               A 0580
C     FOR CONSERVATIVE TRANSPORT DO NOT CALL CHATSOL                    A 0590
            IF (ICT.EQ.0) CALL CHATSOL                                 A 0600
            CALL CHEMBAL                                               A 0610
            IF (SUMT.EQ.TPDAY) GO TO 120                               A 0620
            NCALL = NCALL + 1                                          A 0630
  110    CONTINUE                                                      A 0640
  120    CONTINUE                                                      A 0650
         CALL FLOWOUT                                                  A 0660
         CALL CHEMOUT                                                  A 0670
         ICALL = INT + 1                                               A 0680
         IF (ICALL.GT.NPMP) GO TO 130                                  A 0690
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      CALL INPUT (ICALL)                                              A 0700
  130 CONTINUE                                                        A 0710
C     *******************************************************************  A 0720
      STOP                                                            A 0730
      END                                                             A 0740
      SUBROUTINE INPUT(ICALL)                                         B 0010
      COMMON /BLOCKA/ NUMNP,X(35),Y(35),NUMEL,NI(50),NJ(50),          B 0020
     1NK(50),NUMBS,NBNDYI(18),NBNDYJ(18),COSX(18),COSY(18),           B 0030
     2DHDX(18),DHDY(18),TITLE(20),IBAND,ICT                           B 0040
      COMMON /BLOCKB/ NTIM,NPMP,PINT,TIMX,TINIT,TPDAY,SUMT,TDEL,INT,TIMY  B 0050
     1,TDELMAX                                                        B 0060
      COMMON /BLOCKC/ S,POROS,BETA,DLTRAT,Z1,Z2,ATOMWT1,ATOMWT2,DBYHUK1,  B 0070
     1DBYHUK2,SK                                                      B 0080
      COMMON /BLOCKD/ NCCDNP,NODEID(35),TRANS(35),HYDK(35),THCK(35),   B 0090
     1REC(35),C1REC(35),C2REC(35)                                     B 0100
      COMMON /BLOCKE/ IDELEM(50),RECH(50),C1RECH(50),C2RECH(50),       B 0110
     1VPRM(50),AREA(50)                                               B 0120
      COMMON /BLOCKF/ HEAD(35),HDI(35),C1(35),C2(35),C1HAT(35),        B 0130
     1C2HAT(35),CEC(35)                                               B 0140
      COMMON /BLOCKI/ CM(35,13),RHS(35),RHSU(35),RHSL(35)             B 0150
      COMMON /BLOCKJ/QINRCH,QOUTRCH,QINREC,QOUTREC,QINCHN,QOUTCHN,     B 0160
     1QINLEK,QOUTLEK,QINBDY,QOUTBDY,QSTOR                             B 0170
      COMMON /BLOCKK/ C1INRCH,C2INRCH,C1OTRCH,C2OTRCH,C1INREC,C2INREC, B 0180
     1C1OTREC,C2OTREC,C1INCHN,C2INCHN,C1OTCHN,C2OTCHN,C1INLEK,C2INLEK, B 0190
     2C1OTLEK,C2OTLEK,C1ISTOR,C2ISTOR,C1STOR,C2STOR,C1INBDY,C2INBDY,   B 0200
     3C1OTBDY,C2OTBDY                                                 B 0210
C     *******************************************************************  B 0220
C                                                                     B 0230
C     THIS SUBROUTINE INITIALIZES THE VARIABLES AND READS AND PRINTS ALL  B 0240
C     INPUT DATA.  THESE DATA DEFINE THE MODEL GRID, THE BOUNDARY     B 0250
C     CONDITIONS, TIME-STEP FACTORS, AQUIFER PROPERTIES,INITIAL       B 0260
C     POTENTIOMETRIC HEAD, INITIAL DISSOLVED SOLUTION CONCENTRATIONS, B 0270
C     HYDROLOGIC AND CHEMICAL DEFINITION CF THE STRESSES ON THE       B 0280
C     GROUNDWATER SYSTEM, AND OTHER HYDROLOGIC AND CHEMICAL PARAMETERS.  B 0290
C     THE INITIAL ADSORBED CONCENTRATIONS ARE CALCULATED ASSUMING THAT  B 0300
C     EQUILIBRIUM CONDITIONS HOLD.  THIS SUBROUTINE IS ALSO USED TO   B 0310
C     SELECTIVELY UPDATE SOME OF THE MODEL INPUT DATA AT THE END OF EACH  B 0320
C     PUMPING PERIOD.                                                 B 0330
C                                                                     B 0340
C     *******************************************************************  B 0350
      IF (ICALL.GT.1) GO TO 1020                                      B 0360
C     *******************************************************************  B 0370
C                                                                     B 0380
C     INITIALIZE VARIABLES                                            B 0390
C                                                                     B 0400
      AREATOT = 0.                                                    B 0410
      IBAND = 0                                                       B 0420
      QOUTREC = 0.                                                    B 0430
      QINREC = QOUTREC                                                B 0440
      QOUTRCH = QINREC                                                B 0450
      QINRCH = QOUTRCH                                                B 0460
      QOUTLEK = 0.                                                    B 0470
      QINLEK = QOUTLEK                                                B 0480
      QOUTCHN = QINLEK                                                B 0490
      QINCHN = QOUTCHN                                                B 0500
      QOUTBDY = 0.                                                    B 0510
      QINBDY = QOUTBDY                                                B 0520
      C2OTRCH = 0.                                                    B 0530
      C1OTRCH = C2OTRCH                                               B 0540
      C1INRCH = C1OTRCH                                               B 0550
      C1INRCH = C1INRCH                                               B 0560
      C2OTREC = 0.                                                    B 0570
      C1OTREC = C2OTREC                                               B 0580
      C2INREC = C1OTREC                                               B 0590
      C1INREC = C2INREC                                               B 0600
      C2OTCHN = 0.                                                    B 0610
      C1OTCHN = C2OTCHN                                               B 0620
      C2INCHN = C1OTCHN                                               B 0630
      C1INCHN = C2INCHN                                               B 0640
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          C20TLEK = 0.                                                  B 0650
          C10TLEK = C20TLEK                                             B 0660
          C2INLEK = C10TLEK                                             B 0670
          C1INLEK = C2INLEK                                             B 0680
          C20TBDY = 0.                                                  B 0690
          C10TBDY = C20TBDY                                             B 0700
          C2INBDY = C10TBDY                                             B 0710
          C1INBDY = C2INBDY                                             B 0720
    C     **********************************************************    B 0730
    C                                                                   B 0740
    C     PRINT HEADING                                                 B 0750
    C                                                                   B 0760
          WRITE (6,100)                                                 B 0770
      100 FORMAT (1H15X,108H2-DIMENSIONAL MASS TRANSPORT IN FLOWING GROUNDWA  B 0780
         1TER FOR 2 REACTING SOLUTES SUBJECT TO BINARY CATION EXCHANGE/1H ,5  B 0790
         2X,109HNUMERICAL SOLUTION BY THE GALERKIN FINITE ELEMENT METHOD USI  B 0800
         3NG TRIANGULAR ELEMENTS AND LINEAR SHAPE FUNCTIONS/1H ,5X,38HWRITTE  B 0810
         4N AND PROGRAMMED BY JAMES WARNER)                             B 0820
    C                                                                   B 0830
    C     READ TITLE CARD                                               B 0840
    C                                                                   B 0850
          READ (5,110) TITLE                                            B 0860
      110 FORMAT (20A4)                                                 B 0870
          WRITE (6,120) TITLE                                           B 0880
      120 FORMAT (//1H ,20A4//)                                         B 0890
    C     **********************************************************    B 0900
    C                                                                   B 0910
    C     READ - FOR CONSERVATIVE TRANSPORT, ICT>0                      B 0920
    C             FOR NONCONSERVATIVE TRANSPORT, ICT=0                   B 0930
    C                                                                   B 0940
          READ (5,110) TITLE                                            B 0950
          READ (5,130) ICT                                              B 0960
      130 FORMAT (I5)                                                   B 0970
          IF (ICT.EQ.0) WRITE (6,140)                                   B 0980
      140 FORMAT (33H NONCONSERVATIVE TRANSPORT(ICT=0))                 B 0990
          IF (ICT.GT.0) WRITE (6,150)                                   B 1000
      150 FORMAT (30H CONSERVATIVE TRANSPORT(ICT>0))                    B 1010
          WRITE (6,160)                                                 B 1020
      150 FORMAT (1H0,45X,21HI N P U T    D A T A/1H ,44X,23H-----------  B 1030
         1----------/////)                                              B 1040
    C     **********************************************************    B 1050
    C                                                                   B 1060
    C     LOAD ELEMENT DESCRIPTORS                                      B 1070
    C                                                                   B 1080
    C     NUMNP = NUMBER OF NODAL POINTS                                B 1090
    C     NUMEL = NUMBER OF ELEMENTS                                    B 1100
    C     NUMBS = NUMBER OF BOUNDARY SEGMENTS                           B 1110
    C                                                                   B 1120
          READ (5,110) TITLE                                            B 1130
          READ (5,170) NUMNP,NUMEL,NUMBS                                B 1140
      170 FORMAT (3I5)                                                  B 1150
          WRITE (6,180) NUMNP,NUMEL,NUMBS                               B 1160
      180 FORMAT (1H ,22X,19HELEMENT DISCRIPTORS//13X,48HNUMNP   (NUMBER OF   B 1170
         1NODAL POINTS)        =,2X,I4/13X,48HNUMEL   (NUMBER OF ELEM   B 1180
         2ENTS)               =,2X,I4/13X,48HNUMBS   (NUMBER OF BOUNDARY  B 1190
         3 SEGMENTS)          =,2X,I4)                                  B 1200
    C     **********************************************************    B 1210
    C                                                                   B 1220
    C     LOAD TIME PARAMETERS                                          B 1230
    C                                                                   B 1240
    C     NTIM = MAXIMUM NUMBER OF TIME STEPS                           B 1250
    C     NPMP = NUMBER OF PUMPING PERIODS                              B 1260
    C     PINT = FIRST PUMPING PERIOD IN DAYS                           B 1270
    C     TIMX = TIME INCREMENT MULTIPLIER                              B 1280
    C     TDELMAX = MAXIMUM TIME STEP IN DAYS                           B 1290
    C     TINIT = INITIAL TIME STEP IN SECONDS                         B 1300
    C                                                                   B 1310
          READ (5,110) TITLE                                            B 1320
          READ (5,130) NTIM,NPMP,PINT,TIMX,TDELMAX,TINIT               B 1330
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      190 FORMAT (2I5,4F10.0)                                                  B 1340
          WRITE (6,200) NTIM,NPMP,PINT,TIMX,TCELMAX,TINIT                      B 1350
      200 FORMAT (///,23X,16HTIME  PARAMETERS//13X,48HNTIM    (MAXIMUM NUMBE   B 1360
         1R OF TIME STEPS)              =,2X,I4/13X,48HNPMP    (NUMBER OF PUMPING  B 1370
         2 PERIODS)          =,2X,I4/13X,48HPINT   (FIRST PUMPING PERIOD       B 1380
         3IN DAYS)          =,2X,F7.2/13X,48HTIMX   (TIME INCREMENT MULTIPLI    B 1390
         4ER)              =,2X,F7.2/13X,48HTDELMAX (MAXIMUM TIME STEP IN DAYS  B 1400
         5)              =,2X,F7.2/13X,48HTINIT   (INITIAL TIME STEP IN SECOND  B 1410
         6S)          =,2X,F5.0)                                               B 1420
      C   ***********************************************************************  B 1430
      C                                                                        B 1440
      C                                                                        B 1450
      C   LOAD HYDROLOGIC AND CHEMICAL PARAMETERS                              B 1450
      C                                                                        B 1460
      C   S = STORAGE COEFFICIENT                                              B 1470
      C   POROS = EFFECTIVE POROSITY                                           B 1480
      C   BETA = LONGITUDINAL DISPERSIVITY IN FT                               B 1490
      C   DLTRAT = RATIO OF TRANSVERSE TO LONGITUDINAL DISPERSIVITY            B 1500
      C   Z1 = VALENCE OF SPECIES 1                                            B 1510
      C   Z2 = VALENCE OF SPECIES 2                                            B 1520
      C   ATOMWT1 = ATOMIC WEIGHT IN GRAMS OF SPECIES 1                        B 1530
      C   ATOMWT2 = ATOMIC WEIGHT IN GRAMS OF SPECIES 2                        B 1540
      C   DBYHUK1 = DEBYE HUCKEL PARAMETER FOR SPECIES 1                       B 1550
      C   DBYHUK2 = DEBYE HUCKEL PARAMETER FOR SPECIES 2                       B 1560
      C   SK = SELECTIVITY COEFFICIENT                                         B 1570
      C   NOTE--Z2 MUST BE GREATER THAN OR EQUAL TO Z1                         B 1580
      C                                                                        B 1590
          READ (5,110) TITLE                                                   B 1600
          READ (5,210) S,POROS,BETA,DLTRAT,Z1,Z2,ATOMWT1,ATOMWT2               B 1610
      210 FORMAT (8F10.0)                                                      B 1620
          READ (5,110) TITLE                                                   B 1630
          READ (5,220) DBYHUK1,DBYHUK2,SK                                      B 1640
      220 FORMAT (3F10.0)                                                      B 1650
          WRITE (6,230) S,POROS,BETA,DLTRAT,Z1,Z2,ATOMWT1,ATOMWT2,DBYHUK1,DB   B 1660
         1YHUK2,SK                                                             B 1670
      230 FORMAT (///,14X,34HHYDROLOGIC AND CHEMICAL PARAMETERS//13X,48HS      B 1680
         1    (STORAGE COEFFICIENT)                 =,2X,F10.5/13X,48HPOROS    B 1690
         2    (EFFECTIVE POROSITY)                  =,2X,F10.5/13X,48HBETA     B 1700
         3   (LONGITUDINAL DISPERSIVITY IN FT)      =,2X,F6.1/13X,48HDLTRAT    B 1710
         4(RATIO OF TRANSVERSE TO                   /13X,48H            LONGITUDI  B 1720
         5NAL DISPERSIVITY)            =,2X,F7.2/13X,48HZ1      (VALENCE OF     B 1730
         6SPECIES 1)                =,2X,F5.0/13X,48HZ2      (VALENCE OF SP     B 1740
         7ECIES 2)            =,2X,F5.0/13X,48HATOMWT1 (ATOMIC WEIGHT I         B 1750
         8N GRAMS OF SPECIES 1)  =,2X,F8.3/13X,48HATOMWT2 (ATOMIC WEIGHT IN     B 1760
         9GRAMS OF SPECIES 2)  =,2X,F8.3/13X,48HDBYHUK1 (DEBYE HUCKEL PARAME    B 1770
         OTER FOR SPECIES 1) =,2X,F5.0/13X,48HDBYHUK2 (DEBYE HUCKEL PARAMETE    B 1780
         1R FOR SPECIES 2) =,2X,F5.0/13X,48HSK       (SELECTIVITY COEFFICIENT  B 1790
         2)          =,2X,F10.5)                                               B 1800
      C   ***********************************************************************  B 1810
      C                                                                        B 1820
      C READ NODAL COORDINATES                                                 B 1830
      C                                                                        B 1840
          READ (5,110) TITLE                                                   B 1850
          READ (5,240) FCTR                                                    B 1860
      240 FORMAT (F10.0)                                                       B 1870
          READ (5,250) (NP,X(NP),Y(NP),I = 1,NUMNP)                            B 1880
      250 FORMAT (3(I5,2F10.0))                                                B 1890
      C                                                                        B 1900
          DO 260 NP = 1,NUMNP                                                  B 1910
            X(NP) = X(NP) * FCTR                                               B 1920
            Y(NP) = Y(NP) * FCTR                                               B 1930
      260 CONTINUE                                                             B 1940
      C                                                                        B 1950
          WRITE (6,270)                                                        B 1960
      270 FORMAT (1H1,45X,21HI N P U T    D A T A/1H ,44X,23H--------------    B 1970
         1--------////1H0,5X,16HNODE COORDINATES/1H ,4X,18H---------------     B 1980
         2--/1H0,9X,3(4HNODE,5X,5HX LOC,7X,5HY LOC,16X)/)                      B 1990
          WRITE (6,230) (NP,X(NP),Y(NP),NP = 1,NUMNP)                          B 2000
      280 FORMAT (/(10X,3(I3,F12.2,F12.2,15X)))                                B 2010
      C   ***********************************************************************  B 2020
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PROGRAM LISTING--CONTINUED

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C                                                                    B 2030
C       READ ELEMENT VERTICES                                        B 2040
C                                                                    B 2050
        READ (5,110) TITLE                                           B 2060
        READ (5,290) (NE,NI(NE),NJ(NE),NK(NE),I = 1,NUMEL)           B 2070
    290 FORMAT (4(4I5))                                              B 2080
C                                                                    B 2090
C       CALCULATE BANDWIDTH                                          B 2100
C                                                                    B 2110
        DO 300 I = 1,NUMEL                                           B 2120
            IJ = IABS(NI(I) - NJ(I)) + 1                             B 2130
            IK = IABS(NI(I) - NK(I)) + 1                             B 2140
            JK = IABS(NJ(I) - NK(I)) + 1                             B 2150
    300 IBAND = MAXO(IBAND,IJ,IK,JK)                                 B 2160
C                                                                    B 2170
        WRITE (6,310)                                                B 2180
    310 FORMAT (1H1,45X,21HI N P U T    D A T A/1H ,44X,23H--------------  B 2190
       1----------////1H0,5X,16HELEMENT VERTICES/1H ,4X,18H--------------  B 2200
       2--/1H0,10X,3(7HELEMENT,3X,6HNODE I,2X,6HNODE J,2X,6HNODE K,5X)/)   B 2210
        WRITE (6,320) (NE,NI(NE),NJ(NE),NK(NE),NE = 1,NUMEL)         B 2220
    320 FORMAT (//(10X,3(I5,5X,I5,3X,I5,3X,I5,6X)))                  B 2230
        WRITE (6,330) IBAND                                          B 2240
    330 FORMAT (///,1H ,10X,11HBANDWIDTH =,I5)                       B 2250
C       **********************************************************   B 2260
C                                                                    B 2270
C       READ BOUNDARY SEGMENTS, DIRECTIONAL COSINES AND BOUNDARY GRADIENTS  B 2280
C                                                                    B 2290
        READ (5,110) TITLE                                           B 2300
        READ (5,340) (NBNDYI(I),NBNDYJ(I),COSX(I),COSY(I),DHDX(I),DHDY(I),  B 2310
       1I = 1,NUMBS)                                                 B 2320
    340 FORMAT (2I5,4F10.0)                                          B 2330
C                                                                    B 2340
        WRITE (6,350)                                                B 2350
    350 FORMAT (1H1,45X,21HI N P U T    D A T A/1H ,44X,23H--------------  B 2360
       1----------////1H0,5X,8HBOUNDARY/1H ,4X,10H----------/1H0,12X,2(7HSE  B 2370
       2GMENT,52X)/1H ,10X,2(11HNODE - NODE,5X,2HLX,8X,2HLY,7X,4HDHDX,6X,4   B 2380
       3HDHDY,10X)/)                                                 B 2390
        WRITE (6,360) (NBNDYI(I),NBNDYJ(I),COSX(I),COSY(I),DHDX(I),DHDY(I)  B 2400
       1,I = 1,NUMBS)                                                B 2410
    360 FORMAT (/(9X,2(I5,3H  -,I4,4F10.4,7X)))                      B 2420
C       **********************************************************   B 2430
C                                                                    B 2440
C CALCULATE ELEMENT AREAS                                            B 2450
C                                                                    B 2460
        DO 370 I = 1,NUMEL                                           B 2470
            AREA(I) = ABS((X(NJ(I)) * Y(NK(I)) - X(NK(I)) * Y(NJ(I)) + X(NK  B 2480
       1    (I)) * Y(NI(I)) - X(NI(I)) * Y(NK(I)) + X(NI(I)) * Y(NJ(I)) - X  B 2490
       2    (NJ(I)) * Y(NI(I)))) * .5                                B 2500
    370 AREATOT = AREATOT + AREA(I)                                  B 2510
C       **********************************************************   B 2520
C                                                                    B 2530
C       READ IDELEM ARRAY                                            B 2540
C       RECH =DISTRIBUTED RECHARGE OR DISCHARGE IN FT**3/DAY/FT**2   B 2550
C       POSITIVE IS DISCHARGE(PUMPAGE) AND NEGATIVE IS RECHARGE(INJECTION)  B 2560
C       C1RECH =CONCENTRATION OF C1 IN DISTRIBUTED RECHARGE IN MG/L  B 2570
C       C2RECH =CONCENTRATION OF C2 IN DISTRIBUTED RECHARGE IN MG/L  B 2580
C       VPRM =VERTICAL HYDRAULIC CONDUCTIVITY/THICKNESS OF CONFINING LAYER  B 2590
C       RECH=FCTR1                                                   B 2600
C       C1RECH=FCTR2                                                 B 2610
C       C2RECH=FCTR3                                                 B 2620
C       VPRM=FCTR4                                                   B 2630
C       SPECIFY OTHER CODES TO FIT YOUR NEEDS                        B 2640
C                                                                    B 2650
        READ (5,110) TITLE                                           B 2660
C                                                                    B 2670
C       NCODEL = NUMBER OF ELEMENT ID                                B 2680
        READ (5,380) NCODEL                                          B 2690
    380 FORMAT (I2)                                                  B 2700
        DO 390 NE = 1,NUMEL                                          B 2710
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PROGRAM LISTING--CONTINUED

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            RECH(NE) = 0.                                         B 2720
            C1RECH(NE) = 0.                                       B 2730
            C2RECH(NE) = 0.                                       B 2740
            VPRM(NE) = 0.                                         B 2750
            IDELEM(NE) = 0                                        B 2760
  390 CONTINUE                                                    B 2770
      IF (NCODEL.EQ.0) GO TO 460                                  B 2780
      READ (5,400) (NE,IDELEM(NE),I = 1,NUMEL)                    B 2790
  400 FORMAT (8(2I5))                                             B 2800
      WRITE (6,410)                                               B 2810
  410 FORMAT (1H1,45X,21HI N P U T      D A T A/1H ,44X,23H----------------  B 2820
     1----------////1H0,5X,22HELEMENT IDENTIFICATION/1H ,4X,23H-----------   B 2830
     2--------------/1H0,21X,9HNUMBER OF,/1H ,9X,7HELEM ID,5X,10HOCCURENC     B 2840
     3ES,10X,5HRECH ,9X,6HC1RECH,9X,6HC2RECH,10X,4HVPRM)          B 2850
      READ (5,110) TITLE                                          B 2860
      DO 450 NID = 1,NCODEL                                       B 2870
         KOUNT = 0                                                B 2880
         READ (5,420) ICODE,FCTR1,FCTR2,FCTR3,FCTR4               B 2890
  420 FORMAT (I5,4F10.0)                                          B 2900
         DO 430 I = 1,NUMEL                                       B 2910
            IF (IDELEM(I).NE.ICODE) GO TO 430                     B 2920
            KOUNT = KOUNT + 1                                     B 2930
            RECH(I) = FCTR1                                       B 2940
            C1RECH(I) = FCTR2                                     B 2950
            C2RECH(I) = FCTR3                                     B 2960
            VPRM(I) = FCTR4                                       B 2970
  430    CONTINUE                                                 B 2980
         WRITE (6,440) ICODE,KOUNT,FCTR1,FCTR2,FCTR3,FCTR4        B 2990
  440 FORMAT ((10X,I5,8X,I5,8X,4(F10.0,5X)))                      B 3000
  450 CONTINUE                                                    B 3010
C     ***********************************************************************  B 3020
C                                                                B 3030
C     CONVERT CRECH CONCENTRATIONS FROM MG/L TO MEQ/L            B 3040
C                                                                B 3050
  460 DO 470 NE = 1,NUMEL                                         B 3060
         C1RECH(NE) = C1RECH(NE) * Z1/ATOMWT1                     B 3070
  470 C2RECH(NE) = C2RECH(NE) * Z2/ATOMWT2                        B 3080
C     ***********************************************************************  B 3090
C                                                                B 3100
C     PRINT ELEMENT DATA FOR AREA AND ELEMENT ID                 B 3110
C                                                                B 3120
      WRITE (6,480)                                               B 3130
  480 FORMAT (1H1,45X,21HI N P U T      D A T A/1H ,44X,23H----------------  B 3140
     1----------////1H0,5X,12HELEMENT DATA/1H ,4X,14H--------------/1H0,3     B 3150
     2(9X,7HELEMENT,7X,4HAREA,5X,7HELEM ID,4X))                  B 3160
      WRITE (6,490) (NE,AREA(NE),IDELEM(NE),NE = 1,NUMEL)         B 3170
  490 FORMAT (3(10X,I5,F14.1,4X,I5,5X))                           B 3180
      WRITE (6,500) AREATOT                                       B 3190
  500 FORMAT (///,1H ,10X,18HMODEL AREA(FT**2)=,F20.2)            B 3200
C     ***********************************************************************  B 3210
C                                                                B 3220
C     READ AQUIFER THICKNESS ARRAY IN (FT)                       B 3230
C                                                                B 3240
      READ (5,110) TITLE                                         B 3250
      READ (5,510) INP,FCTR                                      B 3260
  510 FORMAT (I2,F10.0)                                          B 3270
      IF (INP.EQ.1) READ (5,520) (NP,THCK(NP),I = 1,NUMNP)       B 3280
  520 FORMAT (5(I5,F10.0))                                       B 3290
      DO 540 I = 1,NUMNP                                         B 3300
         IF (INP.NE.1) GO TO 530                                 B 3310
         THCK(I) = THCK(I) * FCTR                                B 3320
         GO TO 540                                               B 3330
  530    THCK(I) = FCTR                                          B 3340
  540 CONTINUE                                                   B 3350
C     ***********************************************************************  B 3360
C                                                                B 3370
C     READ TRANSMISSIVITY ARRAY IN (FT**2/DAY)                   B 3380
C                                                                B 3390
      READ (5,110) TITLE                                         B 3400
```

```
      READ (5,550) INP,FCTR                                     B 3410
  550 FORMAT (I2,F10.0)                                         B 3420
      IF (INP.EQ.1) READ (5,560) (NP,TRANS(NP),I = 1,NUMNP)     B 3430
  560 FORMAT (5(I5,F10.0))                                      B 3440
      DO 580 I = 1,NUMNP                                        B 3450
         IF (INP.NE.1) GO TO 570                                B 3460
         TRANS(I) = TRANS(I) * FCTR                             B 3470
         GO TO 580                                              B 3480
  570    TRANS(I) = FCTR                                        B 3490
  580 CONTINUE                                                  B 3500
C                                                               B 3510
C     CALCULATE HYDRAULIC CONDUCTIVITY ARRAY IN (FT/DAY)        B 3520
C                                                               B 3530
      DO 590 I = 1,NUMNP                                        B 3540
  590 HYDK(I) = TRANS(I)/THCK(I)                                B 3550
C     ****************************************************       B 3560
C                                                               B 3570
C                                                               B 3580
C     READ INITIAL HEAD ARRAY IN (FT)                          B 3580
C                                                               B 3590
      READ (5,110) TITLE                                        B 3600
      READ (5,600) INP,FCTR                                     B 3610
  600 FORMAT (I2,F10.0)                                         B 3620
      IF (INP.EQ.1) READ (5,610) (NP,HEAD(NP),I = 1,NUMNP)      B 3630
  610 FORMAT (5(I5,F10.0))                                      B 3640
      DO 630 I = 1,NUMNP                                        B 3650
         IF (INP.NE.1) GO TO 620                                B 3660
         HEAD(I) = HEAD(I) * FCTR                               B 3670
         GO TO 630                                              B 3680
  620    HEAD(I) = FCTR                                         B 3690
  630 CONTINUE                                                  B 3700
C                                                               B 3710
C     SET INITIAL HEAD VALUE                                    B 3720
C                                                               B 3730
      DO 640 I = 1,NUMNP                                        B 3740
  640 HDI(I) = HEAD(I)                                          B 3750
C     ****************************************************       B 3760
C                                                               B 3770
C                                                               B 3780
C     READ INITIAL SOLUTE CONCENTRATION ARRAY FOR SPECIES 1 IN (MG/L)  B 3780
C                                                               B 3790
      READ (5,110) TITLE                                        B 3800
      READ (5,650) INP,FCTR                                     B 3810
  650 FORMAT (I2,F10.0)                                         B 3820
      IF (INP.EQ.1) READ (5,660) (NP,C1(NP),I = 1,NUMNP)        B 3830
  660 FORMAT (5(I5,F10.0))                                      B 3840
      DO 680 I = 1,NUMNP                                        B 3850
         IF (INP.NE.1) GC TO 670                                B 3860
         C1(I) = C1(I) * FCTR                                   B 3870
         GO TO 680                                              B 3880
  670    C1(I) = FCTR                                           B 3890
  680 CONTINUE                                                  B 3900
C     ****************************************************       B 3910
C                                                               B 3920
C     READ INITIAL SOLUTE CONCENTRATION ARRAY FOR SPECIES 2 IN (MG/L)  B 3930
C                                                               B 3940
      READ (5,110) TITLE                                        B 3950
      READ (5,690) INP,FCTR                                     B 3960
  690 FORMAT (I2,F10.0)                                         B 3970
      IF (INP.EQ.1) READ (5,700) (NP,C2(NP),I = 1,NUMNP)        B 3980
  700 FORMAT (5(I5,F10.0))                                      B 3990
      DO 720 I = 1,NUMNP                                        B 4000
         IF (INP.NE.1) GO TO 710                                B 4010
         C2(I) = C2(I) * FCTR                                   B 4020
         GO TO 720                                              B 4030
  710    C2(I) = FCTR                                           B 4040
  720 CONTINUE                                                  B 4050
      DO 730 NP = 1,NUMNP                                       B 4060
      IF (C1(NP).LE..00001) C1(NP) = .00001                     B 4070
  730 IF (C2(NP).LE..00001) C2(NP) = .00001                     B 4080
C     ****************************************************       B 4090
```

