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A Preliminary Evaluation Capability for Some Two-Dimensional Groundwater Contamination Problems

by R. William Nelson and John A. Schur

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A PRELIMINARY EVALUATION CAPABILITY FOR SOME
TWO-DIMENSIONAL GROUNDWATER CONTAMINATION PROBLEMS

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as part of the

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Waste Isolation Safety Assessment Program

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ABSTRACT

There are a variety of two-dimensional groundwater pollution problems where a preliminary evaluation of contaminant transport is needed. A common difficulty in making this first assessment is the meager field data usually available. A preliminary evaluation capability has been developed for two-dimensional contamination problems that is consistent with the limited data initially available. Idealizations and simplifications have been introduced with special care so that worst-case final estimates will be provided.

The preliminary evaluation results are produced using interactive computer programs that utilize "self-help" or "coaching" features for the user's convenience. The self-help programs aid the user by asking for the necessary input parameters and by guiding the user, in selecting the options needed to obtain the required results. If the request for data or option selection is unclear, the user simply responds with "Help", whereupon a more detailed explanation is provided. In this way, any particular situation covered by the evaluation procedure and of interest to the user may be quickly and inexpensively evaluated.

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SUMMARY

A preliminary evaluation capability for two-dimensional subsurface pollution problems has been developed that is both easy to use and inexpensive. This capability is based on a model that was designed to best utilize the limited data usually available in early evaluation of a subsurface pollution problem. At some points, idealization and worst-case approximations were used rather than requiring more elaborate, hard-to-get data. Through the conservative assumptions used, the predictive results should represent the worst-case expectations. Such worst-case estimates can be very useful for an initial evaluation.

A variety of predictive results are provided by the model, which is capable of considering both steady and transient flows either with or without various corrective actions involving pumping or injection wells. Such results include 1) the expected flow paths of the contaminant, 2) the gradual advance of contaminant fronts through the stratum with time, 3) the location where the fluid-transported constituents will first reach the biosphere, and 4) the time necessary for various contaminant quantities to reach the interface with the biosphere. The overall environmental consequences can be evaluated from such results.

Interactive computer programs were developed to make it easy for noncomputer people to use the evaluation capability. These programs aid the user by asking for the necessary input parameters and by guiding the user through selecting the options needed to obtain the required results. If the request for data or option selection is not clear to the user, he simply responds with HELP, and a more detailed explanation is provided. In this way, any particular situation described by the initial predictive model and of specific interest to the user may be quickly and easily evaluated.

A PRELIMINARY EVALUATION CAPABILITY FOR SOME TWO-DIMENSIONAL GROUNDWATER CONTAMINATION PROBLEMS⁽¹⁾

by

R. William Nelson

John A. Schur

INTRODUCTION

There are a variety of two-dimensional groundwater contamination problems where a preliminary evaluation is needed. Some of these cases involve small, localized problems where elaborate evaluations are not feasible. Even in large, complicated problems requiring extensive long-term studies, a preliminary evaluation is usually the first step. Common to all of these problems is the lack of sufficient data to support comprehensive initial evaluations.

Accordingly, there is a real need for assessment procedures that seek a balance between predictive sophistication and the amount and quality of data available. Further, such procedures must be easy to use and must provide the results needed in a moderate amount of time and at minimal cost.

A preliminary evaluation capability for two-dimensional groundwater pollution problems was developed as part of the Transport Modeling Task for the Waste Isolation Safety Assessment Program (WISAP). Our approach was to use the data limitations as a guide in setting the level of modeling detail.

This evaluation capability has grown out of earlier developmental efforts and numerous enhancements made in the process of solving a variety of related problems over the past decade. A project for the Research and Development Department of Atlantic Richfield Hanford Company (Nelson, 1970) in the late sixties provided a simplified single source leakage model. Later, while working with pollution problems of a commercial mining operation,

⁽¹⁾ This report was prepared under Project BCA 640 for the Water and Land Resources Department of Battelle, Pacific Northwest Laboratories, as part of the Transport Modeling Task for the Waste Isolation Safety Assessment Program (WISAP).

the features for considering several injection or pumping wells in addition to the central source were incorporated. Shortly after that, the original central source expression was replaced by the more complete and useful doublet expression used now. Recently, out of an underground siting study of nuclear power plants (Allensworth, et al., 1977), the feature to consider nuclide holdup due to ion exchange of a single component was first included.

In 1977, Battelle, Pacific Northwest Laboratories, as part of WISAP for the Department of Energy, conducted a detailed evaluation of fluid and contaminant transport models for use in assessing the safety of geological repositories for solidified nuclear wastes. The preliminary two-dimensional evaluation tool that had evolved during the previous decade was selected by WISAP as the needed preliminary evaluation capability.

This document describes the preliminary evaluation capability prepared for WISAP, including the enhancements that were made because of the authors' experience using the earlier capability. Appendixes A through D supplement the report as follows: Complete derivations of the background equations are provided in Appendix A. Appendix B is a comprehensive set of instructions for users of PATHS. It is written for users who have little or no experience with computers. Appendix C is for the programmer. It contains information on how input parameters are passed between programs in the system. It also contains program listings and test case listings. Appendix D is a definition of terms.

THE PRELIMINARY EVALUATION MODEL

A preliminary analysis commonly is restricted by lack of field data. In particular, there is insufficient hydraulic conductivity, porosity, or stratum configuration data to enable a detailed description of the actual field situation. Accordingly, the approach used here involved idealizing the model to stay within the available data bounds, followed by selection of conservative alternatives at decision points to assure that the predicted results will represent a worst-case situation.

Several idealizations are involved in the model. The fluid release postulated by the model represents a severe, worst possible failure for the storage structure, if one exists. We are assuming that any metal, concrete or lining material of the structure offers no resistance to flow. In effect, the fluid is assumed to be standing in an unlined, cylindrical, vertical cavity in the porous material. The leakage rate of fluid from the pond or vertical cavern is governed only by the hydraulic conductivity of the material, the hydraulic head in the unlined vertical cavity and the other flow system variables.

The two-dimensional initial-assessment model represents flow in a confined stratum of uniform vertical thickness, and is of large lateral extent in the horizontal plane. The stratum is assumed homogeneous, having isotropic hydraulic conductivity and constant effective porosity. A uniform lateral flow gradient is assumed within the stratum and the superimposed leakage is from a vertical, cylindrical pond or cavern that completely penetrates the entire stratum. A potential energy head is applied at the pond or structure and is completely dissipated at finite radial distance rather than at an infinite distance, thereby introducing a worst-case situation into the evaluation procedure.

The model can consider as many as 35 wells at optional locations. Wells are represented as completely penetrating, vertical line sources with steady or time-dependent flow rates.

The model considers both steady and transient saturated flow systems. The steady cases are evaluated by holding the uniform gradient, the head in

the pond, and the well strengths constant. Under such steady conditions, only one set of flow paths, advancing fronts, and travel times must be calculated since subsequent fluid leaving the pond or wells traverses identical flow paths, gives duplicate contaminant-front configurations, and has the same elapsed travel times. In the transient cases each new set of fluid particles leaving the pond or wells encounters changing velocity effects. Therefore, a range of typical departure times is selected and the flow paths, front configurations, and travel times are calculated successively for each selected set of fluid particles leaving the contaminant source. Usually the moderate extra effort to get the transient results is more than compensated by the more realistic representation provided for practical problems.

The model also considers the effect of equilibrium ion exchange reactions for a single contaminant at trace ion concentration. The approximate equilibrium coefficient, or K_d approach is utilized to give the ion exchange delay effects for a single constituent. There are, however, no dispersion effects considered in the preliminary model, since field dispersion data is seldom, if ever, available for preliminary evaluations. Omitting dispersion effects also yields the worst overall results in terms of the amount of contaminants reaching the biosphere.

The preliminary evaluation capability is based on an idealized analytical expression for the groundwater potential in a two-dimensional flow system and direct numerical solution of the kinematic pathline equations to allow the approximate contaminant transport evaluation. This approach, though idealized, provides a fast, inexpensive first-cut evaluation tool, consistent with the amount of field data usually available.

The basis of the evaluation tools is summarized in the following paragraphs. Complete derivation of these summary relations is provided in Appendix A; symbols are defined in Appendix D.

NEW POTENTIAL DETERMINATION

The potential distribution for the two-dimensional flow system can be approximated satisfactorily by superposition of elementary flows. In particular, a uniform lateral flow of gradient strength, U , inducing flow in the

positive x coordinate direction, is added to a combined source and positive doublet (Shames, 1962) centered at the origin to represent outflow from the completely penetrating cylindrical pond or cavern of radius r_0 . The pumped wells and injection wells are superimposed as vertical line sinks and sources, respectively, with the center of the j th well located at the point x_j, y_j , to yield an expression for the overall groundwater potential, ϕ , throughout the porous stratum. Specifically,

$$\phi = H - \frac{UR}{H_0} x + \frac{URr_0^2}{H_0} \left(\frac{x}{x^2 + y^2} \right) - \frac{M_0}{2\pi H_0} \ln \left(\frac{\sqrt{x^2 + y^2}}{r_0} \right) - \sum_{j=1}^{j=N} \frac{M_j}{2\pi H_0} \ln \sqrt{\frac{(x - x_j)^2 + (y - y_j)^2}{x_j^2 + y_j^2}} \quad (1)$$

with the remaining variables and parameters defined in Appendix D.

The potential, ϕ , is defined by Equation (1) in the region for all locations $(x^2 + y^2) > r_0^2$ (r_0 is the central pond radius) except at the well coordinates x_j and y_j . The potential satisfies the LaPlace Equation describing flow in homogeneous isotropic material. The potential, ϕ , also satisfies the boundary conditions that $\phi = H \pm \epsilon$ when $x^2 + y^2 = r_0^2$. As Appendix A shows, ϵ is negligibly small if

$$\frac{r_0^2}{(x_j^2 + y_j^2)} < 0.01 \quad (2)$$

Equation (1), subject to Equation (2), provides the potential distribution for subsequent use in determining the flow system kinematics.

FLOW SYSTEM KINEMATICS

The flow system kinematics provide the pattern, or geometry of flow, in the subsurface system. The pathlines for individual fluid particles through the flow system provide the points of emergence at outflow boundaries. These locations and the arrival time of fluids at outflow boundaries are determined by the path function. The stream function gives the flux rate

at the outflow boundary, and throughout the entire system. Together, the path function and stream function provide the results needed for the arrival distributions with fluid-coincident contaminants.

The characteristic equations for the pathlines are most useful in generating the flow paths and obtaining the travel times. They come directly from the definition of the macroscopic pore velocity utilizing Darcy's Law, as demonstrated by Equations (A-25) through (A-31) of Appendix A. In particular, from Equations (1) and (A-27), the pair of pathline differential equations are

$$\begin{aligned} \frac{dx}{dt} = & \frac{UR}{PH_0} \left\{ 1 + \frac{r_0^2}{(x^2 + y^2)} \left[\frac{2x^2}{x^2 + y^2} - 1 \right] \right\} + \frac{H}{P \ln\left(\frac{1}{r_0}\right)} \left(\frac{x}{x^2 + y^2} \right) \\ & + \sum_{j=1}^{j=N} \frac{M_j}{2\pi H_0 P} \left[\frac{(x - x_j)}{(x - x_j)^2 + (y - y_j)^2} \right], \end{aligned} \quad (3)$$

and

$$\begin{aligned} \frac{dy}{dt} = & \frac{UR}{PH_0} \left[\frac{2(r_0)^2 xy}{(x^2 + y^2)^2} \right] + \frac{H}{P \ln\left(\frac{1}{r_0}\right)} \left(\frac{y}{x^2 + y^2} \right) \\ & + \sum_{j=1}^{j=N} \frac{M_j}{2\pi PH_0} \left[\frac{y - y_j}{(x - x_j)^2 + (y - y_j)^2} \right] \end{aligned} \quad (4)$$

The contamination departs from the pond or vertical cavern at t_0 ; i.e.,

$$x(t_0) = x_0 \quad (5)$$

and

$$y(t_0) = y_0 \quad (6)$$

where

$$(x_0)^2 + (y_0)^2 = r_0^2. \quad (7)$$

Simultaneous solution of Equations (3) and (4) using the initial conditions in Equations (5) and (6) is accomplished numerically to yield pathlines and

travel times to the pumped wells or to the remote outflow boundary. The calculations, using a fourth-order Runge-Kutta numerical solution scheme, are made using a computer program.

The flux, or fluid flow rate, at any outflow boundary is available from the instantaneous stream function, which is simply the complex conjugation of the potential expressions used in Equation (1). Upon superposition of the simple basic flows, the instantaneous stream function (derived in Equations (A-34) through (A-43) in Appendix A) is

$$\frac{Q_i}{Q_o} = \frac{UR \ln\left(\frac{1}{r_o}\right)}{2\pi H_o} y + \frac{UR \ln\left(\frac{1}{r_o}\right) r_o^2 y}{2\pi H_o (x^2 + y^2)} + \frac{H}{2\pi} \arctan\left(\frac{y}{x}\right) + \sum_{j=1}^{j=N} \left[\frac{M_j \ln\left(\frac{1}{r_o}\right)}{4\pi^2 H_o} \right] \left[\arctan\left(\frac{y - y_j}{x - x_j}\right) - \arctan\left(\frac{-y_j}{x_o - x_j}\right) \right] \quad (8)$$

where

$$Q_o = \frac{2\pi D_o K_o H_o}{\ln\left(\frac{1}{r_o}\right)} \quad (9)$$

from Equation (A-41). Equations (8) and (9) are used to determine the relative flux and are most easily visualized in steady flow systems, although they are equally useful on an instantaneous basis at any specific time in a transient flow system.

Often in transient flow systems it is helpful to calculate the variation of the groundwater unit outflow fluxes along a river, for example, rather than use the cumulative stream function. The instantaneous flux per unit outflow length, q , can be calculated using

$$q = P \frac{dx}{dt} \quad (10)$$

The equation for direct calculation of q is obtained by substituting the expression for $\frac{dx}{dt}$ from Equation (3) into Equation (10).

Equations (8) through (10) provide the outflow rates either as the relative cumulative flux or as the flux per unit length of outflow. These

results provide the outflow quantity component of the location/outflow-quantity distribution required for evaluating the environmental consequences of a subsurface contamination problem. With this data, outflow quantities can be obtained easily on a computer.

The remaining part of the preliminary evaluation capability is a simple extension of the flow kinematics already discussed. It includes the effect of ion sorption on contaminant transport.

CONTAMINANT TRANSPORT WITH SORPTION

A single chemical species at trace concentration with equilibrium sorption is readily considered with only minor modifications of the kinematic equations provided in the preceding section. Without considering dispersion, as shown in Appendix A in Equations (A-44) through (A-52), the characteristic contaminant transport equations are

$$\begin{aligned} \frac{dx}{dt} = & \frac{UR}{PH_0 K} \left\{ 1 + \frac{r_0^2}{(x^2 + y^2)} \left[\frac{2x^2}{x^2 + y^2} - 1 \right] \right\} + \frac{H}{KP \ln\left(\frac{1}{r_0}\right)} \left(\frac{x}{x^2 + y^2} \right) \\ & + \sum_{j=1}^{j=N} \frac{M_j}{2\pi H_0 P K} \left[\frac{(x - x_j)}{(x - x_j)^2 + (y - y_j)^2} \right] \end{aligned} \quad (11)$$

and

$$\begin{aligned} \frac{dy}{dt} = & \frac{UR}{PH_0 K} \left[\frac{2(r_0)^2 xy}{(x^2 + y^2)^2} \right] + \frac{H}{KP \ln\left(\frac{1}{r_0}\right)} \left(\frac{y}{x^2 + y^2} \right) \\ & + \sum_{j=1}^{j=N} \frac{M_j}{2\pi PH_0 K} \left[\frac{y - y_j}{(x - x_j)^2 + (y - y_j)^2} \right] \end{aligned} \quad (12)$$

where

$$K = 1 + \frac{B_d K_d}{P} \quad (13)$$

with B_d as the bulk density of the porous material; K_d , the equilibrium exchange distribution coefficient; and P , the porosity.

Comparing Equations (11) and (12) with the original kinematic characteristic Equations (3) and (4) shows that the idealized transport involved only incorporating the new parameter K defined by Equation (13). Accordingly, the approximate transport results can be readily obtained through applying the same Runge-Kutta numerical integration scheme as previously used.

USE OF THE PRELIMINARY EVALUATION MODELS

The model equations and detailed formulation in Appendix A were utilized to build interactive "self-help" or "coaching" computer programs. These programs allow a user to obtain the results for a specific problem simply and quickly via a remote job entry terminal. Every effort was made to get results to the user quickly and inexpensively. Our intent is to have the user on the computer as quickly as possible, without having to spend time mastering computer programming or learning machine-related details. Interactive programs make using the computer fairly easy. Through the computer terminal, the programs asks questions that the user responds to by typing in YES, NO, or by providing the input value requested. If the question is confusing, the user may at any time type in HELP, whereupon a more complete description or further suggestions are provided by the computer. The question is then repeated and the user must respond before the program proceeds to the next item.

In the course of this interactive process, all the data inputs and controls are provided. When all the necessary data have been entered, at the user's instruction, the program automatically submits a batch computer run to most economically generate the calculations, listings and plots needed. Subsequently, the results from the batch run are automatically stored in files awaiting interrogation from the terminal. Upon request, the summary results are provided to the user--usually within a short time--at the terminal; plots and more extensive printout, if requested, are produced in the computer center and sent to the user. This gives the user summary information in a matter of minutes and the more detailed results in a few hours. Appendix B provides complete instructions for using the interactive self-help computer programs. Example cases are given in the appendix and in the following section to help use the programs.

PREPARING COMPUTER INPUT

There are various ways to assemble the input values one needs to use the interactive computer programs. One of them is to collect the case data on the worksheet in Table 1. Benefits of using the worksheet are that consistent units are used for the various input values and that complete

data are at hand. Another approach is to use the worksheet to collect the first few most pertinent input values and rely more on the coaching features of the programs.

A user may opt to rely exclusively on the coaching programs. This way a user can make a dry run with the programs on a terminal to build an input worksheet. This is done by entering the known input values and making the machine-coached selections. For unknown values or for difficult selections in the dry run, an arbitrary number or choice is made for the trial input. Subsequently, the dry run is terminated using the "escape" feature (as instructed by the program) and no actual batch run is made. In this way, for a few pennies of computer time, the user gets a quick terminal printout that serves as a draft input worksheet. After some checking and a few penciled corrections, the printout becomes a complete and detailed input aid for the actual run. However, the one-page input worksheet in Table 1 is used for the example preliminary evaluation in the following section.

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TABLE 1. Input Parameter Worksheet.

INPUT PARAMETER WORKSHEET

CASE: _____

1. _____ = D_0 is the stratum thickness.
2. _____ = R is the distance to the boundary. Units must be the same as D_0 .
3. _____ = $XMAX/TMAX$ are the stopping distance or time for pathlines.
4. _____ = r_0 is the cavern or pond radius. Units must be the same as D_0 .
5. _____ = H_0 is the head in the cavern. Units must be the same as D_0 .
6. _____ = K_0 is the stratum hydraulic conductivity. Length units must be the same as D_0 .
Whatever time units are in K_0 sets the units of the travel time.
7. _____ = P is the effective porosity.
8. _____ = S or T . A steady (S) or transient (T) case.
9. _____ = UO is the initial uniform gradient value. See Figure 1.
10. _____ = UM is the lateral gradient value. See Figure 1.
11. _____ = TM in time units of K_0 .
12. _____, _____, _____ = A, B, C are three time-related integers.
13. _____ = S or E or C . Use the serpin (S), exponential (E), or cyclic (C) head variation in the cavern.
14. _____ = HI is the initial head.
15. _____ = HM is the maximum head.
16. _____ = TN in time units of K_0 .
17. _____, _____, _____ = D, E, F . See Figure 1.
18. _____ = J is total number of wells.
19. _____ = $\theta 0$ is the angle (deg) around the cavern wall to the starting point for the first pathline.
20. _____ = θM is the maximum angle (deg) to the last pathline starting point along the cavern wall.
21. _____ = $N\theta$ is the number of pathlines to be generated from $\theta 0$ to and including θM .
22. _____ = $K\theta$ is the number of pathlines wanted between θM and $179.99 + \theta$.
23. _____ = t_0 is the departure time of the first fluid particles leaving the cavern.
24. _____ = t_f is the departure time of the final fluid particles.
25. _____ = NT is the number of equally spaced departure times beginning with t_0 and ending with t_f .
26. _____ = K_d is the equilibrium exchange distribution coefficient.
27. _____ = B_d is the bulk density of the porous material.
28. _____ = _____ inch wide plots are desired. Request either a 30" or 11" wide by 30" plot.
29. _____ = $XCENTER$ } The location (x & y in inches) on the plot where
30. _____ = $YCENTER$ } the cavern center is to be located.
31. _____ = $SCALE$ is the scale for the plot. Length in units of D_0 per inch.

INPUT FOR WELLS (J sets are required)

18.05	_____	= j	is the well number.
18.10	_____	= XWELL _j = x' _j	is the x-coordinate location of the center of the well. (Units consistent with D ₀ .)
18.15	_____	= YWELL _j = y' _j	is the y-coordinate location of the center of the well.
18.20	_____	= ROWELL _j	is the stopping radius around the well.
18.25	S	= S or C.	serpin (S) or cyclic (C) option. See Figure 1.
18.30	_____	= QI _j	is initial inflow (+) or outflow (-) rate in length cubed per time units the same as D ₀ and K ₀ .
18.35	_____	= QM _j	is a later inflow (+) or outflow (-) rate of this well option.
18.40	_____	= TN _j	is the time parameter in the serpin option. See Figure 1.
18.45	_____,_____,____	= DW _j , EW _j , FW _j .	serpin well option parameters.

18.50	_____	= j	is the well number.
18.55	_____	= XWELL _j = x' _j	is the x-coordinate location of the center of the well. (Units consistent with D ₀ .)
18.60	_____	= YWELL _j = y' _j	is the y-coordinate location of the center of the well.
18.65	_____	= ROWELL _j	is the stopping radius around the well.
18.70	C	= S or C;	serpin (S) or cyclic (C). See Figure 2.
18.75	_____	= QQ _j	is the mean inflow (+) or outflow (-) rate in length cubed per time units the same as D ₀ and K ₀ .
18.80	_____	= QA _j	is the amplitude of the cyclic inflow (+) or outflow (-) rate.
18.85	_____	= TOWELL _j	is the initial or beginning time for the cyclic well option.
18.90	_____	= TMWELL _j	is the later cyclic time parameter.

(If 00 in Item 19 equals 0M in Item 20 then N0 pathlines will be generated from the individual coordinates provided below.)

21. _____ = N0 is the number of input data sets to be entered for starting pathlines
($1 < i < N0$).

[illegible]

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INPUT FOR AN EXAMPLE TRANSIENT EVALUATION

An example evaluation using the model is included to show what results are obtainable and to help explain the inputs needed. Typical input values using the input parameter worksheet (Table 1) are provided and discussed.

The first seven parameters on the worksheet in Table 2 are the primary variables that must be entered in the model; they should represent the very best measurements or estimates of the respective properties that can be obtained. Parameter 8 simply indicates whether the system involves transient flow or is restricted to steady flow. Parameters 9 through 12 provide the flexibility to represent the change with time of the uniform gradient strength, U (see Figure 1). For this particular example case, the uniform gradient is constant with a value of 0.001. From Figure 1(a), we set $U_0 = 0.001$ and $U_m = 0.001$ for input items 9 and 10, which gives $U = U_0$ for values for $TM = A = B = C = 1$, hence the value of 1 is used in items 11 and 12.

Parameters 13 through 17 allow the user to represent a variety of pond or cavern head variations with time. If the user has detailed information about the time dependence, a programmer can easily build a subroutine for direct use. However, a look at the consequences of various types of time dependence, rather than a specific detailed representation in time, is probably most useful for an initial evaluation. In the latter case, a series of variations that can be easily used are very helpful. Three broad options have been built into the programs for direct use and we have found that they cover most situations.

The three time-dependent options are the serpin, exponential leakage, and cyclic options. Each is discussed in our example case. For input item 13 (in Table 2), the user selects one of the three time-variation options to be applied. The serpin (S) option will be used for the example transient case so S is entered in item 13. The specific time variation chosen for the example case from the several serpin alternatives is in Figure 1(g). The desired pond or cavern head begins at a 4-foot head, gradually increases to a maximum of 8 feet at 50 years and then gradually returns to the original head of 4 feet. Using the schematic in Figure 1(g), the tabular definitions and conditions provide the inputs: $HI = 4$ ft, $HM = 8$ ft, $TN = 50$ yr, $D = 0$, $E = 1$ and $F = 1$, which are entered as input items 14 through 17, respectively, on the example transient input worksheet in Table 2.

TABLE 2. Input Parameter Worksheet for the Example Transient Case

INPUT PARAMETER WORKSHEET

CASE: Example Transient Case (Two Wells)

1. 100 ft. = D_0 is the stratum thickness.
2. 8500 ft. = R is the distance to the boundary. Units must be the same as D_0 .
3. 8500 ft. = X_{MAX}/T_{MAX} are the stopping distance or time for pathlines.
4. 250 ft. = r_0 is the cavern or pond radius. Units must be the same as D_0 .
5. 10 ft. = H_0 is the head in the cavern. Units must be the same as D_0 .
6. 1825 ft/yr. = K_0 is the stratum hydraulic conductivity. Length units must be the same as D_0 . Whatever time units are in K_0 sets the units of the travel time.
7. 0.2 = P is the effective porosity.
8. T = S or T . A steady (S) or transient (T) case.
9. 0.001 = U_0 is the initial uniform gradient value. See Figure 1.
10. 0.001 = U_M is the lateral gradient value. See Figure 1.
11. 1 = T_M in time units of K_0 .
12. 1, 1, 1 = A, B, C are three time-related integers.
13. S = S or E or C . Use the serpin (S), exponential (E), or cyclic (C) head variation in the cavern.
14. 4 ft. = H_I is the initial head.
15. 8 ft. = H_M is the maximum head.
16. 50 yr. = T_N in time units of K_0 .
17. 0, 1, 1 = D, E, F . See Figure 1.
18. 2 = J is total number of wells.
19. 0° = θ_0 is the angle (deg) around the cavern wall to the starting point for the first pathline.
20. 160° = θ_M is the maximum angle (deg) to the last pathline starting point along the cavern wall.
21. 9 = N_θ is the number of pathlines to be generated from θ_0 to and including θ_M .
22. 1 = K_θ is the number of pathlines wanted between θ_M and 179.99° .
23. 0 yr. = t_0 is the departure time of the first fluid particles leaving the cavern.
24. 100 yr. = t_f is the departure time of the final fluid particles.
25. 5 = N_T is the number of equally spaced departure times beginning with t_0 and ending with t_f .
26. _____ = K_d is the equilibrium exchange distribution coefficient.
27. _____ = B_d is the bulk density of the porous material.
28. 30 in. = _____ inch wide plots are desired. Request either a 30" or 11" wide by 30" plot.
29. 3 in. = X_{CENTER} } The location (x & y in inches) on the plot where
30. 2 in. = Y_{CENTER} } the cavern center is to be located.
31. 1000 ft/in. = $SCALE$ is the scale for the plot. Length in units of D_0 per inch.

INPUT FOR WELLS (J sets are required)

SERPIN OPTION

18.05	$\frac{1}{3000 \text{ ft.}}$	$= j$	is the well number.
18.10	$\frac{3000 \text{ ft.}}$	$= \text{XWELL}_j = x'_j$	is the x-coordinate location of the center of the well. (Units consistent with D_0 .)
18.15	$\frac{1000 \text{ ft.}}$	$= \text{YWELL}_j = y'_j$	is the y-coordinate location of the center of the well.
18.20	$\frac{250 \text{ ft.}}$	$= \text{ROWELL}_j$	is the stopping radius around the well.
18.25	S	$= S \text{ or } C.$	serpin (S) or cyclic (C) option. See Figure 1.
18.30	$\frac{4(10^3) \text{ ft}^3/\text{yr}}$	$= \text{QI}_j$	is initial inflow (+) or outflow (-) rate in length cubed per time units the same as D_0 and K_0 .
18.35	$\frac{6(10^5) \text{ ft}^3/\text{yr}}$	$= \text{QM}_j$	is a later inflow (+) or outflow (-) rate of this well option.
18.40	$\frac{25 \text{ yr.}}$	$= \text{TN}_j$	is the time parameter in the serpin option. See Figure 1.
18.45	$\frac{1, 1, 1}{1, 1, 1}$	$= \text{DW}_j, \text{EW}_j, \text{FW}_j.$	serpin well option parameters.

CYCLIC OPTION

18.50	<u>2</u>	= j	is the well number.
18.55	<u>5500 ft.</u>	= XWELL _j = x' _j	is the x-coordinate location of the center of the well. (Units consistent with D ₀ .)
18.60	<u>3000 ft.</u>	= YWELL _j = y' _j	is the y-coordinate location of the center of the well.
18.65	<u>300 ft.</u>	= ROWELL _j	is the stopping radius around the well.
18.70	<u>C</u>	= S or C;	serpin (S) or cyclic (C). See Figure 2.
18.75	<u>0.0</u>	= QQ _j	is the mean inflow (+) or outflow (-) rate in length cubed per time units the same as D ₀ and K ₀ .
18.80	<u>5(10⁵) ft.³/yr.</u>	= QA _j	is the amplitude of the cyclic inflow (+) or outflow (-) rate.
18.85	<u>50 yr.</u>	= TOWELL _j	is the initial or beginning time for the cyclic well option.
18.90	<u>450 yr.</u>	= TMWELL _j	is the later cyclic time parameter.

PATHLINE - IRREGULAR STARTING COORDINATES

(If 00 in Item 19 equals 0M in Item 20 then N0 pathlines will be generated from the individual coordinates provided below.)

21. _____ = N_0 is the number of input data sets to be entered for starting pathlines ($1 \leq i \leq N_0$).

Pathline i	Starting Coordinates		Starting Pathline Length*	Initial Time*
	X	Y		

*Values need not be supplied

$$\text{Serpín Equation } W(t') = w_o + \frac{2(w_m - w_o) \left(\frac{t'}{t'_n} + A \right)}{B \left(\frac{t'}{t'_n} + A \right)^2 + C} \quad (14)$$

Parameters in serpín Equation (14) $W(t')$	Term defined on input worksheet for:		
	Uniform gradient, $U(t')$	Cavern or pond head, $H(t')$	Well flow rate $Q_j(t')$
w_o	UO	HI	QI _j
w_m	UM	HM	QM _j
t'_n	TM	TN	TN _j
A	A	D	DW _j
B	B	E	EW _j
C	C	F	FW _j

FIGURE 1. Serpín Time-Dependent Forms

If the exponential leakage (E) option, which considers the case of the head diminishing as the fluid seeps from the cavern, had been chosen then no special inputs would be required for items 14 through 17. The parameters necessary to calculate the falling head or exponential leakage case have been entered already (see Equations (A-23) and (A-24) in Appendix A).

Input item 18 is the number of wells to be considered in the flow system. Two injection wells are used in the example transient case, so $J = 2$. The specific well data needed are described on the back of the worksheet.

The first injection well with an inflow rate, $Q_j(t')$, is represented by the serpin time dependence illustrated in Figure 1(c). The center of the first well (i.e., $j = 1$ entered in item 18.05 on the back of the worksheet) is located at $x_1 = 3000$ ft and $y_1 = 1000$ ft. The x and y coordinate distances are always measured from the center of the pond or cavern, which has coordinates $x = 0$, $y = 0$. Accordingly, input items 18.10 and 18.15 are 3000 feet and 1000 feet, respectively. The stopping radius, $ROWELL_j$, for item 18.20 is required since the well is represented as a singularity. Numerical difficulties will occur if one approaches a well too closely; two or three hundred feet is a reasonable distance away from such a well, so 250 feet was used in the example.

The injection rate of the first well is represented by the serpin-form time dependence with a lower injection rate $QI_1 = 4000$ ft³/yr, a maximum rate $QM_1 = 600,000$ ft³/yr, with a time parameter $TN_1 = 25$ yr, and integer parameters of $A = B = C = 1$ to complete the input for the first well.

The second well represented by $j = 2$ is located at $x_2 = 5500$ ft and $y_2 = 3000$ ft with a stopping radius of 300 feet. These values provide input items 18.50, 18.55, 18.60 and 18.65. This well is used to illustrate the cyclic option for time dependence, so item 18.70 is specified as C. Figure 2 is convenient in selecting the cyclic parameters. For this example case, Figure 2(b) is used with a mean injection rate $QQ_2 = 0$ beginning at $TO_2 = 50$ yr. The amplitude of the injection rate QA_2 is 500,000 ft³/yr with a maximum cycle time $TM_2 = 450$ yr, which completes the well input parameters for the example transient case.

Cyclic Equation

$$\begin{aligned} W(t') &= W & \text{if } W > 0 \\ W(t') &= 0 & \text{if } W \leq 0 \end{aligned} \quad (15)$$

where:

$$W = w_{mc} + w_{oc} \sin \left[\left(\frac{t' - t_{oc}}{t_{mc} - t_{oc}} \right) 2\pi \right] \quad (16)$$

Parameters in cyclic Equation (16) W	Term defined on input worksheet for:	
	Cavern or pond head, $H(t')$	Well flow rate, $Q_j(t')$
w_{mc}	HMC	QQ_j
w_{oc}	HAC	QA_j
t_{oc}	TOC	TO_j
t_{mc}	TMC	TM_j

FIGURE 2. Cyclic Time-Dependent Forms

The remaining input for the example case involves items 19 through 31 in Table 2. Items 19 through 22 allow the user to select the location for starting the pathlines, thereby allowing the fluid particles to be followed. In item 19, the user selects the angle between the x axis and the point on the cavern or pond wall where the first pathline is to originate. One wants to look at the travel along the shortest pathline so a starting angle $\theta_0 = 0$ is used. The maximum angle of interest was set equal to 160 degrees for θ_M . If $N_\theta = 9$, then a pathline originating at $\theta = 0$ and pathlines beginning every $(160-0)/(9-1) = 20$ deg around the cavern wall, up to and including the last pathline beginning at 160 degrees, are generated. This should provide a good beginning set of fluid particle pathlines. The input parameter K_θ is also set to 1 here to get an additional pathline between 160 and 179.99 degrees. Use of the K_θ parameter is helpful in getting more pathlines near 180 degrees without specifically using the latter value. There is a stagnation point (i.e., a point of zero velocity) upstream of $\theta = 180$ that will use excessive computer time if one attempts to generate a path through or very near it. The K_θ input feature allows pathlines to be generated near 180 degrees while minimizing the difficulties with the stagnation point.

The next three parameters (items 23 through 25) specify the times for which fluid particles leaving the cavern wall will be traced. The first contaminated fluid particles leaving the cavern should be followed so t_0 is set equal to zero (item 23). A useful final set of fluid particles to follow in time are those departing at 100 years, $t_f = 100$ yr (item 24). The value for $NT = 5$ was chosen, which means the fluid particles departing at 0, 25, 50, 75 and 100 years will be generated by the model, so $NT = 5$ is shown for input item 25.

No input values are provided for data items 26 and 27 (the K_d and bulk density) since exchange reactions for a particular ion are not considered in this example case. Individual fluid particles or the movement of a perfect tracer such as tritium, sulfate, or chloride are being evaluated in this example.

The remaining worksheet inputs in Table 2 are needed to generate plots of the results. Item 28 determines the width of the plot. If a rather narrow plot is expected, as in our example case, then 11-inch wide paper is specified. When in doubt, it is usually best to request the 30-inch

width. The XCENTER and YCENTER values in items 29 and 30 specify the location, in inches, from the lower right-hand corner of the plotting sheet where the center of the cavern or pond will be positioned on the plots. In this example, 3 inches to the right of the lower left-hand corner of the plotter paper and 2 inches above should work. The last input item is the plotting scale. It is the number of length units in the real problem to be represented per inch of length on the plot. A plot scale of 1000 ft/in. is used in this case. This scale and the case title are automatically added to the finished computer-generated plot.

This example worksheet (Table 2) contains the major inputs needed by the user. Those few additional questions not specifically covered by the worksheet either will be obvious to the user or readily available using the HELP feature. So, armed with an input worksheet (that reflects the case at hand), a terminal and the Appendix B User's Guide, a computer novice should now be able to get the arrival results needed. (The example transient case is presented in complete detail in Appendix B.)

CONTAMINANT ARRIVAL RESULTS FROM THE MODEL

The contaminant arrival results are available from the interactive and batch runs described in Appendix B. Among the results provided are 1) the fluid or contaminant flow paths and the rate of advance and shape of the contaminant fronts moving through the subsurface region, 2) the location and time of contaminant arrival at the biosphere interface, and 3) the amount of contaminated fluid arriving with passing time. These are the results necessary to evaluate the environmental consequences (Nelson, 1976). The example case results will be used to illustrate the results obtained from the preliminary evaluation methods.

Fluid Pathlines and Advancing Fronts

The fluid pathline provides the expected location of the fluid at various times during the gradual movement from the pond or cavern to the remote boundary (river, in this example). The pattern of the advancing front is developed by following representative fluid particles along the paths traversed with passing time. If, at a specific time, a line is passed through the location of each particle on its pathline, an isochronal line

(i.e., the position of the advancing front of fluid particles at that particular time) is determined. In this way, the changing locations of fluid particles are conveniently indicated by the pathlines and isochronal lines.

The pathlines and isochronal lines for the example transient case, obtained using the PATHS program, are shown in Figures 3 and 4. In Figure 3, the pathlines and advancing fronts in time denoted by the numbers are shown for the fluid departing from the pond at 0 and 50 years. Figure 4 shows the results for fluid particles leaving the pond at 75 and 100 years.

The flow results in the figures were obtained from the type of computer-generated plots shown near the end of Appendix B as example output of the PATHS program. Each number placed along the pathlines in the machine plots corresponds to a time in the individual pathline. For example, the number one is for 100 years, 2 for 200 years. The advancing front isochronal lines at a given time are represented by connecting like numbers on the plots in Figures 3 and 4.

The overall flow pattern and advancing front results provide considerable insight into the system response. The pattern is also very useful in physically interpreting the arrival results provided in the next two sections.

The Location/Arrival-Time Distribution

The location/arrival-time distribution gives the locations where the contaminants will reach the groundwater outflow boundary with passing time. In our example, this is the location, as a function of time, where the contaminated groundwater will enter the river.

The interactive model provides the arrival data as summary results, which are listed in Table 3. The results labeled "Y" in column 3 of the computer output table in the section, Summary File-BQ3VH_ in Appendix C and labeled as S in column 3 of Table 3 are plotted against the travel times in column 2 to provide the location/arrival-time distribution shown in Figure 5. The several curves in the figure represent the arrival along the river bank of contaminated water that departed from the pond at time zero, 25, 50, 75, 100 and 125 years. The opening between 800 and 1200 feet along the river containing no arrival curves results from the injected uncontaminated water entering the first well (see Figures 3 and 4). Similarly, the vug-shaped open area in the arrival curves around 3000 feet in

3(a) 0 years

3(b) 50 years

FIGURE 3. Example Transient Flow Results for Fluid Particles Departing Pond at 0 and 50 Years

FIGURE 4. Example Transient Flow Results for Fluid Particles Departing Pond at 75 and 100 Years

TABLE 3. Contaminant Arrival Time and Outflow Locations
Along River for the Example Transient Case

Departure time from pond, t'_0 , yr	Arrival of contaminant at river	
	Time, T , yr	Location, s , ft
0	593.11	-594.1
	597.58	85.3
	656.09	2147.7
	812.86	4070.8
	908.30	4215.1
	1000.88	4300.3
	1159.64	4495.8
	1409.07	4107.3
	1339.77	-4091.9
	911.16	-4003.0
	709.11	-2912.8
	608.93	-1408.3
	615.85	-544.7
	620.57	146.1
	678.77	2108.8
25	722.55	2471.3
	865.08	4028.9
	935.31	4109.0
	1021.23	4237.0
	1180.65	4483.1
	1412.95	4080.1
	1368.40	-4051.5
	942.29	-3997.2
	736.78	-2921.5
	631.94	-1379.4
	645.00	-508.9
	649.26	169.4
	705.55	1977.3
	760.28	2276.5
	911.22	3759.1
50	953.72	3936.6
	1034.60	4130.1
	1195.69	4448.0
	1420.04	4039.1
	1378.48	-4018.5
	962.79	-3916.4
	763.76	-2851.0
	661.02	-1329.6
	675.54	-479.1
	679.24	180.3
	735.23	1844.4
	797.76	2166.2
	968.37	3757.5
	1046.91	4022.6
	1212.18	4413.0
75	1430.27	3996.8
	1383.19	-3988.9
	980.87	-3822.2
	790.58	-2767.6
	691.26	-1281.9
	705.41	-451.0
	708.82	187.7
	766.27	1739.9
	832.18	2121.7
	981.08	3603.0
	1058.89	3927.5
	1229.78	4377.5
	1433.66	3962.9
	1390.33	-3960.3
	998.78	-3732.8
100	816.61	-2685.1
	720.72	-1234.3

FIGURE 5. The Contaminant Location/Arrival-Time Distribution for the Transient Example Case.

Figure 5 is caused by the fluid injected into the second well. In both instances, the flow system results in Figures 3 and 4 are helpful in understanding the outflow-location/arrival-time response functions shown in Figure 5.

The location/arrival-time results (in Table 3 and shown in Figure 5) are the first results required to evaluate the environmental consequences. The second set of results is discussed in the next section using the example evaluation results. The two sets of results are then used to provide the overall environmental consequences.

The Location/Outflow-Quantity Distribution

The location/outflow-quantity results give the amount of contaminated groundwater outflow at the various locations along the river. The particular unit outflow rates are provided by the interactive LOCQAR program, discussed in detail for the example case in Appendix B.

The LOCQAR program is easy to execute; since it requires very limited input, no special input sheets are needed. As the GROUND program (i.e., batch computer run part of PATHS) is executed, most of the inputs required for LOCQAR are placed on a special file for subsequent use. Few requests for data from the user are made by the LOCQAR program. Those requests utilize the prompting and HELP features, as in PATHS, and can be answered directly from the location/arrival-time curves as in Figure 5. Instructions for using LOCQAR and complete example runs are provided in Appendix B in the section "Executing LOCQAR."

The results from LOCQAR are shown in Table 4. In particular, the arrival times at various locations along the river are provided along with the unit outflow rate of contaminated fluid. The unit outflow rate is the water outflow volume per unit time per unit distance along the river bank. Such a unit outflow rate is required since the rate changes both with location along the river and with time.

From the results in Table 4, the graph of the location/outflow-quantity distribution was prepared as shown in Figure 6. Some caution in using the plotted results is necessary since the curves representing various arrival times can be confusing. The curve for an arrival time, $T = 600$ yr, has a maximum value for q of $228.4 \text{ ft}^3/\text{yr}/\text{ft}$. The outflow rate values for the

TABLE 4. Contaminant Arrival Location Along River and Unit Outflow Rate for Example Transient Case

Arrival time, T, yr	Arrival location, s, ft	Unit outflow rate, q, ft ³ /yr/ft
600	-4000	209.5
600	-2000	215.7
600	0000	221.4
600	1600	227.0
600	2600	228.4
600	4000	223.4
650	-4000	206.4
650	-2000	210.3
650	0000	212.1
650	1600	211.2
650	2600	209.6
900	-4000	208.2
900	-2000	214.0
900	0000	220.1
900	1600	225.2
900	2600	226.8
900	4000	222.4
950	-4000	209.3
950	-2000	215.9
950	0000	223.8
950	1600	231.4
950	2600	234.2
950	4000	229.3
1000	-4000	207.9
1000	-2000	213.7
1000	0000	219.7
1000	1600	224.9
1000	2600	226.4
1000	4000	222.1
1050	-4000	204.9
1050	-2000	208.6
1050	0000	210.2
1050	1600	209.3
1050	2600	207.9
1050	4000	205.1
1300	-4000	207.4
1300	-2000	213.0
1300	0000	219.0
1300	1600	224.1
1300	2600	225.7
1300	4000	221.5
1350	-4000	208.5
1350	-2000	215.0
1350	0000	222.8
1350	1600	230.4
1350	2600	233.3
1350	4000	228.4
1450	-4000	204.4
1450	-2000	207.8
1450	0000	209.4
1450	1600	208.5
1450	2600	207.1
1450	4000	204.4

FIGURE 6. Contaminant Location/Outflow-Quantity Distribution at the River for the Example Transient Case

curve $T = 625$ yr in Figure 6 is smaller or lies to the left of the 600 yr curve as do the curves for 637.5, 650, and 750 yr. The curve for $T = 850$ yr is also displaced slightly to the left and is a local minimum curve. For $T = 900$ yr, the curve is displaced considerably to the right. The 950 yr curve is still further displaced to the right and is the maximum q curve in the Figure over most of the range of s . The 1000 yr curve recedes again to the left, with smaller q values, as do the 1050 yr and 1150 yr curves. Similarly, the 1250 yr curve is slightly left and is another local minimum curve. However, the 1300 yr curve is again significantly displaced to the right with the trend continuing to the local maximum curve for $T = 1350$ yr. The curves recede again to the left passing the 1400 yr curve and ending with $T = 1450$ yr as the most extreme left-hand curve. Such a pattern of initially diminishing unit outflow rates--which later reverse, then increase cyclically until a maximum is reached at $T = 950$ yr and then recede--requires special care in using the plot.