```
C                                                                    B 4100
C      CONVERT SOLUTION  CONCENTRATICNS FROM MG/L TO MEQ/L           B 4110
C                                                                    B 4120
       DO 740 NP = 1,NUMNP                                           B 4130
           C1(NP) = C1(NP) * Z1/ATOMWT1                              B 4140
           C2(NP) = C2(NP) * Z2/ATCMWT2                              B 4150
   740 CONTINUE                                                      B 4160
C      ************************************************************* B 4170
C                                                                    B 4180
C      READ CATION EXCHANGE CAPACITY ARRAY IN (MEQ/L)                B 4190
C                                                                    B 4200
       READ (5,110) TITLE                                           B 4210
       READ (5,750) INP,FCTR                                        B 4220
   750 FORMAT (I2,F10.0)                                            B 4230
       IF (INP.EQ.1) READ (5,760) (NP,CEC(NP),I = 1,NUMNP)          B 4240
   750 FORMAT (5(I5,F10.0))                                         B 4250
       DO 780 I = 1,NUMNP                                           B 4260
           IF (INP.NE.1) GO TO 770                                  B 4270
           CEC(I) = CEC(I) * FCTR                                   B 4280
           GO TO 780                                                B 4290
   770     CEC(I) = FCTR                                            B 4300
   780 CONTINUE                                                      B 4310
C      ************************************************************* B 4320
C                                                                    B 4330
C      CALCULATE INITIAL ADSORBED CONC FOR SPECIES 1 AND 2 IN (MEQ/L) B 4340
C                                                                    B 4350
       DO 790 I = 1,NUMNP                                           B 4360
           C1HAT(I) = 0.                                            B 4370
           C2HAT(I) = 0.                                            B 4380
   790 CONTINUE                                                      B 4390
C      FOR CONSERVATIVE TRANSPORT DO NOT CALL CHATSOL               B 4400
       IF (ICT.EQ.0) CALL CHATSOL                                   B 4410
C      ************************************************************* B 4420
C                                                                    B 4430
C      READ NODEID ARRAY                                             B 4440
C      NODE ID CODES FOR 1 - 10 ARE RESERVED FOR CONSTANT HEAD NODES B 4450
C      REC =POINT RECHARGE CR DISCHARGE IN GPM                      B 4460
C      POSITIVE IS DISCHARGE(PUMPAGE) AND NEGATIVE IS RECHARGE(INJECTION) B 4470
C      C1REC =CONCENTRATION OF C1 IN POINT RECHARGE IN MG/L         B 4480
C      C2REC =CONCENTRATION OF C2 IN POINT RECHARGE IN MG/L         B 4490
C      REC=FCTR1                                                     B 4500
C      C1REC=FCTR2                                                   B 4510
C      C2REC=FCTR3                                                   B 4520
C      SPECIFY OTHER CODES TO FIT YOUR NEEDS                         B 4530
C                                                                    B 4540
       READ (5,110) TITLE                                           B 4550
C                                                                    B 4560
C      NCODNP = NUMBER OF NODE ID                                    B 4570
       READ (5,800) NCODNP                                          B 4580
   800 FORMAT (I2)                                                   B 4590
       DO 810 NP = 1,NUMNP                                           B 4600
           REC(NP) = 0.                                              B 4610
           C1REC(NP) = 0.                                            B 4620
           C2REC(NP) = 0.                                            B 4630
           NODEID(NP) = 0                                            B 4640
   810 CONTINUE                                                      B 4650
       IF (NCODNP.LE.0) GO TO 880                                    B 4660
       READ (5,820) (NP,NODEID(NP),I = 1,NUMNP)                     B 4670
   820 FORMAT (8(2I5))                                               B 4680
       WRITE (6,830)                                                 B 4690
   830 FORMAT (1H1,45X,21HI N P U T    D A T A/1H ,44X,23H--------------- B 4700
      1---------////1H0,5X,19HNODE IDENTIFICATION/1H ,4X,21H--------------- B 4710
      2---------/1H0,21X,9HNUMBER OF,/1H ,5X,7HNODE ID,5X,10HOCCURENCES,11 B 4720
      3X,3HREC,10X,5HC1REC,10X,5HC2REC)                            B 4730
       READ (5,110) TITLE                                           B 4740
       DO 870 NID = 1,NCODNP                                        B 4750
           KOUNT = 0                                                B 4760
           READ (5,840) ICODE,FCTR1,FCTR2,FCTR3                    B 4770
   840 FORMAT (I5,3F10.0)                                           B 4780
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PROGRAM LISTING--CONTINUED

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          DO 850 I = 1,NUMNP                                       B 4790
             IF (NODEID(I).NE.ICODE) GO TO 850                     B 4800
             KOUNT = KOUNT + 1                                     B 4810
             REC(I) = FCTR1                                        B 4820
             C1REC(I) = FCTR2                                      B 4830
             C2REC(I) = FCTR3                                      B 4840
      850 . CONTINUE                                               B 4850
             WRITE (6,860) ICODE,KOUNT,FCTR1,FCTR2,FCTR3           B 4860
      860 FORMAT ((10X,I5,8X,I5,8X,3(F10.0,5X)))                   B 4870
      870 CONTINUE                                                 B 4880
C         ********************************************************* B 4890
C                                                                  B 4900
C         CONVERT REC FROM GPM TO FT**3/DAY                        B 4910
C         CONVERT CREC CONCENTRATIONS FROM MG/L TO MEQ/L           B 4920
C         CONVERT SOLUTION CONCENTRATIONS FROM MEQ/L TO MG/L       B 4930
C         CONVERT ADSORBED CONCENTRATIONS FROM MEQ/L TO FRACTION ADSORBED B 4940
C         TEMPORARILY USE RHSU & RHSL ARRAYS TO PRINT C1HAT & C2HAT IN MG/L B 4950
C                                                                  B 4960
      880 DO 890 NP = 1,NUMNP                                      B 4970
             REC(NP) = REC(NP)/7.48052 * 60 * 24                   B 4980
             C1REC(NP) = C1REC(NP) * Z1/ATOMWT1                    B 4990
             C2REC(NP) = C2REC(NP) * Z2/ATOMWT2                    B 5000
             C1(NP) = C1(NP)/Z1 * ATOMWT1                          B 5010
             C2(NP) = C2(NP)/Z2 * ATOMWT2                          B 5020
             C1HAT(NP) = C1HAT(NP)/CEC(NP)                         B 5030
             C2HAT(NP) = C2HAT(NP)/CEC(NP)                         B 5040
             RHSU(NP) = C1HAT(NP) * CEC(NP)/Z1 * ATOMWT1           B 5050
             RHSL(NP) = C2HAT(NP) * CEC(NP)/Z2 * ATOMWT2           B 5060
      890 CONTINUE                                                 B 5070
C         ********************************************************* B 5080
C                                                                  B 5090
C         PRINT NODE DATA FOR TRANSMISSIVITY, HYDRAULIC CONDUCTIVITY, B 5100
C         SATURATED THICKNESS, CATION EXCHANGE CAPACITY AND NODE ID B 5110
C                                                                  B 5120
          I = 1                                                    B 5130
          J = 50                                                   B 5140
      900 IF (J.GE.NUMNP) J = NUMNP                                B 5150
          WRITE (6,910)                                            B 5160
      910 FORMAT (1H1,45X,21HI N P U T    D A T A/1H ,44X,23H----------------- B 5170
     1---------////1H0,5X,9HNODE DATA/1H ,4X,11H------------/1H0,43X,9HHY B 5180
     2DRAULIC,28X,15HCATION EXCHANGE/10X,4HNODE,9X,14HTRANSMISSIVITY,6X, B 5190
     312HCONDUCTIVITY,9X,9HTHICKNESS,8X,15HCAPACITY(MEQ/L),5X,7HNODE ID) B 5200
          WRITE (6,920) (NP,TRANS(NP),HYDK(NP),THCK(NP),CEC(NP),NODEID(NP),N B 5210
     1P = I,J)                                                     B 5220
      920 FORMAT ((8X,I5,10X,F10.2,9X,F10.3,10X,F10.2,9X,F10.1,10X,I5) B 5230
          IF (J.EQ.NUMNP) GO TO 930                                B 5240
          I = I + 50                                               B 5250
          J = J + 50                                               B 5260
          GO TO 900                                                B 5270
      930 CONTINUE                                                 B 5280
C         ********************************************************* B 5290
C                                                                  B 5300
C         PRINT INITIAL NODE VALUES FOR HEAD AND CONCENTRATION     B 5310
C                                                                  B 5320
          I = 1                                                    B 5330
          J = 50                                                   B 5340
      940 IF (J.GE.NUMNP) J = NUMNP                                B 5350
          WRITE (6,950)                                            B 5360
      950 FORMAT (1H1,45X,21HI N P U T    D A T A/1H ,44X,23H----------------- B 5370
     1---------////1H0,5X,17HINITIAL NODE DATA/1H ,4X,19H------------------ B 5380
     2----/1H0,37X,6HSOLUTE,11X,6HSOLUTE,9X,8HADSORBED,6X,8HADSORBED,7X, B 5390
     38HADSORBED,9X,8HADSORBED/10X,4HNODE,9X,4HHEAD,10X,8HC1(MG/L),9X,8H B 5400
     4C2(MG/L),8X,9HC1HAT/CEC,5X,9HC2HAT/CEC,5X,11HC1HAT(MG/L),6X,11HC2H B 5410
     5AT(MG/L))                                                    B 5420
          WRITE (6,960) (NP,HEAD(NP),C1(NP),C2(NP),C1HAT(NP),C2HAT(NP),RHSU( B 5430
     1NP),RHSL(NP),NP = I,J)                                       B 5440
      960 FORMAT ((8X,I5,5X,F10.1,2(5X,F12.3),2(9X,F5.3),2(5X,F12.3))) B 5450
          IF (J.EQ.NUMNP) GO TO 970                                B 5460
          I = I + 50                                               B 5470
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```
           J = J + 50                                              B 5480
           GO TO 940                                               B 5490
     970 CONTINUE                                                  B 5500
           WRITE (6,980)                                           B 5510
     980 FORMAT (1H1,//////)                                       B 5520
C      ********************************************************    B 5530
C                                                                  B 5540
C      CONVERT ADSORBED CONCENTRATIONS FROM FRACTION ADSORBED TO MG/L  B 5550
C                                                                  B 5560
           DO 990 NP = 1,NUMNP                                     B 5570
              C1HAT(NP) = C1HAT(NP) * CEC(NP)/Z1 * ATOMWT1         B 5580
              C2HAT(NP) = C2HAT(NP) * CEC(NP)/Z2 * ATOMWT2         B 5590
     990 CONTINUE                                                  B 5600
C      ********************************************************    B 5610
C                                                                  B 5620
C      CALCULATE INITIAL MASS STORED IN THE AQUIFER               B 5630
C                                                                  B 5640
           C1ISTOR = 0.                                           B 5650
           C2ISTOR = 0.                                           B 5660
           DO 1000 NE = 1,NUMEL                                   B 5670
              THCKBAR = (THCK(NI(NE)) + THCK(NJ(NE)) + THCK(NK(NE)))/3.  B 5680
              C1TBAR = (C1(NI(NE)) + C1(NJ(NE)) + C1(NK(NE)))/3. + (C1HAT(NI(  B 5690
         1    NE)) + C1HAT(NJ(NE)) + C1HAT(NK(NE)))/3.            B 5700
              C1ISTOR = AREA(NE) * THCKBAR * POROS * C1TBAR + C1ISTOR  B 5710
              C2TBAR = (C2(NI(NE)) + C2(NJ(NE)) + C2(NK(NE)))/3. + (C2HAT(NI(  B 5720
         1    NE)) + C2HAT(NJ(NE)) + C2HAT(NK(NE)))/3.            B 5730
              C2ISTOR = AREA(NE) * THCKBAR * POROS * C2TBAR + C2ISTOR  B 5740
    1000 CONTINUE                                                  B 5750
C      ********************************************************    B 5760
C                                                                  B 5770
C      CONVERT SOLUTION CONCENTRATIONS FROM MG/L TO MEQ/L         B 5780
C      CONVERT ADSORBED CONCENTRATIONS FROM MG/L TO MEQ/L         B 5790
C                                                                  B 5800
           DO 1010 NP = 1,NUMNP                                   B 5810
              C1(NP) = C1(NP) * Z1/ATOMWT1                         B 5820
              C2(NP) = C2(NP) * Z2/ATOMWT2                         B 5830
              C1HAT(NP) = C1HAT(NP) * Z1/ATOMWT1                   B 5840
    1010 C2HAT(NP) = C2HAT(NP) * Z2/ATOMWT2                        B 5850
           GO TO 1160                                              B 5860
C      ********************************************************    B 5870
C      ********************************************************    B 5880
C                                                                  B 5890
C      UPDATE PUMPING PERIOD DATA                                 B 5900
C                                                                  B 5910
    1020 WRITE (6,1030)                                            B 5920
    1030 FORMAT (1H1,45X,23HU P D A T E    D A T A/1H ,44X,25H-------------  B 5930
         1---------------/////)                                    B 5940
           READ (5,110) TITLE                                     B 5950
           WRITE (6,120) TITLE                                    B 5960
C                                                                  B 5970
C      UPDATE TIME PARAMETERS                                     B 5980
C                                                                  B 5990
           READ (5,110) TITLE                                     B 6000
           READ (5,1040) PINT                                     B 6010
    1040 FORMAT (F10.0)                                            B 6020
           WRITE (6,1050) PINT                                    B 6030
    1050 FORMAT (///6X,31HPINT (PUMPING PERIOD IN DAYS) =,2X,F7.2)  B 6040
C                                                                  B 6050
C      UPDATE NODEID ARRAY                                        B 6060
C                                                                  B 6070
           DO 1060 NP = 1,NUMNP                                   B 6080
              REC(NP) = 0.                                         B 6090
              C1REC(NP) = 0.                                       B 6100
              C2REC(NP) = 0.                                       B 6110
    1060 NODEID(NP) = 0                                            B 6120
           READ (5,110) TITLE                                     B 6130
           READ (5,820) (NP,NCDEID(NP),I = 1,NUMNP)               B 6140
           WRITE (6,1070)                                         B 6150
    1070 FORMAT (////1H0,5X,19HNODE IDENTIFICATION/1H ,4X,21H----------------  B 6160
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PROGRAM LISTING--CONTINUED

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       1-------/1H0,21X,9HNUMBER OF,/1H ,9X,7HNODE ID,5X,10HOCCURENCES,11X   B 6170
       2,3HREC,10X,5HC1REC,10X,5HC2REC)                                       B 6180
         READ (5,110) TITLE                                                   B 6190
         DO 1110 NID = 1,NCODNP                                               B 6200
            KOUNT = 0                                                         B 6210
            READ (5,1080) ICODE,FCTR1,FCTR2,FCTR3                             B 6220
 1080 FORMAT (I5,3F10.0)                                                      B 6230
            DO 1090 I = 1,NUMNP                                               B 6240
               IF (NODEID(I).NE.ICODE) GO TO 1090                            B 6250
               KOUNT = KOUNT + 1                                             B 6260
               REC(I) = FCTR1                                                B 6270
               C1REC(I) = FCTR2                                              B 6280
               C2REC(I) = FCTR3                                              B 6290
 1090       CONTINUE                                                         B 6300
            WRITE (6,1100) ICODE,KOUNT,FCTR1,FCTR2,FCTR3                     B 6310
 1100 FORMAT ((10X,I5,8X,I5,8X,3(F10.0,5X)))                                  B 6320
 1110 CONTINUE                                                               B 6330
C                                                                            B 6340
C     CONVERT REC FROM GPM TO FT**3/DAY                                      B 6350
C     CONVERT CREC CONCENTRATIONS FROM MG/L TO MEQ/L                         B 6360
C                                                                            B 6370
         DO 1120 NP = 1,NUMNP                                                B 6380
            REC(NP) = REC(NP)/7.48052 * 60 * 24                             B 6390
            C1REC(NP) = C1REC(NP) * Z1/ATOMWT1                              B 6400
            C2REC(NP) = C2REC(NP) * Z2/ATOMWT2                              B 6410
 1120 CONTINUE                                                               B 6420
         WRITE (6,1030)                                                      B 6430
         WRITE (6,1130)                                                      B 6440
 1130 FORMAT (1H0,5X,13HNODE ID ARRAY/1H ,4X,15H---------------/1H0,11X,    B 6450
       15(4HNODE,4X,7HNODE ID,10X))                                         B 6460
         WRITE (6,1140) (I,NODEID(I),I = 1,NUMNP)                            B 6470
 1140 FORMAT (5(10X,I5,5X,I5))                                               B 6480
         WRITE (6,1150)                                                      B 6490
 1150 FORMAT (1H1,//////)                                                    B 6500
C     ***************************************************************        B 6510
 1160 RETURN                                                                 B 6520
      END                                                                    B 6530
      SUBROUTINE ELINTF(NCALL)                                               C 0010
      COMMON /BLOCKA/ NUMNP,X(35),Y(35),NUMEL,NI(50),NJ(50),                C 0020
      1NK(50),NUMBS,NBNDYI(18),NBNDYJ(18),COSX(18),COSY(18),               C 0030
      2DHDX(18),DHDY(18),TITLE(20),IBAND,ICT                                C 0040
      COMMON /BLOCKC/ S,POROS,BETA,DLTRAT,Z1,Z2,ATOMWT1,ATOMWT2,DBYHUK1,   C 0050
      1DBYHUK2,SK                                                           C 0060
      COMMON /BLOCKD/ NCODNP,NODEID(35),TRANS(35),HYDK(35),THCK(35),       C 0070
      1REC(35),C1REC(35),C2REC(35)                                          C 0080
      COMMON /BLOCKE/ IDELEM(50),RECH(50),C1RECH(50),C2RECH(50),           C 0090
      1VPRM(50),AREA(50)                                                    C 0100
      COMMON /BLOCKF/ HEAD(35),HDI(35),C1(35),C2(35),C1HAT(35),            C 0110
      1C2HAT(35),CEC(35)                                                    C 0120
      COMMON /BLOCKG/ AF(35,7),BF(35,7),DF(35)                             C 0130
C     ***************************************************************        C 0140
C                                                                            C 0150
C     THIS SUBROUTINE PERFORMS THE INTEGRATIONS REQUIRED FOR THE FLOW       C 0160
C     EQUATION.  THESE INTEGRATIONS ARE CARRIED OUT IN A PIECEWISE          C 0170
C     MANNER ON AN ELEMENT BASIS.  GLOBAL MATRICES ARE THEN FORMED BY       C 0180
C     SUMMING FOR A GIVEN NODE THE CONTRIBUTION TO THAT NODE FROM EACH      C 0190
C     ELEMENT.  THESE GLOBAL MATRICES FOR THE FLOW EQUATION ARE BANDED      C 0200
C     AND SYMMETRIC.                                                        C 0210
C                                                                            C 0220
C     ***************************************************************        C 0230
      IF (NCALL.GT.1) GO TO 140                                             C 0240
C     ***************************************************************        C 0250
C                                                                            C 0260
C     PERFORM ELEMENT INTEGRATIONS ( A MATRIX - FLOW)                       C 0270
C                                                                            C 0280
         DO 100 I = 1,NUMNP                                                  C 0290
         DO 100 J = 1,IBAND                                                  C 0300
  100 AF(I,J) = 0.                                                           C 0310
C                                                                            C 0320
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      DO 110 I = 1,NUMEL                                               C 0330
      TA4 = (TRANS(NI(I)) + TRANS(NJ(I)) + TRANS(NK(I)))/(AREA(I) * 1  C 0340
     1  2.)                                                            C 0350
      E1 = ((Y(NJ(I)) - Y(NK(I))) * (Y(NJ(I)) - Y(NK(I))) + (X(NK(I))  C 0360
     1   - X(NJ(I))) * (X(NK(I)) - X(NJ(I)))) * TA4                    C 0370
      E2 = ((Y(NK(I)) - Y(NI(I))) * (Y(NJ(I)) - Y(NK(I))) + (X(NI(I))  C 0380
     1   - X(NK(I))) * (X(NK(I)) - X(NJ(I)))) * TA4                    C 0390
      E3 = ((Y(NI(I)) - Y(NJ(I))) * (Y(NJ(I)) - Y(NK(I))) + (X(NJ(I))  C 0400
     1   - X(NI(I))) * (X(NK(I)) - X(NJ(I)))) * TA4                    C 0410
      E4 = ((Y(NK(I)) - Y(NI(I))) * (Y(NK(I)) - Y(NI(I))) + (X(NI(I))  C 0420
     1   - X(NK(I))) * (X(NI(I)) - X(NK(I)))) * TA4                    C 0430
      E5 = ((Y(NI(I)) - Y(NJ(I))) * (Y(NK(I)) - Y(NI(I))) + (X(NJ(I))  C 0440
     1   - X(NI(I))) * (X(NI(I)) - X(NK(I)))) * TA4                    C 0450
      E6 = ((Y(NI(I)) - Y(NJ(I))) * (Y(NI(I)) - Y(NJ(I))) + (X(NJ(I))  C 0460
     1   - X(NI(I))) * (X(NJ(I)) - X(NI(I)))) * TA4                    C 0470
C                                                                      C 0480
C     LOCATE IN BANDED GLOBAL MATRIX (SYMMETRIC)                       C 0490
C                                                                      C 0500
      IJ = IABS(NI(I) - NJ(I)) + 1                                     C 0510
      IK = IABS(NI(I) - NK(I)) + 1                                     C 0520
      JK = IABS(NJ(I) - NK(I)) + 1                                     C 0530
      AF(NI(I),1) = AF(NI(I),1) + E1                                   C 0540
      IF (NI(I).LT.NJ(I)) AF(NI(I),IJ) = AF(NI(I),IJ) + E2             C 0550
      IF (NJ(I).LT.NI(I)) AF(NJ(I),IJ) = AF(NJ(I),IJ) + E2             C 0560
      IF (NI(I).LT.NK(I)) AF(NI(I),IK) = AF(NI(I),IK) + E3             C 0570
      IF (NK(I).LT.NI(I)) AF(NK(I),IK) = AF(NK(I),IK) + E3             C 0580
      AF(NJ(I),1) = AF(NJ(I),1) + E4                                   C 0590
      IF (NJ(I).LT.NK(I)) AF(NJ(I),JK) = AF(NJ(I),JK) + E5             C 0600
      IF (NK(I).LT.NJ(I)) AF(NK(I),JK) = AF(NK(I),JK) + E5             C 0610
      AF(NK(I),1) = AF(NK(I),1) + E6                                   C 0620
  110 CONTINUE                                                         C 0630
C     *********************************************************        C 0640
C                                                                      C 0650
C     PERFORM ELEMENT INTEGRATIONS ( B MATRIX - FLOW)                  C 0660
C                                                                      C 0670
      DO 120 I = 1,NUMNP                                               C 0680
      DO 120 J = 1,IBAND                                               C 0690
  120 BF(I,J) = 0.                                                     C 0700
C                                                                      C 0710
      DO 130 I = 1,NUMEL                                               C 0720
      E1 = S * AREA(I)/6.                                              C 0730
      E2 = S * AREA(I)/12.                                             C 0740
      E3 = S * AREA(I)/12.                                             C 0750
      E4 = S * AREA(I)/6.                                              C 0760
      E5 = S * AREA(I)/12.                                             C 0770
      E6 = S * AREA(I)/6.                                              C 0780
C                                                                      C 0790
C     LOCATE IN BANDED GLOBAL MATRIX (SYMMETRIC)                       C 0800
C                                                                      C 0810
      IJ = IABS(NI(I) - NJ(I)) + 1                                     C 0820
      IK = IABS(NI(I) - NK(I)) + 1                                     C 0830
      JK = IABS(NJ(I) - NK(I)) + 1                                     C 0840
      BF(NI(I),1) = BF(NI(I),1) + E1                                   C 0850
      IF (NI(I).LT.NJ(I)) BF(NI(I),IJ) = BF(NI(I),IJ) + E2             C 0860
      IF (NJ(I).LT.NI(I)) BF(NJ(I),IJ) = BF(NJ(I),IJ) + E2             C 0870
      IF (NI(I).LT.NK(I)) BF(NI(I),IK) = BF(NI(I),IK) + E3             C 0880
      IF (NK(I).LT.NI(I)) BF(NK(I),IK) = BF(NK(I),IK) + E3             C 0890
      BF(NJ(I),1) = BF(NJ(I),1) + E4                                   C 0900
      IF (NJ(I).LT.NK(I)) BF(NJ(I),JK) = BF(NJ(I),JK) + E5             C 0910
      IF (NK(I).LT.NJ(I)) BF(NK(I),JK) = BF(NK(I),JK) + E5             C 0920
      BF(NK(I),1) = BF(NK(I),1) + E6                                   C 0930
  130 CONTINUE                                                         C 0940
C     *********************************************************        C 0950
C                                                                      C 0960
C     PERFORM ELEMENT INTEGRATION ( MATRICES D,E&F - FLOW)             C 0970
C     LOCATE IN GLOBAL MATRIX                                          C 0980
C                                                                      C 0950
  140 DO 150 NP = 1,NUMNP                                              C 1000
  150 DF(NP) = 0.                                                      C 1010
```

PRCGRAM LISTING--CONTINUED

```
C                                                                      C 1020
      DO 170 NE = 1,NUMEL                                              C 1030
         QLEK = 0.                                                     C 1040
         QRECH = 0.                                                    C 1050
         IF (VPRM(NE).EQ.0.0) GO TO 160                                C 1060
         HEADBAR = (HEAD(NI(NE)) + HEAD(NJ(NE)) + HEAD(NK(NE)))/3.     C 1070
         HDIBAR = (HDI(NI(NE)) + HDI(NJ(NE)) + HDI(NK(NE)))/3.         C 1080
         QLEK = VPRM(NE) * (HEADBAR - HDIBAR) * AREA(NE)/3.            C 1090
  160    QRECH = RECH(NE) * AREA(NE)/3.                                C 1100
         DF(NI(NE)) = DF(NI(NE)) + QRECH + QLEK                        C 1110
         DF(NJ(NE)) = DF(NJ(NE)) + QRECH + QLEK                        C 1120
         DF(NK(NE)) = DF(NK(NE)) + QRECH + QLEK                        C 1130
  170 CONTINUE                                                         C 1140
      DO 180 NP = 1,NUMNP                                              C 1150
         IF (NODEID(NP).GE.1.AND.NODEID(NP).LE.10) REC(NP) = 0.        C 1160
         DF(NP) = DF(NP) + REC(NP)                                     C 1170
  180 CONTINUE                                                         C 1180
      DO 190 NB = 1,NUMBS                                              C 1190
         DX2 = (X(NBNDYI(NB)) - X(NBNDYJ(NB))) *   * 2                 C 1200
         DY2 = (Y(NBNDYI(NB)) - Y(NBNDYJ(NB))) *   * 2                 C 1210
         DL = (DX2 + DY2) *   * .5                                     C 1220
         DHDN = DHDX(NB) * COSX(NB) + DHDY(NB) * COSY(NB)              C 1230
         QBNDYI = DHDN * DL/6. * (2 * TRANS(NBNDYI(NB)) + TRANS(NBNDYJ(N  C 1240
     1   B)))                                                          C 1250
         QBNDYJ = DHDN * DL/6. * (TRANS(NBNDYI(NB)) + 2 * TRANS(NBNDYJ(N  C 1260
     1   B)))                                                          C 1270
         DF(NBNDYI(NB)) = DF(NBNDYI(NB)) - QBNDYI                      C 1280
         DF(NBNDYJ(NB)) = DF(NBNDYJ(NB)) - QBNDYJ                      C 1290
  190 CONTINUE                                                         C 1300
C     *****************************************************************  C 1310
      RETURN                                                           C 1320
      END                                                              C 1330
      SUBROUTINE MATFLOW                                               D 0010
      COMMON /BLOCKA/ NUMNP,X(35),Y(35),NUMEL,NI(50),NJ(50),          D 0020
     1NK(50),NUMBS,NBNDYI(18),NBNDYJ(18),COSX(18),COSY(18),           D 0030
     2DHDX(18),DHDY(18),TITLE(20),IBAND,ICT                           D 0040
      COMMON /BLOCKB/ NTIM,NPMP,PINT,TIMX,TINIT,TPDAY,SUMT,TDEL,INT,TIMY  D 0050
     1,TDELMAX                                                         D 0060
      COMMON /BLOCKC/ S,FCROS,BETA,DLTRAT,Z1,Z2,ATOMWT1,ATOMWT2,DBYHUK1,  D 0070
     1DBYHUK2,SK                                                       D 0080
      COMMON /BLOCKD/ NCODNP,NODEID(35),TRANS(35),HYDK(35),THCK(35),   D 0090
     1REC(35),C1REC(35),C2REC(35)                                     D 0100
      COMMON /BLOCKF/ HEAD(35),HDI(35),C1(35),C2(35),C1HAT(35),        D 0110
     1C2HAT(35),CEC(35)                                               D 0120
      COMMON /BLOCKG/ AF(35,7),BF(35,7),DF(35)                         D 0130
      COMMON /BLOCKI/ CM(35,13),RHS(35),RHSU(35),RHSL(35)              D 0140
C     *****************************************************************  D 0150
C                                                                      D 0160
C     THIS SUBROUTINE ASSEMBLES AND SOLVES THE FLOW EQUATION           D 0170
C     (MATRIX(AF)+(MATRIX(BF)/TDEL))=LHS COEFFICIENT MATRIX            D 0180
C     (((MATRIX(BF)/TDEL) * VECTOR(HEAD)) - VECTOR(DF))=KNOWN RHS VECTOR  D 0190
C     SOLUTION IS BY THE POINT SUCCESIVE OVERRELAXATION ITERATIVE METHOD  D 0200
C                                                                      D 0210
C     *****************************************************************  D 0220
C                                                                      D 0230
C     ABSOLUTE CONVERGENCE TEST                                        D 0240
C                                                                      D 0250
C     (1) ROW                                                          D 0260
      SUM = 0.                                                         D 0270
      DO 100 J = 2,IBAND                                               D 0280
  100 SUM = (AF(1,J) + BF(1,J)/TDEL) + SUM                             D 0290
      IF (SUM.GT.(AF(1,1) + BF(1,1)/TDEL)) GO TO 170                   D 0300
C                                                                      D 0310
C     (2) TO (IBAND) ROW                                               D 0320
      DO 130 I = 2,IBAND                                               D 0330
         SUM = 0.                                                      D 0340
         DO 110 J = 2,IBAND                                            D 0350
  110    SUM = (AF(I,J) + BF(I,J)/TDEL) + SUM                          D 0360
         JC = 1                                                        D 0370
```

PROGRAM LISTING--CONTINUED

```
          IR = I                                                    D 0380
          DO 120 K = 2,I                                            D 0390
             JC = JC + 1                                            D 0400
             IR = IR - 1                                            D 0410
   120    SUM = (AF(IR,JC) + BF(IR,JC)/TDEL) + SUM                  D 0420
C                                                                   D 0430
C     (IBAND+1) TO (NUMNP) ROW                                      D 0440
       IBP1 = IBAND + 1                                             D 0450
       DO 160 I = IBP1,NUMNP                                        D 0460
          SUM = 0.                                                  D 0470
          DO 140 J = 2,IBAND                                        D 0480
   140    SUM = (AF(I,J) + BF(I,J)/TDEL) + SUM                      D 0490
          JC = 1                                                    D 0500
          IR = I                                                    D 0510
          DO 150 K = 2,IBAND                                        D 0520
             JC = JC + 1                                            D 0530
             IR = IR - 1                                            D 0540
   150    SUM = (AF(IR,JC) + BF(IR,JC)/TDEL) + SUM                  D 0550
       GO TO 190                                                    D 0560
   170 WRITE (6,180)                                                D 0570
   180 FORMAT (1H0,5X,105H***WARNING***ABSOLUTE CONVERGENCE TEST FAILED I  D 0580
      1N SUBROUTINE MATFLOW--NEW SOLUTION ALGORITHM MAY BE NEEDED)  D 0590
   190 CONTINUE                                                     D 0600
C     ***********************************************************************  D 0610
C                                                                   D 0620
C     RHS VECTOR                                                    D 0630
C                                                                   D 0640
       CALL MULT (NUMNP,IBAND,BF,HEAD,RHS)                          D 0650
       DO 200 I = 1,NUMNP                                           D 0660
   200 RHS(I) = RHS(I)/TDEL - DF(I)                                 D 0670
C     ***********************************************************************  D 0680
       TOL = .01                                                    D 0690
       ITMAX = 200                                                  D 0700
       RELAX = 1.                                                   D 0710
C     ***********************************************************************  D 0720
       DO 390 IT = 1,ITMAX                                          D 0730
          ERROR = 0.0                                               D 0740
C                                                                   D 0750
C     (1) ROW                                                       D 0760
          SUM = 0.                                                  D 0770
          DO 210 J = 2,IBAND                                        D 0780
   210    SUM = (AF(1,J) + BF(1,J)/TDEL) * HEAD(J) + SUM            D 0790
          IF (NODEID(1).EQ.0.OR.NODEID(1).GT.10) GO TO 220          D 0800
          REC(1) = RHS(1) - SUM - ((AF(1,1) + BF(1,1)/TDEL) * HEAD(1))  D 0810
          GO TO 230                                                 D 0820
   220    HNEW = (RHS(1) - SUM)/(AF(1,1) + BF(1,1)/TDEL)            D 0830
          RESID = HNEW - HEAD(1)                                    D 0840
          HEAD(1) = HEAD(1) + RELAX * RESID                         D 0850
          RESID = ABS(RESID)                                        D 0860
          ERROR = AMAX1(ERROR,RESID)                                D 0870
   230    CONTINUE                                                  D 0880
C                                                                   D 0890
C     (2) TO (IBAND) ROW                                            D 0900
          DO 270 I = 2,IBAND                                        D 0910
             SUM = 0.                                               D 0920
             IR = I                                                 D 0930
             DO 240 J = 2,IBAND                                     D 0940
                IR = IR + 1                                         D 0950
   240       SUM = (AF(I,J) + BF(I,J)/TDEL) * HEAD(IR) + SUM        D 0960
             JC = 1                                                 D 0970
             IR = I                                                 D 0980
             DO 250 K = 2,I                                         D 0990
                JC = JC + 1                                         D 1000
                IR = IR - 1                                         D 1010
   250       SUM = (AF(IR,JC) + BF(IR,JC)/TDEL) * HEAD(IR) + SUM    D 1020
             IF (NODEID(I).EQ.0.OR.NODEID(I).GT.10) GO TO 260       D 1030
             REC(I) = RHS(I) - SUM - ((AF(I,1) + BF(I,1)/TDEL) * HEAD(I))  D 1040
             GO TO 270                                              D 1050
   260       HNEW = (RHS(I) - SUM)/(AF(I,1) + BF(I,1)/TDEL)         D 1060
```

PROGRAM LISTING--CONTINUED