USE OF ARRIVAL DISTRIBUTIONS

The two arrival distributions are easy to use to determine the concentrations and amount of contaminants that will interface with the environment. The concentration along the outflow boundary (the river, in the example) is always available from the location/arrival-time distribution.

The concentration arrival distribution is similar to the results in Figure 5 since only water-coincident contaminants are considered, and the input concentration at the pond is constant. No exchange reactions are considered in the example and the contaminant source concentration, C_0 , is assumed constant over the first 25 years. After the first 25 years, no more contaminant will enter the pond or cavern. Under such conditions and with the worst-case assumption (no dispersion occurs), the concentration arrival distribution involved only using a portion of the location/arrival-time results from Figure 5.

In Figure 7, the concentration/arrival-time distribution is shown and provides the concentration entering the river with passing time. The same concentration as departed from the cavern reaches the river since the contaminant input was uniformly distributed between the zero and 25-year departure-time curves, and no exchange occurred with the porous material.

FIGURE 7. The Concentration of Contamination Entering the River at Various Locations and Times for the Example Transient Case

Through the use of Figure 7, various combinations of locations with times can be considered to yield the worst-case dose of contaminant to the biosphere. Accordingly, the concentration arrival distribution provides the first results required to evaluate the environmental consequences.

The second set of results needed is the outflow rate of contaminant into the river as time passes. Such results are available by using the concentration/arrival-time results and location/outflow-quantity distributions together. By combining the concentration and fluid outflow rate into the river, the actual contaminant outflow rate as a function of time is obtained. Specifically, the rate of contaminant entering the river, W_T , has the integral form

$$W_T = \int_{s_1}^{s_2} C_0 \cdot q \Big|_T ds \quad (17)$$

where W_T is the contaminant outflow rate.

C_0 is the concentration in the pond.

q is the unit outflow rate of groundwater into the river.

T is the particular arrival time at which q , hence W_T , is evaluated.

s_1 is the location (lower limit) where contaminated fluid enters the river.

s_2 is the location (upper limit) where contaminated fluid is entering the river.

Suppose one wanted to evaluate the contaminant outflow rate using Equation (17) at $T = 600$ yr. From Table 3, or more directly from Figure 7, at $T = 600$ yr the contaminated water is seen to enter the river between $s_1 = -1088$ and the location $s_2 = 230$ ft. Use of these locations in Figure 6 indicates the q variation with distance along the river. Using the q variation and the locations in Equation (17) and using $C_0 = 0.1$ lb/ft³ gives

$$W_{600} = 0.1 \int_{-1088}^{230} q \Big|_{600} ds \quad (18)$$

or upon evaluating

$$W_{600} = 28,872 \text{ lb/yr} = 0.0549 \text{ lb/min} \quad (19)$$

As a second example, consider the arrival time $T = 800$ yr. From Figure 7, two outflow intervals are seen at $T = 800$ years. The first outflow length, s , is between -3540 and -3400 feet. The second outflow is between 3973 and 4017 feet. Accordingly, the contaminant outflow is

$$W_{800} = 0.1 \int_{-3540}^{-3400} q \bigg|_{800} ds + 0.1 \int_{3973}^{4017} q \bigg|_{800} ds \quad (20)$$

or

$$W_{800} = 4,336 \text{ lb/yr} = 0.00825 \text{ lb/min} \quad (21)$$

Other evaluations of the type just illustrated provide the complete contaminant outflow rate in time that is shown in Figure 8.

FIGURE 8. The Outflow Rate of Groundwater Contamination for the Example Transient Case.

From the contaminant arrival curve in Figure 8, two consequences for the example are noted that are typical. The peak value is most important and, second, the significantly extended tail of the curve. The peak value of 0.087 pounds per minute is immediately apparent and always considered; however, the tail part of the curve is sometimes overlooked too quickly. By itself, this low value may not be significant, but, if it is combined with the tails of several other contaminant sources on a river or stream, then the additive effect may become important. Therefore, the entire curve is really needed if the environmental consequences are to be considered in any detail.

This completes the example evaluation using the preliminary evaluation capability. If a user wants more experience using the interactive programs, a second example steady case is provided in Appendix B. Our experience shows that the programs are quite helpful in providing preliminary evaluations for a group of two-dimensional subsurface pollution problems.

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APPENDIX A
DERIVATION OF MODEL EQUATIONS

APPENDIX A

DERIVATION OF MODEL EQUATIONS

The equations for the idealized model described in the report are presented here and useful results are derived. The model was designed to enable estimates of expected contaminant transport consequences when limited field data is available. Accordingly, the model is necessarily simplified and idealized as the representation of the real situation. However, special care was exercised to assure that minimum worst-case estimates for the fluid travel times would be provided by the model.

A GROUNDWATER POTENTIAL SOLUTION

The model assumes isothermal conditions and describes the saturated flow of an incompressible fluid through a two-dimensional lateral stratum of thickness or depth, D_0 . The stratum is a porous material that is homogeneous and isotropic with respect to hydraulic conductivity, K_0 , and the effective porosity, P . A uniform lateral gradient, U , of the fluid in the stratum provides a velocity in the x direction. Though the lateral gradient is uniform in direction, the gradient strength, U , may vary with time. A cylindrical cavity of radius r'_0 and length D_0 completely penetrates the stratum or porous slab. The flow from the cylindrical cavity depends upon the cavern head, H' , which generally is some function of time. Wells are introduced into the model as completely penetrating vertical line sources again with time-varying injection or withdrawal rates.

The objective for the idealized model is to consider a range of typical transient situations. The time dependence enters through the uniform gradient, U , the cavern head, H' , and the well flow rates. Each of these are represented by a moderately general variable/functional form for the time dependence. In this way, a variety of transient situations can be evaluated directly and most others can be approximated quite satisfactorily. The transient forms of variation are shown schematically in Figures 1 and 2 of the report; the steady situations are available by setting the time-varying parameters to appropriate constants.

We begin by considering a potential function formed by superposition of elementary flows. A uniform lateral flow is added to a combined source and positive doublet centered at the origin. Away from the origin several pumping or injection wells are superimposed as completely penetrating vertical line sinks and sources. Specifically,

$$\phi' = -Ux' - \frac{M_0}{2\pi} \ln \sqrt{(x')^2 + (y')^2} + \frac{Ux'(r_0')^2}{(x')^2 + (y')^2} - \sum_{j=1}^N \frac{M_j}{2\pi} \ln \sqrt{(x' - x_j')^2 + (y' - y_j')^2} + C_0' \quad (A-1)$$

where

$\phi' = \phi'(x', y', t')$ is the potential energy function that satisfies the Laplace Equation

$U = U(t')$ is time-dependent uniform flow gradient

$M_0 = M_0(t')$ is the major time dependent source strength located at the origin

$r_0' = \sqrt{(x_0')^2 + (y_0')^2}$ is the radius of the major source

$M_j = M_j(t')$ is the source or sink strength of the j th well located with center at (x_j', y_j')

x_j' and y_j' are respectively x' and y' coordinates of the center of the j th well

N is the total number of wells in the flow system

C_0' is a constant to be determined

x' and y' are the Cartesian coordinate variables

t' is time

A convenient set of dimensionless variables is:

$$x = \frac{x'}{R} \quad (A-2)$$

$$y = \frac{y'}{R}$$

$$r_o = \frac{r'_o}{R}$$

$$r_j = \frac{r'_j}{R}$$

$$\phi = \frac{\phi'}{H_o}$$

$$H = \frac{H'}{H_o}$$

$$t = \frac{K_o H_o}{R^2} t' \quad (A-2)$$

Substituting Equation (A-2) into (A-1) provides the potential in dimensionless form

$$\begin{aligned} \phi = & -\frac{UR}{H_o} x - \frac{M_o}{2\pi H_o} \ln \sqrt{R^2(x^2 + y^2)} + \frac{URr_o^2 x}{H_o(x^2 + y^2)} \\ & - \sum_{j=1}^{j=N} \frac{M_j}{2\pi H_o} \ln \sqrt{R^2[(x - x_j)^2 + (y - y_j)^2]} + C_1 \end{aligned} \quad (A-3)$$

C_1 is to be specified such that around the major source wall described by

$$x_o^2 + y_o^2 = r_o^2 \quad (A-4)$$

the condition to be satisfied is

$$\phi = H \quad (A-5)$$

Therefore, upon substituting into (A-3) and solving for C gives

$$C_1 = H + \frac{M_o}{2\pi H_o} \ln (Rr_o) + \sum_{j=1}^{j=N} \frac{M_j}{2\pi H_o} \ln \left[R \sqrt{(x_o - x_j)^2 + (y_o - y_j)^2} \right] \quad (A-6)$$

Substitution of Equation (A-6) into (A-3) yields

$$\phi = H - \frac{UR}{H_0} x + \frac{URr_0^2}{H_0} \left(\frac{x}{x^2 + y^2} \right) - \frac{M_0}{2\pi H_0} \ln \left(\sqrt{\frac{x^2 + y^2}{r_0}} \right) - \sum_{j=1}^{j=N} \frac{M_j}{2\pi H_0} \ln \sqrt{\frac{(x - x_j)^2 + (y - y_j)^2}{x_j^2 \left(1 - \frac{x_0}{x_j}\right)^2 + y_j^2 \left(1 - \frac{y_0}{y_j}\right)^2}} \quad (A-7)$$

The dependence in Equation (A-7) would be simplified considerably if

$$x_0 \ll x_j \text{ and } y_0 \ll y_j \quad (A-8)$$

which would imply that the wells with centers at x_j, y_j cannot be too close to the main source wall defined by Equation (A-4). If (A-8) is true, then

$$\left(1 - \frac{x_0}{x_j}\right)^2 \approx 1$$

and

$$\left(1 - \frac{y_0}{y_j}\right)^2 \approx 1 \quad (A-9)$$

We assume Equations (A-8) and (A-9) are satisfied and then derive the expression for the error introduced. That is, Equation (A-7) becomes

$$\phi = H - \frac{UR}{H_0} x + \frac{URr_0^2}{H_0} \left(\frac{x}{x^2 + y^2} \right) - \frac{M_0}{2\pi H_0} \ln \left(\sqrt{\frac{x^2 + y^2}{r_0}} \right) - \sum_{j=1}^{j=N} \frac{M_j}{2\pi H_0} \ln \sqrt{\frac{(x - x_j)^2 + (y - y_j)^2}{x_j^2 + y_j^2}} \quad (A-10)$$

The error term associated with assuming Equation (A-9) is obtained by setting $x = x_0, y = y_0$ and using Equation (A-4) in (A-10) to give the error introduced by the j th well as

$$(\phi - H)_j = \frac{M_j}{2\pi H_0} \ln \sqrt{\frac{(x_0 - x_j)^2 + (y_0 - y_j)^2}{(x_j^2 + y_j^2)}} \quad (A-11)$$

If we consider part of the expression under the radical and the sketch below, then using the Law of Cosines

$$(x_0 - x_j)^2 + (y_0 - y_j)^2 =$$

$$r_j^2 + r_0^2 - 2r_j r_0 \cos(\theta_0 - \theta_j)$$

or

$$\frac{(x_0 - x_j)^2 + (y_0 - y_j)^2}{r_j^2} = 1 + \frac{r_0^2}{r_j^2} - \frac{2r_0}{r_j} \cos(\theta_0 - \theta_j) \quad (A-12)$$

But the left-hand side is the expression under the radical in Equation (A-11), so substituting and rearranging that equation gives

$$\epsilon \equiv \frac{(\phi - H)_j}{\frac{M_j}{2\pi H_0}} = \ln \sqrt{1 + \frac{r_0}{r_j} \left[\frac{r_0}{r_j} - 2 \cos(\theta_0 - \theta_j) \right]} \quad (A-13)$$

The approximation error, ϵ , is expressed as the ratio of the major source boundary condition to the j th well strength, which by the right-hand side of Equation (A-13) is a function of r_0/r_j and the differences of angles $(\theta_0 - \theta_j)$. The magnitude of error depends primarily on the size of r_0/r_j since the cosine is bounded. That is, if r_0/r_j is small enough then negligible error will be introduced. In Figure A-1, the expression for error given by Equation (A-13) is plotted for a range of r_0/r_j values. As r_0/r_j becomes smaller the error becomes essentially insignificant. For values of r_0/r_j less than 0.01, the error is always less than 1-percent maximum. Such a value is reasonable and is recommended for general use. Accordingly, Equation (A-10) approximately satisfies the boundary conditions so long as:

FIGURE A-1. Approximation Error at the Major Source or Pond Boundary Caused by the Proximity of the jth Well

$$\frac{r_0}{r_j} < 0.01 . \quad (A-14)$$

Equation (A-14) is the criterion used to assure that ϵ is small enough for general use.

We can assure conservatism in the calculated travel times of fluid particles by using the slightly higher gradients associated with flow to a finite remote boundary rather than to an infinite boundary. These slightly higher gradients result if all of the major source head, H , is dissipated at the finite radial distance R . In dimensionless form it is equivalent to stating that H is dissipated at $x^2 + y^2 = 1$, or more specifically,

$$H - \frac{M_0}{2\pi H_0} \ln \left(\frac{1}{r_0} \right) = 0 . \quad (A-15)$$

Solving for $M_0/(2\pi H_0)$ gives

$$\frac{M_0}{2\pi H_0} = \frac{H}{\ln \left(\frac{1}{r_0} \right)} \quad (A-16)$$

Substituting Equation (A-16) into (A-10) gives as the final dimensionless potential function:

$$\begin{aligned} \phi = H - \frac{UR}{H_0} x + \frac{URr_0^2}{H_0} \left(\frac{x}{x^2 + y^2} \right) - \frac{H}{\ln \left(\frac{1}{r_0} \right)} \ln \left(\frac{\sqrt{x^2 + y^2}}{r_0} \right) \\ - \sum_{j=1}^{j=N} \frac{M_j}{2\pi H_0} \ln \sqrt{\frac{(x - x_j)^2 + (y - y_j)^2}{(x_j^2 + y_j^2)}} , \quad \frac{r_0}{r_j} < 0.01 \end{aligned} \quad (A-17)$$

where

$M_j = \frac{Q_j}{D_0 K_0}$ is the well source or sink strength.

Q_j is the volume inflow or outflow rate of the well;

i.e., Q_j is positive for an injection well and negative when a well is pumped.

D_0 is the constant stratum thickness

K_0 is the uniform hydraulic conductivity, and the other terms are as already defined or as shown in Appendix D.

Equation (A-17) can be shown to be a solution of the Laplace Equation that describes flow of an incompressible fluid in a homogeneous isotropic porous medium. Since the fluid is incompressible, the transient flow systems are impulsively generated by boundary conditions that change in time. In Equation (A-17) the variables H , U , and M_j through Q_j may all be time dependent. Under many conditions of expected use for the model, the time dependence may not be known in detail. In these initial evaluations, it is often a matter of considering the consequences of various types of variation rather than detailed representation. Accordingly, considerable flexibility is needed and several functional forms for the time dependence were considered. From this evaluation came some particular functional forms. The most useful form found is a slight modification of the classical serpentine expression of the form

$$W(t') = w_0 + \frac{2(w_0 - w_m) \left(\frac{t'}{t_n} + A \right)}{B \left(\frac{t'}{t_n} + A \right)^2 + C} \quad (A-18)$$

where w_0 , w_m , t'_n , A , B and C are arbitrary parameters. This serpentine equation form was used to describe the time dependence of U , H and Q_j with the specific parameters defined as shown in Table A-1.

TABLE A-1. Definition of Parameters for the Serpentine Equation Form (A-18)

Parameter in Equation (A-18), $W(t')$	Parameter defined in serpentine forms for		
	$U(t')$	$H(t')$	$Q_j(t')$
w_o	UO	HI	QI _j
w_m	UM	HM	QM _j
t'_n	TM	TN	TN _j
A	A	D	DW _j
B	B	E	EW _j
C	C	F	FW _j

The second convenient functional form used to describe the time dependence of H and Q_j is

$$W(t') = w_{mc} + w_{oc} \sin \left[2\pi \frac{(t' - t_{oc})}{(t_{mc} - t_{oc})} \right] \quad (A-19)$$

which provides a continuous cyclic-type fluctuation. The parameters for describing H and Q_j are shown in Table A-2.

TABLE A-2. Definition of Parameters for the Cyclic Equation Form (A-19)

Parameter in Equation A-19 $W(t')$	Parameter defined in cyclic form for	
	$H(t')$	$Q_j(t')$
w_{mc}	HMC	QQ _j
w_{oc}	HAC	QA _j
t_{oc}	TOC	TO _j
t_{mc}	TMC	TM _j

A third form for the time-dependent head H in Equation (A-17) is useful when considering worst-case accidental leakage into the ground from liquid-storage facilities. It is the falling head case where the fluid level diminishes in the storage facility at the rate that fluid seeps

from the structure. Consider the cylindrical fluid volume of radius r'_0 and height H' ; then the instantaneous volume change $\frac{dv'}{dt'}$ or Q' the outflow rate is

$$\frac{dv'}{dt'} = Q' = -\pi(r'_0)^2 \frac{dH'}{dt'} \quad (A-20)$$

but the instantaneous outflow rate, Q_0 , is

$$Q = \frac{2\pi D_0 K_0 H'}{\ln\left(\frac{R}{r'_0}\right)} \quad (A-21)$$

Substituting (A-21) into (A-20) gives upon rearranging

$$\int_{H_0}^{H'} \frac{dH'}{H'} = \int_0^{t'} -\frac{2D_0 K_0}{(r'_0)^2 \ln\left(\frac{R}{r'_0}\right)} dt' \quad (A-22)$$

and upon evaluating the integrals one obtains

$$\frac{H'}{H_0} = \exp \left[-\frac{2D_0 K_0}{(r'_0)^2 \ln\left(\frac{R}{r'_0}\right)} t' \right] \quad (A-23)$$

and using the Equations (A-2) to form the dimensionless equivalent yields

$$H = \exp \left[-\frac{2D_0}{H_0 r_0^2 \ln\left(\frac{1}{r_0}\right)} t \right] \quad (A-24)$$

which is the exponential expression for the declining head in the circular source as leakage occurs from storage facility.

Experience in using the above time-dependent forms shows them usually to be adequate. However, in some instances where specific forms are needed, it may be convenient to write a particular computer subroutine to replace the serpin form. Usually the six parameters

provide sufficient input capacity for any special time-dependent routine that may be needed.

THE KINEMATIC PATHLINES

The equations for the fluid pathlines are available from Darcy's Law expressed as a pore velocity using the potential equations already derived. Specifically, the dimensional pore velocity, $\underline{u}'$, is

$$\underline{u}' = - \frac{K_0}{P} \nabla' \phi' \quad (A-25)$$

If the dimensionless velocity, $\underline{u}$, is

$$\underline{u} = \frac{R}{K_0 H_0} \underline{u}' \quad (A-26)$$

Using Equation (A-2) gives the dimensionless pore velocity expression

$$\underline{u} = - \frac{1}{P} \nabla \phi \quad (A-27)$$

or in components

$$\frac{dx}{dt} = u_x = - \frac{1}{P} \frac{\partial \phi}{\partial x} \quad (A-28)$$

and

$$\frac{dy}{dt} = u_y = - \frac{1}{P} \frac{\partial \phi}{\partial y} \quad (A-29)$$

where the expression for ϕ is provided by the potential solution in Equation (A-17). Differentiation of Equation (A-17) first with respect to x , then with respect to y and substitution into Equations (A-28) and (A-29), respectively, gives the pair of pathline differential equations, i.e.,

$$\begin{aligned} \frac{dx}{dt} = \frac{UR}{PH_0} \left\{ 1 + \frac{r_0^2}{(x^2 + y^2)} \left[\frac{2x^2}{x^2 + y^2} - 1 \right] \right\} + \frac{H}{P \ln \left(\frac{1}{r_0} \right)} \left(\frac{x}{x^2 + y^2} \right) \\ + \sum_{j=1}^{j=N} \frac{M_j}{2\pi H_0 P} \left[\frac{(x - x_j)}{(x - x_j)^2 + (y - y_j)^2} \right], \end{aligned} \quad (A-30)$$

and

$$\begin{aligned} \frac{dy}{dt} = & \frac{UR}{PH_0} \left[\frac{2(r_0)^2 xy}{(x^2 + y^2)^2} \right] + \frac{H}{P \ln \left(\frac{1}{r_0} \right)} \left(\frac{y}{x^2 + y^2} \right) \\ & + \sum_{j=1}^{j=N} \frac{M_j}{2\pi PH_0} \left[\frac{y - y_j}{(x - x_j)^2 + (y - y_j)^2} \right] \end{aligned} \quad (A-31)$$

The simultaneous solution of these two pathline equations beginning from the initial conditions

$$x(t_0) = x_0 \quad (A-32)$$

and

$$y(t_0) = y_0 \quad (A-33)$$

yields the path of the fluid particle that was located at x_0, y_0 at time t_0 . By successively considering other combinations of x_0, y_0 and t_0 , i.e., other starting points and times, the entire field of fluid particle pathlines can be obtained.

The system of equations made up of (A-30) through (A-33) generally cannot be solved in closed form, particularly when U, H and/or M_j take on the time-dependent forms of Equations (A-18), (A-19) and (A-24), therefore, a modified fourth-order Runge-Kutta numerical method is conveniently used to calculate the pathlines (Gill, 1951). In this way the macroscopic flow paths of fluid particles are directly calculated.

The Stream Function

The stream function is needed to provide complete environmental results. The stream function is directly available from the previously derived potential function Equation (A-17) as the complex conjugate. The stream function ψ in dimensionless variables is

$$\psi = -\frac{UR}{H_0} y - \frac{UR r_0^2 y}{H_0 (x^2 + y^2)} - \frac{H}{\ln\left(\frac{1}{r_0}\right)} \arctan\left(\frac{y}{x}\right) - \sum_{j=1}^{j=N} \frac{M_j}{2\pi H_0} \left[\arctan\left(\frac{y - y_j}{x - x_j}\right) - \arctan\left(\frac{-y_j}{x_0 - x_j}\right) \right] \quad (A-34)$$

Equation (A-34) can be rewritten in polar coordinates (r, θ) to give

$$\psi = -\frac{UR}{H_0} r \sin \theta - \frac{UR r_0 \sin \theta}{H_0 r} - \frac{H}{\ln\left(\frac{1}{r_0}\right)} \theta - \sum_{j=1}^{j=N} \frac{M_j}{2\pi H_0} \left[\arctan\left(\frac{r \sin \theta - r_j \sin \theta_j}{r \cos \theta - r_j \cos \theta_j}\right) - \arctan\left(\frac{-r_j \sin \theta_j}{r \cos \theta - r_j \cos \theta_j}\right) \right] \quad (A-35)$$

We note that $\psi = 0$, when $r = r_0$ and $\theta = 0$ and, further, that when $r = r_0$ and $\theta = 2\pi$ so that all of the outflow from the circular source is included, then $\psi = \psi_s$, which gives

$$\psi_s = -\frac{2\pi H}{\ln\left(\frac{1}{r_0}\right)} \quad (A-37)$$

and using Equation (A-16) gives

$$\psi_s = -\frac{M_0}{H_0} \quad (A-38)$$

but the source strength $M_0 = Q/(D_0 K_0)$, so

$$\psi_s = -\frac{Q}{D_0 K_0 H_0} \quad (A-39)$$

where Q is the volume outflow rate from the source. Equating (A-37) with (A-39) and solving for Q gives

$$Q = \frac{2\pi D_o K_o H_o H}{\ln\left(\frac{1}{r_o}\right)} \quad (\text{A-40})$$

which, with all terms reduced to dimensional form, is identical to Equation (A-21).