```
            RESID = HNEW - HEAD(I)                                     D 1070
            HEAD(I) = HEAD(I) + RELAX * RESID                          D 1080
            RESID = ABS(RESID)                                         D 1090
            ERROR = AMAX1(ERROR,RESID)                                 D 1100
  270       CONTINUE                                                   D 1110
C                                                                      D 1120
C     (IBAND+1) TO (NUMNP-(IBAND-1)) ROW                               D 1130
            KR = NUMNP - IBAND + 1                                     D 1140
            IBP1 = IBAND + 1                                           D 1150
            DO 310 I = IBP1,KR                                         D 1160
            SUM = 0.                                                   D 1170
            IR = I                                                     D 1180
            DO 280 J = 2,IBAND                                         D 1190
            IR = IR + 1                                                D 1200
  280       SUM = (AF(I,J) + BF(I,J)/TDEL) * HEAD(IR) + SUM            D 1210
            JC = 1                                                     D 1220
            IR = I                                                     D 1230
            DO 290 K = 2,IBAND                                         D 1240
            JC = JC + 1                                                D 1250
            IR = IR - 1                                                D 1260
  290       SUM = (AF(IR,JC) + BF(IR,JC)/TDEL) * HEAD(IR) + SUM        D 1270
            IF (NODEID(I).EQ.0.OR.NODEID(I).GT.10) GO TO 300           D 1280
            REC(I) = RHS(I) - SUM - ((AF(I,1) + BF(I,1)/TDEL) * HEAD(I)) D 1290
            GO TO 310                                                  D 1300
  300       HNEW = (RHS(I) - SUM)/(AF(I,1) + BF(I,1)/TDEL)             D 1310
            RESID = HNEW - HEAD(I)                                     D 1320
            HEAD(I) = HEAD(I) + RELAX * RESID                          D 1330
            RESID = ABS(RESID)                                         D 1340
            ERROR = AMAX1(ERROR,RESID)                                 D 1350
  310       CONTINUE                                                   D 1360
C                                                                      D 1370
C     (NUMNP-IBAND+2) TO (NUMNP-1) ROW                                 D 1380
            NUMNP1 = NUMNP - 1                                         D 1390
            KR = NUMNP - IBAND + 2                                     D 1400
            KC = IBAND - 1                                             D 1410
            DO 350 I = KR,NUMNP1                                       D 1420
            SUM = 0.                                                   D 1430
            IR = I                                                     D 1440
            DO 320 J = 2,KC                                            D 1450
            IR = IR + 1                                                D 1460
  320       SUM = (AF(I,J) + BF(I,J)/TDEL) * HEAD(IR) + SUM            D 1470
            JC = 1                                                     D 1480
            IR = I                                                     D 1490
            DO 330 K = 2,IBAND                                         D 1500
            JC = JC + 1                                                D 1510
            IR = IR - 1                                                D 1520
  330       SUM = (AF(IR,JC) + BF(IR,JC)/TDEL) * HEAD(IR) + SUM        D 1530
            IF (NODEID(I).EQ.0.OR.NODEID(I).GT.10) GO TO 340           D 1540
            REC(I) = RHS(I) - SUM - ((AF(I,1) + BF(I,1)/TDEL) * HEAD(I)) D 1550
            GO TO 350                                                  D 1560
  340       HNEW = (RHS(I) - SUM)/(AF(I,1) + BF(I,1)/TDEL)             D 1570
            RESID = HNEW - HEAD(I)                                     D 1580
            HEAD(I) = HEAD(I) + RELAX * RESID                          D 1590
            RESID = ABS(RESID)                                         D 1600
            ERROR = AMAX1(ERROR,RESID)                                 D 1610
            KC = KC - 1                                                D 1620
  350       CONTINUE                                                   D 1630
C                                                                      D 1640
C     (NUMNP) ROW                                                      D 1650
            SUM = 0.                                                   D 1660
            JC = 1                                                     D 1670
            IR = NUMNP                                                 D 1680
            DO 360 K = 2,IBAND                                         D 1690
            JC = JC + 1                                                D 1700
            IR = IR - 1                                                D 1710
  360       SUM = (AF(IR,JC) + BF(IR,JC)/TDEL) * HEAD(IR) + SUM        D 1720
            IF (NODEID(NUMNP).EQ.0.OR.NODEID(NUMNP).GT.10) GO TO 370   D 1730
            REC(NUMNP) = RHS(NUMNP) - SUM - ((AF(NUMNP,1) + BF(NUMNP,1)/TDE D 1740
     1      L) * HEAD(NUMNP))                                          D 1750
```

```
         GO TO 390                                                       D 1760
   370   HNEW = (RHS(NUMNP) - SUM)/(AF(NUMNP,1) + BF(NUMNP,1)/TDEL)       D 1770
         RESID = HNEW - HEAD(NUMNP)                                       D 1780
         HEAD(NUMNP) = HEAD(NUMNP) + RELAX * RESID                        D 1790
         RESID = ABS(RESID)                                              D 1800
         ERROR = AMAX1(ERROR,RESID)                                      D 1810
   380   IF (ERROR.LE.TOL) GO TO 410                                     D 1820
   390 CONTINUE                                                           D 1830
       WRITE (6,400)                                                     D 1840
   400 FORMAT (1H1,5X,83HSTOP--MAXIMUM ALLOWABLE NUMBER OF ITERATIONS HAS D 1850
      1 BEEN REACHED IN SUBROUTINE MATFLOW)                              D 1860
       STOP                                                              D 1870
   410 WRITE (6,420) IT,SUMT                                             D 1880
   420 FORMAT (/,5X,19HMATFLOW ITERATIONS=,I3,10X,5HTIME=,F12.7)         D 1890
         GO TO 440                                                       D 1900
       WRITE (6,430) (HEAD(NP),NP = 1,NUMNP)                             D 1910
   430 FORMAT (12F10.3)                                                  D 1920
C      *********************************************************************** D 1930
   440 RETURN                                                            D 1940
       END                                                              D 1950
       SUBROUTINE ELINTT                                                 E 0010
       COMMON /BLOCKA/ NUMNP,X(35),Y(35),NUMEL,NI(50),NJ(50),            E 0020
      1NK(50),NUMBS,NBNDYI(18),NBNDYJ(18),COSX(18),COSY(18),             E 0030
      2DHDX(18),DHDY(18),TITLE(20),IBAND,ICT                             E 0040
       COMMON /BLOCKB/ NTIM,NPMP,PINT,TIMX,TINIT,TPDAY,SUMT,TDEL,INT,TIMY E 0050
      1,TDELMAX                                                          E 0060
       COMMON /BLOCKC/ S,POROS,BETA,DLTRAT,Z1,Z2,ATOMWT1,ATOMWT2,DBYHUK1, E 0070
      1DBYHUK2,SK                                                        E 0080
       COMMON /BLOCKD/ NCCDNP,NODEID(35),TRANS(35),HYDK(35),THCK(35),     E 0090
      1REC(35),C1REC(35),C2REC(35)                                       E 0100
       COMMON /BLOCKE/ IDELEM(50),RECH(50),C1RECH(50),C2RECH(50),         E 0110
      1VPRM(50),AREA(50)                                                 E 0120
       COMMON /BLOCKF/ HEAD(35),HDI(35),C1(35),C2(35),C1HAT(35),          E 0130
      1C2HAT(35),CEC(35)                                                 E 0140
       COMMON /BLOCKH/ AT(35,13),BT1(35,7),BT2(35,7),                     E 0150
      1CT1(35,7),CT2(35,7),DT1(35),DT2(35)                               E 0160
C      *********************************************************************** E 0170
C                                                                        E 0180
C      THIS SUBROUTINE PERFORMS THE INTEGRATIONS REQUIRED FOR THE TWO     E 0190
C      COUPLED TRANSPORT EQUATIONS.  THESE INTEGRATIONS ARE CARRIED OUT   E 0200
C      IN A PIECEWISE MANNER ON AN ELEMENT BASIS.  GLOBAL MATRICES ARE    E 0210
C      THEN FORMED BY SUMMING FOR A GIVEN NODE THE CONTRIBUTION TO THAT   E 0220
C      NODE FROM EACH ELEMENT.  THESE MATRICES FOR THE TRANSPORT          E 0230
C      EQUATIONS ARE BANDED.                                             E 0240
C                                                                        E 0250
C      *********************************************************************** E 0260
C                                                                        E 0270
C      PERFORM ELEMENT INTEGRATIONS ( A MATRIX - TRANSPORT)              E 0280
C                                                                        E 0290
       IBAND2 = IBAND * 2 - 1                                           E 0300
       DO 100 I = 1,NUMNP                                               E 0310
       DO 100 J = 1,IBAND2                                              E 0320
   100 AT(I,J) = 0.                                                     E 0330
       DO 140 I = 1,NUMEL                                               E 0340
C                                                                        E 0350
C      CALCULATE THE INTERSTITTIAL VELOCITIES VX,VY&VR                   E 0360
C                                                                        E 0370
       VXI =  - HYDK(NI(I)) * ((Y(NJ(I)) - Y(NK(I))) * HEAD(NI(I)) + (   E 0380
      1 Y(NK(I)) - Y(NI(I))) * HEAD(NJ(I)) + (Y(NI(I)) - Y(NJ(I))) * HE  E 0390
      2 AD(NK(I)))/(POROS * 2 * AREA(I))                                 E 0400
       VXJ =  - HYDK(NJ(I)) * ((Y(NJ(I)) - Y(NK(I))) * HEAD(NI(I)) + (   E 0410
      1 Y(NK(I)) - Y(NI(I))) * HEAD(NJ(I)) + (Y(NI(I)) - Y(NJ(I))) * HE  E 0420
      2 AD(NK(I)))/(POROS * 2 * AREA(I))                                 E 0430
       VXK =  - HYDK(NK(I)) * ((Y(NJ(I)) - Y(NK(I))) * HEAD(NI(I)) + (   E 0440
      1 Y(NK(I)) - Y(NI(I))) * HEAD(NJ(I)) + (Y(NI(I)) - Y(NJ(I))) * HE  E 0450
      2 AD(NK(I)))/(POROS * 2 * AREA(I))                                 E 0460
       VYI =  - HYDK(NI(I)) * ((X(NK(I)) - X(NJ(I))) * HEAD(NI(I)) + (   E 0470
      1 X(NI(I)) - X(NK(I))) * HEAD(NJ(I)) + (X(NJ(I)) - X(NI(I))) * HE  E 0480
      2 AD(NK(I)))/(POROS * 2 * AREA(I))                                 E 0490
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PROGRAM LISTING--CONTINUED

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         VYJ =  - HYDK(NJ(I)) * ((X(NK(I)) - X(NJ(I))) * HEAD(NI(I)) + (   E 0500
       1 X(NI(I)) - X(NK(I))) * HEAD(NJ(I)) + (X(NJ(I)) - X(NI(I))) * HE   E 0510
       2 AD(NK(I)))/(POROS * 2 * AREA(I))                                  E 0520
         VYK =   - HYDK(NK(I)) * ((X(NK(I)) - X(NJ(I))) * HEAD(NI(I)) + (  E 0530
       1 X(NI(I)) - X(NK(I))) * HEAD(NJ(I)) + (X(NJ(I)) - X(NI(I))) * HE   E 0540
       2 AD(NK(I)))/(POROS * 2 * AREA(I))                                  E 0550
         VRI = (VXI *  * 2 + VYI *  * 2) *  * .5                           E 0560
         VRJ = (VXJ *  * 2 + VYJ *  * 2) *  * .5                           E 0570
         VRK = (VXK *  * 2 + VYK *  * 2) *  * .5                           E 0580
C                                                                          E 0590
C     CALCULATE THE DISPERSIVITY COEFFICIENTS DXX,DYY&DXY                  E 0600
C                                                                          E 0610
         DXYI = 0.                                                         E 0620
         DYYI = DXYI                                                       E 0630
         DXXI = DYYI                                                       E 0640
         DXYJ = 0.                                                         E 0650
         DYYJ = DXYJ                                                       E 0660
         DXXJ = DYYJ                                                       E 0670
         DXYK = 0.                                                         E 0680
         DYYK = DXYK                                                       E 0690
         DXXK = DYYK                                                       E 0700
         IF (VRI.EQ.0.) GO TO 110                                         E 0710
         DXXI = BETA * VXI *  * 2/VRI + BETA * DLTRAT * VYI *  * 2/VRI     E 0720
         DYYI = BETA * DLTRAT * VXI *  * 2/VRI + BETA * VYI *  * 2/VRI     E 0730
         DXYI = BETA * (1 - DLTRAT) * VXI * VYI/VRI                        E 0740
C     DXXI=DXXI - VXI*VXI*TDEL/2.                                          E 0750
C     DYYI=DYYI - VYI*VYI*TDEL/2.                                          E 0760
C     DXYI=DXYI - VXI*VYI*TDEL/2.                                          E 0770
  110    IF (VRJ.EQ.0.) GO TO 120                                         E 0780
         DXXJ = BETA * VXJ *  * 2/VRJ + BETA * DLTRAT * VYJ *  * 2/VRJ     E 0790
         DYYJ = BETA * DLTRAT * VXJ *  * 2/VRJ + BETA * VYJ *  * 2/VRJ     E 0800
         DXYJ = BETA * (1 - DLTRAT) * VXJ * VYJ/VRJ                        E 0810
C     DXXJ=DXXJ - VXJ*VXJ*TDEL/2.                                          E 0820
C     DYYJ=DYYJ - VYJ*VYJ*TDEL/2.                                          E 0830
C     DXYJ=DXYJ - VXJ*VYJ*TDEL/2.                                          E 0840
  120    IF (VRK.EQ.0.) GO TO 130                                         E 0850
         DXXK = BETA * VXK *  * 2/VRK + BETA * DLTRAT * VYK *  * 2/VRK     E 0860
         DYYK = BETA * DLTRAT * VXK *  * 2/VRK + BETA * VYK *  * 2/VRK     E 0870
         DXYK = BETA * (1 - DLTRAT) * VXK * VYK/VRK                        E 0880
C     DXXK=DXXK - VXK*VXK*TDEL/2.                                          E 0890
C     DYYK=DYYK - VYK*VYK*TDEL/2.                                          E 0900
C     DXYK=DXYK - VXK*VYK*TDEL/2.                                          E 0910
  130    DXX = (DXXI + DXXJ + DXXK)/3.                                     E 0920
         DYY = (DYYI + DYYJ + DYYK)/3.                                     E 0930
         DXY = (DXYI + DXYJ + DXYK)/3.                                     E 0940
C                                                                          E 0950
         E1 = (DXX * ((Y(NJ(I)) - Y(NK(I))) * (Y(NJ(I)) - Y(NK(I)))) + D   E 0960
       1 YY * ((X(NK(I)) - X(NJ(I))) * (X(NK(I)) - X(NJ(I)))) + DXY * ((   E 0970
       2 Y(NJ(I)) - Y(NK(I))) * (X(NK(I)) - X(NJ(I))) + (X(NK(I)) - X(NJ   E 0980
       3 (I))) * (Y(NJ(I)) - Y(NK(I)))))/(4 * AREA(I))                     E 0990
         E2 = (DXX * ((Y(NK(I)) - Y(NI(I))) * (Y(NJ(I)) - Y(NK(I)))) + D   E 1000
       1 YY * ((X(NI(I)) - X(NK(I))) * (X(NK(I)) - X(NJ(I)))) + DXY * ((   E 1010
       2 Y(NK(I)) - Y(NI(I))) * (X(NK(I)) - X(NJ(I))) + (X(NI(I)) - X(NK   E 1020
       3 (I))) * (Y(NJ(I)) - Y(NK(I)))))/(4 * AREA(I))                     E 1030
         E3 = (DXX * ((Y(NI(I)) - Y(NJ(I))) * (Y(NJ(I)) - Y(NK(I)))) + D   E 1040
       1 YY * ((X(NJ(I)) - X(NI(I))) * (X(NK(I)) - X(NJ(I)))) + DXY * ((   E 1050
       2 Y(NI(I)) - Y(NJ(I))) * (X(NK(I)) - X(NJ(I))) + (X(NJ(I)) - X(NI   E 1060
       3 (I))) * (Y(NJ(I)) - Y(NK(I)))))/(4 * AREA(I))                     E 1070
         E4 = E2                                                           E 1080
         E5 = (DXX * ((Y(NK(I)) - Y(NI(I))) * (Y(NK(I)) - Y(NI(I)))) + D   E 1090
       1 YY * ((X(NI(I)) - X(NK(I))) * (X(NI(I)) - X(NK(I)))) + DXY * ((   E 1100
       2 Y(NK(I)) - Y(NI(I))) * (X(NI(I)) - X(NK(I))) + (X(NI(I)) - X(NK   E 1110
       3 (I))) * (Y(NK(I)) - Y(NI(I)))))/(4 * AREA(I))                     E 1120
         E6 = (DXX * ((Y(NI(I)) - Y(NJ(I))) * (Y(NK(I)) - Y(NI(I)))) + D   E 1130
       1 YY * ((X(NJ(I)) - X(NI(I))) * (X(NI(I)) - X(NK(I)))) + DXY * ((   E 1140
       2 Y(NI(I)) - Y(NJ(I))) * (X(NI(I)) - X(NK(I))) + (X(NJ(I)) - X(NI   E 1150
       3 (I))) * (Y(NK(I)) - Y(NI(I)))))/(4 * AREA(I))                     E 1160
         E7 = E3                                                           E 1170
         E8 = E6                                                           E 1180
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```
       E9 = (DXX * ((Y(NI(I)) - Y(NJ(I))) * (Y(NI(I)) - Y(NJ(I)))) + D    E 1190
   1   YY * ((X(NJ(I)) - X(NI(I))) * (X(NJ(I)) - X(NI(I)))) + DXY * ((      E 1200
   2   Y(NI(I)) - Y(NJ(I))) * (X(NJ(I)) - X(NI(I))) + (X(NJ(I)) - X(NI      E 1210
   3   (I))) * (Y(NI(I)) - Y(NJ(I)))))/(4 * AREA(I))                       E 1220
C                                                                          E 1230
       VXC1 = 2 * VXI + VXJ + VXK                                          E 1240
       VXC2 = VXI + 2 * VXJ + VXK                                          E 1250
       VXC3 = VXI + VXJ + 2 * VXK                                          E 1260
       VYC1 = 2 * VYI + VYJ + VYK                                          E 1270
       VYC2 = VYI + 2 * VYJ + VYK                                          E 1280
       VYC3 = VYI + VYJ + 2 * VYK                                          E 1290
       E1 = E1 + ( - VXC1 * (Y(NJ(I)) - Y(NK(I))) - VYC1 * (X(NK(I)) -     E 1300
   1   X(NJ(I))))/24.                                                      E 1310
       E2 = E2 + ( - VXC2 * (Y(NJ(I)) - Y(NK(I))) - VYC2 * (X(NK(I)) -     E 1320
   1   X(NJ(I))))/24.                                                      E 1330
       E3 = E3 + ( - VXC3 * (Y(NJ(I)) - Y(NK(I))) - VYC3 * (X(NK(I)) -     E 1340
   1   X(NJ(I))))/24.                                                      E 1350
       E4 = E4 + ( - VXC1 * (Y(NK(I)) - Y(NI(I))) - VYC1 * (X(NI(I)) -     E 1360
   1   X(NK(I))))/24.                                                      E 1370
       E5 = E5 + ( - VXC2 * (Y(NK(I)) - Y(NI(I))) - VYC2 * (X(NI(I)) -     E 1380
   1   X(NK(I))))/24.                                                      E 1390
       E6 = E6 + ( - VXC3 * (Y(NK(I)) - Y(NI(I))) - VYC3 * (X(NI(I)) -     E 1400
   1   X(NK(I))))/24.                                                      E 1410
       E7 = E7 + ( - VXC1 * (Y(NI(I)) - Y(NJ(I))) - VYC1 * (X(NJ(I)) -     E 1420
   1   X(NI(I))))/24.                                                      E 1430
       E8 = E8 + ( - VXC2 * (Y(NI(I)) - Y(NJ(I))) - VYC2 * (X(NJ(I)) -     E 1440
   1   X(NI(I))))/24.                                                      E 1450
       E9 = E9 + ( - VXC3 * (Y(NI(I)) - Y(NJ(I))) - VYC3 * (X(NJ(I)) -     E 1460
   1   X(NI(I))))/24.                                                      E 1470
C                                                                          E 1480
C   LOCATE IN BANDED GLOBAL MATRIX (ASYMMETRIC)                            E 1490
C                                                                          E 1500
       IJ = NJ(I) - NI(I) + IBAND                                          E 1510
       JI = NI(I) - NJ(I) + IBAND                                          E 1520
       IK = NK(I) - NI(I) + IBAND                                          E 1530
       KI = NI(I) - NK(I) + IBAND                                          E 1540
       JK = NK(I) - NJ(I) + IBAND                                          E 1550
       KJ = NJ(I) - NK(I) + IBAND                                          E 1560
       AT(NI(I),IBAND) = AT(NI(I),IBAND) + E1                              E 1570
       AT(NI(I),IJ) = AT(NI(I),IJ) + E2                                    E 1580
       AT(NI(I),IK) = AT(NI(I),IK) + E3                                    E 1590
       AT(NJ(I),JI) = AT(NJ(I),JI) + E4                                    E 1600
       AT(NJ(I),IBAND) = AT(NJ(I),IBAND) + E5                              E 1610
       AT(NJ(I),JK) = AT(NJ(I),JK) + E6                                    E 1620
       AT(NK(I),KI) = AT(NK(I),KI) + E7                                    E 1630
       AT(NK(I),KJ) = AT(NK(I),KJ) + E8                                    E 1640
       AT(NK(I),IBAND) = AT(NK(I),IBAND) + E9                              E 1650
 140 CONTINUE                                                              E 1660
C    *******************************************************************   E 1670
C                                                                          E 1680
C                                                                          E 1680
C   PERFORM ELEMENT INTEGRATIONS ( B&C MATRICES - TRANSPORT)               E 1690
C                                                                          E 1700
     DO 150 I = 1,NUMNP                                                    E 1710
     DO 150 J = 1,IBAND                                                    E 1720
       CT1(I,J) = 0.                                                       E 1730
       CT2(I,J) = 0.                                                       E 1740
       BT1(I,J) = 0.                                                       E 1750
 150 BT2(I,J) = 0.                                                         E 1760
     DO 230 I = 1,NUMEL                                                    E 1770
       F23K = 0.                                                          E 1780
       F23J = F23K                                                        E 1790
       F23I = F23J                                                        E 1800
       F13K = F23I                                                        E 1810
       F13J = F13K                                                        E 1820
       F13I = F13J                                                        E 1830
C   FOR CONSERVATIVE TRANSPORT SKIP G PARAMETER CALCULATIONS               E 1840
       IF (ICT.GT.0) GO TO 160                                            E 1850
       SOLSI = (C1(NI(I)) * (1 + Z1) + C2(NI(I)) * (1 + Z2))/2000.         E 1860
       SOLSJ = (C1(NJ(I)) * (1 + Z1) + C2(NJ(I)) * (1 + Z2))/2000.         E 1870
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PROGRAM LISTING--CONTINUED

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         SOLSK = (C1(NK(I)) * (1 + Z1) + C2(NK(I)) * (1 + Z2))/2000.    E 1880
         AC1I = 10 *  * (( - .5085 * Z1 *  * 2. * SOLSI *  * .5)/(1 + .3  E 1890
       1 281 * DBYHUK1 * SOLSI *  * .5))                                 E 1900
         AC1J = 10 *  * (( - .5085 * Z1 *  * 2. * SOLSJ *  * .5)/(1 + .3  E 1910
       1 281 * DBYHUK1 * SOLSJ *  * .5))                                 E 1920
         AC1K = 10 *  * (( - .5085 * Z1 *  * 2. * SOLSK *  * .5)/(1 + .3  E 1930
       1 281 * DBYHUK1 * SOLSK *  * .5))                                 E 1940
         AC2I = 10 *  * (( - .5085 * Z2 *  * 2. * SOLSI *  * .5)/(1 + .3  E 1950
       1 281 * DBYHUK2 * SOLSI *  * .5))                                 E 1960
         AC2J = 10 *  * (( - .5085 * Z2 *  * 2. * SOLSJ *  * .5)/(1 + .3  E 1970
       1 281 * DBYHUK2 * SOLSJ *  * .5))                                 E 1980
         AC2K = 10 *  * (( - .5085 * Z2 *  * 2. * SOLSK *  * .5)/(1 + .3  E 1990
       1 281 * DBYHUK2 * SOLSK *  * .5))                                 E 2000
C    AC1I=AC1J=AC1K=AC2I=AC2J=AC2K=1                                     E 2010
         G1I =  - (1 - C1HAT(NI(I))/CEC(NI(I))) *  * Z1 * AC1I *  * Z2 *  E 2020
       1 Z2 * C1(NI(I)) *  * (Z2 - 1)                                    E 2030
         G1J =  - (1 - C1HAT(NJ(I))/CEC(NJ(I))) *  * Z1 * AC1J *  * Z2 *  E 2040
       1 Z2 * C1(NJ(I)) *  * (Z2 - 1)                                    E 2050
         G1K =  - (1 - C1HAT(NK(I))/CEC(NK(I))) *  * Z1 * AC1K *  * Z2 *  E 2060
       1 Z2 * C1(NK(I)) *  * (Z2 - 1)                                    E 2070
         G2I =  - SK * (C1HAT(NI(I))/CEC(NI(I))) *  * Z2 * AC2I *  * Z1   E 2080
       1 * Z1 * C2(NI(I)) *  * (Z1 - 1)                                  E 2090
         G2J =  - SK * (C1HAT(NJ(I))/CEC(NJ(I))) *  * Z2 * AC2J *  * Z1   E 2100
       1 * Z1 * C2(NJ(I)) *  * (Z1 - 1)                                  E 2110
         G2K =  - SK * (C1HAT(NK(I))/CEC(NK(I))) *  * Z2 * AC2K *  * Z1   E 2120
       1 * Z1 * C2(NK(I)) *  * (Z1 - 1)                                  E 2130
         G3I =  - SK * AC2I *  * Z1 * C2(NI(I)) *  * Z1 * C1HAT(NI(I)) *  E 2140
       1  * (Z2 - 1) * Z2 * (1/CEC(NI(I))) *  * Z2 - AC1I *  * Z2 * C1(   E 2150
       2 NI(I)) *  * Z2 * Z1/CEC(NI(I)) * (1 - C1HAT(NI(I))/CEC(NI(I)))   E 2160
       3  *  * (Z1 - 1)                                                  E 2170
         G3J =  - SK * AC2J *  * Z1 * C2(NJ(I)) *  * Z1 * C1HAT(NJ(I)) *  E 2180
       1  * (Z2 - 1) * Z2 * (1/CEC(NJ(I))) *  * Z2 - AC1J *  * Z2 * C1(   E 2190
       2 NJ(I)) *  * Z2 * Z1/CEC(NJ(I)) * (1 - C1HAT(NJ(I))/CEC(NJ(I)))   E 2200
       3  *  * (Z1 - 1)                                                  E 2210
         G3K =  - SK * AC2K *  * Z1 * C2(NK(I)) *  * Z1 * C1HAT(NK(I)) *  E 2220
       1  * (Z2 - 1) * Z2 * (1/CEC(NK(I))) *  * Z2 - AC1K *  * Z2 * C1(   E 2230
       2 NK(I)) *  * Z2 * Z1/CEC(NK(I)) * (1 - C1HAT(NK(I))/CEC(NK(I)))   E 2240
       3  *  * (Z1 - 1)                                                  E 2250
         F13I = G1I/G3I                                                  E 2260
         F13J = G1J/G3J                                                  E 2270
         F13K = G1K/G3K                                                  E 2280
         F23I = G2I/G3I                                                  E 2290
         F23J = G2J/G3J                                                  E 2300
         F23K = G2K/G3K                                                  E 2310
   160   E1 = AREA(I)/30.                                                E 2320
         E2 = AREA(I)/60.                                                E 2330
         E3 = AREA(I)/60.                                                E 2340
         E4 = AREA(I)/30.                                                E 2350
         E5 = AREA(I)/60.                                                E 2360
         E6 = AREA(I)/30.                                                E 2370
C                                                                        E 2380
C     LOCATE IN BANDED GLOBAL MATRIX (SYMMETRIC)                         E 2390
C                                                                        E 2400
         IJ = IABS(NI(I) - NJ(I)) + 1                                    E 2410
         IK = IABS(NI(I) - NK(I)) + 1                                    E 2420
         JK = IABS(NJ(I) - NK(I)) + 1                                    E 2430
         BT1(NI(I),1) = BT1(NI(I),1) + E1 * (5 + 3 * F13I + F13J + F13K) E 2440
         BT2(NI(I),1) = BT2(NI(I),1) + E1 * (5 + 3 * F23I + F23J + F23K) E 2450
         CT1(NI(I),1) = CT1(NI(I),1) + E1 * ( - 3 * F23I - F23J - F23K)  E 2460
         CT2(NI(I),1) = CT2(NI(I),1) + E1 * ( - 3 * F13I - F13J - F13K)  E 2470
         IF (NI(I).LT.NJ(I)) GO TO 170                                   E 2480
         BT1(NJ(I),IJ) = BT1(NJ(I),IJ) + E2 * (5 + 2 * F13I + 2 * F13J + E 2490
       1 F13K)                                                          E 2500
         BT2(NJ(I),IJ) = BT2(NJ(I),IJ) + E2 * (5 + 2 * F23I + 2 * F23J + E 2510
       1 F23K)                                                          E 2520
         CT1(NJ(I),IJ) = CT1(NJ(I),IJ) + E2 * ( - 2 * F23I - 2 * F23J -  E 2530
       1 F23K)                                                          E 2540
         CT2(NJ(I),IJ) = CT2(NJ(I),IJ) + E2 * ( - 2 * F13I - 2 * F13J -  E 2550
       1 F13K)                                                          E 2560
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PROGRAM LISTING--CONTINUED