It is convenient to use a single reference outflow Q_o , which is obtained by setting $H = 1$, i.e. $H' = H_o$, in Equation (A-40). That is,

$$Q_o = \frac{2\pi D_o K_o H_o}{\ln\left(\frac{1}{r_o}\right)} \quad (\text{A-41})$$

which corresponds to defining a ψ_o through reducing Equation (A-37) to

$$\psi_o = -\frac{2\pi}{\ln\left(\frac{1}{r_o}\right)} \quad (\text{A-42})$$

If Equation (A-34) is divided by (A-42) and the resulting ψ/ψ_o is equated to Q_i/Q_o , then one obtains

$$\begin{aligned} \frac{Q_i}{Q_o} = & \frac{UR \ln\left(\frac{1}{r_o}\right)}{2\pi H_o} y + \frac{UR \ln\left(\frac{1}{r_o}\right) r_o^2 y}{2\pi H_o (x^2 + y^2)} + \frac{H}{2\pi} \arctan\left(\frac{y}{x}\right) \\ & + \sum_{j=1}^{j=N} \left[\frac{M_j \ln\left(\frac{1}{r_o}\right)}{4\pi^2 H_o} \right] \left[\arctan\left(\frac{y - y_j}{x - x_j}\right) - \arctan\left(\frac{-y_j}{x_o - x_j}\right) \right] \end{aligned} \quad (\text{A-43})$$

SIMPLIFIED CHEMICAL TRANSPORT WITH SORPTION

A single chemical species at trace concentration with equilibrium sorption is readily considered with only minor modification of the kinematic equations already provided. In particular, if the hydrodynamic dispersion is ignored since it is so very small in a homogeneous porous material, then the chemical transport equation using an equilibrium distribution coefficient, K_d , and the bulk density, B_d , of the porous material is

$$\nabla' \cdot (C' \underline{u}') = \left(1 + \frac{B_d K_d}{P}\right) \frac{\partial C'}{\partial t'} \quad (\text{A-44})$$

or the dimensionless equivalent expression upon using Equations (A-2), (A-25) and (A-26) is

$$\nabla \cdot (C^0 \underline{u}) = \left(1 + \frac{B_d K_d}{P}\right) \frac{\partial C^0}{\partial t} \quad (\text{A-45})$$

where $C^0 = C'/C_0$ with the C_0 being the original source concentration at $t = 0$. Expanding the equation gives

$$\underline{u} \cdot \nabla C^0 = K \frac{\partial C^0}{\partial t} \quad (\text{A-46})$$

since

$$\nabla \cdot \underline{u} = \frac{1}{P} \nabla \cdot \underline{q} \equiv 0 \quad (\text{A-47})$$

by conservation of mass in a homogeneous material, and where

$$K = \left(1 + \frac{B_d K_d}{P}\right) \quad (\text{A-48})$$

Inspection of Equation (A-46) shows it to be a first-order partial differential equation, which is reduceable to the set of Characteristic Equations

$$\frac{dx}{dt} = \frac{1}{K} u_x \quad (\text{A-49})$$

and

$$\frac{dy}{dt} = \frac{1}{K} u_y \quad (\text{A-50})$$

But comparison with the kinematic Equations (A-28) and (A-29) shows that characteristic equations for the idealized contaminant transport are within a constant multiplier of the original kinematic expressions. Accordingly, it is no more difficult to solve for the idealized approximate chemicals transport equations; i.e.,

$$\begin{aligned} \frac{dx}{dt} = & \frac{UR}{PH_0 K} \left\{ 1 + \frac{r_0^2}{(x^2 + y^2)} \left[\frac{2x^2}{x^2 + y^2} - 1 \right] \right\} + \frac{H}{KP \ln \left(\frac{1}{r_0} \right)} \left(\frac{x}{x^2 + y^2} \right) \\ & + \sum_{j=1}^{j=N} \frac{M_j}{2\pi H_0 PK} \left[\frac{(x - x_j)}{(x - x_j)^2 + (y - y_j)^2} \right] \end{aligned} \quad (A-51)$$

$$\begin{aligned} \frac{dy}{dt} = & \frac{UR}{PH_0 K} \left[\frac{2(r_0)^2 xy}{(x^2 + y^2)^2} \right] + \frac{H}{KP \ln \left(\frac{1}{r_0} \right)} \left(\frac{y}{x^2 + y^2} \right) \\ & + \sum_{j=1}^{j=N} \frac{M_j}{2\pi PH_0 K} \left[\frac{y - y_j}{(x - x_j)^2 + (y - y_j)^2} \right] \end{aligned} \quad (A-52)$$

Equations (A-51) and (A-52) reduce identically to Equations (A-30) and (A-31) when no exchange occurs. So if there is no exchange then $K_d = 0$ in Equation (A-48); hence $K = 1$ so (A-36) and (A-37) reduce to the kinematic equations of (A-51) and (A-52).

APPENDIX B

USER'S GUIDE FOR THE
PRELIMINARY EVALUATION MODELS.

APPENDIX B

USER'S GUIDE FOR THE PRELIMINARY EVALUATION MODELS

USING THE TERMINAL

The interactive PATHS program was written utilizing a conversational mode; it is tutorial and aids the user in providing the proper reply. Most responses will require a yes (Y) or no (N) answer or some numerical value. Details and examples of this will be given later. Other than knowing how to respond to prompting questions, the user needs little knowledge of computer commands.

Before working with the computer, bureaucratic details of being funded and given a project ID, user ID, password, and account number must be completed. Having these, a terminal and a phone, the Univac 1100/44 may be called by dialing 942-7841. After placing the phone in the acoustic coupler, and without prompting from the Univac, type in the terminal ID (written on the terminal). After the Univac responds to this, follow up with the USERID/PASSWORD, PROJECT-ID, and address, as shown in the example following. Note that the symbol > (greater than) prompts the responses that are entered by the user.

```
DLT106  
ENTER USERID/PASSWORD:
```

```
*DESTROY USERID/PASSWORD ENTRY  
*UNIVAC 1100 OPERATING SYSTEM VER. 33R2*43A00002(RSI)*  
ENTER PROJECT-ID:  
>NELSON
```

```
RUN NUMBER 94
```

```
LAST RUN AT: 042678 082824  
DATE: 042678 TIME: 082943  
TYPE NAME/ADDRESS -  
>NIALI PLINE 703 BLOC
```

At this point, PATHS could be executed. The beginning sequence of this is

```
@XQT NELSON*PATHS.RUN
THIS PROGRAM CALCULATES AND PLOTS THE FLOW PATHS
FROM CAVERN TO BOUNDARY AND CALCULATES THE ARRIVAL TIME
DISTRIBUTION OF FLUID AT THE BOUNDARY.
```

```
PLEASE ENTER THE FOLLOWING FOR THE BATCH PORTION OF
THE RUN. PRESS THE CARRIAGE RETURN AFTER RESPONDING.
ENTER YOUR ACCOUNT NUMBER:
```

```
>ABC123
```

```
ENTER USER ID
```

```
>MYID
```

```
ENTER PROJECT ID
```

```
>PROJID
```

```
ENTER NAME/ADDRESS
```

```
>JOHN DOE/FED. BLDG. RM. 999
```

```
ENTER PASSWORD
```

```
>MYPASSWORD
```

```
NOW ENTER THE TEST CASE NAME--A ONE LINE TITLE
```

```
>ENTER THE TITLE THAT YOU PREFER: (The case title at the top of the
input worksheet can be used.)
```

```
ENTER INPUT VARIABLES AS REQUESTED.
```

```
IN RESPONSE TO ANY REQUEST FOR INPUT, ENTER THE WORD
HELP TO OBTAIN AN EXPLANATION FOR THE REQUIRED INPUT.
```

```
DO
```

```
>100
```

The PATHS program now has control and directs the user to respond appropriately. If you make a mistake while responding to PATHS, it can be erased (backspaced over). To do this, depress the control key and type the letter H. If the carriage has been returned and bad data thereby entered, PATHS can be terminated by typing the master character @. After this, begin again, starting with the @XQT statement. However, you may choose to note the mistake and continue with the intent of later modifying the job stream created. In this instance, continue to respond to all questions until the end. When PATHS asks if the batch job is to be submitted, reply NO. This way a copy of the job stream is saved. Following PATHS, the Univac EDITOR may be entered to modify the job stream appropriately for batch submittal. See "Using EDITOR for Minor Run Changes" for details.

SAMPLE JOB

The following job stream was entered through PATHS as an example. See the input parameter worksheet from Table I in the report.

```
@WAT NELSON*PATHS.MUN
THIS PROGRAM CALCULATES AND PLOTS THE FLOW PATHS
FROM CAVERN TO BOUNDARY AND CALCULATES THE ARRIVAL TIME
DISTRIBUTION OF FLUID AT THE BOUNDARY.
```

```
PLEASE ENTER THE FOLLOWING FOR THE BATCH PORTION OF
THE RUN.  PRESS THE CARRIAGE RETURN AFTER RESPONDING.
ENTER YOUR ACCOUNT NUMBER
```

```
>
ENTER USERID
>
ENTER PROJECT ID
>
ENTER NAME/ADDRESS
>
ENTER PASSWORD
>
```

```
NOW ENTER THE TEST CASE NAME--A ONE LINE TITLE
>EXAMPLE TRANSIENT CASE (TWO WELLS)
```

```
ENTER INPUT VARIABLES AS REQUESTED.
```

```
IN RESPONSE TO ANY REQUEST FOR INPUT, ENTER THE WORD
HELP TO OBTAIN AN EXPLANATION FOR THE REQUIRED INPUT.
```

```
DO
>100
R
>8500
STANDARD * TERMINATION OF PATHLINES
>YES
ENTER XMAX
>8500
RO
>250
HO
>10
KO
>1825
P
>.2
STEADY OR TRANSIENT CASE (S OR T)
>T
UO
>.001
UM
>.001
```

(If the steady case is chosen, you will input HI and UO. HM is automatically set equal to HI and UM is set equal to UO.)

ENTER S, E, OR C FOR COMPUTING
VARIATION IN THE CAVERN HEAD

>S (If exponential were chosen for the time variation,
HI parameters HI, HM, TM, D, E, and F would not be
>4 needed to perform the calculations.)
HM
>8
TM
>50
D
>0
E
>1
F
>1

DO YOU WANT TO ENTER ADDITIONAL WELLS OR CAVERNS?

>YES

J

>2

(Use well input data from the back of Table 2.)

XWELL(1)

>3000

YWELL(1)

>1000

ROWELL(1)

>250

ENTER SERPIN OR CYCLIC OPTION FOR THE WELL (S OR C)

>S

QI

>4000

QM

>600000

TNWELL

>25

EWELL

>1

FWELL

>1

FWELL

>1

XWELL(2)

>5500

YWELL(2)

>3000

ROWELL(2)

>300

ENTER SERPIN OR CYCLIC OPTION FOR THE WELL (S OR C)

>C

QI

>0

QM

>500000

TNWELL

>50

TNWELL

>450

(If a question arises, type in help.)

THE TIME UNITS OF KO ARE IN?
 >YEARS
 THETA0
 >0
 THETA1
 >160
 NTHETA
 >9
 KTHETA
 >1
 T0
 >0
 TF
 >100
 NT
 >5
 IS THERE AN ION EXCHANGE DELAY?
 >NO
 CHOOSE A CONVENIENT ROUNDED DELTA BETWEEN THE NUMBERS 1 AND 3
 >2.5
 ENTER STEP
 >6
 ENTER ITLIM
 >5000
 TO OBTAIN BETWEEN 15 AND 25 ISOCHRONAL LINES,
 CHOOSE NPRINT BETWEEN 7 AND 13
 ENTER NPRINT
 >40 (Note: 40 was used, rather than a number within the range suggested
 by the program, to reduce the length of example case output.)
 ENTER EPSLN
 >.00001
 DO YOU WANT THE FLOW PATHS PLOTTED?
 >YES
 DO YOU WANT 30 INCH PLOTS?
 >NO
 ENTER XCENTER
 >3
 ENTER YCENTER
 >2
 ENTER SCALE (IN FEET /INCH)
 >1000
 DO YOU WANT THE DETAILED COMPUTER PRINTOUT?
 >YES
 ENTER RUN NUMBER OF THE JOB STREAM TO BE SAVED---
 ---OTHERWISE, ESCAPE BY TYPING @
 >1 (Remember this run number for later use.)
 DO YOU WANT THE JOB SUBMITTED.
 >YES
 THE PROGRAM GROUND HAS BEEN SUBMITTED FOR EXECUTION.
 THE BATCH RUNSTREAM HAS BEEN SAVED IN FILE NELSON*GRND1.
 UPON EXECUTION OF THE BATCH PROGRAM, THE SUMMARY
 IS SAVED IN FILE NELSON*GRNDUN

Finally, to quit interacting with the Univac properly, type `@FIN` and follow up with `@@TERM`. The carrier detect light will go off on the terminal and the phone can be taken off the acoustic coupler. However, after finishing with the interactive part of job submittal, it is a good idea to verify the successful entry of the batch portion into the execute queue. Also, you may wish to preview the summary file created by the batch run's (GROUND's) execution, and to execute the program LOCQAR. Discussions of these follow.

The detailed printed output from responding YES to the question: "Do you want the job submitted?" can be seen under the topic "Example Transient Case."

TRACKING JOB EXECUTION

After starting the batch job, type `@@CONS` to check its progress. Follow this by T as shown below.

```

@@CONS
>T
ACTIVE RUNS: ICCRUN+ TAPEA/DLT519 SCHLOS/DLT035
>ACTIVE RUNS: WDC211+/DLT073 UUTT+ WDC515/DLT119 CDRPRT+
ACTIVE RUNS: JUDE+/DLT109 ISCHUR+/DLT035 GDFORT/DOCT002
ACTIVE RUNS: MOCURR+ SDUMP+ MORITZ+/DOCT001 GROUND+

```

All the jobs currently in execution are listed. If another job GROUND is already queued, a later entry will be called GROUNE, and one after that GROUND and so on.

Information on the progress of execution of a particular job can be obtained by typing RC and then the job name. This is shown below for GROUND.

```

>RC GROUND
GROUND,M                                OPEN/SWAP
> BATCH TIME =                          PAGES = 10000/4
  CARDS = 5000/0 SIZE = 6
RC GROUND
GROUND,M BQA640                        OPEN/INCOR
> BATCH TIME = 06:00:00/00:01:30 PAGES = 10000/77
  CARDS = 5000/0 SIZE = 31
RC GROUND
GROUND,M BQA640                        OPEN/INCOR
> BATCH TIME = 06:00:00/00:02:03 PAGES = 10000/105
  CARDS = 5000/0 SIZE = 31
RC GROUND
GROUND HAS FINNED
>GROUND: PR 107 PGS M PR2/PR

```

Notice that progress is monitored until the job has finished. Of course, in normal practice, job monitoring to this detail is not necessary. Type @@END CONS when finished monitoring the job. Once the batched job GROUND has finished successfully, the two files it generates (PROJID*BQ3VH_ and PROJID*LOCQ_) are available for the user. (Note: PROJID is the user project ID and the _ is the run number. For the example transient problem, these are respectively NELSON*BQ3VH1. and NELSON*LOCQ1.).

SUMMARY FILE - BQ3VH_.

With the successful execution of the GROUND program, you may view from the terminal a summary of the flow paths calculated. This way you have the summary results and can partially review calculated results before the longer printed output is delivered. To do this type @ED,R PROJID*BQ3VH_ followed by P!. This is shown with the ensuing results for the example case stored on NELSON*BQ3VH1. .

JOED,R NELSON♦B03VH1.

READ-ONLY MODE

ED 15R2-TUE-04/11/78-14:03:11-(0.)

EDIT

0:>P! (P! means to print all lines in the file.)

EXAMPLE TRANSIENT CASE (TWO WELLS)

THE DEPARTURE TIME IS .000 YEARS
THE INITIAL OUTFLOW RATE IS .13006966+007
CUBIC FEET PER YEARS
THE INITIAL RELATIVE CAVERN HEAD IS .4000

PATH NO.	TRAVEL TIME YEARS	X FEET	Y FEET	PATH LENGTH FEET
1	5.93105+002	9.50000+003	-5.94146+002	8.29076+003
2	5.97578+002	8.49998+003	8.53198+001	8.31150+003
3	1.50781+002	2.75648+003	1.05426+003	2.74278+003
4	6.56093+002	8.49992+003	2.14770+002	8.87105+003
5	4.52500+002	5.52440+003	2.70168+003	6.33241+003
6	8.12856+002	8.49996+003	4.07076+003	1.09956+004
7	9.08300+002	8.49993+003	4.21505+003	1.08034+004
8	1.00088+003	8.49996+003	4.30026+003	1.12869+004
9	1.15964+003	8.49999+003	4.49577+003	1.21774+004
10	1.40907+003	8.49992+003	4.10734+003	1.26985+004

THE DEPARTURE TIME IS 25.000 YEARS
 THE INITIAL OUTFLOW RATE IS .23412538+007
 CUBIC FEET PER YEARS
 THE INITIAL RELATIVE CAVERN HEAD IS .7200

PATH NO.	TRAVEL TIME YEARS	X FEET	Y FEET	PATH LENGTH FEET
1	6.15849+002	8.49999+003	-5.44676+002	8.27626+003
2	6.20566+002	8.49996+003	1.46096+002	8.31424+003
3	1.73750+002	2.76808+003	1.08996+003	2.76965+003
4	6.78774+002	8.49996+003	2.10882+003	8.89020+003
5	7.22548+002	8.49994+003	2.47132+003	9.36523+003
6	8.65077+002	8.49995+003	4.02887+003	1.01362+004
7	9.35311+002	8.49995+003	4.10902+003	1.06107+004
8	1.02123+003	8.49992+003	4.23700+003	1.12974+004
9	1.18065+003	8.50000+003	4.48307+003	1.21531+004
10	1.41295+003	8.49995+003	4.08009+003	1.26239+004

THE DEPARTURE TIME IS 50.000 YEARS
 THE INITIAL OUTFLOW RATE IS .26013932+007
 CUBIC FEET PER YEARS
 THE INITIAL RELATIVE CAVERN HEAD IS .8000

PATH NO.	TRAVEL TIME YEARS	X FEET	Y FEET	PATH LENGTH FEET
1	6.45004+002	8.49996+003	-5.08899+002	8.27236+003
2	6.49257+002	8.49995+003	1.69379+002	8.31094+003
3	1.97969+002	2.75369+003	1.04029+003	2.74411+003
4	7.05546+002	8.49992+003	1.97734+003	8.87098+003
5	7.60277+002	8.49995+003	2.27654+003	9.35390+003
6	9.11215+002	8.49996+003	3.75909+003	1.00119+004
7	9.53724+002	8.49997+003	3.93656+003	1.05183+004
8	1.03460+003	8.50000+003	4.13010+003	1.12026+004
9	1.19569+003	8.50000+003	4.44799+003	1.20519+004
10	1.42004+003	8.49993+003	4.03909+003	1.25146+004

THE DEPARTURE TIME IS 75.000 YEARS
 THE INITIAL OUTFLOW RATE IS .25013396+007
 CUBIC FEET PER YEARS
 THE INITIAL RELATIVE CAVERN HEAD IS .7692

PATH NO.	TRAVEL TIME YEARS	X FEET	Y FEET	PATH LENGTH FEET
1	6.75536+002	8.49998+003	-4.79104+002	8.26912+003
2	6.79238+002	8.49997+003	1.30307+002	8.30669+003
3	2.23750+002	2.75079+003	9.93653+002	2.72904+003
4	7.35234+002	8.49993+003	1.84440+003	8.34856+003
5	7.97763+002	8.49999+003	2.16618+003	9.31621+003
6	6.25312+002	5.20091+003	3.00368+003	6.49025+003
7	9.68368+002	8.49993+003	3.75754+003	1.04142+004
8	1.04691+003	8.49992+003	4.02259+003	1.10226+004
9	1.21212+003	8.49993+003	4.41300+003	1.19453+004
10	1.43027+003	8.49996+003	3.99681+003	1.24079+004

THE DEPARTURE TIME IS 100.000 YEARS
 THE INITIAL OUTFLOW RATE IS .23412539+007
 CUBIC FEET PER YEARS
 THE INITIAL RELATIVE CAVERN HEAD IS .7200

PATH NO.	TRAVEL TIME YEARS	X FEET	Y FEET	PATH LENGTH FEET
1	7.05409+002	8.49994+003	-4.50975+002	8.26644+003
2	7.08822+002	8.49996+003	1.87686+002	8.30357+003
3	2.49375+002	2.75395+003	9.64524+002	2.72337+003
4	7.66269+002	8.49994+003	1.73988+003	8.33857+003
5	9.32177+002	8.49994+003	2.12171+003	9.26736+003
6	6.40781+002	5.29290+003	2.78342+003	6.50668+003
7	9.81083+002	8.49993+003	3.60303+003	1.03224+004
8	1.05889+003	8.49996+003	3.92747+003	1.09901+004
9	1.22978+003	8.49996+003	4.37746+003	1.18447+004
10	1.43966+003	8.49999+003	3.96292+003	1.23099+004

EOF:111
 0:> Exit

After the summary file has been listed on the terminal and control is returned to the user, i.e.; when the system prints the symbol >, type in EXIT to get out of the editor.

These summary results are the basic arrival data required to evaluate the contamination problem. Specifically, the above results are contained in Table 3 in the body of the report.

EXECUTING LOCQAR

After GROUND has completed execution and after the summary file BQ3VH_ has been reviewed, the LOCQAR program can be executed to calculate fluid arrival locations and outflow quantities. To execute LOCQAR from the terminal, type @XQT NELSON*LOCQAR.RUN . Now LOCQAR asks for the information it needs. Like PATHS, LOCQAR is tutorial and aids in answering its questions. Typing HELP solicits clarification of LOCQAR's questions, as shown below.

```
XMAX
>HELP
XMAX IS THE VALUE OF X AT WHICH THE FLUX IS EVALUATED.
XMAX
>8500

SMIN
>HELP
SMIN IS THE MINIMUM VALUE OF Y ALONG THE LINE X=XMAX
AT WHICH THE FLUX IS TO BE EVALUATED.

IF SMIN EQUALS SMAX THE USER CAN MANUALLY INPUT NOS VALUES
SMIN
>1000
```

Following is an execution of LOCQAR using the file created by the transient case.

PAOT NELSON+LOCQAR.RUN

ENTER RUN NUMBER USED IN PROGRAM PATHS, IF PATHS NOT
PREVIOUSLY RUN, DO NOT CONTINUE WITH THIS PROGRAM

>1

ENTER TEST CASE NAME

>EXAMPLE TRANSIENT CASE (TWO WELLS)

SMAK

>2500

SMIN

>-4000

(If SMIN and SMAK are input as the same number,
NQS irregular locations of s can be input.)

SMAK

>4000

NQS

>3

ATMIN IN UNITS OF YEARS

>600

ATMAX IN UNITS OF YEARS

>650

(If ATMIN and ATMAX are input as the same number,
NAT irregular times can be input.)

NAT

>2

FLUID ARRIVAL LOCATIONS AND OUTFLOW QUANTITIES FOR
EXAMPLE TRANSIENT CASE (TWO WELLS)

ARRIVAL TIME YEARS	S, LOCATIONS OF OUTFLOW FEET	OUTFLOW RATE IN CUBIC FEET / YEARS / FEET
.600000+003	-.400000+004	.209556+003
.600000+003	.000000	.221375+003
.600000+003	.400000+004	.223860+003
.650000+003	-.400000+004	.206351+003
.650000+003	.000000	.212106+003
.650000+003	.400000+004	.206661+003

(These results are the arrival outflow data required to evaluate the
contamination problem. They are contained in Table 4 in the report.)

USING EDITOR FOR MINOR RUN CHANGES

Often it is quicker for the user to edit the batch run stream created by PATHS rather than to create a new job stream by rerunning PATHS. To facilitate this, the following flow diagram shows the data names read by the GROUND program. Most of these names can be recognized from the input parameter worksheet data in Table 1 of the report. The others, superscripted by an asterisk (*), are variables set by PATHS. They are primarily used to direct the flow of execution of the GROUND program.

```
1. @RUN . . .
2. @IDENT . . .
3. @PASSWD
4. @ASG,UP . . .
5. @USE 4., . . .
6. @TP,W PLOT*BP400./8
7. @XT NELSON*GROUND.RUN


---


8. TEST CASE NAME (A one line title)
9. R, R , HO, KO
10. RO, RO, Do, UO
11. UM, P, TM
12. PATH*,KD,BD
13. CHEM, PROJ, VH3*, IPROJ*
14. A, B, C, KTHETA
15. THETAO, THETAM, TO, NTHETA
16. TF, TMAX,EPSLN,ITLIM
17. DELTA, TN, STEP, NT
18. XMAX, XCENTER, YCENTER, NPRINT
19. SCALE, D, E, F
20. HI, HM, P9
21. HMC, HAC, TOC, TMC
22. SS, J, P1*


---


23. ROWELL(J), XWELL(J)
24. YWELL(J), TNWELL(J)
25. QI(J), QM(J), DWELL(J)
26. EWELL(J), FWELL(J), QA(J), QQ(J)
27. TOWELL(J), TMWELL(J)
28. WSS(J)*


---


```

Note: The variable VH3 contains the run number used by the PATHS system for a particular job. In the example, transient case, the value of VH3 is 1.

Skips if J=0. Otherwise, loops through these

```
35. VS
36. WS
37. CS
```

(When THETAO = THETAM, a list of XSTART and YSTART values are printed out here.)

TPSAV8

To explicate further, the batch run stream of the sample problem for the transient case is shown below.

```

@ED:U NELSON*GRND1.
ED 15R2-WED-04/26/78-14:45:57-(0,1)
EDIT
0:>LNP!
1:@RUN GROUND, / , NELSON,20
2:@IDENT
3:@PASSWD
4:@ASQ,UP B03UH1.
5:@USE 4.,B03UH1.
6:@TP,W PLOT*BP400./8
7:@XOT NELSON*GROUND.RUN
8:EXAMPLE TRANSIENT CASE (TWO WELLS)
9: .85000+004 .85000+004 .10000+002 .18250+004
10: .25000+003 .25000+003 .10000+003 .10000-002
11: .10000-002 .20000+000 .10000+001
12: .00000 .00000 .00000
13: NELSON 1. 6
14: .10000+001 .10000+001 .10000+001 1
15: .00000 .16000+003 .00000 9
16: .10000+003 .00000 .10000-004 5000
17: .25000+001 .50000+002 .60000+001 5
18: .85000+004 .30000+001 .20000+001 40
19: .10000+004 .00000 .10000+001 .10000+001
20: .40000+001 .80000+001 .10000+001 .00000
21: .00000 .00000 .00000 .00000
22: SERPIN 2 .00000
23: .25000+003 .30000+004
24: .10000+004 .25000+002
25: .40000+004 .60000+006 .10000+001
26: .10000+001 .10000+001 .00000 .00000
27: .00000 .00000
28: SERPIN
29: .30000+003 .55000+004
30: .30000+004 .00000
31: .00000 .00000 .00000
32: .00000 .00000 .50000+006 .00000
33: .50000+002 .45000+003
34: CYCLIC
35: FEET
36: YEARS
37: T
38:@TPSAU 0
EOF:38
0:>

```

This can be compared with the sample data entered earlier in the PATHS program. (Already shown under "Sample Job.")

Note the first command on this listing: @ED, UQ NELSON*GRND1. . This brings the run stream generated to the Univac EDITOR. NELSON is the PROJECT ID entered in PATHS under which the batch file is cataloged. GRND1 is the file name. GRND is always the prefix, and the number appended, 1 in this case, is the number of the job stream the user gave PATHS. (See the note near the end of topic "Sample Job" or item 78 in the detailed run stream, Appendix C). Next, the edit command LNP! lists the entire run stream for viewing. With this list the data can be checked and modified as desired. For example to change variable .85000+004 on line 18 to .96000+003, one can do the following:

18 (Positions to line 18)

C /.85000+004/.96000+003/ 1

This would make the change. The tailing 1 says to make the change only to the first line. If this change were to be made to any like variables in the ensuing 10 lines, you should enter C-/.85000+004/.96000+003/1 .

STARTING JOB EXECUTION

After the batch stream has been modified, type EXIT. This frees the file with all the changes that have been made and control leaves the EDITOR. (To leave EDITOR with the batch stream left in its original state, type OMIT.) To submit the file into the input stream for execution, type @START NESLON*GRND1.

[Note: For additional detailed information on most of the available EDITOR commands and system control commands refer to UNIVAC 1100 Series EXEC 8 Hardware/Software Summary (UP-7824 Rev. 1).]

CAUTION

When starting an execution of GROUND, it is important to realize that GROUND itself will generate and catalog two files: the summary file PROJID*BQ3VH_. and the data file read by LOCQAR, cataloged PROJID*LOCQ_. (Once again PROJID is the user project ID, and the _ stands for the job run number.) If these files should exist from a prior run of GROUND, they will precipitate a fatal error should GROUND be reexecuted. Two alternatives are available to the user: the first, and simplest, is to delete these files if they exist. This is done by typing @DELETE followed by the file name. The example below shows the deletion of the file NELSON*BQ3VH8..

```
@DELETE NELSON*BQ3VH8.  
FURPUR 27R2 RL72R1 01/10/78 14:56:56
```

Alternatively, you could change the number of the file BQ3VH_ that is used on cards 4, 5 and 13 of the run stream (see "Using EDITOR"). Thus BQ3VH1. could be changed to BQ3VH9. if BQ3VH9. does not already exist. Along with this, the internally assigned and cataloged file LOCQ_., should have its file number changed appropriately. It is set by variable VH3.. (See line 13, in "Using EDITOR".)

As BQ3VH1. was changed to BQ3VH9., VH3 should be changed from 1. to 9..

FILES

Keeping track of the files accumulated by the PATHS program can be done by taking an audit of the files cataloged. Do this by typing @AUDIT as shown in the following example.

>>AUDIT

CATALOG 208 14 APR 78-07:44:47

TRACK COUNT	HIGH REF	TRK MAX	# OF ASG	FLAGS	DATE CREATED	LAST ASG	FILE NAME
35	61	128T	35	P B	01/24/78	04/13	NELSON♦LOC00A(1)
45	71	155T	255	P B	01/25/78	04/13	NELSON♦GRND(1)
41	67	141T	94	P B	01/24/78	04/13	NELSON♦PATHS(1)
1	0	128T	1	P B	04/13/78	04/13	NELSON♦BO3VH1(1)
1	0	128T	2	P B	04/11/78	04/11	NELSON♦BO3VH5(1)
2	1	128T	3	P B	04/12/78	04/12	NELSON♦GRND9(1)
1	0	128T	1	P B	04/12/78	04/12	NELSON♦LOC09(1)
2	1	128T	4	P B	04/12/78	04/12	NELSON♦GRND8(1)
1	0	128T	1	P B	04/12/78	04/12	NELSON♦LOC08(1)
1	0	128T	1	P B	04/12/78	04/12	NELSON♦BO3VH8(1)
1	0	128T	4	P B	04/07/78	04/12	NELSON♦10(1)
34	33	128T	1	P B	04/11/78	04/11	NELSON♦TEMP(1)
36	62	500T	9	P B	04/13/78	04/13	NELSON♦REVISION(1)
3	29	128T	10	P B	04/07/78	04/12	NELSON♦UTIL(1)
1	0	128T	14	P B	04/07/78	04/13	NELSON♦GRND6(1)
1	0	128T	2	P B	04/07/78	04/11	NELSON♦LOC06(1)
1	0	128T	14	P B	04/11/78	04/13	NELSON♦GRND1(1)
34	33	128T	1	P B	04/11/78	04/11	NELSON♦GTEMP(1)
10	9	128T	1	P B	04/11/78	04/11	NELSON♦LTEMP(1)
1	0	128T	2	P B	04/11/78	04/11	NELSON♦LOC01(1)
1	0	128T	4	P B	04/12/78	04/12	NELSON♦GRND7(1)
1	0	128T	1	P B	04/12/78	04/12	NELSON♦LOC07(1)
1	0	128T	9	P B	04/12/78	04/13	NELSON♦MEDIAT(1)
1	0	128T	1	P B	04/12/78	04/12	NELSON♦BO3VH9(1)
1	0	128T	14	P B	04/04/78	04/11	NELSON♦GRND5(1)
1	0	128T	1	P B	04/04/78	04/04	NELSON♦LOC05(1)
1	0	128T	1	P B	04/12/78	04/12	NELSON♦BO3VH7(1)

TOTAL: 27 FILES (0 DISABLED, 0 UNLOADED) USING 259 TRACKS.

Files should be deleted when they are no longer needed. This avoids paying for unneeded disc storage, and reduces the likelihood of trying to create files with file names already cataloged.

EXAMPLE TRANSIENT CASE

The printed output following comes from entering information to the PATHS program shown in "Sample Job". Notice the individual path histories for each of the 10 paths followed by the summary page. This would be repeated five

times for the transient cases for the years 0, 25, 50, 75, and 100. However, to save space only the first is completely shown and primarily summary information is subsequently shown. This summary information, incidentally, is the same as that obtained from file BQ3VH1, under "Summary File - BQ3VH_" previously. The complete output for the example transient case is provided on microfiche near the end of Appendix C.

The five plots that follow are also from this run. Normal production plots need not have such large numbers along the pathlines. They have been made larger here so they will be legible.

Following the output of the example transient case, a steady case is presented to further illustrate some additional alternatives. Among these features are the ion exchange delay and the input of irregularly located starting coordinates for the pathlines.

CASE = EXAMPLE TRANSIENT CASE (TWO WELLS)

DO	=	.10000+003	EFFECTIVE STRATUM THICKNESS
R	=	.25000+004	MAXIMUM RADIUS FOR TRAVEL TIME CALCULATIONS--ALSO LENGTH SCALING PARAMETER
RO	=	.25000+003	EFFECTIVE RADIUS OF CAVERN
HO	=	.10000+002	INITIAL HEAD IN CAVITY STORAGE TANK
KO	=	.10250+004	HYDRAULIC CONDUCTIVITY OF STRATUM MATERIAL
P	=	.25000+000	THE EFFECTIVE POROSITY
UG	=	.10000+002	INITIAL UNIFORM FIELD STRENGTH AT TIME=0
UH	=	.10000+002	VALUE OF UNIFORM FIELD STRENGTH AT TIME=TH
OPTION	=	SERPIN	EXPONENT FOR EXPONENTIAL VARIATION. SERPIN FOR SERPENTINE VARIATION
TR	=	.10000+001	PARAMETER FOR SERPENTINE VARIATION CALCULATION OF U (IN TIME UNIT)
A	=	.10000+001	PARAMETER USED BY SERPIN IN THE CALCULATION OF U
B	=	.10000+001	PARAMETER USED BY SERPIN IN THE CALCULATION OF U
C	=	.10000+001	PARAMETER USED BY SERPIN IN THE CALCULATION OF U
H1	=	.40000+001	MINIMUM VALUE OF H IN SERPEN CALCULATION
H2	=	.10000+001	MAXIMUM VALUE OF H IN SERPEN CALCULATION
IN	=	.50000+002	PARAMETER FOR SERPENTINE VARIATION CALCULATION OF H (IN TIME UNIT)
G	=	.10000	PARAMETER USED BY SERPIN IN THE CALCULATION OF H
E	=	.10000+001	PARAMETER USED BY SERPIN IN THE CALCULATION OF H
F	=	.10000+001	PARAMETER USED BY SERPIN IN THE CALCULATION OF H
XMAX	=	.25000+004	X-ABSCISSA VALUE AT WHICH TRAVEL TIME CALCULATIONS WILL BE TERMINATED
THAX	=	.00000	MAXIMUM TRAVEL TIME BEFORE TERMINATION OF FLOW PATHS
THETA0	=	.00000	MINIMUM CONTROL ANGLE FOR PATHLINE STARTING POINTS ALONG CAVERN WALL
THETA1	=	.16000+003	MAXIMUM CONTROL ANGLE FOR PATHLINE STARTING LINE ALONG CAVERN WALL
NTHETA	=	9	NUMBER OF PATHLINE: WANTED BETWEEN THETA0 AND THETA1
ATHETA	=	0	NUMBER OF PATHLINE: WANTED BETWEEN THETA1 AND 180 DEGREES
IG	=	.00000	STARTING DEPARTURE TIME FOR CALCULATING FLOW PATHS
IF	=	.10000+003	FINAL DEPARTURE TIME FOR CALCULATING FLOW PATHS
NI	=	5	NUMBER OF TIME INCREMENTS WANTED BETWEEN IG AND IF PLUS ONE
CHEN	=		NAME OF CHEMICAL SPECIE INVOLVED IN ION EXCHANGE REACTIONS.
KC	=	.00000	EQUILIBRIUM DISTRIBUTION COEFFICIENT FOR THE ION EXCHANGE SPECIE
DC	=	.00000	BULK DENSITY OF THE SOIL OR POROUS MATERIAL
DLTA	=	.12500+001	TRAVEL TIME INCREMENT USED IN SOLVING FOR FLOW PATHS
STEP	=	.60000+001	NUMBER TO BE DIVIDED INTO DLTA TO GET ACTUAL STEP SIZE FOR INTERGRATION
ILIM	=	5000	MAXIMUM NUMBER OF INCREMENTS AND INTERACTIONS ALONG ANY PATHLINE
NPRINT	=	80	CONTROLS PRINTOUT FREQUENCY. NPRINT-1 TIME INCREMENTS ARE OMITTED
EPSLN	=	.10000+004	NEAR ZERO CONVERGENCE TOLERANCE FOR STOPPING AT R OR XMAX
XCENTER	=	.30000+001	X-ABSCISSA IN INCHES TO DEFINE ORIGIN FOR PLOT
YCENTER	=	.20000+001	Y-ORDINATE IN INCHES TO DEFINE ORIGIN FOR PLOT
SCALE	=	.10000+004	SCALE IN LENGTH UNITS PER INCH ON THE PLOT

INPUT FOR WELL 1

WELLOP	=	SEPPIN	
XWELL	=	.36000+004	X-COORDINATE OF THE WELL
YWELL	=	.10000+004	Y-COORDINATE OF THE WELL
ROWELL	=	.25000+003	STOPPING RADIUS OF THE WELL
QO	=	.00000	THE MEAN INFLOW(+) (R OUTFLOW(-) RATE OF THE WELL
C	=	.00000	THE MAXIMUM INFLOW(+)OR OUTFLOW (-) RATE OF THE WELL
TOWELL	=	.00000	THE BEGINING TIME OF THE CYCLIC FLOW FOR THE WELL
TWELL	=	.00000	THE ENDING TIME OF THE CYCLIC FLOW FOR THE WELL
OI	=	.40000+004	THE INITIAL FLOW RATE OF THE WELL
OM	=	.01000+006	THE MAXIMUM FLOW RATE OF THE WELL
INWELL	=	.25000+002	PARAMETER USED IN CALCULATING WELL FLOW RATE
OWELL	=	.10000+001	PARAMETER USED IN CALCULATING WELL FLOW RATE
FWELL	=	.10000+001	PARAMETER USED IN CALCULATING WELL FLOW RATE
FWELL	=	.10000+001	PARAMETER USED IN CALCULATING WELL FLOW RATE

INPUT FOR WELL 2

WELLOP	=	CYCLIC	
XWELL	=	.55000+004	X-COORDINATE OF THE WELL
YWELL	=	.30000+004	Y-COORDINATE OF THE WELL
ROWELL	=	.30000+003	STOPPING RADIUS OF THE WELL
QO	=	.00000	THE MEAN INFLOW(+) (R OUTFLOW(-) RATE OF THE WELL
C	=	.50000+006	THE MAXIMUM INFLOW(+)OR OUTFLOW (-) RATE OF THE WELL
TOWELL	=	.51000+002	THE BEGINING TIME OF THE CYCLIC FLOW FOR THE WELL
TWELL	=	.45000+003	THE ENDING TIME OF THE CYCLIC FLOW FOR THE WELL
OI	=	.00000	THE INITIAL FLOW RATE OF THE WELL
OM	=	.00000	THE MAXIMUM FLOW RATE OF THE WELL
INWELL	=	.00000	PARAMETER USED IN CALCULATING WELL FLOW RATE
OWELL	=	.00000	PARAMETER USED IN CALCULATING WELL FLOW RATE
FWELL	=	.00000	PARAMETER USED IN CALCULATING WELL FLOW RATE
FWELL	=	.00000	PARAMETER USED IN CALCULATING WELL FLOW RATE

AT THE SUCCESSFUL CONCLUSION OF GROUND THE FOLLOWING FILES ARE CATALOGUED:
 NELSON+LOCUI. AND NELSON+BO3VH1.

THE RATIO OF TRAVEL TIME TO WATER TRAVEL TIME (1/K) = (1/ .10000+001)

PATHLINE NO. 1 OF FLUID PARTICLES DEPARTING THE CAVERN WALL AT TI = .00000 YEARS
 THETA = .00000 DEGREES
 HEAD(H/H0) = .40000+000

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	.00000	2.94118-002	.00000	.00000	2.50000+002	.00000	.00000
1	2.52595-002	2.96454-001	-1.85233-002	1.00000+002	2.51986+003	-1.57448+002	2.27688+003 .00000
2	5.05190-002	4.61129-001	-4.41471-002	2.00000+002	3.91959+003	-3.75250+002	3.69357+003 .00000
3	7.57785-002	6.08646-001	-5.34281-002	3.00000+002	5.17349+003	-4.54139+002	4.95044+003 .00000
4	1.01038-001	7.45440-001	-5.68986-002	4.00000+002	6.33624+003	-4.83638+002	6.11357+003 .00000
5	1.26297-001	8.76849-001	-6.10537-002	4.99999+002	7.45322+003	-5.18957+002	7.23128+003 .00000
5+	1.49965-001	9.99995-001	-7.00682-002	5.93300+002	8.49996+003	-5.95580+002	8.28084+003 .00000

PATHLINE NO. 2 OF FLUID PARTICLES DEPARTING THE CAVERN WALL AT TI = .00000 YEARS
 THETA = .20000+002 DEGREES
 HEAD(H/H0) = .40000+000

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	.00000	2.76390-002	1.00594-002	.00000	2.34923+002	8.55050+001	.00000
1	2.52595-002	2.85159-001	4.52434-002	1.00000+002	2.42385+003	3.84569+002	2.21991+003 .12257+000
2	5.05190-002	4.48972-001	7.45019-002	2.00000+002	3.81626+003	2.08266+002	3.62395+003 .10462+000
3	7.57785-002	5.99121-001	2.02137-002	3.00000+002	5.09253+003	1.71816+002	4.90122+003 .97226-001
4	1.01038-001	7.36932-001	2.01965-002	4.00000+002	6.26392+003	1.71670+002	6.07262+003 .92960-001
5	1.26297-001	8.69197-001	1.80770-002	4.99999+002	7.38818+003	1.53654+002	7.19727+003 .89746-001
6	1.59965-001	9.99971-001	9.77566-003	5.97733+002	8.49976+003	8.30931+001	8.31112+003 .87986-001
6+	1.50989-001	9.99997-001	9.77455-003	5.97753+002	8.49997+003	8.30837+001	8.31134+003 .87985-001

PATHLINE NO. 3 OF FLUID PARTICLES DEPARTING THE CAVERN WALL AT $T_1 = .00000$ YEARS
 $\theta = .40000 \times 10^{-2}$ DEGREES
 $HEAD(H/H_0) = .40000 \times 10^0$

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	.00000	2.25307-002	1.89055-002	.00000	1.91511+002	1.60697+002	.00000
1	2.52595-002	2.58160-001	1.11248-001	1.00000+002	2.19436+003	9.45605+002	2.16970+003 .24222+000
1+	3.81261-002	3.24270-001	1.23702-001	1.50937+002	2.75630+003	1.05146+003	2.74173+003 .21961+000

PATHLINE NO. 4 OF FLUID PARTICLES DEPARTING THE CAVERN WALL AT $T_1 = .00000$ YEARS
 $\theta = .60000 \times 10^{-2}$ DEGREES
 $HEAD(H/H_0) = .40000 \times 10^0$