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            GO TO 180                                                      E 2570
   170      BT1(NI(I),IJ) = BT1(NI(I),IJ) + E2 * (5 + 2 * F13I + 2 * F13J +  E 2580
      1     F13K)                                                         E 2590
            BT2(NI(I),IJ) = BT2(NI(I),IJ) + E2 * (5 + 2 * F23I + 2 * F23J +  E 2600
      1     F23K)                                                         E 2610
            CT1(NI(I),IJ) = CT1(NI(I),IJ) + E2 * ( - 2 * F23I - 2 * F23J -   E 2620
      1     F23K)                                                         E 2630
            CT2(NI(I),IJ) = CT2(NI(I),IJ) + E2 * ( - 2 * F13I - 2 * F13J -   E 2640
      1     F13K)                                                         E 2650
   180      IF (NI(I).LT.NK(I)) GO TO 190                                 E 2660
            BT1(NK(I),IK) = BT1(NK(I),IK) + E3 * (5 + 2 * F13I + F13J + 2 *  E 2670
      1     F13K)                                                         E 2680
            BT2(NK(I),IK) = BT2(NK(I),IK) + E3 * (5 + 2 * F23I + F23J + 2 *  E 2690
      1     F23K)                                                         E 2700
            CT1(NK(I),IK) = CT1(NK(I),IK) + E3 * ( - 2 * F23I - F23J - 2 *   E 2710
      1     F23K)                                                         E 2720
            CT2(NK(I),IK) = CT2(NK(I),IK) + E3 * ( - 2 * F13I - F13J - 2 *   E 2730
      1     F13K)                                                         E 2740
            GO TO 200                                                      E 2750
   190      BT1(NI(I),IK) = BT1(NI(I),IK) + E3 * (5 + 2 * F13I + F13J + 2 *  E 2760
      1     F13K)                                                         E 2770
            BT2(NI(I),IK) = BT2(NI(I),IK) + E3 * (5 + 2 * F23I + F23J + 2 *  E 2780
      1     F23K)                                                         E 2790
            CT1(NI(I),IK) = CT1(NI(I),IK) + E3 * ( - 2 * F23I - F23J - 2 *   E 2800
      1     F23K)                                                         E 2810
            CT2(NI(I),IK) = CT2(NI(I),IK) + E3 * ( - 2 * F13I - F13J - 2 *   E 2820
      1     F13K)                                                         E 2830
   200      BT1(NJ(I),1) = BT1(NJ(I),1) + E4 * (5 + F13I + 3 * F13J + F13K)  E 2840
            BT2(NJ(I),1) = BT2(NJ(I),1) + E4 * (5 + F23I + 3 * F23J + F23K)  E 2850
            CT1(NJ(I),1) = CT1(NJ(I),1) + E4 * ( - F23I - 3 * F23J - F23K)   E 2860
            CT2(NJ(I),1) = CT2(NJ(I),1) + E4 * ( - F13I - 3 * F13J - F13K)   E 2870
            IF (NJ(I).LT.NK(I)) GO TO 210                                 E 2880
            BT1(NK(I),JK) = BT1(NK(I),JK) + E5 * (5 + F13I + 2 * F13J + 2 *  E 2890
      1     F13K)                                                         E 2900
            BT2(NK(I),JK) = BT2(NK(I),JK) + E5 * (5 + F23I + 2 * F23J + 2 *  E 2910
      1     F23K)                                                         E 2920
            CT1(NK(I),JK) = CT1(NK(I),JK) + E5 * ( - F23I - 2 * F23J - 2 *   E 2930
      1     F23K)                                                         E 2940
            CT2(NK(I),JK) = CT2(NK(I),JK) + E5 * ( - F13I - 2 * F13J - 2 *   E 2950
      1     F13K)                                                         E 2960
            GO TO 220                                                      E 2970
   210      BT1(NJ(I),JK) = BT1(NJ(I),JK) + E5 * (5 + F13I + 2 * F13J + 2 *  E 2980
      1     F13K)                                                         E 2990
            BT2(NJ(I),JK) = BT2(NJ(I),JK) + E5 * (5 + F23I + 2 * F23J + 2 *  E 3000
      1     F23K)                                                         E 3010
            CT1(NJ(I),JK) = CT1(NJ(I),JK) + E5 * ( - F23I - 2 * F23J - 2 *   E 3020
      1     F23K)                                                         E 3030
            CT2(NJ(I),JK) = CT2(NJ(I),JK) + E5 * ( - F13I - 2 * F13J - 2 *   E 3040
      1     F13K)                                                         E 3050
   220      BT1(NK(I),1) = BT1(NK(I),1) + E6 * (5 + F13I + F13J + 3 * F13K)  E 3060
            BT2(NK(I),1) = BT2(NK(I),1) + E6 * (5 + F23I + F23J + 3 * F23K)  E 3070
            CT1(NK(I),1) = CT1(NK(I),1) + E6 * ( - F23I - F23J - 3 * F23K)   E 3080
            CT2(NK(I),1) = CT2(NK(I),1) + E6 * ( - F13I - F13J - 3 * F13K)   E 3090
   230 CONTINUE                                                           E 3100
C     ******************************************************************  E 3110
C                                                                         E 3120
C     PERFORM ELEMENT INTEGRATION ( MATRICES D,E&F - TRANSPORT)           E 3130
C     CALCULATE CRECH AND CREC FOR DISCHARGE                             E 3140
C     LOCATE IN GLOBAL MATRIX                                             E 3150
C                                                                         E 3160
      DO 240 NP = 1,NUMNP                                                 E 3170
         DT1(NP) = 0.                                                     E 3180
         DT2(NP) = 0.                                                     E 3190
   240 CONTINUE                                                           E 3200
C                                                                         E 3210
      DO 290 NE = 1,NUMEL                                                 E 3220
         IF (RECH(NE).EQ.0.0) GO TO 290                                  E 3230
         IF (RECH(NE).LT.0.0) GO TO 250                                  E 3240
         CRECH1 = (C1(NI(NE)) + C1(NJ(NE)) + C1(NK(NE)))/3.              E 3250
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PROGRAM LISTING--CONTINUED

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            CRECH2 = (C2(NI(NE)) + C2(NJ(NE)) + C2(NK(NE)))/3.        E 3260
            GO TO 260                                                 E 3270
    250     CRECH1 = C1RECH(NE)                                       E 3280
            CRECH2 = C2RECH(NE)                                       E 3290
    260     IF (NODEID(NI(NE)).GE.1.AND.NODEID(NI(NE)).LE.10) GO TO 270  E 3300
            THCKI = (1/THCK(NI(NE)) + 1/(THCK(NJ(NE)) * 2) + 1/(THCK(NK(NE)  E 3310
        1    ) * 2))                                                  E 3320
            DT1(NI(NE)) = DT1(NI(NE)) + (CRECH1 * RECH(NE) * AREA(NE))/(6 *  E 3330
        1     POROS * THCKI)                                          E 3340
            DT2(NI(NE)) = DT2(NI(NE)) + (CRECH2 * RECH(NE) * AREA(NE))/(6 *  E 3350
        1     POROS * THCKI)                                          E 3360
    270     IF (NODEID(NJ(NE)).GE.1.AND.NODEID(NJ(NE)).LE.10) GO TO 280  E 3370
            THCKJ = (1/(THCK(NI(NE)) * 2) + 1/THCK(NJ(NE)) + 1/(THCK(NK(NE)  E 3380
        1    ) * 2))                                                  E 3390
            DT1(NJ(NE)) = DT1(NJ(NE)) + (CRECH1 * RECH(NE) * AREA(NE))/(6 *  E 3400
        1     POROS * THCKJ)                                          E 3410
            DT2(NJ(NE)) = DT2(NJ(NE)) + (CRECH2 * RECH(NE) * AREA(NE))/(6 *  E 3420
        1     POROS * THCKJ)                                          E 3430
    280     IF (NODEID(NK(NE)).GE.1.AND.NODEID(NK(NE)).LE.10) GO TO 290  E 3440
            THCKK = (1/(THCK(NI(NE)) * 2) + 1/(THCK(NJ(NE)) * 2) + 1/THCK(N  E 3450
        1    K(NE)))                                                  E 3460
            DT1(NK(NE)) = DT1(NK(NE)) + (CRECH1 * RECH(NE) * AREA(NE))/(6 *  E 3470
        1     POROS * THCKK)                                          E 3480
            DT2(NK(NE)) = DT2(NK(NE)) + (CRECH2 * RECH(NE) * AREA(NE))/(6 *  E 3490
        1     POROS * THCKK)                                          E 3500
    290 CONTINUE                                                      E 3510
        DO 340 NE = 1,NUMEL                                           E 3520
            IF (VPRM(NE).EQ.0.0) GO TO 340                            E 3530
            HEADBAR = (HEAD(NI(NE)) + HEAD(NJ(NE)) + HEAD(NK(NE)))/3.  E 3540
            HDIBAR = (HDI(NI(NE)) + HDI(NJ(NE)) + HDI(NK(NE)))/3.     E 3550
            VLEK = VPRM(NE) * (HEADBAR - HDIBAR) * AREA(NE)           E 3560
            IF (VLEK.LE.0.0) GO TO 300                                E 3570
            CLEK1 = (C1(NI(NE)) + C1(NJ(NE)) + C1(NK(NE)))/3.         E 3580
            CLEK2 = (C2(NI(NE)) + C2(NJ(NE)) + C2(NK(NE)))/3.         E 3590
            GO TO 310                                                 E 3600
    300     CLEK1 = C1RECH(NE)                                        E 3610
            CLEK2 = C2RECH(NE)                                        E 3620
    310     IF (NODEID(NI(NE)).GE.1.AND.NODEID(NI(NE)).LE.10) GO TO 320  E 3630
            THCKI = (1/THCK(NI(NE)) + 1/(THCK(NJ(NE)) * 2) + 1/(THCK(NK(NE)  E 3640
        1    ) * 2))                                                  E 3650
            DT1(NI(NE)) = DT1(NI(NE)) + (CLEK1 * VLEK)/(6 * POROS * THCKI)  E 3660
            DT2(NI(NE)) = DT2(NI(NE)) + (CLEK2 * VLEK)/(6 * POROS * THCKI)  E 3670
    320     IF (NODEID(NJ(NE)).GE.1.AND.NODEID(NJ(NE)).LE.10) GO TO 330  E 3680
            THCKJ = (1/(THCK(NI(NE)) * 2) + 1/THCK(NJ(NE)) + 1/(THCK(NK(NE)  E 3690
        1    ) * 2))                                                  E 3700
            DT1(NJ(NE)) = DT1(NJ(NE)) + (CLEK1 * VLEK)/(6 * POROS * THCKJ)  E 3710
            DT2(NJ(NE)) = DT2(NJ(NE)) + (CLEK2 * VLEK)/(6 * POROS * THCKJ)  E 3720
    330     IF (NODEID(NK(NE)).GE.1.AND.NODEID(NK(NE)).LE.10) GO TO 340  E 3730
            THCKK = (1/(THCK(NI(NE)) * 2) + 1/(THCK(NJ(NE)) * 2) + 1/THCK(N  E 3740
        1    K(NE)))                                                  E 3750
            DT1(NK(NE)) = DT1(NK(NE)) + (CLEK1 * VLEK)/(6 * POROS * THCKK)  E 3760
            DT2(NK(NE)) = DT2(NK(NE)) + (CLEK2 * VLEK)/(6 * POROS * THCKK)  E 3770
    340 CONTINUE                                                      E 3780
        DO 370 NP = 1,NUMNP                                           E 3790
            IF (REC(NP).LE.0.0) GO TO 350                             E 3800
            CREC1 = C1(NP)                                            E 3810
            CREC2 = C2(NP)                                            E 3820
            GO TO 360                                                 E 3830
    350     CREC1 = C1REC(NP)                                         E 3840
            CREC2 = C2REC(NP)                                         E 3850
    360     DT1(NP) = DT1(NP) + (CREC1 * REC(NP))/(POROS * THCK(NP))  E 3860
            DT2(NP) = DT2(NP) + (CREC2 * REC(NP))/(POROS * THCK(NP))  E 3870
    370 CONTINUE                                                      E 3880
C   ***************************************************************   E 3890
        RETURN                                                        E 3900
        END                                                           E 3910
        SUBROUTINE MATCHEM                                            F 0010
        COMMON /BLOCKA/ NUMNP,X(35),Y(35),NUMEL,NI(50),NJ(50),        F 0020
       1NK(50),NUMBS,NBNDYI(18),NBNDYJ(18),COSX(18),COSY(18),         F 0030
```

```
      2DHDX(18),DHDY(18),TITLE(20),IBAND,ICT                            F 0040
       COMMON /BLOCKB/ NTIM,NPMP,PINT,TIMX,TINIT,TPDAY,SUMT,TDEL,INT,TIMY  F 0050
      1,TDELMAX                                                         F 0060
       COMMON /BLOCKC/ S,POROS,BETA,DLTRAT,Z1,Z2,ATOMWT1,ATOMWT2,DBYHUK1, F 0070
      1DBYHUK2,SK                                                       F 0080
       COMMON /BLOCKD/ NCCDNP,NODEID(35),TRANS(35),HYDK(35),THCK(35),   F 0090
      1PEC(35),C1REC(35),C2REC(35)                                      F 0100
       COMMON /BLOCKF/ HEAD(35),HOI(35),C1(35),C2(35),C1HAT(35),        F 0110
      1C2HAT(35),CEC(35)                                                F 0120
       COMMON /BLOCKH/ AT(35,13),BT1(35,7),BT2(35,7),                   F 0130
      1CT1(35,7),CT2(35,7),DT1(35),DT2(35)                              F 0140
       COMMON /BLOCKI/ CM(35,13),RHS(35),RHSU(35),RHSL(35)              F 0150
C      *************************************************************** F 0160
C                                                                      F 0170
C      THIS SUBROUTINE ASSEMBLES AND SOLVES THE TWO COUPLED TRANSPORT  F 0180
C      EQUATIONS.  SOLUTION IS BY A BLOCK ITERATIVE GAUSSIAN ELIMINATION F 0190
C      PROCEDURE.                                                      F 0200
C                                                                      F 0210
C      *************************************************************** F 0220
C                                                                      F 0230
C      RHS VECTOR                                                      F 0240
C                                                                      F 0250
       CALL MULT (NUMNP,IBAND,BT1,C1,RHS)                              F 0260
       CALL MULT (NUMNP,IBAND,CT1,C2,RHSU)                             F 0270
       DO 100 I = 1,NUMNP                                              F 0280
  100 RHSU(I) = (RHS(I) + RHSU(I))/TDEL - DT1(I)                       F 0290
       CALL MULT (NUMNP,IBAND,CT2,C1,RHS)                              F 0300
       CALL MULT (NUMNP,IBAND,BT2,C2,RHSL)                             F 0310
       DO 110 I = 1,NUMNP                                              F 0320
  110 RHSL(I) = (RHS(I) + RHSL(I))/TDEL - DT2(I)                       F 0330
C      *************************************************************** F 0340
       TOL = .1                                                        F 0350
       TOL1 = TOL * Z1/ATOMWT1                                         F 0360
       TOL2 = TOL * Z2/ATOMWT2                                         F 0370
       ITMAX = 100                                                     F 0380
C      *************************************************************** F 0390
C                                                                      F 0400
C      BEGIN ITERATIONS                                                F 0410
C                                                                      F 0420
       DO 380 IT = 1,ITMAX                                             F 0430
           ERROR1 = 0.0                                                F 0440
           ERROR2 = 0.0                                                F 0450
C                                                                      F 0460
C      MODIFY RHS VECTOR                                               F 0470
           CALL MULT (NUMNP,IBAND,CT1,C2,RHS)                          F 0480
           DO 120 I = 1,NUMNP                                          F 0490
  120      RHS(I) = RHSU(I) - RHS(I)/TDEL                              F 0500
C                                                                      F 0510
C      COEFFICIENT MATRIX                                              F 0520
           IBAND2 = IBAND * 2 - 1                                      F 0530
           DO 130 J = 1,IBAND2                                         F 0540
           DO 130 I = 1,NUMNP                                          F 0550
  130      CM(I,J) = 0.                                                F 0560
C                                                                      F 0570
C      (1) ROW                                                         F 0580
           DO 140 J = 1,IBAND                                          F 0590
             LC = IBAND - 1 + J                                        F 0600
  140        CM(1,LC) = AT(1,LC) + BT1(1,J)/TDEL                       F 0610
C                                                                      F 0620
C      (2) TO (IBAND) ROW                                             F 0630
           DO 170 I = 2,IBAND                                          F 0640
             DO 150 J = 1,IBAND                                        F 0650
               LC = IBAND - 1 + J                                      F 0660
  150          CM(I,LC) = AT(I,LC) + BT1(I,J)/TDEL                     F 0670
             IR = I                                                    F 0680
             JC = 1                                                    F 0690
             LC = IBAND                                                F 0700
             DO 160 K = 2,I                                            F 0710
               IR = IR - 1                                             F 0720
```

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              JC = JC + 1                                           F 0730
              LC = LC - 1                                           F 0740
 160          CM(I,LC) = AT(I,LC) + BT1(IR,JC)/TDEL                 F 0750
 170      CONTINUE                                                  F 0760
C                                                                   F 0770
C     (IBAND+1) TO (NUMNP-(IBAND-1)) ROW                            F 0780
          KR = NUMNP - IBAND + 1                                    F 0790
          IBP1 = IBAND + 1                                          F 0800
          DO 200 I = IBP1,KR                                        F 0810
              DO 180 J = 1,IBAND                                    F 0820
              LC = IBAND - 1 + J                                    F 0830
 180          CM(I,LC) = AT(I,LC) + BT1(I,J)/TDEL                   F 0840
              IR = I                                                F 0850
              JC = 1                                                F 0860
              LC = IBAND                                            F 0870
              DO 190 K = 2,IBAND                                    F 0880
                 IR = IR - 1                                        F 0890
                 JC = JC + 1                                        F 0900
                 LC = LC - 1                                        F 0910
 190          CM(I,LC) = AT(I,LC) + BT1(IR,JC)/TDEL                 F 0920
 200      CONTINUE                                                  F 0930
C                                                                   F 0940
C     (NUMNP-IBAND+2) TO (NUMNP) ROW                                F 0950
          KR = NUMNP - IBAND + 2                                    F 0960
          KC = IBAND                                                F 0970
          DO 230 I = KR,NUMNP                                       F 0980
              KC = KC - 1                                           F 0990
              DO 210 J = 1,KC                                       F 1000
              LC = IBAND - 1 + J                                    F 1010
 210          CM(I,LC) = AT(I,LC) + BT1(I,J)/TDEL                   F 1020
              IR = I                                                F 1030
              JC = 1                                                F 1040
              LC = IBAND                                            F 1050
              DO 220 K = 2,IBAND                                    F 1060
                 IR = IR - 1                                        F 1070
                 JC = JC + 1                                        F 1080
                 LC = LC - 1                                        F 1090
 220          CM(I,LC) = AT(I,LC) + BT1(IR,JC)/TDEL                 F 1100
 230      CONTINUE                                                  F 1110
          CALL BSOLVE (CM,RHS,NUMNP,IBAND2)                         F 1120
          IR = 0                                                    F 1130
          DO 240 I = 1,NUMNP                                        F 1140
              DIFF = ABS(RHS(I) - C1(I))                            F 1150
              ERROR1 = AMAX1(ERROR1,DIFF)                           F 1160
 240      C1(I) = RHS(I)                                            F 1170
C                                                                   F 1180
C     MODIFY RHS VECTOR                                             F 1190
          CALL MULT (NUMNP,IBAND,CT2,C1,RHS)                        F 1200
          DO 250 I = 1,NUMNP                                        F 1210
 250      RHS(I) = RHSL(I) - RHS(I)/TDEL                            F 1220
C                                                                   F 1230
C     COEFFICIENT MATRIX                                            F 1240
          DO 260 J = 1,IBAND2                                       F 1250
          DO 260 I = 1,NUMNP                                        F 1260
 260      CM(I,J) = 0.                                              F 1270
C                                                                   F 1280
C     (1) ROW                                                       F 1290
          DO 270 J = 1,IBAND                                        F 1300
              LC = IBAND - 1 + J                                    F 1310
 270      CM(1,LC) = AT(1,LC) + BT2(1,J)/TDEL                       F 1320
C                                                                   F 1330
C     (2) TO (IBAND) ROW                                            F 1340
          DO 300 I = 2,IBAND                                        F 1350
              DO 280 J = 1,IBAND                                    F 1360
              LC = IBAND - 1 + J                                    F 1370
 280          CM(I,LC) = AT(I,LC) + BT2(I,J)/TDEL                   F 1380
              IR = I                                                F 1390
              JC = 1                                                F 1400
              LC = IBAND                                            F 1410
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                DO 290 K = 2,I                                       F 1420
                    IP = IR - 1                                      F 1430
                    JC = JC + 1                                      F 1440
                    LC = LC - 1                                      F 1450
  290           CM(I,LC) = AT(I,LC) + BT2(IR,JC)/TDEL                F 1460
  300       CONTINUE                                                 F 1470
C                                                                    F 1480
C      (IBAND+1) TO (NUMNP-(IBAND-1)) ROW                            F 1490
            KR = NUMNP - IBAND + 1                                   F 1500
            IBP1 = IBAND + 1                                         F 1510
            DO 330 I = IBP1,KR                                       F 1520
                DO 310 J = 1,IBAND                                   F 1530
                    LC = IBAND - 1 + J                               F 1540
  310           CM(I,LC) = AT(I,LC) + BT2(I,J)/TDEL                  F 1550
                IR = I                                               F 1560
                JC = 1                                               F 1570
                LC = IBAND                                           F 1580
                DO 320 K = 2,IBAND                                   F 1590
                    IR = IR - 1                                      F 1600
                    JC = JC + 1                                      F 1610
                    LC = LC - 1                                      F 1620
  320           CM(I,LC) = AT(I,LC) + BT2(IR,JC)/TDEL                F 1630
  330       CONTINUE                                                 F 1640
C                                                                    F 1650
C      (NUMNP-IBAND+2) TO (NUMNP) ROW                                F 1660
            KR = NUMNP - IBAND + 2                                   F 1670
            KC = IBAND                                               F 1680
            DO 360 I = KR,NUMNP                                      F 1690
                KC = KC - 1                                          F 1700
                DO 340 J = 1,KC                                      F 1710
                    LC = IBAND - 1 + J                               F 1720
  340           CM(I,LC) = AT(I,LC) + BT2(I,J)/TDEL                  F 1730
                IR = I                                               F 1740
                JC = 1                                               F 1750
                LC = IBAND                                           F 1760
                DO 350 K = 2,IBAND                                   F 1770
                    IR = IR - 1                                      F 1780
                    JC = JC + 1                                      F 1790
                    LC = LC - 1                                      F 1800
  350           CM(I,LC) = AT(I,LC) + BT2(IR,JC)/TDEL                F 1810
  360       CONTINUE                                                 F 1820
            CALL BSOLVE (CM,RHS,NUMNP,IBAND2)                        F 1830
            IR = 0                                                   F 1840
            DO 370 I = 1,NUMNP                                       F 1850
                DIFF = ABS(RHS(I) - C2(I))                           F 1860
                ERROR2 = AMAX1(ERROR2,DIFF)                          F 1870
  370       C2(I) = RHS(I)                                           F 1880
            IF (ERROR1.LE.TOL1.AND.ERROR2.LE.TOL2) GO TO 400         F 1890
C      FOR CONSERVATIVE TRANSPORT NO ITERATIONS GOTO 500             F 1900
            IF (ICT.EQ.1) GO TO 400                                  F 1910
  380 CONTINUE                                                       F 1920
      WRITE (6,390)                                                  F 1930
  390 FORMAT (1H1,5X,83HSTOP--MAXIMUM ALLOWABLE NUMBER OF ITERATIONS HAS F 1940
     1 BEEN REACHED IN SUBROUTINE MATCHEM)                           F 1950
      STOP                                                           F 1960
  400 CONTINUE                                                       F 1970
      DO 410 I = 1,NUMNP                                             F 1980
          IF (C1(I).LE..00001) C1(I) = .00001                       F 1990
          IF (C2(I).LE..00001) C2(I) = .00001                       F 2000
  410 CONTINUE                                                       F 2010
      WRITE (6,420) IT,SUMT                                          F 2020
  420 FORMAT (5X,19HMATCHEM ITERATIONS=,I3,10X,5HTIME=,F12.7)        F 2030
      GO TO 460                                                      F 2040
C     CONVERT SOLUTION CONCENTRATIONS FROM MEQ/L TO MG/L             F 2050
      DO 430 NP = 1,NUMNP                                            F 2060
          C1(NP) = C1(NP)/Z1 * ATOMWT1                               F 2070
  430 C2(NP) = C2(NP)/Z2 * ATOMWT2                                   F 2080
      WRITE (6,440) (C1(NP),NP = 1,NUMNP)                            F 2090
      WRITE (6,440) (C2(NP),NP = 1,NUMNP)                            F 2100
```

PROGRAM LISTING--CONTINUED

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    440 FORMAT (12F10.3/)                                              F 2110
 C     CONVERT SOLUTION CONCENTRATIONS FROM MG/L TO MEQ/L              F 2120
        DO 450 NP = 1,NUMNP                                            F 2130
            C1(NP) = C1(NP) * Z1/ATOMWT1                               F 2140
    450 C2(NP) = C2(NP) * Z2/ATOMWT2                                   F 2150
 C     ******************************************************************  F 2160
    460 RETURN                                                        F 2170
        END                                                           F 2180
        SUBROUTINE CHATSOL                                            G 0010
        COMMON /BLOCKA/ NUMNP,X(35),Y(35),NUMEL,NI(50),NJ(50),        G 0020
       1NK(50),NUMBS,NBNDYI(18),NBNDYJ(18),COSX(18),COSY(18),         G 0030
       2DHDX(18),DHDY(18),TITLE(20),IBAND,ICT                         G 0040
        COMMON /BLOCKC/ S,PCROS,BETA,DLTRAT,Z1,Z2,ATOMWT1,ATOMWT2,DBYHUK1, G 0050
       1DBYHUK2,SK                                                    G 0060
        COMMON /BLOCKF/ HEAD(35),HDI(35),C1(35),C2(35),C1HAT(35),     G 0070
       1C2HAT(35),CEC(35)                                             G 0080
 C     ******************************************************************  G 0090
 C                                                                    G 0100
 C     THIS SUBROUTINE SOLVES FOR THE VALUES OF C1HAT AND C2HAT       G 0110
 C     Z2 MUST BE GREATER THAN OR EQUAL TO Z1                         G 0120
 C                                                                    G 0130
 C     ******************************************************************  G 0140
        RATIO = Z2/Z1                                                 G 0150
        Z1INV = 1/Z1                                                  G 0160
        IF (RATIO.EQ.1.) GO TO 130                                    G 0170
        IF (RATIO.EQ.2.) GO TO 110                                    G 0180
        WRITE (6,100)                                                 G 0190
    100 FORMAT (1H1,5X,24HSTOP--SUBROUTINE CHATSOL)                   G 0200
        STOP                                                          G 0210
 C     ******************************************************************  G 0220
 C                                                                    G 0230
 C     MONOVALENT-DIVALENT EXCHANGE                                   G 0240
 C                                                                    G 0250
    110 DO 120 NP = 1,NUMNP                                           G 0260
        SOLS = (C1(NP) * (1 + Z1) + C2(NP) * (1 + Z2))/2000.          G 0270
        AC1 = 10 *  * (( - .5085 * Z1 *  * 2. * SOLS *  * .5)/(1 + .328 G 0280
       1  1 * DBYHUK1 * SOLS *  * .5))                                G 0290
        AC2 = 10 *  * (( - .5085 * Z2 *  * 2. * SOLS *  * .5)/(1 + .328 G 0300
       1  1 * DBYHUK2 * SOLS *  * .5))                                G 0310
 C      AC1=AC2=1                                                     G 0320
        SKP = 1./((SK * AC2 *  * Z1 * C2(NP) *  * Z1)/(AC1 *  * Z2 * C1 G 0330
       1  (NP) *  * Z2)) *  * Z1INV                                   G 0340
        C1HAT(NP) = ( - SKP + (SKP *  * 2. + 4 * SKP) *  * .5)/2. * CEC G 0350
       1  (NP)                                                        G 0360
        C2HAT(NP) = CEC(NP) - C1HAT(NP)                               G 0370
    120 CONTINUE                                                      G 0380
        GO TO 150                                                     G 0390
 C     ******************************************************************  G 0400
 C                                                                    G 0410
 C     MONOVALENT-MONOVALENT EXCHANGE OR DIVALENT-DIVALENT EXCHANGE   G 0420
 C                                                                    G 0430
    130 DO 140 NP = 1,NUMNP                                           G 0440
        SOLS = (C1(NP) * (1 + Z1) + C2(NP) * (1 + Z2))/2000.          G 0450
        AC1 = 10 *  * (( - .5085 * Z1 *  * 2. * SOLS *  * .5)/(1 + .328 G 0460
       1  1 * DBYHUK1 * SOLS *  * .5))                                G 0470
        AC2 = 10 *  * (( - .5085 * Z2 *  * 2. * SOLS *  * .5)/(1 + .328 G 0480
       1  1 * DBYHUK2 * SOLS *  * .5))                                G 0490
        SKP = 1./((SK * AC2 *  * Z1 * C2(NP) *  * Z1)/(AC1 *  * Z2 * C1 G 0500
       1  (NP) *  * Z2)) *  * Z1INV                                   G 0510
        C1HAT(NP) = SKP * CEC(NP)/(1 + SKP)                           G 0520
        C2HAT(NP) = CEC(NP) - C1HAT(NP)                               G 0530
    140 CONTINUE                                                      G 0540
        GO TO 150                                                     G 0550
 C     ******************************************************************  G 0560
    150 RETURN                                                        G 0570
        END                                                           G 0580
        SUBROUTINE BSOLVE(C,V,N,M)                                    H 0010
        DIMENSION C(35,13),V(35)                                      H 0020
 C     ******************************************************************  H 0030
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C                                                                          H 0040
C       THIS SUBROUTINE SOLVES A BANDED MATRIX BY GAUSSIAN ELIMINATION     H 0050
C                                                                          H 0060
C       ****************************************************************** H 0070
        LR = (M - 1)/2                                                     H 0080
        DO 110 L = 1,LR                                                    H 0090
          IM = LR - L + 1                                                  H 0100
          DO 110 I = 1,IM                                                  H 0110
            DO 100 J = 2,M                                                 H 0120
  100       C(L,J - 1) = C(L,J)                                            H 0130
            KN = N - L                                                     H 0140
            KM = M - I                                                     H 0150
            C(L,M) = 0.                                                    H 0160
  110   C(KN + 1,KM + 1) = 0.                                              H 0170
        LR = LR + 1                                                        H 0180
        IM = N - 1                                                        H 0190
        DO 180 I = 1,IM                                                    H 0200
          NPIV = I                                                         H 0210
          LS = I + 1                                                       H 0220
          DO 120 L = LS,LR                                                 H 0230
            IF (ABS(C(L,1)).GT.ABS(C(NPIV,1))) NPIV = L                    H 0240
  120     CONTINUE                                                         H 0250
          IF (NPIV.LE.I) GO TO 140                                         H 0260
          DO 130 J = 1,M                                                   H 0270
            TEMP = C(I,J)                                                  H 0280
            C(I,J) = C(NPIV,J)                                             H 0290
  130     C(NPIV,J) = TEMP                                                 H 0300
          TEMP = V(I)                                                      H 0310
          V(I) = V(NPIV)                                                   H 0320
          V(NPIV) = TEMP                                                   H 0330
  140     V(I) = V(I)/C(I,1)                                               H 0340
          DO 150 J = 2,M                                                   H 0350
  150     C(I,J) = C(I,J)/C(I,1)                                           H 0360
          DO 170 L = LS,LR                                                 H 0370
            TEMP = C(L,1)                                                  H 0380
            V(L) = V(L) - TEMP * V(I)                                      H 0390
            DO 160 J = 2,M                                                 H 0400
  160       C(L,J - 1) = C(L,J) - TEMP * C(I,J)                            H 0410
  170     C(L,M) = 0.                                                      H 0420
          IF (LR.LT.N) LR = LR + 1                                         H 0430
  180   CONTINUE                                                           H 0440
        V(N) = V(N)/C(N,1)                                                 H 0450
        JM = 2                                                             H 0460
        DO 200 I = 1,IM                                                    H 0470
          L = N - I                                                        H 0480
          DO 190 J = 2,JM                                                  H 0490
            KM = L + J                                                     H 0500
  190     V(L) = V(L) - C(L,J) * V(KM - 1)                                 H 0510
          IF (JM.LT.M) JM = JM + 1                                         H 0520
  200   CONTINUE                                                           H 0530
C       ****************************************************************** H 0540
        RETURN                                                             H 0550
        END                                                               H 0560
        SUBROUTINE MULT(NUMNP,IBAND,A,X,Y)                                 I 0010
        DIMENSION A(35,7),X(35),Y(35)                                      I 0020
C       ****************************************************************** I 0030
C                                                                          I 0040
C       THIS SUBROUTINE MULTIPLIES A BANDED SYMMETRIC MATRIX TIMES A       I 0050
C       VECTOR. THE PRODUCT OF MATRIX(A) AND VECTOR(X) IS VECTOR(Y).       I 0060
C                                                                          I 0070
C       ****************************************************************** I 0080
C                                                                          I 0090
C       IBAND MUST BE .LE. (NUMNP/2)                                       I 0100
C       CHECK LIMITS ON IBAND                                              I 0110
C                                                                          I 0120
        IBT2 = IBAND * 2                                                   I 0130
        IF (IBT2.LE.NUMNP) GO TO 110                                       I 0140
        WRITE (6,100)                                                      I 0150
  100   FORMAT (1H0,4X,77H***ERROR***   IN SUBROUTINE MULT IBAND MUST BE LE I 0160
```