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	.00000	1.47059-002	2.54713-002	.00000	1.25000+002	2.16506+002	.00000
1	2.52595-002	2.19540-001	1.65291-001	1.00000+002	1.86609+003	1.46497+003	2.14331+003 .35661+000
2	5.05190-002	3.61200-001	2.11835-001	2.00000+002	3.07020+003	1.80060+003	3.41126+003 .30270+000
3	7.57785-002	5.06577-001	2.37810-001	3.00000+002	4.30591+003	2.02139+003	4.66728+003 .28051+000
4	1.01038-001	6.44297-001	2.51485-001	4.00000+002	5.47652+003	2.13762+003	5.84375+003 .26770+000
5	1.26297-001	7.80736-001	2.55287-001	4.99999+002	6.63625+003	2.16994+003	7.00529+003 .25802+000
6	1.51557-001	9.27072-001	2.51043-001	5.99999+002	7.88011+003	2.13387+003	8.24983+003 .25270+000
6+	1.65758-001	9.99994-001	2.52533-001	6.56219+002	8.49995+003	2.14653+003	8.86983+003 .25219+000

PATHLINE NO. 5 OF FLUID PARTICLES DEPARTING THE CAVERN WALL AT TI = .00000 YEARS
 THETA = .80000+002 DEGREES
 HEAD(H/H0) = .40000+000

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	.00000	5.10730-003	2.89649-002	.00000	4.34120+001	2.46202+002	.00000
1	2.52595-002	1.66787-001	2.03136-001	1.00000+002	1.41769+003	1.72666+003	2.08199+003 .46402+000
2	5.05190-002	3.04581-001	2.58933-001	2.00000+002	2.58894+003	2.20093+003	3.34746+003 .39201+000
3	7.57785-002	4.44078-001	2.91824-001	3.00000+002	3.77466+003	2.48050+003	4.56647+003 .36223+000
4	1.01038-001	5.80573-001	3.10834-001	4.00000+002	4.93487+003	2.64209+003	5.73808+003 .34512+000
5	1.26297-001	7.23612-001	3.10628-001	4.99999+002	6.15071+003	2.64034+003	6.95997+003 .33234+000
6	1.51557-001	8.81241-001	3.08097-001	5.99999+002	7.49055+003	2.61883+003	8.30047+003 .32523+000
6*	1.74956-001	9.99997-001	3.12586-001	6.92635+002	8.49998+003	2.65698+003	9.31063+003 .32268+000

PATHLINE NO. 6 OF FLUID PARTICLES DEPARTING THE CAVERN WALL AT TI = .00000 YEARS
 THETA = .10000+003 DEGREES
 HEAD(H/H0) = .40000+000

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	.00000	-5.10730-003	2.89649-002	.00000	-4.34120+001	2.46202+002	.00000
1	2.52595-002	1.00748-001	2.23614-001	1.00000+002	8.56356+002	1.90072+003	1.97487+003 .56355+000
2	5.05190-002	2.30536-001	2.92098-001	2.00000+002	1.95957+003	2.48283+003	3.22597+003 .47332+000
3	7.57785-002	3.65215-001	3.31784-001	3.00000+002	3.10432+003	2.82016+003	4.42038+003 .43572+000
4	1.01038-001	4.99691-001	3.56572-001	4.00000+002	4.24738+003	3.03087+003	5.58298+003 .41428+000
5	1.26297-001	6.12213-001	3.81572-001	4.99999+002	5.20381+003	3.24336+003	6.57807+003 .39857+000
6	1.51557-001	7.35089-001	4.56091-001	5.99999+002	6.24825+003	3.87677+003	7.83108+003 .38966+000
7	1.76816-001	8.63304-001	4.70316-001	6.99999+002	7.33808+003	3.99768+003	8.92881+003 .38576+000
8	2.02076-001	9.85198-001	4.77905-001	7.99998+002	8.37418+003	4.06219+003	9.96692+003 .38093+000
8*	2.05162-001	9.99990-001	4.78722-001	8.12215+002	8.49992+003	4.06914+003	1.00928+004 .38042+000

PATHLINE NO. 7 OF FLUID PARTICLES DEPARTING THE CAVERN WALL AT TI = .00000 YEARS
 THETA = .12000+003 DEGREES
 HEAD(H/H0) = .40000+000

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	.00000	-1.47059-002	2.54713-002	.00000	-1.25000+002	2.16506+002	.00000
1	2.52595-002	2.31459-002	2.21881-001	1.00000+002	1.96740+002	1.88599+003	1.81383+003 .65523+000
2	5.05190-002	1.37053-001	3.04864-001	2.00000+002	1.16495+003	2.59135+003	3.01861+003 .54667+000
3	7.57785-002	2.65565-001	3.53485-001	3.00000+002	2.25731+003	3.00463+003	4.18809+003 .50100+000
4	1.01038-001	3.97027-001	3.85171-001	4.00000+002	3.37473+003	3.27395+003	5.33791+003 .47521+000
5	1.26297-001	5.20582-001	4.08904-001	4.99999+002	4.42495+003	3.47568+003	6.40773+003 .45675+000
6	1.51557-001	6.18425-001	4.55539-001	5.99999+002	5.25661+003	3.87208+003	7.33126+003 .44603+000
7	1.76816-001	7.47274-001	4.76838-001	6.99999+002	6.30933+003	4.05312+003	8.40476+003 .44090+000
8	2.02076-001	8.65159-001	4.86371-001	7.99998+002	7.35385+003	4.13416+003	9.45243+003 .43509+000
9	2.27335-001	9.89327-001	4.95153-001	8.99998+002	8.40928+003	4.20880+003	1.05105+004 .42798+000
10	2.29392-001	9.99990-001	4.96043-001	9.08142+002	8.49992+003	4.21636+003	1.06015+004 .42734+000

PATHLINE NO. 8 OF FLUID PARTICLES DEPARTING THE CAVERN WALL AT $T = .00000$ YEARS
 $\theta_{FTA} = .14000+003$ DEGREES
 $HEAD(H/H_0) = .40000+000$

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	.00000	-2.25307-002	1.89055-002	.00000	-1.91511+002	1.60697+002	.00000
1	2.52595-002	-6.13580-002	1.88398-001	1.00000+002	-5.21543+002	1.60138+003	1.58863+003 .74004+000
2	5.05190-002	2.01750-002	2.83505-001	2.00000+002	1.71488+002	2.40979+003	2.66525+003 .61304+000
3	7.57785-002	1.35506-001	3.45452-001	3.00000+002	1.15180+003	2.93634+003	3.76085+003 .55904+000
4	1.01038-001	2.61436-001	3.87442-001	4.00000+002	2.22221+003	3.29325+003	4.90989+003 .52888+000
5	1.26297-001	3.85976-001	4.17512-001	4.99999+002	3.28046+003	3.54885+003	5.99864+003 .50787+000
6	1.51557-001	4.92506-001	4.47261-001	5.99999+002	4.18630+003	3.80172+003	6.93921+003 .49533+000
7	1.76816-001	6.13459-001	4.66938-001	6.99999+002	5.21440+003	3.96897+003	7.98225+003 .48875+000
8	2.02076-001	7.37616-001	4.79121-001	7.99998+002	6.26975+003	4.07253+003	9.04270+003 .48196+000
9	2.27335-001	8.63863-001	4.91141-001	8.99998+002	7.34284+003	4.17470+003	1.01208+004 .47421+000
10	2.52594-001	9.98792-001	5.05890-001	9.99997+002	8.48973+003	4.30006+003	1.12746+004 .46996+000
10+	2.52829-001	9.99994-001	5.05988-001	1.00092+003	8.49995+003	4.30090+003	1.12848+004 .46996+000

PATHLINE NO. 9 OF FLUID PARTICLES DEPARTING THE CAVERN WALL AT TI = .00000 YEARS
 THETA = .16000+003 DEGREES
 HEAD(H/H0) = .40000+000

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	.00000	-2.76380-002	1.00594-002	.00000	-2.34923+002	6.55050+001	.00000
1	2.52595-002	-1.36723-001	1.10335-001	1.00000+002	-1.16215+003	9.37849+002	1.31610+003 .81979+000
2	5.05197-002	-1.16278-001	1.91828-001	2.00000+002	-9.82366+002	1.63054+003	2.04734+003 .67426+000
3	7.57785-002	-4.25323-002	2.66699-001	3.00000+002	-3.61525+002	2.26694+003	2.94519+003 .61173+000
4	1.01038-001	6.25345-002	3.28840-001	4.00000+002	5.31543+002	2.79514+003	3.98457+003 .57718+000
5	1.26297-001	1.80396-001	3.75238-001	4.99999+002	1.53336+003	3.18952+003	5.06175+003 .55379+000
6	1.51557-001	2.93557-001	4.10417-001	5.99999+002	2.49523+003	3.48855+003	6.06923+003 .53942+000
7	1.76816-001	4.17025-001	4.36029-001	6.99999+002	3.54471+003	3.70624+003	7.14148+003 .53120+000
8	2.02076-001	5.42582-001	4.54418-001	7.99998+002	4.61534+003	3.86255+003	8.22354+003 .52342+000
9	2.27335-001	6.67468-001	4.76987-001	8.99998+002	5.67348+003	4.05439+003	9.30210+003 .51523+000
10	2.52594-001	8.04018-001	5.13433-001	9.99997+002	6.83416+003	4.36418+003	1.05051+004 .51036+000
11	2.77854-001	9.28186-001	5.24648-001	1.10000+003	7.88958+003	4.45951+003	1.15653+004 .50849+000
11*	2.92943-001	9.99999-001	5.28901-001	1.15973+003	8.49999+003	4.49566+003	1.21767+004 .50643+000

SUMMARY OF FLUID PARTICLE ARRIVAL LOCATIONS AND TIMES AT THE OUTFLOW BOUNDRIES

WITH DEPARTURE TIME OF .000YEARS AND AT THAT TIME
 THE OUTFLOW RATE IS .13006966+007 CUBIC FEET PER YEARS
 AND THE RELATIVE CAVERN HEAD IS .40000

PATH NO	REL. ARR. TIME X YEARS	FEET	Y FEET	PATH LENGTH FEET
1	5.93300+002	8.49996+003	-5.95580+002	8.26084+003
2	5.97753+002	8.49997+003	8.30837+001	8.31134+003
3	1.50937+002	2.75630+003	1.05146+003	2.74170+003
4	6.56210+002	8.49995+003	2.14653+003	8.86983+003
5	6.92635+002	8.49996+003	2.65646+003	9.31063+003
6	8.12215+002	8.49992+003	4.06914+003	1.00928+004
7	9.08142+002	8.49992+003	4.21636+003	1.06015+004
8	1.00092+003	8.49995+003	4.30090+003	1.12848+004
9	1.15973+003	8.49999+003	4.49566+003	1.21767+004

PATHLINE NO. 1 OF FLUID PARTICLES DEPARTING THE CAVERN WALL AT TI = .25000+002YEARS
 THETA = .00000 DEGREES
 HEAD(H/H0) = .72000+000

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	6.31488-003	2.94118-002	.00000	2.50000+001	2.50000+002	.00000	.00000
1	3.15744-002	3.03530-001	-1.70246-002	1.25000+002	2.58001+003	-1.44711+002	2.33656+003 .00000
2	5.68339-002	4.65192-001	-3.98131-002	2.25000+002	3.95413+003	-3.38412+002	3.72457+003 .00000
3	8.29933-002	6.12056-001	-4.65618-002	3.25000+002	5.20256+003	-3.95776+002	4.97447+003 .00000
4	1.07353-001	7.48287-001	-4.95835-002	4.25000+002	6.36044+003	-4.21460+002	6.13264+003 .00000
5	1.32612-001	8.80479-001	-5.58196-002	5.24999+002	7.48407+003	-4.74466+002	7.25785+003 .00000
6	1.55549-001	9.99996-001	-6.42062-002	6.15805+002	8.49997+003	-5.45752+002	8.27634+003 .00000

PATHLINE NO. 2 OF FLUID PARTICLES DEPARTING THE CAVERN WALL AT TI = .25000+002YEARS
 THETA = .20000+002 DEGREES
 HEAD(H/H0) = .72000+000

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	6.31488-003	2.76380-002	1.00594-002	2.50000+001	2.34923+002	8.55050+001	.00000
1	3.15744-002	2.91319-001	4.83996-002	1.25000+002	2.47621+003	4.11397+002	2.27788+003 .11639+000
2	5.68339-002	4.57539-001	3.02855-002	2.25000+002	3.84658+003	2.57427+002	3.65749+003 .10232+000
3	8.20933-002	6.02071-001	2.87840-002	3.25000+002	5.11760+003	2.44664+002	4.92879+003 .95930-001
4	1.07353-001	7.39213-001	2.92355-002	4.25000+002	6.20331+003	2.48502+002	6.09442+003 .92192-001
5	1.32612-001	8.72645-001	2.46702-002	5.24999+002	7.41748+003	2.09697+002	7.22975+003 .89061-001
6	1.56742-001	9.99996-001	1.70790-002	6.20526+002	8.49991+003	1.45172+002	8.31424+003 .87894-001
6*	1.56743-001	9.99996-001	1.70789-002	6.20531+002	8.49996+003	1.45170+002	8.31429+003 .87894-001

SUMMARY OF FLUID PARTICLE ARRIVAL LOCATIONS AND TIMES AT THE OUTFLOW BOUNDRIES

WITH DEPARTURE TIME OF 25.000YEARS AND AT THAT TIME
 THE OUTFLOW RATE IS .23412536+007 CUBIC FEET PER YEARS
 AND THE RELATIVE CAVERN HEAD IS .7200

PATH NO	REL.ARR.TIME X YEARS	FEET	Y FEET	PATH LENGTH FEET
1	6.15805+002	8.49997+003	-5.45752+002	3.27634+003
2	6.20531+002	8.49996+003	-1.45170+002	8.31429+003
3	1.73750+002	2.76709+003	1.09058+003	2.76971+003
4	6.76788+002	8.49997+003	2.11145+003	8.89054+003
5	7.22298+002	8.49996+003	2.47694+003	9.36508+003
6	8.64470+002	8.49996+003	4.03255+003	1.01374+004
7	9.35417+002	8.49992+003	4.11275+003	1.06124+004
8	1.02149+003	8.49992+003	4.23936+003	1.12991+004
9	1.18090+003	8.49994+003	4.48383+003	1.21552+004

SUMMARY OF FLUID PARTICLE ARRIVAL LOCATIONS AND TIMES AT THE OUTFLOW BOUNDRIES

WITH DEPARTURE TIME OF 50.000YEARS AND AT THAT TIME
 THE OUTFLOW RATE IS .26013932+007 CUBIC FEET PER YEARS
 AND THE RELATIVE CAVERN HEAD IS .8000

PATH NO	REL.ARR.TIME X YEARS	FEET	Y FEET	PATH LENGTH FEET
1	6.44872+002	8.49997+003	-5.09674+002	8.27246+003
2	6.49139+002	8.49996+003	1.69000+002	8.31108+003
3	1.97969+002	2.75401+003	1.04166+003	2.74483+003
4	7.05467+002	8.50000+003	1.98081+003	8.87172+003
5	7.59940+002	8.49992+003	2.28031+003	9.35466+003
6	9.10862+002	8.49996+003	3.76889+003	1.00172+004
7	9.53943+002	8.49995+003	3.94113+003	1.05210+004
8	1.03490+003	8.49997+003	4.13285+003	1.12053+004
9	1.19591+003	8.49992+003	4.44686+003	1.20545+004

SUMMARY OF FLUID PARTICLE ARRIVAL LOCATIONS AND TIMES AT THE OUTFLOW BOUNDRIES

WITH DEPARTURE TIME OF 75.000YEARS AND AT THAT TIME
THE OUTFLOW RATE IS .25013396+007 CUBIC FEET PER YEARS
AND THE RELATIVE CAVERN HEAD IS .7692

PATH NO	REL. ARR. TIME X YEARS	FEET	Y FEET	PATH LENGTH FEET
1	6.75408+002	8.50000+003	-4.79828+002	8.26922+003
2	6.79122+002	8.49998+003	1.80083+002	8.30681+003
3	2.23750+002	2.75100+003	9.94651+002	2.72958+003
4	7.39101+002	8.49995+003	1.84740+003	8.84921+003
5	7.97468+002	8.49996+003	2.16796+003	9.31745+003
6	6.25780+002	5.20115+003	3.01284+003	6.48338+003
7	9.68669+002	8.49998+003	3.76178+003	1.04175+004
8	1.04724+003	8.49994+003	4.02515+003	1.10963+004
9	1.21739+003	8.49995+003	4.41386+003	1.19479+004

SUMMARY OF FLUID PARTICLE ARRIVAL LOCATIONS AND TIMES AT THE OUTFLOW BOUNDRIES

WITH DEPARTURE TIME OF 100.000YEARS AND AT THAT TIME
THE OUTFLOW RATE IS .23412535+007 CUBIC FEET PER YEARS
AND THE RELATIVE CAVERN HEAD IS .7200

PATH NO	REL. ARR. TIME X YEARS	FEET	Y FEET	PATH LENGTH FEET
1	7.05301+002	8.49995+003	-4.51686+002	8.26650+003
2	7.08719+002	8.49998+003	1.87493+002	8.30397+003
3	2.49297+002	2.75317+003	9.84981+002	2.72273+003
4	7.66116+002	8.49995+003	1.74204+003	8.82916+003
5	8.31990+002	8.49996+003	2.12219+003	9.26877+003
6	6.40936+002	5.28993+003	2.78649+003	6.50529+003
7	9.81404+002	8.49994+003	3.60651+003	1.03247+004
8	1.05921+003	8.49995+003	3.92967+003	1.09926+004
9	1.22957+003	8.49995+003	4.37838+003	1.18471+004

EXAMPLE TRANSIENT CASE (TWO WELLS)

DEPARTURE TIME = 0.00 YEARS

SCALE 1 INCH = 1000 FEET

EXAMPLE TRANSIENT CASE (TWO WELLS)

DEPARTURE TIME = 25.00 YEARS

SCALE 1 INCH = 1000 FEET

EXAMPLE TRANSIENT CASE (TWO WELLS)

DEPARTURE TIME = 50.00 YEARS

SCALE 1 INCH = 1000 FEET

EXAMPLE TRANSIENT CASE (TWO WELLS)

DEPARTURE TIME = 75.00 YEARS

SCALE 1 INCH = 1000 FEET

TABLE B-1. Input Parameter Worksheet for Example Steady Case with Tc-99 Exchange

INPUT PARAMETER WORKSHEET

CASE: Steady Flow with Tc-99 Exchange

1. 100 ft. = D_0 is the stratum thickness.
2. 8500 ft. = R is the distance to the boundary. Units must be the same as D_0 .
3. 8500 ft. = X_{MAX}/T_{MAX} are the stopping distance or time for pathlines.
4. 250 ft. = r_0 is the cavern or pond radius. Units must be the same as D_0 .
5. 4 ft. = H_0 is the head in the cavern. Units must be the same as D_0 .
6. 1825 ft./yr. = K_0 is the stratum hydraulic conductivity. Length units must be the same as D_0 .
Whatever time units are in K_0 sets the units of the travel time.
7. 0.2 = P is the effective porosity.
8. S = S or T . A steady (S) or transient (T) case.
9. 0.001 = U_0 is the initial uniform gradient value. See Figure 1.
10. _____ = U_M is the lateral gradient value. See Figure 1.
11. _____ = T_M in time units of K_0 .
12. _____ = A, B, C are three time-related integers.
13. _____ = S or E or C . Use the serpin (S), exponential (E), or cyclic (C) head variation in the cavern.
14. 4 ft. = H_I is the initial head.
15. _____ = H_M is the maximum head.
16. _____ = T_N in time units of K_0 .
17. _____ = D, E, F . See Figure 1.
18. 1 = J is total number of wells.
19. 5° = Θ_0 is the angle (deg) around the cavern wall to the starting point for the first pathline.
20. 5° = Θ_M is the maximum angle (deg) to the last pathline starting point along the cavern wall.
21. 18 = N_0 is the number of pathlines to be generated
See back of form from Θ_0 to and including Θ_M .
22. _____ = K_Θ is the number of pathlines wanted between Θ_M and 179.99° .
23. _____ = t_0 is the departure time of the first fluid particles leaving the cavern.
24. _____ = t_f is the departure time of the final fluid particles.
25. _____ = N_T is the number of equally spaced departure times beginning with t_0 and ending with t_f .
26. 0.5 ml/gr. = K_d is the equilibrium exchange distribution coefficient.
27. 1.9 gr/cc = B_d is the bulk density of the porous material.
28. 11 in. = _____ inch wide plots are desired. Request either a 30" or 11" wide by 30" plot.
29. 3 in. = X_{CENTER} } The location (x & y in inches) on the plot where
30. 4 in. = Y_{CENTER} } the cavern center is to be located.
31. 1000 ft./in. = $SCALE$ is the scale for the plot. Length in units of D_0 per inch.

TABLE B-1. Continued
INPUT FOR WELLS (J sets are required)

SERPIN OPTION

- 18.05 1 = j is the well number.
- 18.10 3000 ft. = $XWELL_j = x'_j$ is the x-coordinate location of the center of the well. (Units consistent with D_0 .)
- 18.15 1000 ft. = $YWELL_j = y'_j$ is the y-coordinate location of the center of the well.
- 18.20 50 ft. = $ROWELL_j$ is the stopping radius around the well.
- 18.25 S = S or C. serpin (S) or cyclic (C) option. See Figure 1.
- 18.30 2(10⁵) ft³/yr. = QI_j is initial inflow (+) or outflow (-) rate in length cubed per time units the same as D_0 and K_0 .
- 18.35 _____ = QM_j is a later inflow (+) or outflow (-) rate of this well option.
- 18.40 _____ = TN_j is the time parameter in the serpin option. See Figure 1.
- 18.45 _____ = DW_j, EW_j, FW_j . serpin well option parameters.

CYCLIC OPTION

- 18.50 _____ = j is the well number.
- 18.55 _____ = $XWELL_j = x'_j$ is the x-coordinate location of the center of the well. (Units consistent with D_0 .)
- 18.60 _____ = $YWELL_j = y'_j$ is the y-coordinate location of the center of the well.
- 18.65 _____ = $ROWELL_j$ is the stopping radius around the well.
- 18.70 C = S or C; serpin (S) or cyclic (C). See Figure 2.
- 18.75 _____ = QQ_j is the mean inflow (+) or outflow (-) rate in length cubed per time units the same as D_0 and K_0 .
- 18.80 _____ = QA_j is the amplitude of the cyclic inflow (+) or outflow (-) rate.
- 18.85 _____ = $TOWELL_j$ is the initial or beginning time for the cyclic well option.
- 18.90 _____ = $TMWELL_j$ is the later cyclic time parameter.

PATHLINE - IRREGULAR STARTING COORDINATES

(If 00 in Item 19 equals 0M in Item 20 then N0 pathlines will be generated from the individual coordinates provided below.)

21. 18 = N0 is the number of input data sets to be entered for starting pathlines ($1 \leq i \leq N0$).

Pathline i	Starting Coordinates		Starting Pathline Length*	Initial Time*
	X	Y		
1	-1500'	250'	9 250' 0'	
2	3100'	1000'	10 235' 85.5'	
3	3070.7	1070.7	11 191.5' 160.7'	
4	3000'	1100'	12 125.0'	
5	2929.3	1070.7	13 43.4' 246.2'	
6	2923.3	929.3	14 - 43.4' 246.2'	
7	3000'	908'	15 - 125' 216.5'	
8	3070.7	929.3	16 - 191.5' 160.7'	
			17 - 234.5' 85.5'	
			18 - 248.3' 29.0'	

*Values need not be supplied

EXAMPLE STEADY CASE

The second example case involves a steady flow system but the ion exchange delay for a single contaminant is illustrated. Also the special irregular starting location feature for pathlines is used. The completed input parameter worksheet for the example steady case in Table B-1 is shown.

After signing on the Univac and providing user ID, passwords, etc., then PATHS can be executed as follows using the input values from the worksheet or as requested by the program.

```
EXOT NELSON*PATHS.RUN
THIS PROGRAM CALCULATES AND PLOTS THE FLOW PATH
FROM CAVERN TO BOUNDARY AND CALCULATES THE ARRIVAL TIME
DISTRIBUTION OF FLUID AT THE BOUNDARY.

PLEASE ENTER THE FOLLOWING FOR THE BATCH PORTION OF
THE RUN.  PRESS THE CARRIAGE RETURN AFTER RESPONDING.
ENTER YOUR ACCOUNT NUMBER
>ABC123
ENTER USERID
>MYID
ENTER PROJECT ID
>NELSON
ENTER NAME/ADDRESS
>NIRALL KLINE/703 BLDG. RM.227
ENTER PASSWORD
>PASS

NOW ENTER THE TEST CASE NAME--A ONE LINE TITLE
>STEADY FLOW WITH TC-99 EXCHANGE

ENTER INPUT VARIABLES AS REQUESTED.

IN RESPONSE TO ANY REQUEST FOR INPUT, ENTER THE WORD
HELP TO OBTAIN AN EXPLANATION FOR THE REQUIRED INPUT.

DO
>100
R
>8500
STANDARD X TERMINATION OF PATHLINES ?
>YES
```

```

ENTER XMAX
>8500
PD
>250
HD
>4
PD
>1825
P
>.2
STEADY OR TRANSIENT CASE (S OR T)
>S
UO
.001
H1
4
DO YOU WANT TO ENTER ADDITIONAL WELLS OR CAVERNS?
YES
J
WELL( 1)
.000
WELL( 1)
.1000
ROWELL( 1)
>50
Q1
>200000
THE LENGTH OF DO ARE IN -- (DO NOT EXCEED 12 CHARACTERS)
>FEET
THE TIME UNITS OF UO ARE IN?
>YEARS
THETAO
>5
THETAM
>5

```

When THETAO and THETAM are input as the same value, there are two additional options for providing starting coordinates for pathlines.

1. If NTHETA is input as an integer greater than zero, then the program will request NTHETA sets of starting coordinates, (X_i, Y_i) . This option is illustrated in this steady case but may also be used in any transient cases.
2. If NTHETA is input as zero and the case involves steady flow, then a predetermined set of starting coordinates for the streamlines is automatically set such that each of the streamtubes conveys a fraction of the total steady flow. The "HELP" feature in the PATHS program associated with THETAO, THETAM or NTHETA will provide more particulars.

```

NTHETA
>18
ARE THE INITIAL PATH LENGTHS ZERO?
YES
END

```



```

>-1500
  ENTER Y(I)
>250
FOR I = 2  ENTER X(I)

>3100
  ENTER Y(I)
>1000
FOR I = 3  ENTER X(I)

>3070.7
  ENTER Y(I)
>1070.7
FOR I = 4  ENTER X(I)

>3000
  ENTER Y(I)
>1100
FOR I = 5  ENTER X(I)

>2029.3
  ENTER Y(I)
>1070.7
FOR I = 6  ENTER X(I)

>2929.3
  ENTER Y(I)
>929.3
FOR I = 7  ENTER X(I)

>3000
  ENTER Y(I)
>900
FOR I = 8  ENTER X(I)

>3070.7
  ENTER Y(I)
>929.3
FOR I = 9  ENTER X(I)

>250
  ENTER Y(I)
>0
FOR I = 10  ENTER X(I)

>235
  ENTER Y(I)
>85.5
FOR I = 11  ENTER X(I)

>191.5
  ENTER Y(I)
>160.7
FOR I = 12  ENTER X(I)

>125

```

The control key and letter H
erase and back up option was
used in X(I) for I=5.

```

ENTER Y(I)
>216.5
FOR I = 13 ENTER X(I)

>43.4
ENTER Y(I)
>246.2
FOR I = 14 ENTER X(I)

>-43.4
ENTER Y(I)
>246.2
FOR I = 15 ENTER X(I)

>-125.0
ENTER Y(I)
>216.5
FOR I = 16 ENTER X(I)

>-191.5
ENTER Y(I)
>160.7
FOR I = 17 ENTER X(I)

>-234.9
ENTER Y(I)
>85.5
FOR I = 18 ENTER X(I)

>-248.3
ENTER Y(I)
>29
IS THERE AN ION EXCHANGE DELAY?
>YES
CHEMICAL NAME?
>TECHNETIUM
KID?
>.5
DO?
>1.9
CHOOSE A CONVENIENT ROUNDED DELTA BETWEEN THE NUMBERS 7 AND 25
>10
ENTER STEP
>6
ENTER ITLIN
>5000
TO OBTAIN BETWEEN 15 AND 25 ISOCHRONAL LINES,
CHOOSE NPRINT BETWEEN 15 AND 25
ENTER NPRINT
>50
ENTER EPSLN
>.00001
DO YOU WANT THE FLOW PATHS PLOTTED?
>YES
DO YOU WANT 30 INCH PLOTS?
>NO

```

```

ENTER XCENTER
>3
ENTER YCENTER
>4
ENTER SCALE (IN FEET          /INCH)
>1000
DO YOU WANT THE DETAILED COMPUTER PRINTOUT?
>YES
ENTER RUN NUMBER OF THE JOB STREAM TO BE SAVED--
--OTHERWISE, ESCAPE BY TYPING @
>8
DO YOU WANT THE JOB SUBMITTED ?
>YES
THE PROGRAM GROUND HAS BEEN SUBMITTED FOR EXECUTION.
THE BATCH RUNSTREAM HAS BEEN SAVED IN FILE NELSON*GRND8.
UPON EXECUTION OF THE BATCH PROGRAM, THE SUMMARY
IS SAVED IN FILE NELSON*BQ3UH8.
>

```

The last computer output indicates the summary input file was completed and the batch run submitted. The summary file is:

```

@ED,R NELSON*GRND8.
READ-ONLY MODE
ED 15R2-THU-05/25/78-15:06:34-(0.)
EDIT
0:>LNP!
1:BRUN GROUND,          ,NELSON,20 , NIAL KLINE/703 BLDG. RM.227
2:IDENT , NIAL KLINE/703 BLDG. RM.227
3:BPASSWD
4:BPASC,UP BQ3UH8.
5:BOUSE 4.,BQ3UH8.
6:OTP,W PLOT*BP400./8
7:BXOT NELSON*GROUND.RUN
8:STEADY FLOW WITH TC-99 EXCHANGE
9: .85000+004 .25000+004 .40000+001 .18250+004
10: .25000+003 .25000+003 .10000+003 .10000-002
11: .10000-002 .20000+000 .10000+001
12: .00000 .50000+000 .19000+001
13:TECHNETIUM NELSON 8. 6
14: .10000+001 .10000+001 .10000+001 . 0
15: .00000 .00000 .00000 18
16: .00000 .00000 .10000-004 5000
17: .10000+002 .10000+001 .60000+001 0
18: .85000+004 .30000+001 .40000+001 50
19: .10000+004 .10000+001 .10000+001 .10000+001
20: .40000+001 .40000+001 .10000+001 .00000
21: .00000 .00000 .00000 .00000
22:SERPIN 1 .00000
23: .50000+002 .30000+004
24: .10000+004 .10000+001

```

```

25: .20000+006 .20000+006 .10000+001
26: .10000+001 .10000+001 .00000 .00000
27: .00000 .00000
28: SERPIN
29: FEET
30: YEARS
31: 3
32: -.15000+004 .25000+003
33: .31000+004 .10000+004
34: .30707+004 .10707+004
35: .30000+004 .11000+004
36: .29293+004 .10707+004
37: .29293+004 .92930+003
38: .30000+004 .90000+003
39: .30707+004 .92930+003
40: .25000+003 .00000
41: .20500+003 .05500+002
42: .19150+003 .16070+003
43: .12500+003 .21650+003
44: .43400+002 .24620+003
45: -.43400+002 .24620+003
46: -.12500+003 .21650+003
47: -.19150+003 .16070+003
48: -.20490+003 .05500+002
49: -.24830+003 .29000+002
50: @TPSAU 8

```

ECF:50

0:>EXIT

NO CORRECTIONS APPLIED.

>

With the successful completion of the batch run GROUND, the user may obtain the summary arrival results over the terminal. To do this, you type @ED,R PROJID*BQ3VH_ (use 8 in the blank for this example) followed by P!.

The results obtained are:

@ED,R NELSON*BQ3VH2.

READ-ONLY MODE

ED 1582-THU-05/25/78-14:18:49-(0,)

EDIT

0:>P!

STEADY FLOW WITH TC-99 EXCHANGE

THE DEPARTURE TIME IS .000 YEARS
THE INITIAL OUTFLOW RATE IS .13006966+007
CUBIC FEET PER YEARS
THE INITIAL RELATIVE CAVERN HEAD IS 1.0000

PATH NO.	TRAVEL TIME YEARS	X FEET	Y FEET	CUM FLUX 0/00	PATH LENGTH FEET
1	7.09939+003	8.49996+003	3.66636+003	5.92124-001	1.10242+004
2	2.60996+003	8.49996+003	1.19431+003	1.92262-001	5.40405+003
3	2.63660+003	8.49999+003	1.39617+003	2.15197-001	5.44850+003
4	2.69242+003	8.49996+003	1.55522+003	2.41123-001	5.55244+003
5	2.76461+003	8.49999+003	1.64711+003	2.56091-001	5.67900+003
6	2.72738+003	8.49997+003	7.76091+002	1.13947-001	5.63973+003
7	2.66218+003	8.49996+003	8.52858+002	1.26493-001	5.52556+003
8	2.62043+003	8.49996+003	9.97939+002	1.50196-001	5.43518+003
9	3.71984+003	8.49993+003	-3.91366+002	9.23118-001	8.26442+003
10	3.73679+003	8.49999+003	9.08907+001	1.92158-003	8.29923+003
11	3.84378+003	8.49995+003	5.55590+002	7.79015-002	8.43904+003
12	4.05101+003	8.49993+003	1.93095+003	3.02275-001	8.72495+003
13	4.23655+003	8.49995+003	2.32218+003	3.65770-001	9.00049+003
14	4.48843+003	8.49995+003	2.66444+003	4.21143-001	9.34066+003
15	4.79952+003	8.49997+003	2.95771+003	4.68443-001	9.73179+003
16	5.20045+003	8.49994+003	3.20748+003	5.08614-001	1.01810+004
17	5.82404+003	8.50000+003	3.42508+003	5.43521-001	1.07400+004
18	6.78896+003	8.49992+003	3.55977+003	5.65083-001	1.12922+004

EOF:31

0:>EXIT

NO CORRECTIONS APPLIED.

>

The detailed computer printout for the example steady case is provided on the following pages. Also at the end of the printout, the plot for the steady flow system is shown.

CASE : STEADY FLOW WITH TC-99 EXCHANGE

DC	=	.10000+003	EFFECTIVE STRATUM THICKNESS
R	=	.85000+004	MAXIMUM RADIUS FOR TRAVEL TIME CALCULATIONS--ALSO LENGTH SCALING PARAMETER
RO	=	.25000+003	EFFECTIVE RADIUS OF CAVERN
H0	=	.40000+001	INITIAL HEAD IN CAVITY STORAGE TANK
K0	=	.18250+004	HYDRAULIC CONDUCTIVITY OF STRATUM MATERIAL
P	=	.20000+000	THE EFFECTIVE POROSITY
UC	=	.10000+002	INITIAL UNIFORM FIELD STRENGTH AT TIME=0
UM	=	.10000+002	VALUE OF UNIFORM FIELD STRENGTH AT TIME=TM
OPTION	=	SERPIN	EXPERT FOR EXPONENTIAL VARIATION. SERPIN FOR SERPENTINE VARIATION
TR	=	.10000+001	PARAMETER FOR SERPENTINE VARIATION CALCULATION OF U (IN TIME UNIT)
A	=	.10000+001	PARAMETER USED BY SERPIN IN THE CALCULATION OF U
B	=	.10000+001	PARAMETER USED BY SERPIN IN THE CALCULATION OF U
C	=	.10000+001	PARAMETER USED BY SERPIN IN THE CALCULATION OF U
H1	=	.40000+001	MINIMUM VALUE OF H IN SERPEN CALCULATION
H2	=	.40000+001	MAXIMUM VALUE OF H IN SERPEN CALCULATION
TH	=	.10000+001	PARAMETER FOR SERPENTINE VARIATION CALCULATION OF H (IN TIME UNIT)
D	=	.10000+001	PARAMETER USED BY SERPIN IN THE CALCULATION OF H
E	=	.10000+001	PARAMETER USED BY SERPIN IN THE CALCULATION OF H
F	=	.10000+001	PARAMETER USED BY SERPIN IN THE CALCULATION OF H
XMAX	=	.85000+004	X-ABSCISSA VALUE AT WHICH TRAVEL TIME CALCULATIONS WILL BE TERMINATED
TRAX	=	.00000	MAXIMUM TRAVEL TIME BEFORE TERMINATION OF FLOW PATHS
THETA0	=	.00000	MINIMUM CONTROL ANGLE FOR PATHLINE STARTING POINTS ALONG CAVERN WALL
THETA1	=	.00000	MAXIMUM CONTROL ANGLE FOR PATHLINE STARTING LINE ALONG CAVERN WALL
NTHETA	=	18	NUMBER OF PATHLINES WANTED BETWEEN THETA0 AND THETA1
NTHETA	=	0	NUMBER OF PATHLINES WANTED BETWEEN THETA1 AND 180 DEGREES
TO	=	.00000	STARTING DEPARTURE TIME FOR CALCULATING FLOW PATHS
TF	=	.00000	FINAL DEPARTURE TIME FOR CALCULATING FLOW PATHS
NT	=	0	NUMBER OF TIME INCREMENTS WANTED BETWEEN TO AND TF PLUS ONE
CHEM	=	TECHNETIUM	NAME OF CHEMICAL SPECIE INVOLVED IN ION EXCHANGE REACTIONS.
KD	=	.50000+000	EQUILIBRIUM DISTRIBUTION COEFFICIENT FOR THE ION EXCHANGE SPECIE.
BP	=	.19000+001	PULK DENSITY OF THE SOIL OR POROUS MATERIAL
DELTA	=	.10000+002	TRAVEL TIME INCREMENT USED IN SOLVING FOR FLOW PATHS
SIFP	=	.60000+001	NUMBER TO BE DIVIDED INTO DELTA TO GET ACTUAL STEP SIZE FOR INTEGRATION
ILIM	=	5000	MAXIMUM NUMBER OF INCREMENTS AND INTERACTIONS ALONG ANY PATHLINE
NPRINT	=	50	CONTROLS PRINTOUT FREQUENCY. NPRINT-1 TIME INCREMENTS ARE OMITTED
EPSLN	=	.10000+004	NEAR ZERO CONVERGENCE TOLERANCE FOR STOPPING AT R OR XMAX
XCENTER	=	.30000+001	X-ABSCISSA IN INCHES TO DEFINE ORIGIN FOR PLOT
YCENTER	=	.40000+001	Y-ORDINATE IN INCHES TO DEFINE ORIGIN FOR PLOT
SCALE	=	.10000+004	SCALE IN LENGTH UNITS PER INCH ON THE PLOT

INPUT FOR WELL 1

WELLOP	=	SERPIN	
XWELL	=	.30000+004	X-COORDINATE OF THE WELL
YWELL	=	.10000+004	Y-COORDINATE OF THE WELL
ROWELL	=	.50000+002	STOPPING RADIUS OF THE WELL
Q0	=	.00000	THE MEAN INFLOW(+) (OR OUTFLOW(-)) RATE OF THE WELL
Q	=	.00000	THE MAXIMUM INFLOW(+) OR OUTFLOW (-) RATE OF THE WELL
TOWELL	=	.00000	THE BEGINNING TIME OF THE CYCLIC FLOW FOR THE WELL
TINWELL	=	.00000	THE ENDING TIME OF THE CYCLIC FLOW FOR THE WELL
QI	=	.20000+006	THE INITIAL FLOW RATE OF THE WELL
QM	=	.20000+006	THE MAXIMUM FLOW RATE OF THE WELL
TNWELL	=	.10000+001	PARAMETER USED IN CALCULATING WELL FLOW RATE
OWELL	=	.10000+001	PARAMETER USED IN CALCULATING WELL FLOW RATE
FWELL	=	.10000+001	PARAMETER USED IN CALCULATING WELL FLOW RATE
FWELL	=	.10000+001	PARAMETER USED IN CALCULATING WELL FLOW RATE

THE DIRECT INPUT STARTING POINTS XY COORDINATES, P LENGTHS AND TIMES FOLLOW

X	Y	P LENGTH	TIME
-1500.0000	250.0000		
3100.0000	1000.0000		
3070.7000	1070.7000		
3000.0000	1100.0000		
2929.3000	1070.7000		
2829.3000	929.3000		
3000.0000	900.0000		
3070.7000	929.3000		
250.0000	.0000		
235.0000	85.5000		
191.5000	160.7000		
125.0000	216.5000		
43.4000	246.2000		
-43.4000	246.2000		
-125.0000	216.5000		
-191.5000	160.7000		
-234.9000	85.5000		
-240.3000	29.0000		

AT THE SUCCESSFUL CONCLUSION OF GROUND THE FOLLOWING FILES ARE CATALOGUED:
NELSON*10008. AND NELSON*0030H8.

THE RATIO OF TECHNETIUM TRAVEL TIME TO WATER TRAVEL TIME ($1/K$) = (1/

.57500+0011

PATHLINE NO. 1 OF TECHNICTIONS DEPARTING THE CAVERN WALL AT T1 = .00000 YEARS
 THETA = .00000 DEGREES
 HEAD(H/H0) = .10000+001

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	.00000	-1.76471-001	2.94118-002	.00000	-1.50000+003	2.50000+002	.00000
1	5.05190-002	-1.55970-001	4.32386-002	5.00000+002	-1.32574+003	3.67528+002	2.11592+002 .50525+000
2	1.01038-001	-1.38125-001	6.82794-002	9.99999+002	-1.17406+003	5.80375+002	4.73643+002 .50525+000
3	1.51557-001	-1.13572-001	1.10373-001	1.50000+003	-9.64770+002	9.38167+002	8.88208+002 .50525+000
4	2.02076-001	-6.69736-002	1.68848-001	2.00000+003	-5.69276+002	1.43521+003	1.52460+003 .50525+000
5	2.52595-001	9.44802-003	2.29358-001	2.50000+003	8.03082+001	1.94954+003	2.35500+003 .50525+000
6	3.03114-001	1.06084-001	2.78849-001	3.00000+003	9.01714+002	2.37022+003	3.27886+003 .50525+000
7	3.53633-001	2.10808-001	3.17107-001	3.49999+003	1.79187+003	2.69541+003	4.22688+003 .50525+000
8	4.04151-001	3.19144-001	3.48094-001	3.99999+003	2.71273+003	2.95880+003	5.18480+003 .50525+000
9	4.54670-001	4.30325-001	3.72807-001	4.49999+003	3.65776+003	3.16886+003	6.15305+003 .58213+000
10	5.05189-001	5.42374-001	3.91294-001	4.99999+003	4.61018+003	3.32600+003	7.11843+003 .58213+000
11	5.55708-001	6.53571-001	4.04985-001	5.49998+003	5.55536+003	3.44238+003	8.07079+003 .58213+000
12	6.06226-001	7.63361-001	4.15400-001	5.99998+003	6.48857+003	3.53090+003	9.00821+003 .58213+000
13	6.56745-001	8.71735-001	4.23576-001	6.49998+003	7.40975+003	3.60040+003	9.93202+003 .58213+000
14	7.07264-001	9.78837-001	4.30173-001	6.99997+003	8.32012+003	3.65647+003	1.08441+004 .58212+000
14*	7.17308-001	9.99995-001	4.31337-001	7.09939+003	8.49996+003	3.66636+003	1.10242+004 .58212+000

PATHLINE NO. 2 OF TECHNETIUM IONS DEPARTING THE CAVERN WALL AT TI = .00000 YEARS
 THETA = .00000 DEGREES
 HEAD(H/H0) = .10000+001

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	.00000	3.64706-001	1.17647-001	.00000	3.10000+003	1.00000+003	.00000
1	5.05190-002	5.13927-001	1.26323-001	5.00000+002	4.36838+003	1.07374+003	1.27054+003 .18226+000
2	1.01038-001	6.36924-001	1.31533-001	9.99999+002	5.41386+003	1.11803+003	2.31696+003 .18226+000
3	1.51557-001	7.53368-001	1.35188-001	1.50000+003	6.40363+003	1.14910+003	3.30722+003 .18226+000
4	2.02076-001	8.66015-001	1.37936-001	2.00000+003	7.36112+003	1.17246+003	4.26501+003 .18226+000
5	2.52595-001	9.76067-001	1.40093-001	2.50000+003	8.29657+003	1.19079+003	5.20063+003 .18226+000
6	2.63705-001	9.99995-001	1.40508-001	2.60996+003	8.49996+003	1.19431+003	5.40405+003 .18226+000

PATHLINE NO. 3 OF TECHNETIUM IONS DEPARTING THE CAVERN WALL AT TI = .00000 YEARS
 THETA = .00000 DEGREES
 HEAD(H/H0) = .10000+001