```
      1SS THAN OR EQUAL TO (NUMNP/2))                              I 0170
      STOP                                                         I 0180
C     ********************************************************     I 0190
C                                                                  I 0200
C     (1) ROW                                                      I 0210
  110 Y(1) = 0.                                                    I 0220
      DO 120 J = 1,IBAND                                           I 0230
  120 Y(1) = A(1,J) * X(J) + Y(1)                                  I 0240
C                                                                  I 0250
C     (2) TO (IBAND) ROW                                           I 0260
      DO 150 I = 2,IBAND                                           I 0270
         Y(I) = 0.                                                 I 0280
         IR = I - 1                                                I 0290
         DO 130 J = 1,IBAND                                        I 0300
            IR = IR + 1                                            I 0310
  130    Y(I) = A(I,J) * X(IR) + Y(I)                              I 0320
         JC = 1                                                    I 0330
         IR = I                                                    I 0340
         DO 140 K = 2,I                                            I 0350
            JC = JC + 1                                            I 0360
            IR = IR - 1                                            I 0370
  140    Y(I) = A(IR,JC) * X(IR) + Y(I)                            I 0380
  150 CONTINUE                                                     I 0390
C                                                                  I 0400
C     (IBAND+1) TO (NUMNP-(IBAND-1)) ROW                           I 0410
      KR = NUMNP - IBAND + 1                                       I 0420
      IBP1 = IBAND + 1                                             I 0430
      DO 180 I = IBP1,KR                                           I 0440
         Y(I) = 0.                                                 I 0450
         IR = I - 1                                                I 0460
         DO 160 J = 1,IBAND                                        I 0470
            IR = IR + 1                                            I 0480
  150    Y(I) = A(I,J) * X(IR) + Y(I)                              I 0490
         JC = 1                                                    I 0500
         IR = I                                                    I 0510
         DO 170 K = 2,IBAND                                        I 0520
            JC = JC + 1                                            I 0530
            IR = IR - 1                                            I 0540
  170    Y(I) = A(IR,JC) * X(IR) + Y(I)                            I 0550
  180 CONTINUE                                                     I 0560
C                                                                  I 0570
C     (NUMNP-IBAND+2) TO (NUMNP) ROW                               I 0580
      KR = NUMNP - IBAND + 2                                       I 0590
      KC = IBAND - 1                                               I 0600
      DO 210 I = KR,NUMNP                                          I 0610
         Y(I) = 0.                                                 I 0620
         IR = I - 1                                                I 0630
         DO 190 J = 1,KC                                           I 0640
            IR = IR + 1                                            I 0650
  190    Y(I) = A(I,J) * X(IR) + Y(I)                              I 0660
         JC = 1                                                    I 0670
         IR = I                                                    I 0680
         DO 200 K = 2,IBAND                                        I 0690
            JC = JC + 1                                            I 0700
            IR = IR - 1                                            I 0710
  200    Y(I) = A(IR,JC) * X(IR) + Y(I)                            I 0720
         KC = KC - 1                                               I 0730
  210 CONTINUE                                                     I 0740
C     ********************************************************     I 0750
      RETURN                                                       I 0760
      END                                                          I 0770
      SUBROUTINE WATBAL                                            J 0010
      COMMON /BLOCKA/ NUMNP,X(35),Y(35),NUMEL,NI(50),NJ(50),       J 0020
     1NK(50),NUMBS,NBNDYI(18),NBNDYJ(18),COSX(18),COSY(18),        J 0030
     2DHDX(18),DHDY(18),TITLE(20),IBAND,ICT                        J 0040
      COMMON /BLOCKB/ NTIM,NPMP,PINT,TIMX,TINIT,TPDAY,SUMT,TDEL,INT,TIMY  J 0050
     1,TDELMAX                                                     J 0060
      COMMON /BLOCKC/ S,POROS,BETA,DLTRAT,Z1,Z2,ATOMWT1,ATOMWT2,DBYHUK1, J 0070
     1DBYHUK2,SK                                                   J 0080
```

```
          COMMON /BLOCKD/ NCCDNP,NODEID(35),TRANS(35),HYDK(35),THCK(35),      J 0090
         1REC(35),C1REC(35),C2REC(35)                                        J 0100
          COMMON /BLOCKE/ IDELEM(50),RECH(50),C1RECH(50),C2RECH(50),          J 0110
         1VPRM(50),AREA(50)                                                   J 0120
          COMMON /BLOCKF/ HEAD(35),HDI(35),C1(35),C2(35),C1HAT(35),           J 0130
         1C2HAT(35),CEC(35)                                                   J 0140
          COMMON /BLOCKJ/QINRCH,QOUTRCH,QINREC,QOUTREC,QINCHN,QOUTCHN,        J 0150
         1QINLEK,QOUTLEK,QINBDY,QOUTBDY,QSTOR                                 J 0160
C      ***********************************************************************  J 0170
C                                                                             J 0180
C      THIS SUBROUTINE CALCULATES A WATER BALANCE                             J 0190
C                                                                             J 0200
C      ***********************************************************************  J 0210
C                                                                             J 0220
C      CALCULATE FLUX FROM DISTRIBUTED RECHARGE AND DISCHARGE SOURCES         J 0230
C                                                                             J 0240
          DO 110 NE = 1,NUMEL                                                 J 0250
             IF (RECH(NE).GT.0.0) GO TO 100                                   J 0260
             QINRCH = RECH(NE) * AREA(NE) * TDEL + QINRCH                     J 0270
             GO TO 110                                                        J 0280
      100    QOUTRCH = RECH(NE) * AREA(NE) * TDEL + QOUTRCH                   J 0290
      110 CONTINUE                                                            J 0300
C      ***********************************************************************  J 0310
C                                                                             J 0320
C      CALCULATE FLUX FROM POINT RECHARGE AND DISCHARGE SOURCES               J 0330
C      (EXCLUDING CONSTANT HEAD NODES)                                        J 0340
C                                                                             J 0350
          DO 130 NP = 1,NUMNP                                                 J 0360
             IF (NODEID(NP).GE.1.AND.NODEID(NP).LE.10) GO TO 130              J 0370
             IF (REC(NP).GT.0.0) GO TO 120                                    J 0380
             QINREC = REC(NP) * TDEL + QINREC                                 J 0390
             GO TO 130                                                        J 0400
      120    QOUTREC = REC(NP) * TDEL + QOUTREC                              J 0410
      130 CONTINUE                                                            J 0420
C      ***********************************************************************  J 0430
C                                                                             J 0440
C      CALCULATE FLUX FROM POINT RECHARGE AND DISCHARGE SOURCES               J 0450
C      (AT CONSTANT HEAD NODES ONLY)                                          J 0460
C                                                                             J 0470
          DO 150 NP = 1,NUMNP                                                 J 0480
             IF (NODEID(NP).EQ.0.OR.NODEID(NP).GT.10) GO TO 150               J 0490
             IF (REC(NP).GT.0.0) GO TO 140                                    J 0500
             QINCHN = REC(NP) * TDEL + QINCHN                                 J 0510
             GO TO 150                                                        J 0520
      140    QOUTCHN = REC(NP) * TDEL + QOUTCHN                              J 0530
      150 CONTINUE                                                            J 0540
C      ***********************************************************************  J 0550
C                                                                             J 0560
C      CALCULATE FLUX FROM VERTICAL LEAKAGE                                   J 0570
C                                                                             J 0580
          DO 170 NE = 1,NUMEL                                                 J 0590
             IF (VPRM(NE).EQ.0.0) GO TO 170                                   J 0600
             HEADBAR = (HEAD(NI(NE)) + HEAD(NJ(NE)) + HEAD(NK(NE)))/3.        J 0610
             HDIBAR = (HDI(NI(NE)) + HDI(NJ(NE)) + HDI(NK(NE)))/3.            J 0620
             VLEK = VPRM(NE) * (HEADBAR - HDIBAR) * AREA(NE)                  J 0630
             IF (VLEK.GT.0.0) GO TO 160                                       J 0640
             QINLEK = VLEK * TDEL + QINLEK                                    J 0650
             GO TO 170                                                        J 0660
      160    QOUTLEK = VLEK * TDEL + QOUTLEK                                 J 0670
      170 CONTINUE                                                            J 0680
C      ***********************************************************************  J 0690
C                                                                             J 0700
C      CALCULATE FLUX ACROSS MODEL BOUNDARIES                                 J 0710
C                                                                             J 0720
          DO 180 NB = 1,NUMBS                                                 J 0730
             DX2 = (X(NBNDYI(NB)) - X(NBNDYJ(NB))) * * 2                      J 0740
             DY2 = (Y(NBNDYI(NB)) - Y(NBNDYJ(NB))) * * 2                      J 0750
             DL = (DX2 + DY2) * * .5                                          J 0760
             TBAR = (TRANS(NBNDYI(NB)) + TRANS(NBNDYJ(NB)))/2.               J 0770
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PROGRAM LISTING--CONTINUED

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                QXBNDY =  - DHDX(NB) * COSX(NB) * DL * TBAR                  J 0780
                QYBNDY =  - DHDY(NB) * COSY(NB) * DL * TBAR                  J 0790
                IF (QXBNDY.GT.0.) QOUTBDY = QOUTBDY + QXBNDY                 J 0800
                IF (QYBNDY.GT.0.) QOUTBDY = QOUTBDY + QYBNDY                 J 0810
                IF (QXBNDY.LT.0.) QINBDY = QINBDY + QXBNDY                   J 0820
      180 IF (QYBNDY.LT.0.) QINBDY = QINBDY + QYBNDY                         J 0830
    C     ********************************************************************  J 0840
    C                                                                       J 0850
    C     ADJUST QRECH, QLEK AND QBNDY FOR FLOW FROM CONSTANT HEAD NODES     J 0860
    C                                                                       J 0870
          AOUTBDY = 0.                                                      J 0880
          AINBDY = AOUTBDY                                                  J 0890
          AOUTLEK = AINBDY                                                  J 0900
          AINLEK = AOUTLEK                                                  J 0910
          AOUTRCH = AINLEK                                                  J 0920
          AINRCH = AOUTRCH                                                  J 0930
          DO 250 NP = 1,NUMNP                                               J 0940
              IF (NODEID(NP).EQ.0.OR.NODEID(NP).GT.10) GO TO 250            J 0950
              DO 220 NE = 1,NUMEL                                           J 0960
                  IF (NI(NE).NE.NP.AND.NJ(NE).NE.NP.AND.NK(NE).NE.NP) GO TO 22  J 0970
        1         0                                                         J 0980
                  NC = 0                                                    J 0990
                  IF (NI(NE).EQ.NP) NC = NC + 1                             J 1000
                  IF (NJ(NE).EQ.NP) NC = NC + 1                             J 1010
                  IF (NK(NE).EQ.NP) NC = NC + 1                             J 1020
                  IF (VPRM(NE).EQ.0.0) GO TO 200                            J 1030
                  HEADBAR = (HEAD(NI(NE)) + HEAD(NJ(NE)) + HEAD(NK(NE)))/3. J 1040
                  HDIBAR = (HDI(NI(NE)) + HDI(NJ(NE)) + HDI(NK(NE)))/3.     J 1050
                  VLEK = VPRM(NE) * (HEADBAR - HDIBAR) * AREA(NE)/3. * NC   J 1060
                  IF (VLEK.GT.0.0) GO TO 190                                J 1070
                  AINLEK = VLEK * TDEL + AINLEK                             J 1080
                  GO TO 200                                                 J 1090
        190       AOUTLEK = VLEK * TDEL + AOUTLEK                           J 1100
        200       ARECH = RECH(NE) * AREA(NE)/3. * NC                       J 1110
                  IF (ARECH.GT.0.0) GO TO 210                               J 1120
                  AINRCH = ARECH * TDEL + AINRCH                            J 1130
                  GO TO 220                                                 J 1140
        210       AOUTRCH = ARECH * TDEL + AOUTRCH                          J 1150
        220   CONTINUE                                                      J 1160
              DO 240 NB = 1,NUMBS                                           J 1170
                  IF (NBNDYI(NB).NE.NP.AND.NBNDYJ(NB).NE.NP) GO TO 240      J 1180
                  DX2 = (X(NBNDYI(NB)) - X(NBNDYJ(NB))) *   * 2             J 1190
                  DY2 = (Y(NBNDYI(NB)) - Y(NBNDYJ(NB))) *   * 2             J 1200
                  DL = (DX2 + DY2) *   * .5                                 J 1210
                  DHDN = DHDX(NB) * COSX(NB) + DHDY(NB) * COSY(NB)          J 1220
                  IF (NBNDYI(NB).NE.NP) GO TO 230                           J 1230
                  ABNDYI = ABNDYI - DHDN * DL/6. * (2 * TRANS(NBNDYI(NB)) + TR  J 1240
        1         ANS(NBNDYJ(NB)))                                         J 1250
        230       IF (NBNDYJ(NP).NE.NP) GO TO 240                           J 1260
                  ABNDYJ = ABNDYJ - DHDN * DL/6. * (TRANS(NBNDYI(NB)) + 2 * TR  J 1270
        1         ANS(NBNDYJ(NB)))                                         J 1280
        240   CONTINUE                                                      J 1290
      250 CONTINUE                                                          J 1300
          QINRCH = QINRCH - AINRCH                                         J 1310
          QOUTRCH = QOUTRCH - AOUTRCH                                      J 1320
          QINLEK = QINLEK - AINLEK                                         J 1330
          QOUTLEK = QOUTLEK - AOUTLEK                                      J 1340
          QINBDY = QINBDY - AINBDY                                         J 1350
          QOUTBDY = QOUTBDY - AOUTBDY                                      J 1360
    C     ********************************************************************  J 1370
    C                                                                       J 1380
    C     CALCULATE CHANGE IN STORAGE IN THE AQUIFER                        J 1390
    C                                                                       J 1400
          QSTOR = 0.                                                       J 1410
          DO 260 NE = 1,NUMEL                                              J 1420
              HEADBAR = (HEAD(NI(NE)) + HEAD(NJ(NE)) + HEAD(NK(NE)))/3.    J 1430
              HDIBAR = (HDI(NI(NE)) + HDI(NJ(NE)) + HDI(NK(NE)))/3.        J 1440
      260 QSTOR = S * (HDIBAR - HEADBAR) * AREA(NE) + QSTOR                J 1450
    C     ********************************************************************  J 1460
```

```
      RETURN                                                            J 1470
      END                                                               J 1480
      SUBROUTINE CHEMBAL                                                K 0010
      COMMON /BLOCKA/ NUMNP,X(35),Y(35),NUMEL,NI(50),NJ(50),            K 0020
     1NK(50),NUMBS,NBNDYI(18),NBNDYJ(18),COSX(18),COSY(18),             K 0030
     2DHDX(18),DHDY(18),TITLE(20),IBAND,ICT                             K 0040
      COMMON /BLOCKB/ NTIM,NPMP,PINT,TIMX,TINIT,TPDAY,SUMT,TDEL,INT,TIMY K 0050
     1,TDELMAX                                                          K 0060
      COMMON /BLOCKC/ S,POROS,BETA,DLTRAT,Z1,Z2,ATOMWT1,ATOMWT2,DBYHUK1, K 0070
     1DBYHUK2,SK                                                        K 0080
      COMMON /BLOCKD/ NCCDNP,NODEID(35),TRANS(35),HYDK(35),THCK(35),     K 0090
     1REC(35),C1PEC(35),C2REC(35)                                       K 0100
      COMMON /BLOCKE/ IDELEM(50),RECH(50),C1RECH(50),C2RECH(50),         K 0110
     1VPRM(50),AREA(50)                                                 K 0120
      COMMON /BLOCKF/ HEAD(35),HDI(35),C1(35),C2(35),C1HAT(35),          K 0130
     1C2HAT(35),CEC(35)                                                 K 0140
      COMMON /BLOCKK/ C1INRCH,C2INRCH,C1OTRCH,C2OTRCH,C1INREC,C2INREC,   K 0150
     1C1OTREC,C2OTREC,C1INCHN,C2INCHN,C1OTCHN,C2OTCHN,C1INLEK,C2INLEK,   K 0160
     2C1OTLEK,C1ISTOR,C2ISTOR,C1STOR,C2STOR,C1INBDY,C2INBDY,             K 0170
     3C1OTBDY,C2OTBDY                                                    K 0180
C     ********************************************************************  K 0190
C                                                                       K 0200
C     THIS SUBROUTINE CALCULATES A CHEMICAL MASS BALANCE                K 0210
C                                                                       K 0220
C     ********************************************************************  K 0230
C                                                                       K 0240
C     CONVERT CRECH,CREC,SOLUTION AND ADSORBED CONC FROM MEQ/L TO MG/L  K 0250
C                                                                       K 0260
      DO 100 NE = 1,NUMEL                                               K 0270
         C1RECH(NE) = C1RECH(NE)/Z1 * ATOMWT1                           K 0280
  100 C2RECH(NE) = C2RECH(NE)/Z2 * ATOMWT2                              K 0290
      DO 110 NP = 1,NUMNP                                               K 0300
         C1REC(NP) = C1REC(NP)/Z1 * ATOMWT1                             K 0310
         C2REC(NP) = C2REC(NP)/Z2 * ATOMWT2                             K 0320
         C1(NP) = C1(NP)/Z1 * ATOMWT1                                   K 0330
         C2(NP) = C2(NP)/Z2 * ATOMWT2                                   K 0340
         C1HAT(NP) = C1HAT(NP)/Z1 * ATOMWT1                             K 0350
  110 C2HAT(NP) = C2HAT(NP)/Z2 * ATOMWT2                                K 0360
C     ********************************************************************  K 0370
C                                                                       K 0380
C     CALCULATE MASS FROM DISTRIBUTED RECHARGE AND DISCHARGE SOURCES    K 0390
C                                                                       K 0400
      DO 130 NE = 1,NUMEL                                               K 0410
         IF (RECH(NE).GT.0.0) GO TO 120                                 K 0420
         C1INRCH = RECH(NE) * AREA(NE) * TDEL * C1RECH(NE) + C1INRCH    K 0430
         C2INRCH = RECH(NE) * AREA(NE) * TDEL * C2RECH(NE) + C2INRCH    K 0440
         GO TO 130                                                      K 0450
  120    CRECH1 = (C1(NI(NE)) + C1(NJ(NE)) + C1(NK(NE)))/3.             K 0460
         CRECH2 = (C2(NI(NE)) + C2(NJ(NE)) + C2(NK(NE)))/3.             K 0470
         C1OTRCH = RECH(NE) * AREA(NE) * TDEL * CRECH1 + C1OTRCH        K 0480
         C2OTRCH = RECH(NE) * AREA(NE) * TDEL * CRECH2 + C2OTRCH        K 0490
  130 CONTINUE                                                          K 0500
C     ********************************************************************  K 0510
C                                                                       K 0520
C     CALCULATE MASS FROM POINT RECHARGE AND DISCHARGE SOURCES          K 0530
C     (EXCLUDING CONSTANT HEAD NODES)                                   K 0540
C                                                                       K 0550
      DO 150 NP = 1,NUMNP                                               K 0560
         IF (NODEID(NP).GE.1.AND.NODEID(NP).LE.10) GO TO 150            K 0570
         IF (REC(NP).GT.0.0) GO TO 140                                  K 0580
         C1INREC = REC(NP) * TDEL * C1REC(NP) + C1INREC                 K 0590
         C2INREC = REC(NP) * TDEL * C2REC(NP) + C2INREC                 K 0600
         GO TO 150                                                      K 0610
  140    C1OTREC = REC(NP) * TDEL * C1(NP) + C1OTREC                    K 0620
         C2OTREC = REC(NP) * TDEL * C2(NP) + C2OTREC                    K 0630
  150 CONTINUE                                                          K 0640
C     ********************************************************************  K 0650
C                                                                       K 0660
C     CALCULATE MASS FROM POINT RECHARGE AND DISCHARGE SOURCES          K 0670
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PROGRAM LISTING--CONTINUED

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C     (AT CONSTANT HEAD NODES ONLY)                                    K 0680
C                                                                      K 0690
      DO 170 NP = 1,NUMNP                                              K 0700
          IF (NODEID(NP).EQ.0.OR.NODEID(NP).GT.10) GO TO 170          K 0710
          IF (REC(NP).GT.0.0) GO TO 160                               K 0720
          C1INCHN = REC(NP) * TDEL * C1REC(NP) + C1INCHN              K 0730
          C2INCHN = REC(NP) * TDEL * C2REC(NP) + C2INCHN              K 0740
          GO TO 170                                                   K 0750
  160     C1OTCHN = REC(NP) * TDEL * C1(NP) + C1OTCHN                 K 0760
          C2OTCHN = REC(NP) * TDEL * C2(NP) + C2OTCHN                 K 0770
  170 CONTINUE                                                        K 0780
C     ***************************************************************  K 0790
C                                                                      K 0800
C     CALCULATE MASS FROM VERTICAL LEAKAGE                            K 0810
C                                                                      K 0820
      DO 190 NE = 1,NUMEL                                             K 0830
          IF (VPRM(NE).EQ.0.0) GO TO 190                              K 0840
          HEADBAR = (HEAD(NI(NE)) + HEAD(NJ(NE)) + HEAD(NK(NE)))/3.   K 0850
          HDIBAR = (HDI(NI(NE)) + HDI(NJ(NE)) + HDI(NK(NE)))/3.       K 0860
          VLEK = VPRM(NE) * (HEADBAR - HDIBAR) * AREA(NE)             K 0870
          IF (VLEK.GT.0.0) GO TO 180                                  K 0880
          C1INLEK = VLEK * TDEL * C1RECH(NE) + C1INLEK                K 0890
          C2INLEK = VLEK * TDEL * C2RECH(NE) + C2INLEK                K 0900
          GO TO 190                                                   K 0910
  180     CRECH1 = (C1(NI(NE)) + C1(NJ(NE)) + C1(NK(NE)))/3.          K 0920
          CRECH2 = (C2(NI(NE)) + C2(NJ(NE)) + C2(NK(NE)))/3.          K 0930
          C1OTLEK = VLEK * TDEL * CRECH1 + C1OTLEK                    K 0940
          C2OTLEK = VLEK * TDEL * CRECH2 + C2OTLEK                    K 0950
  190 CONTINUE                                                        K 0960
C     ***************************************************************  K 0970
C                                                                      K 0980
C     ADJUST CRECH, CLEK AND CBNDY FOR MASS FROM CONSTANT HEAD NODES  K 0990
C                                                                      K 1000
      A2OTRCH = 0.                                                    K 1010
      A2INRCH = A2OTRCH                                               K 1020
      A1OTRCH = A2INRCH                                               K 1030
      A1INRCH = A1OTRCH                                               K 1040
      A2OTLEK = 0.                                                    K 1050
      A2INLEK = A2OTLEK                                               K 1060
      A1OTLEK = A2INLEK                                               K 1070
      A1INLEK = A1OTLEK                                               K 1080
      DO 240 NP = 1,NUMNP                                             K 1090
          IF (NODEID(NP).EQ.0.OR.NODEID(NP).GT.10) GO TO 240         K 1100
          DO 230 NE = 1,NUMEL                                         K 1110
          IF (NI(NE).NE.NP.AND.NJ(NE).NE.NP.AND.NK(NE).NE.NP) GO TO 23 K 1120
    1     0                                                            K 1130
          IF (VPRM(NE).EQ.0.0) GO TO 210                              K 1140
          HEADBAR = (HEAD(NI(NE)) + HEAD(NJ(NE)) + HEAD(NK(NE)))/3.   K 1150
          HDIBAR = (HDI(NI(NE)) + HDI(NJ(NE)) + HDI(NK(NE)))/3.       K 1160
          VLEK = VPRM(NE) * (HEADBAR - HDIBAR) * AREA(NE)/3.          K 1170
          IF (VLEK.GT.0.0) GO TO 200                                  K 1180
          A1INLEK = VLEK * TDEL * C1RECH(NE) + A1INLEK                K 1190
          A2INLEK = VLEK * TDEL * C2RECH(NE) + A2INLEK                K 1200
          GO TO 210                                                   K 1210
  200     CRECH1 = (C1(NI(NE)) + C1(NJ(NE)) + C1(NK(NE)))/3.          K 1220
          CRECH2 = (C2(NI(NE)) + C2(NJ(NE)) + C2(NK(NE)))/3.          K 1230
          A1OTLEK = VLEK * TDEL * CRECH1 + A1OTLEK                    K 1240
          A2OTLEK = VLEK * TDEL * CRECH2 + A2OTLEK                    K 1250
  210     ARECH = RECH(NE) * AREA(NE)/3.                              K 1260
          IF (ARECH.GT.0.0) GO TO 220                                 K 1270
          A1INRCH = ARECH * TDEL * C1RECH(NE) + A1INRCH              K 1280
          A2INRCH = ARECH * TDEL * C2RECH(NE) + A2INRCH              K 1290
          GO TO 230                                                   K 1300
  220     CRECH1 = (C1(NI(NE)) + C1(NJ(NE)) + C1(NK(NE)))/3.          K 1310
          CRECH2 = (C2(NI(NE)) + C2(NJ(NE)) + C2(NK(NE)))/3.          K 1320
          A1OTRCH = ARECH * TDEL * CRECH1 + A1OTRCH                   K 1330
          A2OTRCH = ARECH * TDEL * CRECH2 + A2OTRCH                   K 1340
  230     CONTINUE                                                    K 1350
  240 CONTINUE                                                        K 1360
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PROGRAM LISTING--CONTINUED

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        C1INRCH = C1INRCH - A1INRCH                                    K 1370
        C2INRCH = C2INRCH - A2INRCH                                    K 1380
        C1OTRCH = C1OTRCH - A1OTRCH                                    K 1390
        C2OTRCH = C2OTRCH - A2OTRCH                                    K 1400
        C1INLEK = C1INLEK - A1INLEK                                    K 1410
        C2INLEK = C2INLEK - A2INLEK                                    K 1420
        C1OTLEK = C1OTLEK - A1OTLEK                                    K 1430
        C2OTLEK = C2OTLEK - A2OTLEK                                    K 1440
C       ***********************************************************    K 1450
C                                                                      K 1460
C       CALCULATE CHANGE IN MASS STORED IN THE AQUIFER                 K 1470
C                                                                      K 1480
        C1STOR = 0.                                                    K 1490
        C2STOR = 0.                                                    K 1500
        DO 250 NE = 1,NUMEL                                            K 1510
          THCKBAR = (THCK(NI(NE)) + THCK(NJ(NE)) + THCK(NK(NE)))/3.    K 1520
          C1TBAR = (C1(NI(NE)) + C1(NJ(NE)) + C1(NK(NE)))/3. + (C1HAT(NI( K 1530
     1    NE)) + C1HAT(NJ(NE)) + C1HAT(NK(NE)))/3.                     K 1540
          C1STOR = AREA(NE) * THCKBAR * PCROS * C1TBAR + C1STOR        K 1550
          C2TBAR = (C2(NI(NE)) + C2(NJ(NE)) + C2(NK(NE)))/3. + (C2HAT(NI( K 1560
     1    NE)) + C2HAT(NJ(NE)) + C2HAT(NK(NE)))/3.                     K 1570
    250 C2STOR = AREA(NE) * THCKBAR * POROS * C2TBAR + C2STOR          K 1580
C       ***********************************************************    K 1590
C                                                                      K 1600
C       CONVERT CRECH,CREC,SOLUTION AND ADSCRBED CONC FROM MG/L TO MEQ/L K 1610
C                                                                      K 1620
        DO 260 NE = 1,NUMEL                                            K 1630
          C1RECH(NE) = C1RECH(NE) * Z1/ATOMWT1                         K 1640
    260 C2RECH(NE) = C2RECH(NE) * Z2/ATOMWT2                           K 1650
        DO 270 NP = 1,NUMNP                                            K 1660
          C1REC(NP) = C1REC(NP) * Z1/ATOMWT1                           K 1670
          C2REC(NP) = C2REC(NP) * Z2/ATOMWT2                           K 1680
          C1(NP) = C1(NP) * Z1/ATOMWT1                                 K 1690
          C2(NP) = C2(NP) * Z2/ATOMWT2                                 K 1700
          C1HAT(NP) = C1HAT(NP) * Z1/ATOMWT1                           K 1710
    270 C2HAT(NP) = C2HAT(NP) * Z2/ATOMWT2                             K 1720
C       ***********************************************************    K 1730
        RETURN                                                         K 1740
        END                                                            K 1750
        SUBROUTINE FLOWOUT                                             L 0010
        COMMON /BLOCKA/ NUMNP,X(35),Y(35),NUMEL,NI(50),NJ(50),        L 0020
     1NK(50),NUMBS,NBNDYI(18),NBNDYJ(18),COSX(18),COSY(18),           L 0030
     2DHDX(18),DHDY(18),TITLE(20),IBAND,ICT                           L 0040
        COMMON /BLOCKB/ NTIM,NPMP,PINT,TIMX,TINIT,TPDAY,SUMT,TDEL,INT,TIMY L 0050
     1,TDELMAX                                                         L 0060
        COMMON /BLOCKC/ S,POROS,BETA,DLTRAT,Z1,Z2,ATOMWT1,ATOMWT2,DBYHUK1, L 0070
     1DBYHUK2,SK                                                       L 0080
        COMMON /BLOCKD/ NCODNP,NODEID(35),TRANS(35),HYDK(35),THCK(35), L 0090
     1REC(35),C1PEC(35),C2REC(35)                                      L 0100
        COMMON /BLOCKF/ HEAD(35),HDI(35),C1(35),C2(35),C1HAT(35),      L 0110
     1C2HAT(35),CEC(35)                                                L 0120
        COMMON /BLOCKJ/QINRCH,QOUTRCH,QINREC,QOUTREC,QINCHN,QOUTCHN,   L 0130
     1QINLEK,QOUTLEK,QINBDY,QOUTBDY,GSTOR                              L 0140
        DIMENSION ND(4),DRWDN(4)                                       L 0150
C       ***********************************************************    L 0160
C                                                                      L 0170
C       THIS SUBROUTINE PRINTS THE OUTPUT FCR THE FLOW PART OF THE MODEL L 0180
C                                                                      L 0190
C       ***********************************************************    L 0200
C                                                                      L 0210
C       PRINT HEAD VALUES -- FT                                        L 0220
C                                                                      L 0230
        WRITE (6,100)                                                  L 0240
    100 FORMAT (1H1,4X,23HHEAD DISTRIBUTION -- FT/5X,23H-------------- L 0250
     1-----)                                                           L 0260
        WRITE (6,110) SUMT                                             L 0270
    110 FORMAT (1H0,4X,13HTIME(DAYS) = ,F10.3)                         L 0280
        WRITE (6,120) TIMY                                             L 0290
    120 FORMAT (5X,13HTIME(YEARS)= ,F10.5)                             L 0300
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```
      WRITE (6,130)                                                  L 0310
  130 FORMAT (///1H ,9X,4HNODE,10X,4HHEAD,12X,4HNODE,10X,4HHEAD,12X,4HNO L 0320
     1DE,10X,4HHEAD,12X,4HNODE,10X,4HHEAD)                            L 0330
      WRITE (6,140) (NP,HEAD(NP),NP = 1,NUMNP)                        L 0340
  140 FORMAT (4(10X,I3,5X,F12.3))                                     L 0350
C     ******************************************************************* L 0360
C                                                                     L 0370
C     PRINT DRAWDOWN VALUES -- FT                                     L 0380
C                                                                     L 0390
      WRITE (6,150)                                                   L 0400
  150 FORMAT (1H1,4X,27HDRAWDOWN DISTRIBUTION -- FT/5X,27H------------ L 0410
     1------------)                                                   L 0420
      WRITE (6,110) SUMT                                              L 0430
      WRITE (6,120) TIMY                                              L 0440
      WRITE (6,160)                                                   L 0450
  160 FORMAT (///1H ,9X,4HNODE,9X,8HDRAWDOWN,9X,4HNODE,9X,8HDRAWDOWN,9X, L 0460
     14HNODE,9X,8HDRAWDOWN,9X,4HNODE,9X,8HDRAWDOWN)                   L 0470
      IR = 0                                                          L 0480
      KR = 1                                                          L 0490
      KC = 4                                                          L 0500
  170 DO 180 NP = KR,KC                                               L 0510
      IR = IR + 1                                                     L 0520
      ND(IR) = NP                                                     L 0530
  180 DRWDN(IR) = HDI(NP) - HEAD(NP)                                  L 0540
      WRITE (6,190) (ND(I),DRWDN(I),I = 1,IR)                         L 0550
  190 FORMAT (4(10X,I3,5X,F12.3))                                     L 0560
      IF (KC.EQ.NUMNP) GO TO 200                                      L 0570
      IR = 0                                                          L 0580
      KR = KC + 1                                                     L 0590
      KC = KC + 4                                                     L 0600
      IF (KC.GT.NUMNP) KC = NUMNP                                     L 0610
      GO TO 170                                                       L 0620
C     ******************************************************************* L 0630
C                                                                     L 0640
C     PRINT CUMULATIVE WATER BALANCE -- FT**3                         L 0650
C                                                                     L 0660
  200 WRITE (6,210)                                                   L 0670
  210 FORMAT (///1H1,4X,33HCUMULATIVE WATER BALANCE -- FT**3/5X,33H----- L 0680
     1------------------------------)                                 L 0690
      WRITE (6,110) SUMT                                              L 0700
      WRITE (6,120) TIMY                                              L 0710
      WRITE (6,220) QINRCH,QOUTRCH                                    L 0720
  220 FORMAT (//,15X,38HQINRCH  (RECHARGE-DISTRIBUTED)      =,F15.3,/,1 L 0730
     15X,38HQOUTRCH (DISCHARGE-DISTRIBUTED)     =,F15.3)              L 0740
      WRITE (6,230) QINREC,QOUTREC                                    L 0750
  230 FORMAT (/,15X,38HQINREC  (RECHARGE-POINT)           =,F15.3,/,15 L 0760
     1X,38HQOUTREC (DISCHARGE-POINT)          =,F15.3)                L 0770
      WRITE (6,240) QINLEK,QOUTLEK                                    L 0780
  240 FORMAT (/,15X,38HQINLEK  (RECHARGE-LEAKAGE)          =,F15.3,/,15 L 0790
     1X,38HQOUTLEK (DISCHARGE-LEAKAGE)        =,F15.3)                L 0800
      WRITE (6,250) QINBDY,QOUTBDY                                    L 0810
  250 FORMAT (/,15X,38HQINBDY  (RECHARGE-BOUNDARY)         =,F15.3,/,15 L 0820
     1X,38HQOUTBDY (DISCHARGE-BOUNDARY)       =,F15.3)                L 0830
      WRITE (6,260) QINCHN,QOUTCHN                                    L 0840
  250 FORMAT (/,15X,38HQINCHN  (RECHARGE-CONST HEAD NODES) =,F15.3,/,15 L 0850
     1X,38HQOUTCHN (DISCHARGE-CONST HEAD NODES) =,F15.3)              L 0860
C                                                                     L 0870
      QIN = QINRCH + QINREC + QINLEK + QINCHN + QINBDY                L 0880
      QOUT = QOUTRCH + QOUTREC + QOUTLEK + QOUTCHN + QOUTBDY          L 0850
      WRITE (6,270) QIN,QOUT                                          L 0900
  270 FORMAT (56X,12H------------/,40X,13HTOTAL QIN   =,F15.3/,40X,13HTO L 0910
     1TAL QOUT  =,F15.3)                                             L 0920
      WRITE (6,280) QSTOR                                             L 0930
  280 FORMAT (/,15X,38HQSTOR   (WATER RELEASED FROM STORAGE) =,F15.3)  L 0940
C                                                                     L 0950
C     CALCULATE AND PRINT MASS BALANCE RESIDUAL AND ERROR AS A PER CENT L 0960
C                                                                     L 0970
      QRESID = QIN + QOUT - QSTOR                                     L 0980
      QRESID = ABS(QRESID)                                            L 0990
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      WRITE (6,290) QRESID                                            L 1000
  290 FORMAT (//,25X,28HMASS BALANCE RESIDUAL      =,F15.3)           L 1010
      QERRIN = 0.                                                     L 1020
      IF (QIN.NE.0.0) QERRIN = ABS(QRESID)/( - QIN) * 100.            L 1030
      QERROUT = 0.                                                    L 1040
      IF (QOUT.NE.0.0) QERROUT = ABS(QRESID)/QOUT * 100.              L 1050
      QERRSTR = 0.                                                    L 1060
      IF (QSTOR.NE.0.0) QERRSTR = ABS(QRESID)/ABS(QSTOR) * 100.       L 1070
      WRITE (6,300) QERRIN,QERROUT,QERRSTR                            L 1080
  300 FORMAT (25X,29HERRCR AS PERCENT OF QIN     =,F15.3/,25X,28HERROR AS  L 1090
     1 PERCENT OF QOUT   =,F15.3/,25X,28HERROR AS PERCENT OF QSTOR   =,F1  L 1100
     25.3)                                                           L 1110
C     ******************************************************************  L 1120
C                                                                    L 1130
C                                                                    L 1130
C     PRINT FLOW BY NODE ID -- GPM                                   L 1140
C                                                                    L 1150
      WRITE (6,310)                                                  L 1160
  310 FORMAT (///1H0,4X,22HFLOW BY NODE ID -- GPM/3X,24H---------------   L 1170
     1--------)                                                      L 1180
      DO 350 NC = 1,NCODNP                                           L 1190
         QINNID = 0.                                                 L 1200
         QOUTNID = 0.                                                L 1210
         DO 330 NP = 1,NUMNP                                         L 1220
            IF (NODEID(NP).NE.NC) GO TO 330                          L 1230
            IF (REC(NP).LE.0.) GO TO 320                             L 1240
            QOUTNID = QOUTNID + REC(NP) * 7.48052/1440.              L 1250
            GO TO 330                                                L 1260
  320       QINNID = QINNID + REC(NP) * 7.48052/1440.                L 1270
  330    CONTINUE                                                    L 1280
         IF (QINNID.EQ.0.0.AND.QOUTNID.EQ.0.0) GO TO 350             L 1290
         WRITE (6,340) NC,QINNID,NC,QOUTNID                          L 1300
  340 FORMAT (/5X,5HQIN (,I3,2H)=,5X,F12.3/5X,5HQOUT(,I3,2H)=,5X,F12.3)   L 1310
  350 CONTINUE                                                       L 1320
C     ******************************************************************  L 1330
C                                                                    L 1340
C     PRINT FLOW FROM CONSTANT HEAD NODES -- GPM                     L 1350
C                                                                    L 1360
      WRITE (6,360)                                                  L 1370
  360 FORMAT (///1H0,4X,42HFLOW FROM CONSTANT HEAD NODES -- GPM      /,5  L 1380
     1X,31HPOSITIVE IS DISCHARGE (PUMPAGE)/,5X,32HNEGATIVE IS RECHARGE (  L 1390
     2INJECTION))                                                   L 1400
      DO 380 NP = 1,NUMNP                                            L 1410
         IF (NODEID(NP).EQ.0.OR.NODEID(NF).GT.10) GO TO 380          L 1420
         REC(NP) = REC(NP) * 7.48052/60/24                          L 1430
         WRITE (6,370) NP,REC(NP)                                    L 1440
         REC(NP) = REC(NP)/7.48052 * 60 * 24                        L 1450
  370 FORMAT (5X,5HNODE(,I3,2H)=,5X,F12.3)                           L 1460
  380 CONTINUE                                                       L 1470
C     ******************************************************************  L 1480
      RETURN                                                         L 1490
      END                                                            L 1500
      SUBROUTINE CHEMOUT                                             M 0010
      COMMON /BLOCKA/ NUMNP,X(35),Y(35),NUMEL,NI(50),NJ(50),         M 0020
     1NK(50),NUMBS,NBNDYI(18),NBNDYJ(18),COSX(18),COSY(18),          M 0030
     2DHDX(18),DHDY(18),TITLE(20),IBAND,ICT                          M 0040
      COMMON /BLOCKB/ NTIM,NPMP,PINT,TIMX,TINIT,TPDAY,SUMT,TDEL,INT,TIMY  M 0050
     1,TDELMAX                                                       M 0060
      COMMON /BLOCKC/ S,PCROS,BETA,DLTRAT,Z1,Z2,ATOMWT1,ATOMWT2,DBYHUK1,  M 0070
     1DBYHUK2,SK                                                     M 0080
      COMMON /BLOCKF/ HEAD(35),HDI(35),C1(35),C2(35),C1HAT(35),       M 0090
     1C2HAT(35),CEC(35)                                             M 0100
      COMMON /BLOCKK/ C1INRCH,C2INRCH,C10TRCH,C20TRCH,C1INREC,C2INREC,    M 0110
     1C10TREC,C20TREC,C1INCHN,C2INCHN,C1CTCHN,C20TCHN,C1INLEK,C2INLEK,    M 0120
     2C10TLEK,C20TLEK,C1ISTOR,C2ISTOR,C1STOR,C2STOR,C1INBDY,C2INBDY,      M 0130
     3C10TBDY,C20TBDY                                                M 0140
C     ******************************************************************  M 0150
C                                                                    M 0160
C     THIS SUBROUTINE PRINTS THE OUTPUT FOR THE TRANSPORT PART OF MODEL   M 0170
C                                                                    M 0180
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PROGRAM LISTING--CONTINUED

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C     ******************************************************************     M 0190
C                                                                           M 0200
C         CONVERT SOLUTION CONCENTRATIONS FROM MEQ/L TO MG/L               M 0210
C                                                                           M 0220
      DO 100 NP = 1,NUMNP                                                   M 0230
         C1(NP) = C1(NP)/Z1 * ATOMWT1                                      M 0240
         C2(NP) = C2(NP)/Z2 * ATOMWT2                                      M 0250
  100 CONTINUE                                                              M 0260
C     ******************************************************************     M 0270
C                                                                           M 0280
C         PRINT SOLUTE CONCENTRATION OF SPECIES 1 (C1) -- MG/L             M 0290
C                                                                           M 0300
      WRITE (6,110)                                                         M 0310
  110 FORMAT (1H1,4X,46HSOLUTE CONCENTRATION OF SPECIES 1 (C1) -- MG/L/5   M 0320
     1X,46H----------------------------------------------)                 M 0330
      WRITE (6,120) SUMT                                                    M 0340
  120 FORMAT (1H0,4X,13HTIME(DAYS) = ,F10.3)                               M 0350
      WRITE (6,130) TIMY                                                    M 0360
  130 FORMAT (5X,13HTIME(YEARS)= ,F10.5)                                   M 0370
      WRITE (6,140)                                                        M 0380
  140 FORMAT (///1H ,9X,4HNODE,10X,4HCONC,12X,4HNODE,10X,4HCONC,12X,4HNO   M 0390
     1DE,10X,4HCONC,12X,4HNODE,10X,4HCONC)                                 M 0400
      WRITE (6,150) (NP,C1(NP),NP = 1,NUMNP)                               M 0410
  150 FORMAT (4(10X,I3,5X,F12.3))                                          M 0420
C     ******************************************************************     M 0430
C                                                                           M 0440
C         PRINT SOLUTE CONCENTRATION OF SPECIES 2 (C2) -- MG/L             M 0450
C                                                                           M 0460
      WRITE (6,160)                                                         M 0470
  160 FORMAT (1H1,4X,46HSOLUTE CONCENTRATION OF SPECIES 2 (C2) -- MG/L/5   M 0480
     1X,46H----------------------------------------------)                 M 0490
      WRITE (6,120) SUMT                                                    M 0500
      WRITE (6,130) TIMY                                                    M 0510
      WRITE (6,140)                                                        M 0520
      WRITE (6,150) (NP,C2(NP),NP = 1,NUMNP)                               M 0530
C     ******************************************************************     M 0540
C                                                                           M 0550
C         CONVERT SOLUTION  CONCENTRATIONS FROM MG/L TO MEQ/L              M 0560
C         CONVERT ADSORBED CONCENTRATIONS FROM MEQ/L TO FRACTION ADSORBED  M 0570
C                                                                           M 0580
      DO 170 NP = 1,NUMNP                                                   M 0590
         C1(NP) = C1(NP) * Z1/ATOMWT1                                      M 0600
         C2(NP) = C2(NP) * Z2/ATOMWT2                                      M 0610
         C1HAT(NP) = C1HAT(NP)/CEC(NP)                                     M 0620
  170 C2HAT(NP) = C2HAT(NP)/CEC(NP)                                        M 0630
C     ******************************************************************     M 0640
C         IF CONSERVATIVE TRANSPORT SKIP PRINTOUT OF CHAT                  M 0650
      IF (ICT.GT.0) GO TO 250                                              M 0660
C     ******************************************************************     M 0670
C                                                                           M 0680
C         PRINT FRACTION ADSORBED OF SPECIES 1 (C1HAT/CEC) -- DIMENSIONLESS M 0690
C                                                                           M 0700
      WRITE (6,180)                                                         M 0710
  180 FORMAT (1H1,4X,70HEQUIVALENT FRACTION ADSORBED OF SPECIES 1 (C1HAT   M 0720
     1/CEC) -- DIMENSIONLESS/5X,70H-----------------------------------     M 0730
     2----------------------------)                                        M 0740
      WRITE (6,120) SUMT                                                    M 0750
      WRITE (6,130) TIMY                                                    M 0760
      WRITE (6,140)                                                        M 0770
      WRITE (6,190) (NP,C1HAT(NP),NP = 1,NUMNP)                            M 0780
  190 FORMAT (4(10X,I3,10X,F5.3,2X))                                       M 0790
C     ******************************************************************     M 0800
C                                                                           M 0810
C         PRINT FRACTION ADSORBED OF SPECIES 2 (C2HAT/CEC) -- DIMENSIONLESS M 0820
C                                                                           M 0830
      WRITE (6,200)                                                         M 0840
  200 FORMAT (1H1,4X,70HEQUIVALENT FRACTION ADSORBED OF SPECIES 2 (C2HAT   M 0850
     1/CEC) -- DIMENSIONLESS/5X,70H-----------------------------------     M 0860
     2----------------------------)                                        M 0870
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PROGRAM LISTING--CONTINUED

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         WRITE (6,120) SUMT                                              M 0880
         WRITE (6,130) TIMY                                              M 0850
         WRITE (6,140)                                                   M 0900
         WRITE (6,190) (NP,C2HAT(NP),NP = 1,NUMNP)                       M 0910
C     ***********************************************************        M 0920
C                                                                        M 0930
C     CONVERT ADSORBED CONCENTRATICNS FROM FRACTION ADSORBED TO MG/L     M 0940
C                                                                        M 0950
         DO 210 NP = 1,NUMNP                                             M 0960
            C1HAT(NP) = C1HAT(NP) * CEC(NP)/Z1 * ATOMWT1                 M 0970
            C2HAT(NP) = C2HAT(NP) * CEC(NP)/Z2 * ATOMWT2                 M 0980
     210 CONTINUE                                                        M 0990
C     ***********************************************************        M 1000
C                                                                        M 1010
C     PRINT ADSORBED CONCENTRATICN CF SPECIES 1 (C1HAT) -- MG/L          M 1020
C                                                                        M 1030
         WRITE (6,220)                                                   M 1040
     220 FORMAT (1H1,4X,51HADSORBED CONCENTRATION OF SPECIES 1 (C1HAT) -- M 1050
        1G/L/5X,51H----------------------------------------------------) M 1060
         WRITE (6,120) SUMT                                              M 1070
         WRITE (6,130) TIMY                                              M 1080
         WRITE (6,140)                                                   M 1090
         WRITE (6,150) (NP,C1HAT(NP),NP = 1,NUMNP)                       M 1100
C     ***********************************************************        M 1110
C                                                                        M 1120
C     PRINT ADSORBED CONCENTRATICN OF SPECIES 2 (C2HAT) -- MG/L          M 1130
C                                                                        M 1140
         WRITE (6,230)                                                   M 1150
     230 FORMAT (1H1,4X,51HADSORBED CONCENTRATION OF SPECIES 2 (C2HAT) -- M 1160
        1G/L/5X,51H----------------------------------------------------) M 1170
         WRITE (6,120) SUMT                                              M 1180
         WRITE (6,130) TIMY                                              M 1190
         WRITE (6,140)                                                   M 1200
         WRITE (6,150) (NP,C2HAT(NP),NP = 1,NUMNP)                       M 1210
C     ***********************************************************        M 1220
C                                                                        M 1230
C     CONVERT ADSORBED  CONCENTRATIONS FROM MG/L TO MEQ/L                M 1240
         DO 240 NP = 1,NUMNP                                             M 1250
            C1HAT(NP) = C1HAT(NP) * Z1/ATOMWT1                           M 1260
            C2HAT(NP) = C2HAT(NP) * Z2/ATOMWT2                           M 1270
     240 CONTINUE                                                        M 1280
C     ***********************************************************        M 1290
C                                                                        M 1300
C     PRINT CUM CHEMICAL BALANCE FCR SPECIES 1 (C1 & C1HAT) -- MG/L*FT**3 M 1310
C                                                                        M 1320
     250 WRITE (6,260)                                                   M 1330
     260 FORMAT (///1H1,4X,66HCUMULATIVE CHEMICAL BALANCE FOR SPECIES 1 (C1 M 1340
        1&C1HAT) -- MG/L*FT**3/5X,66H---------------------------------- M 1350
        2--------------------------)                                    M 1360
         WRITE (6,120) SUMT                                              M 1370
         WRITE (6,130) TIMY                                              M 1380
         WRITE (6,270) C1INRCH,C1OTRCH                                   M 1390
     270 FORMAT (//,15X,38HC1INRCH (DISTRIBUTED RECHARGE)      =,F15.3,/,1 M 1400
        15X,38HC1OTRCH (DISTRIBUTED DISCHARGE)     =,F15.3)             M 1410
         WRITE (6,280) C1INREC,C1OTREC                                   M 1420
     280 FORMAT (/,15X,38HC1INREC (POINT RECHARGE)             =,F15.3,/,15 M 1430
        1X,38HC1OTREC (POINT DISCHARGE)            =,F15.3)             M 1440
         WRITE (6,290) C1INLEK,C1OTLEK                                   M 1450
     290 FORMAT (/,15X,38HC1INLEK (RECHARGE-LEAKAGE)           =,F15.3,/,15 M 1460
        1X,38HC1OTLEK (DISCHARGE-LEAKAGE)          =,F15.3)             M 1470
         WRITE (6,300) C1INCHN,C1OTCHN                                   M 1480
     300 FORMAT (/,15X,38HC1INCHN (RECHARGE-CONST HEAD NODES)   =,F15.3,/,15 M 1490
        1X,38HC1OTCHN (DISCHARGE-CONST HEAD NODES) =,F15.3)             M 1500
         WRITE (6,310) C1INBDY,C1OTBDY                                   M 1510
     310 FORMAT (/,15X,38HC1INBDY (INFLOW-MODEL BOUNDARY)       =,F15.3,/,15 M 1520
        1X,38HC1OTBDY (OUTFLOW-MODEL BOUNDARY)     =,F15.3)             M 1530
C                                                                        M 1540
         C1IN = C1INRCH + C1INREC + C1INLEK + C1INCHN + C1INBDY          M 1550
         C1OUT = C1OTRCH + C1OTREC + C1OTLEK + C1OTCHN + C1OTBDY         M 1560
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         WRITE (6,320) C1IN,C1OUT                                       M 1570
     320 FORMAT (56X,12H------------/,39X,14HTOTAL C1IN    =,F15.3/,39X,14HT M 1580
        1OTAL C1OUT  =,F15.3)                                           M 1590
         WRITE (6,330) C1STOR                                           M 1600
     330 FORMAT (/,18X,35HC1STOR   (PRESENT MASS STORED)    =,F15.3)     M 1610
         WRITE (6,340) C1ISTOR                                          M 1620
     340 FORMAT (18X,35HC1ISTOR (INITIAL MASS STORED)     =,F15.3)       M 1630
         C1DELST = C1STOR - C1ISTOR                                     M 1640
         WRITE (6,350) C1DELST                                          M 1650
     350 FORMAT (56X,12H------------/,18X,35HC1DELST (CHANGE IN MASS STORED M 1660
        1)   =,F15.3)                                                   M 1670
C                                                                       M 1680
C        CALCULATE AND PRINT MASS BALANCE RESIDUAL AND ERROR AS A PER CENT M 1690
C                                                                       M 1700
         C1RESID = C1IN + C1OUT + C1DELST                               M 1710
         C1RESID = ABS(C1RESID)                                         M 1720
         WRITE (6,360) C1RESID                                          M 1730
     360 FORMAT (//,25X,28HMASS BALANCE RESIDUAL       =,F15.3)         M 1740
         C1ERRIN = 0.                                                   M 1750
         IF (C1IN.NE.0.0) C1ERRIN = C1RESID/( - C1IN) * 100.            M 1760
         C1ERROT = 0.                                                   M 1770
         IF (C1OUT.NE.0.0) C1ERROT = C1RESID/C1OUT * 100.               M 1780
         C1ERRST = 0.                                                   M 1790
         IF (C1DELST.NE.0.0) C1ERRST = C1RESID/ABS(C1DELST) * 100.      M 1800
         C1ERIST = 0.                                                   M 1810
         IF (C1ISTOR.NE.0.0) C1ERIST = ABS(C1RESID)/C1ISTOR * 100.      M 1820
         WRITE (6,370) C1ERRIN,C1ERROT,C1ERRST,C1ERIST                  M 1830
     370 FORMAT (24X,29HERROR AS PERCENT OF C1IN    =,F15.3/,24X,29HERROR A M 1840
        1S PERCENT OF C1OUT   =,F15.3/,24X,29HERROR AS PERCENT OF C1DELST = M 1850
        2,F15.3/,24X,29HERROR AS PERCENT OF C1ISTOR =,F15.3)            M 1860
C        **************************************************************** M 1870
C                                                                       M 1880
C        PRINT CUM CHEMICAL BALANCE FOR SPECIES 2 (C2 & C2HAT) -- MG/L*FT**3 M 1890
C                                                                       M 1900
         WRITE (6,380)                                                  M 1910
     380 FORMAT (///1H1,4X,66HCUMULATIVE CHEMICAL BALANCE FOR SPECIES 2 (C2 M 1920
        1&C2HAT) -- MG/L*FT**3/5X,66H--------------------------------- M 1930
        2----------------------)                                       M 1940
         WRITE (6,120) SUMT                                             M 1950
         WRITE (6,130) TIMY                                             M 1960
         WRITE (6,390) C2INRCH,C2OTRCH                                  M 1970
     390 FORMAT (//,15X,38HC2INRCH (DISTRIBUTED RECHARGE)       =,F15.3,/,1 M 1980
        15X,38HC2OTRCH (DISTRIBUTED DISCHARGE)      =,F15.3)            M 1990
         WRITE (6,400) C2INREC,C2OTREC                                  M 2000
     400 FORMAT (/,15X,38HC2INREC (POINT RECHARGE)             =,F15.3,/,15 M 2010
        1X,38HC2OTREC (POINT DISCHARGE)            =,F15.3)             M 2020
         WRITE (6,410) C2INLEK,C2OTLEK                                  M 2030
     410 FORMAT (/,15X,38HC2INLEK (RECHARGE-LEAKAGE)            =,F15.3,/,15 M 2040
        1X,38HC2OTLEK (DISCHARGE-LEAKAGE)          =,F15.3)             M 2050
         WRITE (6,420) C2INCHN,C2OTCHN                                  M 2060
     420 FORMAT (/,15X,38HC2INCHN (RECHARGE-CONST HEAD NODES) =,F15.3,/,15 M 2070
        1X,38HC2OTCHN (DISCHARGE-CONST HEAD NODES) =,F15.3)             M 2080
         WRITE (6,430) C2INBDY,C2OTBDY                                  M 2090
     430 FORMAT (/,15X,38HC2INBDY (INFLOW-MODEL BOUNDARY)       =,F15.3,/,15 M 2100
        1X,38HC2OTBDY (OUTFLOW-MODEL BOUNDARY)     =,F15.3)             M 2110
C                                                                       M 2120
         C2IN = C2INRCH + C2INREC + C2INLEK + C2INCHN + C2INBDY         M 2130
         C2OUT = C2OTRCH + C2OTREC + C2OTLEK + C2OTCHN + C2OTBDY        M 2140
         WRITE (6,440) C2IN,C2OUT                                       M 2150
     440 FORMAT (56X,12H------------/,39X,14HTOTAL C2IN    =,F15.3/,39X,14HT M 2160
        1OTAL C2OUT  =,F15.3)                                           M 2170
         WRITE (6,450) C2STOR                                           M 2180
     450 FORMAT (/,18X,35HC2STOR   (PRESENT MASS STORED)    =,F15.3)     M 2190
         WRITE (6,460) C2ISTOR                                          M 2200
     460 FORMAT (18X,35HC2ISTOR (INITIAL MASS STORED)     =,F15.3)       M 2210
         C2DELST = C2STOR - C2ISTOR                                     M 2220
         WRITE (6,470) C2DELST                                          M 2230
     470 FORMAT (56X,12H------------/,18X,35HC2DELST (CHANGE IN MASS STORED M 2240
        1)   =,F15.3)                                                   M 2250
```

PROGRAM LISTING--CONTINUED

```
C                                                                        M 2260
C        CALCULATE AND PRINT MASS BALANCE RESIDUAL AND ERROR AS A PER CENT   M 2270
C                                                                        M 2280
         C2RESID = C2IN + C2OUT + C2DELST                                M 2290
         C2RESID = ABS(C2RESID)                                          M 2300
         WRITE (6,480) C2RESID                                           M 2310
     480 FORMAT (//,25X,28HMASS BALANCE RESIDUAL      =,F15.3)           M 2320
         C2ERRIN = 0.                                                    M 2330
         IF (C2IN.NE.0.0) C2ERRIN = C2RESID/( - C2IN) * 100.             M 2340
         C2ERROT = 0.                                                    M 2350
         IF (C2OUT.NE.0.0) C2ERROT = C2RESID/C2OUT * 100.                M 2360
         C2ERRST = 0.                                                    M 2370
         IF (C2DELST.NE.0.0) C2ERRST = C2RESID/ABS(C2DELST) * 100.       M 2380
         C2ERIST = 0.                                                    M 2390
         IF (C2ISTOR.NE.0.0) C2ERIST = ABS(C2RESID)/C2ISTOR * 100.       M 2400
         WRITE (6,490) C2ERRIN,C2ERROT,C2ERRST,C2ERIST                   M 2410
     490 FORMAT (24X,29HERROR AS PERCENT OF C2IN    =,F15.3/,24X,29HERROR A  M 2420
        1S PERCENT OF C2OUT   =,F15.3/,24X,29HERROR AS PERCENT OF C2DELST =  M 2430
        2,F15.3/,24X,29HERROR AS PERCENT OF C2ISTOR =,F15.3)             M 2440
C        ***********************************************************************  M 2450
         RETURN                                                          M 2460
         END                                                             M 2470
```

DEFINITION OF PROGRAM VARIABLES--CONTINUED

	BOUNDARY SEGMENT
DBYHUK1	DEBYE HUCKEL PARAMETER FOR CATION 1
DBYHUK2	DEBYE HUCKEL PARAMETER FOR CATION 2
DHDX	GRADIENT OF THE GROUNDWATER IN THE X-DIRECTION ACROSS THE SPECIFIED BOUNDARY SEGMENT
DHDY	GRADIENT OF THE GROUNDWATER IN THE Y-DIRECTION ACROSS THE SPECIFIED BOUNDARY SEGMENT
DLTRAT	RATIO OF TRANSVERSE TO LONGITUDINAL DISPERSIVITY
HOI	INITIAL POTENTIOMETRIC HEAD AT THE SPECIFIED NODE(IN FEET)
HEAD	CALCULATED POTENTIOMETRIC HEAD AT THE END OF THE CURRENT TIME STEP AT THE SPECIFIED NODE(IN FEET)
HYDK	HYDRAULIC CONDUCTIVITY OF THE AQUIFER AT THE SPECIFIED NODE(IN FT/DAY)
IBAND	BANDWIDTH
ICT	INDICATOR VARIABLE FOR CONSERVATIVE/NONCONSERVATIVE TRANSPORT
IDELEM	ELEMENT IDENTIFICATION CODE FOR THE SPECIFIED ELEMENT
INT	CURRENT PUMPING PERIOD NUMBER
NBNDYI	NODE I OF THE SPECIFIED BOUNDARY SEGMENT
NBNDYJ	NODE J OF THE SPECIFIED BOUNDARY SEGMENT
NCODNP	NUMBER OF NODE IDENTIFICATION CODES
NI	NODE I OF THE SPECIFIED ELEMENT
NJ	NODE J OF THE SPECIFIED ELEMENT
NK	NODE K OF THE SPECIFIED ELEMENT
NODEID	NODE IDENTIFICATION NUMBER FOR THE SPECIFIED NODE
NPMP	NUMBER OF PUMPING PERIODS
NT	CURRENT TIME STEP NUMBER
NTIM	MAXIMUM NUMBER OF TIME STEPS
NUMBS	NUMBER OF BOUNDARY SEGMENTS
NUMEL	NUMBER OF ELEMENTS
NUMNP	NUMBER OF NODAL POINTS
PINT	LENGTH OF CURRENT PUMPING PERIOD(IN DAYS)
POROS	EFFECTIVE POROSITY OF THE AQUIFER
QINBDY	CUMULATIVE VOLUME OF WATER AS INFLOW ACROSS MODEL BOUNDARIES(IN FT**3)
QINCHN	CUMULATIVE VOLUME OF WATER RECHARGED THROUGH CONSTANT HEAD NODES(IN FT**3)
QINLEK	CUMULATIVE VOLUME OF WATER RECHARGED FROM VERTICAL LEAKAGE(IN FT**3)
QINRCH	CUMULATIVE VOLUME OF WATER RECHARGED FROM DISTRIBUTED SOURCES(IN FT**3)
QINREC	CUMULATIVE VOLUME OF WATER RECHARGED FROM POINT SOURCES(IN FT**3)
QOUTBDY	CUMULATIVE VOLUME OF WATER AS OUTFLOW ACROSS MODEL BOUNDARIES(IN FT**3)
QOUTCHN	CUMULATIVE VOLUME OF WATER DISCHARGED THROUGH CONSTANT HEAD NODES(IN FT**3)
QOUTLEK	CUMULATIVE VOLUME OF WATER DISCHARGED FROM VERTICAL LEAKAGE(IN FT**3)
QOUTRCH	CUMULATIVE VOLUME OF WATER DISCHARGED TO DISTRIBUTED SINKS(IN FT**3)
QOUTREC	CUMULATIVE VOLUME OF WATER DISCHARGED TO POINT SINKS(IN FT**3)
QSTOR	CHANGE IN VOLUME OF WATER STORED IN THE AQUIFER(IN FT**3)
REC	POINT SOURCE OR SINK AT THE SPECIFIED NODE(IN GPM)
RECH	DISTRIBUTED SOURCE OR SINK FOR SPECIFIED ELEMENT(IN FT**3/DAY/FT**2)
S	STORAGE COEFFICIENT OF THE AQUIFER
SK	SELECTIVITY COEFFICIENT(IN MEQ/L)
SUMT	TOTAL ELAPSED TIME(IN DAYS)
TDEL	LENGTH OF CURRENT TIME STEP(IN DAYS)
TDELMAX	MAXIMUM LENGTH FOR ANY TIME STEP(IN DAYS)
THCK	SATURATED THICKNESS OF THE AQUIFER AT THE SPECIFIED NODE(IN FEET)
TIM	POTENTIAL LENGTH OF CURRENT TIME STEP(IN DAYS)
TIMX	TIME STEP MULTIPLIER
TIMY	TOTAL ELAPSED TIME(IN YEARS)
TINIT	INITIAL TIME STEP(IN SECONDS)
TPDAY	TOTAL TIME AT THE END OF THE CURRENT PUMPING PERIOD(IN DAYS)
TITLE	OPTIONAL USER COMMENT
TRANS	TRANSMISSIVITY OF THE AQUIFER AT THE SPECIFIED NODE(IN FT**2/DAY)
VPRM	LEAKANCE DEFINED AS VERTICAL HYDRAULIC CONDUCTIVITY/THICKNESS OF CONFINING LAYER(IN FT/DAY/FT)
X	X-COORDINATE OF THE SPECIFIED NODE(IN FEET)
Y	Y-COORDINATE OF THE SPECIFIED NODE(IN FEET)
Z1	VALENCE OF CATION 1
Z2	VALENCE OF CATION 2

DEFINITION OF SELECTED PROGRAM VARIABLES

AREA	AREA OF THE SPECIFIED ELEMENT(IN FT**2)
ATOMWT1	ATOMIC WEIGHT OF CATION 1(IN GRAMS)
ATOMWT2	ATOMIC WEIGHT OF CATION 2(IN GRAMS)
BETA	LONGITUDINAL DISPERSIVITY OF THE AQUIFER(IN FEET)
CEC	CATION EXCHANGE CAPACITY OF THE AQUIFER AT THE SPECIFIED NODE (IN MEQ/L OF SOLUTION)
C1	CALCULATED DISSOLVED CONCENTRATION OF CATION 1 AT THE END OF THE CURRENT TIME PERIOD AT THE SPECIFIED NODE (IN MG/L)
C1HAT	CALCULATED ADSORBED CONCENTRATION OF CATION 1 AT THE END OF THE CURRENT TIME PERIOD AT THE SPECIFIED NODE (IN MG/L)
C1INBDY	CUMULATIVE MASS OF CATION 1 IN INFLOW ACROSS MODEL BOUNDARIES (IN MG/L*FT**3)
C1INCHN	CUMULATIVE MASS OF CATION 1 IN RECHARGE THROUGH CONSTANT HEAD NODES (IN MG/L*FT**3)
C1INLEK	CUMULATIVE MASS OF CATION 1 IN RECHARGE FROM VERTICAL LEAKAGE (IN MG/L*FT**3)
C1INRCH	CUMULATIVE MASS OF CATION 1 IN RECHARGE FROM DISTRIBUTED SOURCES (IN MG/L*FT**3)
C1INREC	CUMULATIVE MASS OF CATION 1 IN RECHARGE FROM POINT SOURCES (IN MG/L*FT**3)
C1ISTOR	INITIAL MASS OF CATION 1 STORED IN THE AQUIFER (IN MG/L*FT**3)
C1OTBDY	CUMULATIVE MASS OF CATION 1 IN OUTFLOW ACROSS MODEL BOUNDARIES (IN MG/L*FT**3)
C1OTCHN	CUMULATIVE MASS OF CATION 1 IN DISCHARGE THROUGH CONSTANT HEAD NODES (IN MG/L*FT**3)
C1OTLEK	CUMULATIVE MASS OF CATION 1 IN DISCHARGE FROM VERTICAL LEAKAGE (IN MG/L*FT**3)
C1OTRCH	CUMULATIVE MASS OF CATION 1 IN DISCHARGE TO DISTRIBUTED SINKS (IN MG/L*FT**3)
C1OTREC	CUMULATIVE MASS OF CATION 1 IN DISCHARGE TO POINT SINKS (IN MG/L*FT**3)
C1STOR	MASS OF CATION 1 STORED IN THE AQUIFER AT THE END OF THE CURRENT TIME PERIOD(IN MG/L*FT**3)
C2	CALCULATED DISSOLVED CONCENTRATION OF CATION 2 AT THE END OF THE CURRENT TIME PERIOD AT THE SPECIFIED NODE (IN MG/L)
C2HAT	CALCULATED ADSORBED CONCENTRATION OF CATION 2 AT THE END OF THE CURRENT TIME PERIOD AT THE SPECIFIED NODE (IN MG/L)
C2INBDY	CUMULATIVE MASS OF CATION 2 IN INFLOW ACROSS MODEL BOUNDARIES (IN MG/L*FT**3)
C2INCHN	CUMULATIVE MASS OF CATION 2 IN RECHARGE THROUGH CONSTANT HEAD NODES (IN MG/L*FT**3)
C2INLEK	CUMULATIVE MASS OF CATION 2 IN RECHARGE FROM VERTICAL LEAKAGE (IN MG/L*FT**3)
C2INRCH	CUMULATIVE MASS OF CATION 2 IN RECHARGE FROM DISTRIBUTED SOURCES (IN MG/L*FT**3)
C2INREC	CUMULATIVE MASS OF CATION 2 IN RECHARGE FROM POINT SOURCES (IN MG/L*FT**3)
C2ISTOR	INITIAL MASS OF CATION 2 STORED IN THE AQUIFER (IN MG/L*FT**3)
C2OTBDY	CUMULATIVE MASS OF CATION 2 IN OUTFLOW ACROSS MODEL BOUNDARIES (IN MG/L*FT**3)
C2OTCHN	CUMULATIVE MASS OF CATION 2 IN DISCHARGE THROUGH CONSTANT HEAD NODES (IN MG/L*FT**3)
C2OTLEK	CUMULATIVE MASS OF CATION 2 IN DISCHARGE FROM VERTICAL LEAKAGE (IN MG/L*FT**3)
C2OTRCH	CUMULATIVE MASS OF CATION 2 IN DISCHARGE TO DISTRIBUTED SINKS (IN MG/L*FT**3)
C2OTREC	CUMULATIVE MASS OF CATION 2 IN DISCHARGE TO POINT SINKS (IN MG/L*FT**3)
C2STOR	MASS OF CATION 2 STORED IN THE AQUIFER AT THE END OF THE CURRENT TIME PERIOD(IN MG/L*FT**3)
C1REC	CONCENTRATION OF CATION 1 IN POINT SOURCE OR SINK(IN MG/L)
C2REC	CONCENTRATION OF CATION 2 IN POINT SOURCE OR SINK(IN MG/L)
C1RECH	CONCENTRATION OF CATION 1 IN DISTRIBUTED SOURCE OR SINK(IN MG/L)
C2RECH	CONCENTRATION OF CATION 2 IN DISTRIBUTED SOURCE OR SINK(IN MG/L)
COSX	X-COMPONENT OF THE OUTWARD POINTING NORMAL FROM THE SPECIFIED BOUNDARY SEGMENT
COSY	Y-COMPONENT OF THE OUTWARD POINTING NORMAL FROM THE SPECIFIED

APPENDIX F. -- Data Deck Instructions

DATA DECK INSTRUCTIONS

The following group of cards is read by the first call of subroutine input.

Parameter Card	Format	Variable	Description
1	20A4	TITLE	Description of problem
2	20A4	TITLE	Optional user comment.
3	I5	ICT	Set ICT=0 for nonconservative transport. Set ICT>0 for conservative transport.
4	20A4	TITLE	Optional user comment.
5	3I5	NUMNP NUMEL NUMBS	Number of nodal points. Number of elements. Number of boundary segments.
6	20A4	TITLE	Optional user comment.
7	2I5,4F10.0	NTIM	Maximum number of time steps in a pumping period.
		NPMP	Number of pumping periods. Note that if NPMP>1 then update data must be provided.
		PINT	Length of first pumping period in days.
		TIMX	Time increment multiplier.
		TDELMAX	Maximum allowable time step in days.
		TINIT	Length of initial time step in seconds.
8	20A4	TITLE	Optional user comment.
9	8F10.0	S	Storage coefficient. Set S=0 for steady flow problems.
		POROS	Effective porosity.
		BETA	Longitudinal dispensivity in feet.
		DLTRAT	Ratio of transverse to longitudinal dispersivity.
		Z1	Valence of the first cation.
		Z2	Valence of the second cation. Note Z2 must $\geq$ Z1.
		ATOMWT1	Atomic weight in grams of cation 1.
		ATOMWT2	Atomic weight in grams of cation 2.
10	20A4	TITLE	Optional user comment.
11	3(F10.0)	DBYHUK1	Debye Huckel parameter for cation 1.
		DBYHUK2	Debye Huckel parameter for cation 2.
		SK	Selectivity coefficient.

Data Deck Instructions - continued

Data Set	Number of Cards	Format	Variable	Description
1	1	20A4	TITLE	Optional user comment.
	1	F10.0	FCTR	Multiplication factor for nodal coordinates read below. Set FCTR=1 if no data conversion is required.
	NUMNP/3	3(I5,2F10.0)	NP	Node number.
			X(NP)	X coordinate of node NP in feet.
			Y(NP)	Y coordinate of node NP in feet.
2	1	20A4	TITLE	Optional user comment.
	NUMEL/4	4(4I5)	NE	Element number.
			NI(NE)	Node I of element NE.
			NJ(NE)	Node J of element NE.
			NK(NE)	Node K of element NE. Note nodes must be sequenced in a counter-clockwise manner around the element.
3	1	20A4	TITLE	Optional user comment.
	NUMBS	2I5,4F10.0	NBNDYI(I)	Node I for boundary segment I.
			NBNDYJ(I)	Node J for boundary segment I.
			COSX(I)	Component of outward-pointing normal from boundary in x-direction for boundary segment I.
			COSY (I)	Component of outward-pointing normal from boundary in y-direction for boundary segment I.
			DHDX(I)	Gradient of the groundwater in the x-direction for boundary segment I.
			DHDY(I)	Gradient of the groundwater in the y-direction for boundary segment I. For no-flow boundary both DHDX=0 and DHDY=0.
4	1	20A4	TITLE	Optional user comment.
	1	I2	NCODEL	Number of element identification codes to be specified. If NCODEL=0 then program skips the remainder of data set 4.
	NUMEL/8	8(2I5)	NE	Element number.
			IDELEM(NE)	Element identification number. The IDELEM array is used to input diffuse recharge/discharge sources such as from infiltration of precipitation, evapotranspiration or from vertical leakage.

Data Deck Instructions - continued

Data Set	Number of Cards	Format	Variable	Description
	1	20A4	TITLE	Optional user comment.
	NCODEL	I5,4F10.0	ICODE	Element identification code.
			FCTR1	When IDELEM=ICODE, program sets
			FCTR2	diffuserecharge/discharge
			FCTR3	(RECH)=FCTR1 in Ft**3/day/
			FCTR4	Ft**2,concentration of species 1 in RECH(C1RECH)=FCTR2 in MG/L, concentration of species 2 in RECH(C2RECH)=FCTR3 in MG/L, and leakage (VPRM)= FCTR4 in Ft/day/Ft. Note recharge is (−) and discharge (+).
5	1	20A4	TITLE	Optional user comment.
	1	I2,F10.0	INP	*
			FCTR	*
	NUMNP/5*	5(I5,F10.0)	NP	Node number.
			THCK(NP)	Saturated thickness of aquifer at Node NP in feet.
6	1	20A4	TITLE	Optional user comment.
	1	I2,F10.0	INP	*
			FCTR	*
	NUMNP/5*	5(I5,F10.0)	NP	Node number.
			TRANS(NP)	Transmissivity of aquifer at node NP in Ft**2/day. Note, from saturated thickness and transmissivity data, program calculates the hydraulic conductivity of the aquifer.
7	1	20A4	TITLE	Optional user comment.
	1	I2,F10.0	INP	*
			FCTR	*
	NUMNP/5*	5(I5,F10.0)	NP	Node number.
			HEAD(NP)	Initial potentiometric head in the aquifer at node NP in feet.
8	1	20A4	TITLE	Optional user comment.
	1	I2,F10.0	INP	*
			FCT	*
	NUMNP/5*	5(I5,F0.0)	NP	Node number.
			C1(NP)	Initial concentration of cation 1 in the groundwater at node NP in MG/L.

Data Deck Instructions - continued

Data Set	Number of Cards	Format	Variable	Description
9	1	20A4	TITLE	Optional user comment.
	1	I2,F10.0	INP	*
			FCTR	*
	NUMNP/5*	5(I5,F10.0)	NP	Node number.
			C2(NP)	Initial concentration of cation 2 in the groundwater at node NP in MG/L. Note, from C1 and C2 data, program calculates adsorbed concentrations in the aquifer assuming equilibrium conditions.
10	1	20A4	TITLE	Optional user comment.
	1	I2,F10.0	INP	*
			FCTR	*
	NUMNP/5*	5(I5,F10.0)	NP	Node number.
			CEC(NP)	Cation exchange capacity of the aquifer at node NP in MEQ/Liter of solution.
11	1	20A4	TITLE	Optional user comment.
	1	I2	NCODNP	Number of node identification codes to be specified. If NCODNP=0 then program skips the remainder of data set 11.
	NUMNP/8	8(2I5)	NP	Node number.
			NODEID(NP)	Node identification number. The node ID array is used to input point recharge/discharge sources such as at wells, springs, etc.
	1	20A4	TITLE	Optional user comment.
	NCODNP	I5,3F10.0	ICODE	Node identification code. When NODEID=ICODE, program sets point recharge/discharge (REC)=FCTR1 in GPM, concentration of species 1 in REC (C1Rec)=FCTR2 in MG/L, concentration of species 2 in REC (C2REC)=FCTR3 in MG/L. Note recharge/injection is (−) and discharge/withdrawal is (+).
			FCTR1	
			FCTR2	
			FCTR3	

The following update data is read by additional calls of subroutine input. There should be 1 group of cards for each additional call or a total of (NPMP-1) groups.

Data Deck Instructions - continued

Parameter Card		Format	Variable	Description
1		20A4	TITLE	Description of pumping period.
2		20A4	TITLE	Optional user comment.
3		F10.0	PINT	Length of current pumping period in days.

Data Set	Number of Cards	Format	Variable	Description
1	1	20A4	TITLE	Optional user comment.
	NUMNP/8	8(2I5)	NP	Update of node ID array.
			NODEID(NP)	See above description in data set 11.
	1	20A4	TITLE	Optional user comment.
	NCODNP	I5,3F10.0	ICODE	Update node identification
			FCTR1	codes. See above des-
			FCTR2	cription in data set 11.
			FCTR3	

*This parameter card preceeds the indicated data sets. It is used to specify whether the parameter is constant and uniform, and can be defined by a single value, or whether it varies in space and must be defined at each node. If INP=0, the data set has a constant value, which is defined by FCTR, and the program skips the remainder of the data set. If INP≠0, then FCTR is used as a multiplication factor for the values read in the data set. Set FCTR=1 if no data conversion is required.

APPENDIX G. -- Sample Data Deck

INPUT DATA FOR SAMPLE OUTPUT

```
EXAMPLE DATA
ICT (I5)
    0
NUMNP,NUMEL,NUMBS (3I5)
   35    50    18
NTIM,NPMP,FINT,TIMX,TDELMAX,TINIT (2I5,4F10.0)
  200    02        1.0         1.5        0.5         60.
S,POROS,BETA,DLTRAT,Z1,Z2,ATOMWT1,ATOMWT2 (8F10.)
   .00003           .35         20.         .3          1.         2.       18.04      40.09
DBYHUK1,DBYHUK2,SK (3F10.0)
          3.          6.        38.0
NODAL COORDINATES (F10.0),3(I5,2F10.0)
          1.
    1         0.        120.    2        40.        120.    3        80.        120.
    4       120.        120.    5         0.        100.    6        30.        100.
    7        60.        100.    8        90.        100.    9       120.        100.
   10         0.         80.   11        20.         80.   12        40.         80.
   13        80.         80.   14       100.         80.   15       120.         80.
   16         0.         60.   17        30.         60.   18        60.         60.
   19        90.         60.   20       120.         60.   21         0.         40.
   22        20.         40.   23        40.         40.   24        80.         40.
   25       100.         40.   26       120.         40.   27         0.         20.
   28        30.         20.   29        60.         20.   30        90.         20.
   31       120.         20.   32         0.          0.   33        40.          0.
   34        80.          0.   35       120.          0.
ELEMENT VERTICES 4(4I5)
    1    5    6    1    2    6    2    1    3    6    7    2    4    7    3    2
    5    7    8    3    6    8    4    3    7    8    9    4    8   10   11    5
    9   11    6    5   10   11   12    6   11   12    7    6   12   12   13    7
   13   13    8    7   14   13   14    8   15   14    9    8   16   14   15    9
   17   16   11   10   18   16   17   11   19   17   12   11   20   17   18   12
   21   18   13   12   22   18   19   13   23   19   14   13   24   19   20   14
   25   20   15   14   26   21   22   16   27   22   17   16   28   22   23   17
   29   23   18   17   30   23   24   18   31   24   19   18   32   24   25   19
   33   25   20   19   34   25   26   20   35   27   22   21   36   27   28   22
   37   28   23   22   38   28   29   23   39   29   24   23   40   29   30   24
   41   30   25   24   42   30   31   25   43   31   26   25   44   32   28   27
   45   32   33   28   46   33   29   28   47   33   34   29   48   34   30   29
   49   34   35   30   50   35   31   30
BOUNDARY SEGMENTS, DIRECTIONAL COSINES AND BOUNDARY GRADIENTS (2I5,4F10.0)
    1    2        0.          1.          0.          0.
    2    3        0.          1.          0.          0.
    3    4        0.          1.          0.          0.
    4    9        1.          0.          0.          0.
    9   15        1.          0.          0.          0.
   15   20        1.          0.          0.          0.
   20   26        1.          0.          0.          0.
   26   31        1.          0.          0.          0.
   31   35        1.          0.          0.          0.
   35   34        0.         -1.          0.          0.
   34   33        0.         -1.          0.          0.
   33   32        0.         -1.          0.          0.
   32   27       -1.          0.          0.          0.
   27   21       -1.          0.          0.          0.
   21   16       -1.          0.          0.          0.
   16   10       -1.          0.          0.          0.
   10    5       -1.          0.          0.          0.
    5    1       -1.          0.          0.          0.
IDELEM ARRAY (I2),8(2I5)
 3
    1    0    2    0    3    0    4    0    5    0    6    0    7    0    8    0
    9    0   10    0   11    0   12    0   13    0   14    0   15    0   16    0
   17    0   18    0   19    0   20    0   21    0   22    0   23    0   24    0
   25    0   26    0   27    0   28    0   29    0   30    0   31    0   32    0
   33    0   34    0   35    0   36    0   37    0   38    0   39    0   40    0
   41    0   42    0   43    0   44    0   45    0   46    0   47    0   48    0
   49    0   50    0
ICODE,FCTR1,FCTR2,FCTR3,FCTR4 (I5,4F10.0)
    1        0.          0.          0.          0.
```

INPUT DATA FOR SAMPLE OUTPUT--CONTINUED

```
    2         0.          0.          0.          0.
    3         0.          0.          0.          0.
AQUIFER THICKNESS ARRAY (I2,F10.0),5(I5,F10.0)
         50.
TRANSMISSIVITY ARRAY (I2,F10.0),5(I5,F10.0)
        100.
INITIAL HEAD ARRAY (I2,F10.0),5(I5,F10.0)
  1        1.
    1        50.     2        50.     3        50.     4        50.     5        49.5
    6        49.5    7        49.5    8        49.5    9        49.5   10        49.
   11        49.    12        49.    13        49.    14        49.    15        49.
   16        48.5   17        48.5   18        48.5   19        48.5   20        48.5
   21        48.    22        48.    23        48.    24        48.    25        48.
   26        48.    27        47.5   28        47.5   29        47.5   30        47.5
   31        47.5   32        47.    33        47.    34        47.    35        47.
INITIAL CONCENTRATION C1 ARRAY (I2,F10.0),5(I5,F10.0)
        200.
INITIAL CONCENTRATION C2 ARRAY (I2,F10.0),5(I5,F10.0)
        200.
CATION EXCHANGE CAPACITY ARRAY (I2,F10.0),5(I5,F10.0)
        300.
NODEID ARRAY (I2),8(2I5)
 20
    1   1    2   1    3   1    4   1    5   1    6   0    7   0    8   0
    9   1   10   1   11   0   12   0   13   0   14   0   15   1   16   1
   17   0   18  16   19   0   20   1   21   1   22   0   23   0   24   0
   25   1   26   1   27   1   28   0   29   0   30   0   31   1   32   1
   33   1   34   1   35   1
ICODE,FCTR1,FCTR2,FCTR3 (I5,3F10.0)
    1        0.       200.       200.
    2        0.         0.         0.
    3        0.         0.         0.
    4        0.         0.         0.
    5        0.         0.         0.
    6        0.         0.         0.
    7        0.         0.         0.
    8        0.         0.         0.
    9        0.         0.         0.
   10        0.         0.         0.
   11        0.         0.         0.
   12        0.         0.         0.
   13        0.         0.         0.
   14        0.         0.         0.
   15        0.         0.         0.
   16       -5.      1000.         0.
   17        0.         0.         0.
   18        0.         0.         0.
   19        0.         0.         0.
   20        0.         0.         0.
PUMPING PERIOD 2
PINT (F10.0)
        .5
NODEID ARRAY 8(2I5)
    1   1    2   1    3   1    4   1    5   0    6   0    7   0    8   0
    9   0   10   0   11   0   12   0   13   0   14   0   15   0   16   0
   17   0   18  16   19   0   20   0   21   0   22   0   23   0   24   0
   25   0   26   0   27   0   28   0   29   0   30   0   31   0   32   1
   33   1   34   1   35   1
ICODE,FCTR1,FCTR2,FCTR3 (I5,3F10.0)
    1        0.       200.       200.
    2        0.         0.         0.
    3        0.         0.         0.
    4        0.         0.         0.
    5        0.         0.         0.
    6        0.         0.         0.
    7        0.         0.         0.
    8        0.         0.         0.
    9        0.         0.         0.
   10        0.         0.         0.
```

INPUT DATA FOR SAMPLE OUTPUT--CONTINUED

11	0.	0.	0.
12	0.	0.	0.
13	0.	0.	0.
14	0.	0.	0.
15	0.	0.	0.
16	-10.	500.	0.
17	0.	0.	0.
18	0.	0.	0.
19	0.	0.	0.
20	0.	0.	0.

APPENDIX H. -- Sample Output From Computer Program

2-DIMENSIONAL MASS TRANSPORT IN FLOWING GROUNDWATER FOR 2 REACTING SOLUTES SUBJECT TO BINARY CATION EXCHANGE
NUMERICAL SOLUTION BY THE GALERKIN FINITE ELEMENT METHOD USING TRIANGULAR ELEMENTS AND LINEAR SHAPE FUNCTIONS
WRITTEN AND PROGRAMMED BY JAMES WARNER

EXAMPLE DATA

NONCONSERVATIVE TRANSPORT(ICT=0)

INPUT DATA

ELEMENT DISCRIPTORS

NUMNP	(NUMBER OF NODAL POINTS)	=	35
NUMEL	(NUMBER OF ELEMENTS)	=	50
NUMES	(NUMBER OF BOUNDARY SEGMENTS)	=	18

TIME PARAMETERS

NTIM	(MAXIMUM NUMBER OF TIME STEPS)	=	200
NPMP	(NUMBER OF PUMPING PERIODS)	=	2
PINT	(FIRST PUMPING PERIOD IN DAYS)	=	1.00
TIMX	(TIME INCREMENT MULTIPLIER)	=	1.50
TDELMAX	(MAXIMUM TIME STEP IN DAYS)	=	.50
TINIT	(INITIAL TIME STEP IN SECONDS)	=	60.

HYDROLOGIC AND CHEMICAL PARAMETERS

S	(STORAGE COEFFICIENT)	=	.00003
POROS	(EFFECTIVE POROSITY)	=	.35000
BETA	(LONGITUDINAL DISPERSIVITY IN FT)	=	20.0
DLTRAT	(RATIO OF TRANSVERSE TO LONGITUDINAL DISPERSIVITY)	=	.30
Z1	(VALENCE OF SPECIES 1)	=	1.
Z2	(VALENCE OF SPECIES 2)	=	2.
ATOMWT1	(ATOMIC WEIGHT IN GRAMS OF SPECIES 1)	=	18.040
ATOMWT2	(ATOMIC WEIGHT IN GRAMS OF SPECIES 2)	=	40.080
DBYHUK1	(DEBYE HUCKEL PARAMETER FOR SPECIES 1)	=	3.
DBYHUK2	(DEBYE HUCKEL PARAMETER FOR SPECIES 2)	=	6.
SK	(SELECTIVITY COEFFICIENT)	=	38.00000

I N P U T   D A T A

NODE COORDINATES

NODE	X LOC	Y LOC	NODE	X LOC	Y LOC	NODE	X LOC	Y LOC
1	0.00	120.00	2	40.00	120.00	3	80.00	120.00
4	120.00	120.00	5	0.00	100.00	6	30.00	100.00
7	60.00	100.00	8	90.00	100.00	9	120.00	100.00
10	0.00	80.00	11	20.00	80.00	12	40.00	80.00
13	80.00	80.00	14	100.00	80.00	15	120.00	80.00
16	0.00	60.00	17	30.00	60.00	18	60.00	60.00
19	90.00	60.00	20	120.00	60.00	21	0.00	40.00
22	20.00	40.00	23	40.00	40.00	24	80.00	40.00
25	100.00	40.00	26	120.00	40.00	27	0.00	20.00
28	30.00	20.00	29	60.00	20.00	30	90.00	20.00
31	120.00	20.00	32	0.00	0.00	33	40.00	0.00
34	80.00	0.00	35	120.00	0.00			

I N P U T   D A T A

ELEMENT VERTICES

ELEMENT	NODE I	NODE J	NODE K	ELEMENT	NODE I	NODE J	NODE K	ELEMENT	NODE I	NODE J	NODE K
1	5	6	1	2	6	2	1	3	6	7	2
4	7	3	2	5	7	8	3	6	8	4	3
7	8	9	4	8	10	11	5	9	11	6	5
10	11	12	6	11	12	7	6	12	12	13	7
13	13	8	7	14	13	14	8	15	14	9	8
16	14	15	9	17	16	11	10	18	16	17	11
19	17	12	11	20	17	18	12	21	18	13	12
22	18	19	13	23	19	14	13	24	19	20	14
25	20	15	14	26	21	22	16	27	22	17	16
28	22	23	17	29	23	18	17	30	23	24	18
31	24	19	18	32	24	25	19	33	25	20	19
34	25	26	20	35	27	22	21	36	27	28	22
37	28	23	22	38	28	29	23	39	29	24	23
40	29	30	24	41	30	25	24	42	30	31	25
43	31	26	25	44	32	28	27	45	32	33	28
46	33	29	28	47	33	34	29	48	34	30	29
49	34	35	30	50	35	31	30				

BANDWIDTH =   7

INPUT   DATA

BOUNDARY

SEGMENT NODE - NODE	LX	LY	DHDX	DHDY	SEGMENT NODE - NODE	LX	LY	DHDX	DHDY
1 - 2	0.0000	1.0000	0.0000	0.0000	2 - 3	0.0000	1.0000	0.0000	0.0000
3 - 4	0.0000	1.0000	0.0000	0.0000	4 - 9	1.0000	0.0000	0.0000	0.0000
9 - 15	1.0000	0.0000	0.0000	0.0000	15 - 20	1.0000	0.0000	0.0000	0.0000
20 - 26	1.0000	0.0000	0.0000	0.0000	26 - 31	1.0000	0.0000	0.0000	0.0000
31 - 35	1.0000	0.0000	0.0000	0.0000	35 - 34	0.0000	-1.0000	0.0000	0.0000
34 - 33	0.0000	-1.0000	0.0000	0.0000	33 - 32	0.0000	-1.0000	0.0000	0.0000
32 - 27	-1.0000	0.0000	0.0000	0.0000	27 - 21	-1.0000	0.0000	0.0000	0.0000
21 - 16	-1.0000	0.0000	0.0000	0.0000	16 - 10	-1.0000	0.0000	0.0000	0.0000
10 - 5	-1.0000	0.0000	0.0000	0.0000	5 - 1	-1.0000	0.0000	0.0000	0.0000

```
                                      I N P U T    D A T A
                                      ------------------------


ELEMENT IDENTIFICATION
----------------------

                   NUMBER OF
       ELEM ID     OCCURENCES        RECH          C1RECH         C2RECH         VPRM
          1            0             0.             0.             C.             0.
          2            0             0.             0.             C.             0.
          3            0             0.             0.             C.             0.
```

I N P U T   D A T A

ELEMENT DATA

ELEMENT	AREA	ELEM ID		ELEMENT	AREA	ELEM ID		ELEMENT	AREA	ELEM ID
1	300.8	0		2	400.0	0		3	300.0	0
4	400.0	0		5	300.0	0		6	400.0	0
7	300.0	0		8	200.0	0		9	300.0	0
10	200.0	0		11	300.0	0		12	400.0	0
13	300.0	0		14	200.0	0		15	300.0	0
16	200.0	0		17	200.0	0		18	300.0	0
19	200.0	0		20	300.0	0		21	400.0	0
22	300.8	0		23	200.0	0		24	300.0	0
25	200.0	0		26	200.0	0		27	300.0	0
28	200.0	0		29	300.0	0		30	400.0	0
31	300.8	0		32	200.0	0		33	300.0	0
34	200.0	0		35	200.0	0		36	300.0	0
37	200.0	0		38	300.0	0		39	400.0	0
40	300.8	0		41	200.0	0		42	300.0	0
43	200.0	0		44	300.0	0		45	400.0	0
46	300.8	0		47	400.0	0		48	300.0	0
49	400.0	0		50	300.0	0				

MODEL AREA(FT**2)=   14400.00

NODE IDENTIFICATION

NODE ID	NUMBER OF OCCURENCES	REC	C1REC	C2REC
1	18	0.	200.	200.
2	0	0.	0.	0.
3	0	0.	0.	0.
4	0	0.	0.	0.
5	0	0.	0.	0.
6	0	0.	0.	0.
7	0	0.	0.	0.
8	0	0.	0.	0.
9	0	0.	0.	0.
10	0	0.	0.	0.
11	0	0.	0.	0.
12	0	0.	0.	0.
13	0	0.	0.	0.
14	0	0.	0.	0.
15	0	0.	0.	0.
16	1	-5.	1000.	0.
17	0	0.	0.	0.
18	0	0.	0.	0.
19	0	0.	0.	0.
20	0	0.	0.	0.

I N P U T   D A T A

NOCE DATA

NODE	TRANSMISSIVITY	HYDRAULIC CONDUCTIVITY	THICKNESS	CATION EXCHANGE CAPACITY(MEQ/L)	NODE ID
1	100.00	2.000	50.00	300.0	1
2	100.00	2.000	50.00	300.0	1
3	100.00	2.000	50.00	300.0	1
4	100.00	2.000	50.00	300.0	1
5	100.00	2.000	50.00	300.0	1
6	100.00	2.000	50.00	300.0	0
7	100.00	2.000	50.00	300.0	0
8	100.00	2.000	50.00	300.0	0
9	100.00	2.000	50.00	300.0	1
10	100.00	2.000	50.00	300.0	1
11	100.00	2.000	50.00	300.0	0
12	100.00	2.000	50.00	300.0	0
13	100.00	2.000	50.00	300.0	0
14	100.00	2.000	50.00	300.0	0
15	100.00	2.000	50.00	300.0	1
16	100.00	2.000	50.00	300.0	1
17	100.00	2.000	50.00	300.0	0
18	100.00	2.000	50.00	300.0	16
19	100.00	2.000	50.00	300.0	0
20	100.00	2.000	50.00	300.0	1
21	100.00	2.000	50.00	300.0	1
22	100.00	2.000	50.00	300.0	0
23	100.00	2.000	50.00	300.0	0
24	100.00	2.000	50.00	300.0	0
25	100.00	2.000	50.00	300.0	0
26	100.00	2.000	50.00	300.0	1
27	100.00	2.000	50.00	300.0	1
28	100.00	2.000	50.00	300.0	0
29	100.00	2.000	50.00	300.0	0
30	100.00	2.000	50.00	300.0	0
31	100.00	2.000	50.00	300.0	1
32	100.00	2.000	50.00	300.0	1
33	100.00	2.000	50.00	300.0	1
34	100.00	2.000	50.00	300.0	1
35	100.00	2.000	50.00	300.0	1

INITIAL NODE DATA

NODE	HEAD	SOLUTE C1(MG/L)	SOLUTE C2(MG/L)	ADSORBED C1HAT/CEC	ADSORBED C2HAT/CEC	ADSORBED C1HAT (MG/L)	ADSORBED C2HAT (MG/L)
1	50.0	200.000	200.000	.469	.531	2540.083	3190.306
2	50.0	200.000	200.000	.469	.531	2540.083	3190.306
3	50.0	200.000	200.000	.469	.531	2540.083	3190.306
4	50.0	200.000	200.000	.469	.531	2540.083	3190.306
5	49.5	200.000	200.000	.469	.531	2540.083	3190.306
6	49.5	200.000	200.000	.469	.531	2540.083	3190.306
7	49.5	200.000	200.000	.469	.531	2540.083	3190.306
8	49.5	200.000	200.000	.469	.531	2540.083	3190.306
9	49.5	200.000	200.000	.469	.531	2540.083	3190.306
10	49.0	200.000	200.000	.469	.531	2540.083	3190.306
11	49.0	200.000	200.000	.469	.531	2540.083	3190.306
12	49.0	200.000	200.000	.469	.531	2540.083	3190.306
13	49.0	200.000	200.000	.469	.531	2540.083	3190.306
14	49.0	200.000	200.000	.469	.531	2540.083	3190.306
15	49.0	200.000	200.000	.469	.531	2540.083	3190.306
16	48.5	200.000	200.000	.469	.531	2540.083	3190.306
17	48.5	200.000	200.000	.469	.531	2540.083	3190.306
18	48.5	200.000	200.000	.469	.531	2540.083	3190.306
19	48.5	200.000	200.000	.469	.531	2540.083	3190.306
20	48.5	200.000	200.000	.469	.531	2540.083	3190.306
21	48.0	200.000	200.000	.469	.531	2540.083	3190.306
22	48.0	200.000	200.000	.469	.531	2540.083	3190.306
23	48.0	200.000	200.000	.469	.531	2540.083	3190.306
24	48.0	200.000	200.000	.469	.531	2540.083	3190.306
25	48.0	200.000	200.000	.469	.531	2540.083	3190.306
26	48.0	200.000	200.000	.469	.531	2540.083	3190.306
27	47.5	200.000	200.000	.469	.531	2540.083	3190.306
28	47.5	200.000	200.000	.469	.531	2540.083	3190.306
29	47.5	200.000	200.000	.469	.531	2540.083	3190.306
30	47.5	200.000	200.000	.469	.531	2540.083	3190.306
31	47.5	200.000	200.000	.469	.531	2540.083	3190.306
32	47.0	200.000	200.000	.469	.531	2540.083	3190.306
33	47.0	200.000	200.000	.469	.531	2540.083	3190.306
34	47.0	200.000	200.000	.469	.531	2540.083	3190.306
35	47.0	200.000	200.000	.469	.531	2540.083	3190.306

```
MATFLOW ITERATIONS=   9        TIME=    .0006944
MATCHEM ITERATIONS=   1        TIME=    .0006944

MATFLOW ITERATIONS=   7        TIME=    .0017361
MATCHEM ITERATIONS=   1        TIME=    .0017361

MATFLOW ITERATIONS=   4        TIME=    .0032986
MATCHEM ITERATIONS=   1        TIME=    .0032986

MATFLOW ITERATIONS=   1        TIME=    .0056424
MATCHEM ITERATIONS=   1        TIME=    .0056424

MATFLOW ITERATIONS=   1        TIME=    .0091580
MATCHEM ITERATIONS=   1        TIME=    .0091580

MATFLOW ITERATIONS=   1        TIME=    .0144314
MATCHEM ITERATIONS=   2        TIME=    .0144314

MATFLOW ITERATIONS=   1        TIME=    .0223416
MATCHEM ITERATIONS=   3        TIME=    .0223416

MATFLOW ITERATIONS=   1        TIME=    .0342068
MATCHEM ITERATIONS=   4        TIME=    .0342068

MATFLOW ITERATIONS=   1        TIME=    .0520047
MATCHEM ITERATIONS=   6        TIME=    .0520047

MATFLOW ITERATIONS=   1        TIME=    .0787014
MATCHEM ITERATIONS=   7        TIME=    .0787014

MATFLOW ITERATIONS=   1        TIME=    .1187466
MATCHEM ITERATIONS=   8        TIME=    .1187466

MATFLOW ITERATIONS=   1        TIME=    .1788144
MATCHEM ITERATIONS=  10        TIME=    .1788144

MATFLOW ITERATIONS=   1        TIME=    .2689160
MATCHEM ITERATIONS=  11        TIME=    .2689160

MATFLOW ITERATIONS=   1        TIME=    .4040684
MATCHEM ITERATIONS=  12        TIME=    .4040684

MATFLOW ITERATIONS=   1        TIME=    .6067971
MATCHEM ITERATIONS=  13        TIME=    .6067971

MATFLOW ITERATIONS=   1        TIME=    .9108900
MATCHEM ITERATIONS=  13        TIME=    .9108900

MATFLOW ITERATIONS=   1        TIME=   1.0000000
MATCHEM ITERATIONS=  10        TIME=   1.0000000
```

HEAD DISTRIBUTION -- FT

TIME(DAYS) =   1.000
TIME(YEARS)=   .00274

NODE	HEAD	NODE	HEAD	NODE	HEAD	NODE	HEAD
1	50.000	2	50.000	3	50.000	4	50.000
5	49.500	6	49.933	7	50.129	8	49.933
9	49.500	10	49.000	11	49.585	12	50.346
13	50.346	14	49.585	15	49.000	16	48.500
17	49.648	18	52.435	19	49.648	20	48.500
21	48.000	22	48.585	23	49.346	24	49.346
25	48.585	26	48.000	27	47.500	28	47.933
29	48.129	30	47.933	31	47.500	32	47.000
33	47.000	34	47.000	35	47.000		

DRAWDOWN DISTRIBUTION -- FT

TIME(DAYS) =   1.000
TIME(YEARS)=   .00274

NODE	DRAWDOWN	NODE	DRAWDOWN	NODE	DRAWDOWN	NODE	DRAWDOWN
1	0.000	2	0.000	3	0.000	4	0.000
5	0.000	6	-.433	7	-.629	8	-.433
9	0.000	10	0.000	11	-.585	12	-1.346
13	-1.346	14	-.585	15	0.000	16	0.000
17	-1.148	18	-3.935	19	-1.148	20	0.000
21	0.000	22	-.585	23	-1.346	24	-1.346
25	-.585	26	0.000	27	0.000	28	-.433
29	-.629	30	-.433	31	0.000	32	0.000
33	0.000	34	0.000	35	0.000		

CUMULATIVE WATER BALANCE -- FT**3

TIME(DAYS) =   1.000
TIME(YEARS)=   .00274

                QINRCH   (RECHARGE-DISTRIBUTED)   =   0.000
                GOUTRCH (DISCHARGE-DISTRIBUTED)   =   0.000

                QINREC   (RECHARGE-POINT)   =   -962.500
                QOUTREC (DISCHARGE-POINT)   =   0.000

                QINLEK   (RECHARGE-LEAKAGE)   =   0.000
                QOUTLEK (DISCHARGE-LEAKAGE)   =   0.000

                QINBDY   (RECHARGE-BOUNDARY)   =   0.000
                GOUTBDY (DISCHARGE-BOUNDARY)   =   0.000

                QINCHN   (RECHARGE-CONST HEAD NODES)   =   -78.469
                GOUTCHN (DISCHARGE-CONST HEAD NODES) =   1040.296

                               TOTAL QIN   =   -1040.969
                               TOTAL GOUT   =   1040.296

                GSTOR   (WATER RELEASED FROM STORAGE) =   -.301

                        MASS BALANCE RESIDUAL   =   .372
                        ERROR AS PERCENT OF QIN   =   .036
                        ERROR AS PERCENT OF QOUT   =   .036
                        ERROR AS PERCENT OF GSTOR   =   123.286

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```
FLOW BY NODE ID -- GPM
-----------------------

    QIN (  1)=            -.407
    QOUT(  1)=            5.407

    QIN ( 16)=           -5.000
    QOUT( 16)=            0.000


FLOW FROM CONSTANT HEAD NODES -- GPM
POSITIVE IS DISCHARGE (PUMPAGE)
NEGATIVE IS RECHARGE (INJECTION)
NODE(  1)=               -.204
NODE(  2)=                .007
NODE(  3)=                .007
NODE(  4)=               -.204
NODE(  5)=                .188
NODE(  9)=                .188
NODE( 10)=                .304
NODE( 15)=                .304
NODE( 16)=                .351
NODE( 20)=                .351
NODE( 21)=                .304
NODE( 26)=                .304
NODE( 27)=                .188
NODE( 31)=                .188
NODE( 32)=                .316
NODE( 33)=               1.046
NODE( 34)=               1.046
NODE( 35)=                .316
```

SOLUTE CONCENTRATION OF SPECIES 1 (C1) -- MG/L

TIME(DAYS) =   1.000
TIME(YEARS)=   .00274

NODE	CONC	NODE	CONC	NODE	CONC	NODE	CONC
1	200.128	2	199.284	3	199.284	4	200.128
5	199.366	6	200.409	7	202.196	8	200.409
9	199.366	10	199.043	11	201.866	12	194.004
13	194.004	14	201.866	15	199.042	16	201.128
17	193.636	18	242.741	19	193.636	20	201.128
21	199.129	22	201.682	23	194.594	24	194.595
25	201.682	26	199.129	27	199.479	28	200.301
29	201.808	30	200.301	31	199.479	32	200.109
33	199.471	34	199.471	35	200.109		

SOLUTE CONCENTRATION OF SPECIES 2 (C2) -- MG/L

TIME(DAYS) =   1.000
TIME(YEARS)=   .00274

NODE	CONC	NODE	CONC	NODE	CONC	NODE	CONC
1	200.171	2	199.002	3	199.002	4	200.171
5	199.122	6	200.573	7	203.070	8	200.573
9	199.122	10	198.724	11	202.573	12	191.562
13	191.563	14	202.573	15	198.723	16	201.614
17	190.924	18	262.645	19	190.924	20	201.614
21	198.895	22	202.212	23	192.726	24	192.726
25	202.211	26	198.893	27	199.343	28	200.362
29	202.306	30	200.362	31	199.343	32	200.134
33	199.370	34	199.370	35	200.134		

EQUIVALENT FRACTION ADSORBED OF SPECIES 1 (C1HAT/CEC) -- DIMENSIONLESS

TIME(DAYS) =   1.000
TIME(YEARS)=   .00274

NODE	CONC	NODE	CONC	NODE	CONC	NODE	CONC
1	.469	2	.469	3	.469	4	.469
5	.469	6	.470	7	.471	8	.470
9	.469	10	.469	11	.470	12	.466
13	.466	14	.470	15	.469	16	.470
17	.466	18	.491	19	.466	20	.470
21	.469	22	.470	23	.466	24	.466
25	.470	26	.469	27	.469	28	.470
29	.471	30	.470	31	.469	32	.469
33	.469	34	.469	35	.469		

EQUIVALENT FRACTION ADSORBED OF SPECIES 2 (C2HAT/CEC) -- DIMENSIONLESS

TIME(DAYS) =   1.000
TIME(YEARS)=   .00274

NODE	CONC	NODE	CONC	NODE	CONC	NODE	CONC
1	.531	2	.531	3	.531	4	.531
5	.531	6	.530	7	.529	8	.530
9	.531	10	.531	11	.530	12	.534
13	.534	14	.530	15	.531	16	.530
17	.534	18	.509	19	.534	20	.530
21	.531	22	.530	23	.534	24	.534
25	.530	26	.531	27	.531	28	.530
29	.529	30	.530	31	.531	32	.531
33	.531	34	.531	35	.531		

ADSORBED CONCENTRATION OF SPECIES 1 (C1HAT) -- MG/L

TIME(DAYS) =   1.000
TIME(YEARS)=   .00274

NODE	CONC	NODE	CONC	NODE	CONC	NODE	CONC
1	2540.514	2	2537.876	3	2537.876	4	2540.514
5	2538.109	6	2541.336	7	2546.816	8	2541.336
9	2538.109	10	2536.885	11	2545.954	12	2521.910
13	2521.910	14	2545.954	15	2536.885	16	2543.393
17	2521.324	18	2658.676	19	2521.324	20	2543.393
21	2536.944	22	2545.829	23	2522.255	24	2522.255
25	2545.829	26	2536.944	27	2538.185	28	2541.263
29	2546.550	30	2541.263	31	2538.185	32	2540.501
33	2538.004	34	2538.004	35	2540.501		

ADSORBED CONCENTRATION OF SPECIES 2 (C2HAT) -- MG/L

TIME(DAYS) =   1.000
TIME(YEARS)=   .00274

NODE	CONC	NODE	CONC	NODE	CONC	NODE	CONC
1	3189.832	2	3192.763	3	3192.763	4	3189.832
5	3192.504	6	3188.920	7	3182.831	8	3188.920
9	3192.504	10	3193.863	11	3183.789	12	3210.499
13	3210.499	14	3183.789	15	3193.864	16	3186.634
17	3211.150	18	3058.570	19	3211.150	20	3186.634
21	3193.798	22	3183.928	23	3210.116	24	3210.116
25	3183.928	26	3193.799	27	3192.420	28	3189.001
29	3183.128	30	3189.001	31	3192.420	32	3189.847
33	3192.621	34	3192.621	35	3189.847		

CUMULATIVE CHEMICAL BALANCE FOR SPECIES 1 (C1&C1HAT) -- MG/L*FT**3

TIME(DAYS) =   1.000
TIME(YEARS)=   .00274

```
        C1INRCH (DISTRIBUTED RECHARGE)       =          0.000
        C1OTRCH (DISTRIBUTED DISCHARGE)      =          0.000

        C1INREC (POINT RECHARGE)             =    -962499.933
        C1OTREC (POINT DISCHARGE)            =          0.000

        C1INLEK (RECHARGE-LEAKAGE)           =          0.000
        C1OTLEK (DISCHARGE-LEAKAGE)          =          0.000

        C1INCHN (RECHARGE-CONST HEAD NODES)  =     -15693.809
        C1OTCHN (DISCHARGE-CONST HEAD NODES) =     207828.152

        C1INBDY (INFLOW-MODEL BOUNDARY)      =          0.000
        C1OTBDY (OUTFLOW-MODEL BOUNDARY)     =          0.000
                                                 ------------
                        TOTAL C1IN           =    -978193.742
                        TOTAL C1OUT          =     207828.152

    C1STOR  (PRESENT MASS STORED)      =     691337762.701
    C1ISTOR (INITIAL MASS STORED)      =     690502127.265
                                             ------------
    C1DELST (CHANGE IN MASS STORED)    =        835635.436


        MASS BALANCE RESIDUAL            =       65269.846
        ERROR AS PERCENT OF C1IN         =           6.672
        ERROR AS PERCENT OF C1OUT        =          31.406
        ERROR AS PERCENT OF C1DELST      =           7.811
        ERROR AS PERCENT OF C1ISTOR      =            .009
```

CUMULATIVE CHEMICAL BALANCE FOR SPECIES 2 (C2&C2HAT) -- MG/L*FT**3

TIME(DAYS) =   1.000
TIME(YEARS)=   .00274

```
          C2INRCH (DISTRIBUTED RECHARGE)        =          0.000
          C2OTRCH (DISTRIBUTED DISCHARGE)       =          0.000

          C2INREC (POINT RECHARGE)              =          0.000
          C2OTREC (POINT DISCHARGE)             =          0.000

          C2INLEK (RECHARGE-LEAKAGE)            =          0.000
          C2OTLEK (DISCHARGE-LEAKAGE)           =          0.000

          C2INCHN (RECHARGE-CONST HEAD NODES)   =      -15693.809
          C2OTCHN (DISCHARGE-CONST HEAD NODES)  =      207761.934

          C2INBOY (INFLOW-MODEL BOUNDARY)       =          0.000
          C2OTBOY (OUTFLOW-MODEL BOUNDARY)      =          0.000
                                                        ------------
                        TOTAL C2IN     =      -15693.809
                        TOTAL C2OUT    =      207761.934

      C2STOR  (PRESENT MASS STORED)    =     854062195.327
      C2ISTOR (INITIAL MASS STORED)    =     854357113.615
                                             ------------
      C2DELST (CHANGE IN MASS STORED)  =      -294918.288


                MASS BALANCE RESIDUAL       =      102850.163
                ERROR AS PERCENT OF C2IN    =         655.355
                ERROR AS PERCENT OF C2OUT   =          49.504
                ERROR AS PERCENT OF C2DELST =          34.874
                ERROR AS PERCENT OF C2ISTOR =            .012
```

PUMPING PERIOD 2

PINT (PUMPING PERIOD IN DAYS) =   .50

NODE IDENTIFICATION

NODE ID	NUMBER OF OCCURENCES	REC	C1REC	C2REC
1	8	0.	200.	200.
2	0	0.	0.	0.
3	0	0.	0.	0.
4	0	0.	0.	0.
5	0	0.	0.	0.
6	0	0.	0.	0.
7	0	0.	0.	0.
8	0	0.	0.	0.
9	0	0.	0.	0.
10	0	0.	0.	0.
11	0	0.	0.	0.
12	0	0.	0.	0.
13	0	0.	0.	0.
14	0	0.	0.	0.
15	0	0.	0.	0.
16	1	-10.	500.	0.
17	0	0.	0.	0.
18	0	0.	0.	0.
19	0	0.	0.	0.
20	0	0.	0.	0.

U P D A T E   D A T A

NODE ID ARRAY

NODE	NODE ID	NODE	NODE ID	NODE	NODE ID	NODE	NODE ID	NODE	NODE ID
1	1	2	1	3	1	4	1	5	0
6	0	7	0	8	0	9	0	10	0
11	0	12	0	13	0	14	0	15	0
16	0	17	0	18	16	19	0	20	0
21	0	22	0	23	0	24	0	25	0
26	0	27	0	28	0	29	0	30	0
31	0	32	1	33	1	34	1	35	1

```
MATFLOW ITERATIONS= 15        TIME=   1.00 06944
MATCHEM ITERATIONS=  1        TIME=   1.00 06944

MATFLOW ITERATIONS= 13        TIME=   1.0017361
MATCHEM ITERATIONS=  1        TIME=   1.0017361

MATFLOW ITERATIONS= 10        TIME=   1.0032986
MATCHEM ITERATIONS=  1        TIME=   1.0032986

MATFLOW ITERATIONS=  4        TIME=   1.0056424
MATCHEM ITERATIONS=  1        TIME=   1.0056424

MATFLOW ITERATIONS=  1        TIME=   1.0091580
MATCHEM ITERATIONS=  1        TIME=   1.0091580

MATFLOW ITERATIONS=  1        TIME=   1.0144314
MATCHEM ITERATIONS=  1        TIME=   1.0144314

MATFLOW ITERATIONS=  1        TIME=   1.0223416
MATCHEM ITERATIONS=  1        TIME=   1.0223416

MATFLOW ITERATIONS=  1        TIME=   1.0342068
MATCHEM ITERATIONS=  2        TIME=   1.0342068

MATFLOW ITERATIONS=  1        TIME=   1.0520047
MATCHEM ITERATIONS=  2        TIME=   1.0520047

MATFLOW ITERATIONS=  1        TIME=   1.0787014
MATCHEM ITERATIONS=  2        TIME=   1.0787014

MATFLOW ITERATIONS=  1        TIME=   1.1187466
MATCHEM ITERATIONS=  3        TIME=   1.1187466

MATFLOW ITERATIONS=  1        TIME=   1.1788144
MATCHEM ITERATIONS=  4        TIME=   1.1788144

MATFLOW ITERATIONS=  1        TIME=   1.2689160
MATCHEM ITERATIONS=  5        TIME=   1.2689160

MATFLOW ITERATIONS=  1        TIME=   1.4040684
MATCHEM ITERATIONS=  7        TIME=   1.4040684

MATFLOW ITERATIONS=  1        TIME=   1.50 00000
MATCHEM ITERATIONS=  5        TIME=   1.50 00000
```

HEAD DISTRIBUTION -- FT

TIME(DAYS) =   1.500
TIME(YEARS)=   .00411

NODE	HEAD	NODE	HEAD	NODE	HEAD	NODE	HEAD
1	50.000	2	50.000	3	50.000	4	50.000
5	50.839	6	51.110	7	51.343	8	51.111
9	50.839	10	51.381	11	51.732	12	52.790
13	52.790	14	51.733	15	51.382	16	51.223
17	52.237	18	57.530	19	52.237	20	51.224
21	50.382	22	50.733	23	51.791	24	51.791
25	50.734	26	50.383	27	48.840	28	49.112
29	49.344	30	49.112	31	48.840	32	47.000
33	47.000	34	47.000	35	47.000		

DRAWDOWN DISTRIBUTION -- FT

TIME(DAYS) =   1.500
TIME(YEARS)=   .00411

NODE	DRAWDOWN	NODE	DRAWDOWN	VODE	DRAWDOWN	NODE	DRAWDOWN
1	0.000	2	0.000	3	-0.000	4	0.000
5	-1.339	6	-1.610	7	-1.843	8	-1.611
9	-1.339	10	-2.381	11	-2.732	12	-3.790
13	-3.790	14	-2.733	15	-2.382	16	-2.723
17	-3.737	18	-9.030	19	-3.737	20	-2.724
21	-2.382	22	-2.733	23	-3.791	24	-3.791
25	-2.734	26	-2.383	27	-1.340	28	-1.612
29	-1.844	30	-1.612	31	-1.340	32	0.000
33	0.000	34	0.000	35	-0.000		

CUMULATIVE WATER BALANCE -- FT**3

TIME(DAYS) =   1.500
TIME(YEARS)=   .00411

        QINRCH   (RECHARGE-DISTRIBUTED)   =   0.000
        QOUTRCH (DISCHARGE-DISTRIBUTED)   =   0.000

        QINREC   (RECHARGE-FCINT)   =   -1925.000
        QOUTREC (DISCHARGE-POINT)   =   0.000

        QINLEK   (RECHARGE-LEAKAGE)   =   0.000
        GOUTLEK (DISCHARGE-LEAKAGE)   =   0.000

        QINBDY   (RECHARGE-BOUNDARY)   =   0.000
        GOUTBDY (DISCHARGE-BOUNDARY)   =   0.000

        GINCHN   (RECHARGE-CONST HEAD NODES) =   -78.469
        GOUTCHN (DISCHARGE-CONST HEAD NODES) =   1998.567

                              TOTAL QIN   =   -2003.469
                              TOTAL GOUT   =   1998.567

        QSTOR   (WATER RELEASED FROM STORAGE) =   -1.051

                MASS BALANCE RESIDUAL   =   3.851
                ERROR AS PERCENT OF QIN   =   .192
                ERROR AS PERCENT OF QOUT   =   .193
                ERROR AS PERCENT OF QSTOR   =   366.280

```
FLOW BY NODE ID -- GPM
----------------------

  QIN (  1)=            0.000
  QOUT(  1)=            9.580

  QIN ( 16)=          -10.000
  QOUT( 16)=            0.000



FLOW FROM CONSTANT HEAD NODES -- GPM
POSITIVE IS DISCHARGE (PUMPAGE)
NEGATIVE IS RECHARGE (INJECTION)
  NODE(  1)=             .470
  NODE(  2)=            1.243
  NODE(  3)=            1.244
  NODE(  4)=             .471
  NODE( 32)=             .991
  NODE( 33)=            2.284
  NODE( 34)=            2.284
  NODE( 35)=             .991
```

SOLUTE CONCENTRATION OF SPECIES 1 (C1) -- MG/L

TIME(DAYS) =   1.50C
TIME(YEARS)=   .00411

NODE	CONC	NODE	CONC	NODE	CONC	NODE	CONC
1	200.106	2	199.446	3	199.446	4	200.106
5	199.467	6	200.314	7	201.858	8	200.314
9	199.466	10	199.104	11	201.704	12	194.557
13	194.558	14	201.706	15	199.094	16	201.213
17	193.544	18	245.749	19	193.543	20	201.213
21	199.273	22	201.408	23	195.441	24	195.442
25	201.409	26	199.265	27	199.621	28	200.179
29	201.315	30	200.179	31	199.620	32	200.070
33	199.688	34	199.688	35	200.070		

SOLUTE CONCENTRATICN OF SPECIES 2 (C2) -- MG /L

TIME(DAYS) =   1.500
TIME(YEARS)=   .00411

NODE	CONC	NODE	CONC	NODE	CONC	NODE	CONC
1	200.083	2	199.552	3	199.552	4	200.083
5	199.522	6	200.258	7	201.719	8	200.257
9	199.520	10	199.167	11	201.665	12	194.440
13	194.443	14	201.669	15	199.146	16	201.476
17	192.506	18	257.183	19	192.503	20	201.476
21	199.506	22	201.073	23	196.215	24	196.218
25	201.076	26	199.490	27	199.827	28	199.990
29	200.641	30	199.990	31	199.826	32	200.012
33	200.026	34	200.026	35	200.013		

EQUIVALENT FRACTION ADSORBED OF SPECIES 1 (C1HAT/CEC) -- DIMENSIONLESS

TIME(DAYS) =   1.500
TIME(YEARS)=   .00411

NODE	CONC	NODE	CONC	NODE	CONC	NODE	CONC
1	.469	2	.469	3	.469	4	.469
5	.469	6	.470	7	.471	8	.470
9	.469	10	.469	11	.471	12	.465
13	.465	14	.471	15	.469	16	.470
17	.464	18	.499	19	.464	20	.470
21	.469	22	.471	23	.465	24	.465
25	.471	26	.469	27	.469	28	.470
29	.471	30	.470	31	.469	32	.469
33	.469	34	.469	35	.469		

EQUIVALENT FRACTION ADSORBED OF SPECIES 2 (C2HAT/CEC) -- DIMENSIONLESS

TIME(DAYS) =   1.500
TIME(YEARS)=   .00411

NODE	CONC	NODE	CONC	NODE	CONC	NODE	CONC
1	.531	2	.531	3	.531	4	.531
5	.531	6	.530	7	.529	8	.530
9	.531	10	.531	11	.529	12	.535
13	.535	14	.529	15	.531	16	.530
17	.536	18	.501	19	.536	20	.530
21	.531	22	.529	23	.535	24	.535
25	.529	26	.531	27	.531	28	.530
29	.529	30	.530	31	.531	32	.531
33	.531	34	.531	35	.531		

ADSORBED CONCENTRATION OF SPECIES 1 (C1HAT) -- MG/L

TIME(DAYS) =   1.500
TIME(YEARS)=   .00411

NODE	CONC	NODE	CONC	NODE	CONC	NODE	CONC
1	2540.686	2	2537.014	3	2537.013	4	2540.686
5	2537.324	6	2541.816	7	2549.448	8	2541.816
9	2537.323	10	2535.563	11	2548.301	12	2514.480
13	2514.481	14	2548.302	15	2535.561	16	2544.726
17	2513.560	18	2699.200	19	2513.560	20	2544.726
21	2535.650	22	2548.148	23	2514.948	24	2514.948
25	2548.148	26	2535.648	27	2537.420	28	2541.729
29	2549.132	30	2541.729	31	2537.420	32	2540.662
33	2537.182	34	2537.182	35	2540.662		

ADSORBED CONCENTRATION OF SPECIES 2 (C2HAT) -- MG/L

TIME(DAYS) =   1.500
TIME(YEARS)=   .00411

NODE	CONC	NODE	CONC	NODE	CONC	NODE	CONC
1	3189.642	2	3193.721	3	3193.721	4	3189.642
5	3193.377	6	3188.396	7	3179.908	8	3188.386
9	3193.377	10	3195.332	11	3181.182	12	3218.753
13	3218.752	14	3181.182	15	3195.334	16	3185.153
17	3219.774	18	3013.554	19	3219.775	20	3185.153
21	3195.236	22	3181.352	23	3218.233	24	3218.233
25	3181.352	26	3195.238	27	3193.269	28	3188.483
29	3180.259	30	3188.483	31	3193.269	32	3189.668
33	3193.534	34	3193.534	35	3189.668		

CUMULATIVE CHEMICAL BALANCE FOR SPECIES 1 (C1&C1HAT) -- MG/L*FT**3

```
TIME(DAYS) =      1.500
TIME(YEARS)=       .00411


          C1INRCH (DISTRIBUTED RECHARGE)        =          0.000
          C1OTRCH (DISTRIBUTED DISCHARGE)       =          0.000

          C1INREC (POINT RECHARGE)              =   -1443749.900
          C1OTREC (POINT DISCHARGE)             =          0.000

          C1INLEK (RECHARGE-LEAKAGE)            =          0.000
          C1OTLEK (DISCHARGE-LEAKAGE)           =          0.000

          C1INCHN (RECHARGE-CONST HEAD NODES)   =     -15693.809
          C1OTCHN (DISCHARGE-CONST HEAD NODES)  =     399177.313

          C1INBDY (INFLOW-MODEL BOUNDARY)       =          0.000
          C1OTBDY (OUTFLOW-MODEL BOUNDARY)      =          0.000
                                                   ------------
                       TOTAL C1IN   =   -1459443.709
                       TOTAL C1OUT  =     399177.313

      C1STOR  (PRESENT MASS STORED)  =   691533023.581
      C1ISTOR (INITIAL MASS STORED)  =   690502127.265
                                         ------------
      C1DELST (CHANGE IN MASS STORED) =     1030896.316


          MASS BALANCE RESIDUAL         =      29370.080
          ERROR AS PERCENT OF C1IN      =          2.012
          ERROR AS PERCENT OF C1OUT     =          7.358
          ERROR AS PERCENT OF C1DELST   =          2.849
          ERROR AS PERCENT OF C1ISTOR   =           .004
```

CUMULATIVE CHEMICAL BALANCE FOR SPECIES 2 (C2&C2HAT) -- MG/L*FT**3

TIME(DAYS) =   1.500
TIME(YEARS)=   .00411

                C2INRCH (DISTRIBUTED RECHARGE)   =   0.000
                C2OTRCH (DISTRIBUTED DISCHARGE)   =   0.000

                C2INREC (POINT RECHARGE)   =   0.000
                C2OTREC (POINT DISCHARGE)   =   0.000

                C2INLEK (RECHARGE-LEAKAGE)   =   0.000
                C2OTLEK (DISCHARGE-LEAKAGE)   =   0.000

                C2INCHN (RECHARGE-CONST HEAD NODES) =   -15693.809
                C2OTCHN (DISCHARGE-CONST HEAD NODES) =   399160.489

                C2INBDY (INFLOW-MODEL BOUNDARY)   =   0.000
                C2OTBDY (OUTFLOW-MODEL BOUNDARY)   =   0.000

                             TOTAL C2IN   =   -15693.809
                             TOTAL C2OUT   =   399160.489

         C2STOR (PRESENT MASS STORED)   = 853942570.868
         C2ISTOR (INITIAL MASS STORED)   = 854357113.615

         C2DELST (CHANGE IN MASS STORED)   =   -414542.747

                MASS BALANCE RESIDUAL   =   31076.067
                ERROR AS PERCENT OF C2IN   =   198.015
                ERROR AS PERCENT OF C2OUT   =   7.785
                ERROR AS PERCENT OF C2DELST =   7.496
                ERROR AS PERCENT OF C2ISTOR =   .004

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