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	.00000	3.61259-001	1.25965-001	.00000	3.07070+003	1.07070+003	.00000
1	5.05190-002	5.08362-001	1.46088-001	5.00000+002	4.32108+003	1.24175+003	1.26639+003 .21520+000
2	1.01038-001	6.31241-001	1.52966-001	9.99999+002	5.36555+003	1.30021+003	2.31252+003 .21520+000
3	1.51557-001	7.47628-001	1.57573-001	1.50000+003	6.35484+003	1.33937+003	3.30259+003 .21520+000
4	2.02076-001	8.60246-001	1.60979-001	2.00000+003	7.31210+003	1.36832+003	4.26029+003 .21520+000
5	2.52595-001	9.70288-001	1.63629-001	2.50000+003	8.24745+003	1.39085+003	5.19593+003 .21520+000
6	2.66397-001	9.99998-001	1.64256-001	2.63660+003	8.49999+003	1.39617+003	5.44853+003 .21520+000

PATHLINE NO. 4 OF TECHNETIUM IONS DEPARTING THE CAVERN WALL AT TI = .00000 YEARS
 THETA = .00000 DEGREES
 HEAD(H/H0) = .10000+001

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	.00000	3.52941-001	1.29412-001	.00000	3.00000+003	1.10000+003	.00000
1	5.05190-002	4.95360-001	1.60877-001	5.00000+002	4.21056+003	1.36741+003	1.25832+003 .24112+000
2	1.01038-001	6.18600-001	1.69370-001	9.99999+002	5.25810+003	1.43964+003	2.30640+003 .24112+000
3	1.51557-001	7.25204-001	1.74861-001	1.50000+003	6.24924+003	1.48632+003	3.30064+003 .24112+000
4	2.02076-001	8.47980-001	1.78863-001	2.00000+003	7.20783+003	1.52033+003	4.25984+003 .24112+000
5	2.52595-001	9.58142-001	1.81953-001	2.50000+003	8.14421+003	1.54660+003	5.19659+003 .24112+000
5+	2.72037-001	9.99996-001	1.82967-001	2.69242+003	8.49996+003	1.55522+003	5.55244+003 .24112+000

PATHLINE NO. 5 OF TECHNETIUM IONS DEPARTING THE CAVERN WALL AT TI = .00000 YEARS
 THETA = .00000 DEGREES
 HEAD(H/H0) = .10000+001

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	.00000	3.44624-001	1.25965-001	.00000	2.92930+003	1.07070+003	.00000
1	5.05190-002	4.77670-001	1.68226-001	5.00000+002	4.06020+003	1.42992+003	1.23296+003 .25609+000
2	1.01038-001	6.01600-001	1.78184-001	9.99999+002	5.11537+003	1.51456+003	2.29163+003 .25609+000
3	1.51557-001	7.18900-001	1.84389-001	1.50000+003	6.11065+003	1.56730+003	3.28829+003 .25609+000
4	2.02076-001	8.32003-001	1.88848-001	2.00000+003	7.07203+003	1.60521+003	4.25041+003 .25609+000
5	2.52595-001	9.42407-001	1.92265-001	2.50000+003	8.01046+003	1.63425+003	5.18930+003 .25609+000
5+	2.79330-001	9.99999-001	1.93777-001	2.76461+003	8.49999+003	1.64711+003	5.67900+003 .25609+000

PATHLINE NO. 6 OF TECHNETIUM IONS DEPARTING THE CAVERN WALL AT TJ = .00000 YEARS
 THETA = .00000 DEGREES
 HEAD(H/H0) = .10000+001

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	.00000	3.44624-001	1.09329-001	.00000	2.92930+003	9.29300+002	.00000
1	5.05197-002	4.81935-001	8.44249-002	5.00000+002	4.09645+003	7.17612+002	1.23580+003 .11395+000
2	1.01038-001	6.07871-001	8.62168-002	9.99999+002	5.16691+003	7.32843+002	2.30637+003 .11395+000
3	1.51557-001	7.25897-001	8.80692-002	1.50000+003	6.17013+003	7.48586+002	3.30972+003 .11395+000
4	2.02076-001	8.39569-001	8.95866-002	2.00000+003	7.13634+003	7.61486+002	4.27601+003 .11395+000
5	2.52595-001	9.50347-001	9.08195-002	2.50000+003	8.07795+003	7.71966+002	5.21769+003 .11395+000
6*	2.75569-001	9.99997-001	9.13048-002	2.72738+003	8.49997+003	7.76091+002	5.63973+003 .11395+000

PATHLINE NO. 7 OF TECHNETIUM IONS DEPARTING THE CAVERN WALL AT TJ = .00000 YEARS
 THETA = .00000 DEGREES
 HEAD(H/H0) = .10000+001

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	.00000	3.52941-001	1.05882-001	.00000	3.00000+003	9.00000+002	.00000
1	5.05190-002	4.99181-001	9.21079-002	5.00000+002	4.24304+003	7.82917+002	1.26805+003 .12649+000
2	1.01038-001	6.23693-001	9.46527-002	9.99999+002	5.30139+003	8.04546+002	2.32662+003 .12649+000
3	1.51557-001	7.40984-001	9.68285-002	1.50000+003	6.29837+003	8.23042+002	3.32377+003 .12649+000
4	2.02076-001	8.54185-001	9.85552-002	2.00000+003	7.26057+003	8.37719+002	4.28609+003 .12649+000
5	2.52595-001	9.64629-001	9.99432-002	2.50000+003	8.19934+003	8.49517+002	5.22493+003 .12649+000
6*	2.68982-001	9.99995-001	1.00336-001	2.66218+003	8.49996+003	8.52858+002	5.52555+003 .12649+000

PATHLINE NO. 8 OF TECHNETIUM IONS DEPARTING THE CAVERN WALL AT TI = .00000 YEARS
 THETA = .00000 DEGREES
 HEAD(H/H0) = .10000+001

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	.00000	3.61259-001	1.09329-001	.00000	3.07070+003	9.29300+002	.00000
1	5.05190-002	5.10395-001	1.06683-001	5.00000+002	4.33836+003	9.06808+002	1.27252+003 .15020+000
2	1.01038-001	6.33953-001	1.10387-001	9.99999+002	5.38860+003	9.38290+002	2.32323+003 .15020+000
3	1.51557-001	7.57715-001	1.13184-001	1.50000+003	6.38107+003	9.62067+002	3.31599+003 .15020+000
4	2.02076-001	8.63568-001	1.15337-001	2.00000+003	7.34033+003	9.80361+002	4.27542+003 .15020+000
5	2.52595-001	9.73765-001	1.17044-001	2.50000+003	8.27700+003	9.94877+002	5.21221+003 .15020+000
5+	2.64763-001	9.99995-001	1.17405-001	2.62043+003	8.49996+003	9.97939+002	5.43518+003 .15020+000

PATHLINE NO. 9 OF TECHNETIUM IONS DEPARTING THE CAVERN WALL AT TI = .00000 YEARS
 THETA = .00000 DEGREES
 HEAD(H/H0) = .10000+001

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	.00000	2.54118-002	.00000	.00000	2.50000+002	.00000	.00000
1	5.05190-002	2.28714-001	-5.54646-003	5.00000+002	1.94407+002	-4.71449+001	1.69496+003 .10000+001
2	1.01038-001	3.61862-001	-1.91098-002	9.99999+002	3.06903+003	-1.62433+002	2.82602+003 .92312+000
3	1.51557-001	4.89821-001	-3.15406-002	1.50000+003	4.15668+003	-2.68095+002	3.91894+003 .92312+000
4	2.02076-001	6.11280-001	-3.78499-002	2.00000+003	5.19588+003	-3.21724+002	4.95956+003 .92312+000
5	2.52595-001	7.28239-001	-4.14298-002	2.50000+003	6.19003+003	-3.52154+002	5.95418+003 .92312+000
6	3.03114-001	8.41477-001	-4.37707-002	3.00000+003	7.15256+003	-3.72051+002	6.91692+003 .92312+000
7	3.53633-001	9.52643-001	-4.54450-002	3.49999+003	8.09236+003	-3.86283+002	7.85683+003 .92312+000
7+	3.75845-001	9.99992-001	-4.60431-002	3.71984+003	8.49993+003	-3.91366+002	8.26442+003 .92312+000

PATHLINE NO. 10 OF TECHNETIUM IONS DEPARTING THE CAVERN WALL AT T1 = .00000 YEARS
 THETA = .00000 DEGREES
 HEAD(H/H0) = .10000+001

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	.00000	2.76471-002	1.00588-002	.00000	2.35000+002	8.55000+001	.00000
1	5.05190-002	2.21893-001	3.85003-002	5.00000+002	1.86609+003	3.27253+002	1.67495+003 .78803-001
2	1.01038-001	3.56032-001	3.00443-002	9.99999+002	2.97527+003	2.55376+002	2.76823+003 .78804-001
3	1.51557-001	4.81472-001	1.74539-002	1.50000+003	4.09251+003	1.48358+002	3.89112+003 .19215-002
4	2.02076-001	6.05874-001	1.37152-002	2.00000+003	5.14993+003	1.16579+002	4.94905+003 .19215-002
5	2.52595-001	7.23727-001	1.21868-002	2.50000+003	6.15168+003	1.03588+002	5.95089+003 .19215-002
6	3.03114-001	8.37428-001	1.13725-002	3.00000+003	7.11813+003	9.66664+001	6.91737+003 .19215-002
7	3.53633-001	9.46271-001	1.08695-002	3.49999+003	8.06030+003	9.23903+001	7.85954+003 .19216-002
7*	3.77558-001	9.99999-001	1.06930-002	3.73679+003	8.49999+003	9.08907+001	8.29923+003 .19216-002

PATHLINE NO. 11 OF TECHNETIUM IONS DEPARTING THE CAVERN WALL AT T1 = .00000 YEARS
 THETA = .00000 DEGREES
 HEAD(H/H0) = .10000+001

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	.00000	2.25294-002	1.89059-002	.00000	1.91500+002	1.60700+002	.00000
1	5.05190-002	2.03384-001	6.02903-002	5.00000+002	1.72877+003	6.82468+002	1.64261+003 .15478+000
2	1.01038-001	3.29190-001	8.55363-002	9.99999+002	2.72085+003	7.27058+002	2.63904+003 .15478+000
3	1.51557-001	4.50455-001	6.37751-002	1.50000+003	3.83312+003	5.42089+002	3.77205+003 .77903-001
4	2.02076-001	5.79335-001	6.27883-002	2.00000+003	4.92435+003	5.33701+002	4.86337+003 .77903-001
5	2.52595-001	6.98751-001	6.34663-002	2.50000+003	5.93938+003	5.39463+002	5.87842+003 .77902-001
6	3.03114-001	8.13322-001	6.42433-002	3.00000+003	6.91324+003	5.46068+002	6.85229+003 .77902-001
7	3.53633-001	9.24737-001	6.49404-002	3.49999+003	7.86026+003	5.51994+002	7.79934+003 .77902-001
7*	3.88368-001	9.99995-001	6.53635-002	3.84378+003	8.49995+003	5.55590+002	8.43904+003 .77901-001

PATHLINE NO. 12 OF TECHNETIUM IONS DEPARTING THE CAVERN WALL AT TI = .00000 YEARS
 THETA = .00000 DEGREES
 HEAD(H/H0) = .10000+001

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	.00000	1.47059-002	2.54706-002	.00000	1.25000+002	2.16500+002	.00000
1	5.05190-002	1.74401-001	1.15539-001	5.00000+002	1.48241+003	9.82083+002	1.59703+003 .22540+000
2	1.01038-001	2.92751-001	1.42364-001	9.99999+002	2.48243+003	1.21009+003	2.62284+003 .22539+000
3	1.51557-001	4.06891-001	1.84641-001	1.50000+003	3.45857+003	1.56945+003	3.66608+003 .30228+000
4	2.02076-001	5.34442-001	2.02703-001	2.00000+003	4.54276+003	1.72298+003	4.76167+003 .30228+000
5	2.52595-001	6.53705-001	2.12107-001	2.50000+003	5.55649+003	1.80291+003	5.77859+003 .30228+000
6	3.03114-001	7.68253-001	2.18456-001	3.00000+003	6.53015+003	1.85688+003	6.75376+003 .30228+000
7	3.53633-001	8.79714-001	2.23164-001	3.49999+003	7.47757+003	1.89690+003	7.70202+003 .30227+000
8	4.04151-001	9.88949-001	2.26840-001	3.99999+003	8.40606+003	1.92814+003	8.63104+003 .30227+000
9	4.09306-001	9.99992-001	2.27171-001	4.05101+003	8.49993+003	1.93095+003	8.72495+003 .30227+000

PATHLINE NO. 13 OF TECHNETIUM IONS DEPARTING THE CAVERN WALL AT TI = .00000 YEARS
 THETA = .00000 DEGREES
 HEAD(H/H0) = .10000+001

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	.00000	5.10578-003	2.89647-002	.00000	4.34000+001	2.46200+002	.00000
1	5.05190-002	1.35423-001	1.41110-001	5.00000+002	1.15534+003	1.19943+003	1.52806+003 .28889+000
2	1.01038-001	2.55985-001	1.78121-001	9.99999+002	2.17587+003	1.51403+003	2.59633+003 .28889+000
3	1.51557-001	3.70091-001	2.14198-001	1.50000+003	3.14577+003	1.82068+003	3.61369+003 .36577+000
4	2.02076-001	4.93624-001	2.38529-001	2.00000+003	4.19581+003	2.02750+003	4.68471+003 .36577+000
5	2.52595-001	6.12755-001	2.51595-001	2.50000+003	5.20842+003	2.13856+003	5.70353+003 .36577+000
6	3.03114-001	7.27554-001	2.60181-001	3.00000+003	6.18421+003	2.21154+003	6.68203+003 .36577+000
7	3.53633-001	8.39303-001	2.66439-001	3.49999+003	7.13407+003	2.26474+003	7.63340+003 .36577+000
8	4.04151-001	9.48810-001	2.71268-001	3.99999+003	8.06488+003	2.30578+003	8.56511+003 .36577+000
9	4.28053-001	9.99994-001	2.73198-001	4.23655+003	8.45995+003	2.32216+003	9.00049+003 .36577+000

PATHLINE NO. 14 OF TECHNETIUM IONS DEPARTING THE CAVERN WALL AT T1 = .00000 YEARS
 THETA = .00000 DEGREES
 HEAD(H/H0) = .10000+001

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	.00000	-5.10588-003	2.89647-002	.00000	-4.34000+001	2.46200+002	.00000
1	5.05190-002	3.91821-002	1.54662-001	5.00000+002	7.58047+002	1.31463+003	1.42530+003 .34427+000
2	1.01038-001	2.67047-001	2.01447-001	9.99999+002	1.75990+003	1.71230+003	2.50461+003 .34427+000
3	1.51557-001	3.19954-001	2.36302-001	1.50000+003	2.71961+003	2.00857+003	3.50901+003 .34427+000
4	2.02076-001	4.38231-001	2.65283-001	2.00000+003	3.72497+003	2.25490+003	4.54462+003 .42115+000
5	2.52595-001	5.56849-001	2.82940-001	2.50000+003	4.73322+003	2.40499+003	5.56417+003 .42115+000
6	3.03114-001	6.72053-001	2.94342-001	3.00000+003	5.71245+003	2.50191+003	6.54824+003 .42115+000
7	3.53633-001	7.84305-001	3.02481-001	3.49999+003	6.66660+003	2.57109+003	7.50490+003 .42114+000
8	4.04151-001	8.94281-001	3.08667-001	3.99999+003	7.60139+003	2.62367+003	8.44118+003 .42114+000
9	4.53407-001	9.99792-001	3.13455-001	4.48749+003	8.49824+003	2.66437+003	9.33895+003 .42114+000
9.	4.53502-001	9.99994-001	3.13464-001	4.48843+003	8.49995+003	2.66444+003	9.34066+003 .42114+000

PATHLINE NO. 15 OF TECHNETIUM IONS DEPARTING THE CAVERN WALL AT T1 = .00000 YEARS
 THETA = .00000 DEGREES
 HEAD(H/H0) = .10000+001

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	.00000	-1.47059-002	2.54706-002	.00000	-1.25000+002	2.16500+002	.00000
1	5.05190-002	3.55447-002	1.53212-001	5.00000+002	3.02130+002	1.30230+003	1.27691+003 .39157+000
2	1.01038-001	1.45638-001	2.12147-001	9.99999+002	1.23792+003	1.80325+003	2.34181+003 .39157+000
3	1.51557-001	2.57466-001	2.50303-001	1.50000+003	2.16848+003	2.12758+003	3.34642+003 .39157+000
4	2.02076-001	3.76903-001	2.82056-001	2.00000+003	3.15268+003	2.39748+003	4.34784+003 .46845+000
5	2.52595-001	4.87745-001	3.05108-001	2.50000+003	4.14583+003	2.59342+003	5.36042+003 .46845+000
6	3.03114-001	6.07229-001	3.20253-001	3.00000+003	5.12745+003	2.72215+003	6.35053+003 .46845+000
7	3.53633-001	7.16135-001	3.30836-001	3.49999+003	6.08715+003	2.81211+003	7.31447+003 .46845+000
8	4.04151-001	8.26770-001	3.38725-001	3.99999+003	7.02755+003	2.67916+003	8.25726+003 .46844+000
9	4.54670-001	9.35560-001	3.44877-001	4.49999+003	7.95226+003	2.93146+003	9.18346+003 .46844+000
9+	4.84934-001	9.99996-001	3.47966-001	4.79952+003	8.49997+003	2.95771+003	9.73179+003 .46844+000

PATHLINE NO. 16 OF TECHNETIUM IONS DEPARTING THE CAVERN WALL AT T1 = .00000 YEARS
 THETA = .00000 DEGREES
 HEAD(H/H0) = .10000+001

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	.00000	-2.25254-002	1.89059-002	.00000	-1.91500+002	1.60700+002	.00000
1	5.05199-002	-2.24575-002	1.31271-001	5.00000+002	-1.90889+002	1.11581+003	1.06750+003 .43174+000
2	1.01030-001	6.81599-002	2.04716-001	9.99999+002	5.79359+002	1.74008+003	2.06609+003 .43174+000
3	1.51557-001	1.75521-001	2.51901-001	1.50000+003	1.49533+003	2.14116+003	3.06710+003 .43174+000
4	2.02076-001	2.85949-001	2.87080-001	2.00000+003	2.43057+003	2.44018+003	4.04914+003 .43174+000
5	2.52555-001	3.99090-001	3.15719-001	2.50000+003	3.39226+003	2.68361+003	5.04136+003 .50862+000
6	3.03114-001	5.14054-001	3.36333-001	3.00000+003	4.36946+003	2.85883+003	6.03432+003 .50862+000
7	3.53633-001	6.27701-001	3.50625-001	3.49999+003	5.33546+003	2.98031+003	7.00799+003 .50862+000
8	4.04151-001	7.39281-001	3.61006-001	3.99999+003	6.28389+003	3.06855+003	7.96054+003 .50862+000
9	4.54670-001	8.48963-001	3.68922-001	4.49999+003	7.21618+003	3.13584+003	8.89527+003 .50862+000
10	5.05189-001	9.57045-001	3.75187-001	4.99999+003	8.13488+003	3.18909+003	9.81551+003 .50861+000
10+	5.25444-001	9.99993-001	3.77351-001	5.20045+003	8.49994+003	3.20748+003	1.01810+004 .50861+000

PATHLINE NO. 17 OF TECHNIQUE TONS DEPARTING THE CAVERN WALL AT TI = .00000 YEARS
 THETA = .00000 DEGREES
 HEAD(H/H0) = .10000+001

N	TIME DIMENSIONLESS	X-COORD. DIMENSIONLESS	Y-COORD. DIMENSIONLESS	TIME YEARS	X-COORD. FEET	Y-COORD. FEET	PATH LENGTH FEET
0	.00000	-2.76353-002	1.00588-002	.00000	-2.34900+002	8.55000+001	.00000
1	5.05190-002	-7.59217-002	7.96035-002	5.00000+002	-6.45844+002	6.76629+002	7.92442+002 .46664+000
2	1.01039-001	-3.42476-002	1.56956-001	9.99999+002	-2.91104+002	1.33412+003	1.55050+003 .46664+000
3	1.51557-001	5.21627-002	2.22725-001	1.50000+003	4.43383+002	1.89316+003	2.47725+003 .46664+000
4	2.02076-001	1.55969-001	2.69844-001	2.00000+003	1.32574+003	2.29367+003	3.44722+003 .46664+000
5	2.52595-001	2.64146-001	3.05499-001	2.50000+003	2.24524+003	2.59674+003	4.41558+003 .46664+000
6	3.03114-001	3.75362-001	3.34494-001	3.00000+003	3.19057+003	2.84320+003	5.39268+003 .54352+000
7	3.53633-001	4.88778-001	3.56363-001	3.49999+003	4.15461+003	3.02908+003	6.37463+003 .54352+000
8	4.04151-001	6.01699-001	3.72009-001	3.99999+003	5.11444+003	3.16207+003	7.34370+003 .54352+000
9	4.54670-001	7.12991-001	3.83482-001	4.49999+003	6.06042+003	3.25960+003	8.29472+003 .54352+000
10	5.05189-001	8.22577-001	3.92246-001	4.99999+003	6.99191+003	3.33409+003	9.22920+003 .54352+000
11	5.55708-001	9.35655-001	3.99177-001	5.49998+003	7.91057+003	3.39300+003	1.01497+004 .54352+000
11*	5.88450-001	1.00000+000	4.02951-001	5.82404+003	8.50000+003	3.42506+003	1.07400+004 .54352+000

PATHLINE NO. 1° OF TECHNETIUM IONS DEPARTING THE CAVERN WALL AT T1 = .00000 YEARS
 THEIA = .00000 DEGREES
 HEAD(H/H0) = .10000+001

N	TIME DIMENSIONLESS .00000	X-COORD. DIMENSIONLESS -2.92118-002	Y-COORD. DIMENSIONLESS 3.41176-003	TIME YEARS .00000	X-COORD. FEET -2.48300+002	Y-COORD. FEET 2.90000+001	PATH LENGTH FEET .00000
1	5.05190-002	-9.70539-002	2.66074-002	5.00000+002	-8.24958+002	2.26163+002	6.22793+002 .48821+000
2	1.01038-001	-1.05592-001	6.33367-002	9.99999+002	-8.97529+002	5.38379+002	9.52282+002 .48821+000
3	1.51557-001	-8.46453-002	1.20491-001	1.50000+003	-7.19485+002	1.02418+003	1.47350+003 .48821+000
4	2.02076-001	-2.57039-002	1.88011-001	2.00000+003	-2.18483+002	1.59809+003	2.23883+003 .48821+000
5	2.52595-001	6.42035-002	2.46234-001	2.50000+003	5.45730+002	2.09299+003	3.15130+003 .48821+000
6	3.03114-001	1.67501-001	2.89925-001	3.00000+003	1.42376+003	2.46436+003	4.10527+003 .48821+000
7	3.53633-001	2.75128-001	3.24101-001	3.49999+003	2.33859+003	2.75486+003	5.06529+003 .48821+000
8	4.04151-001	3.85906-001	3.51841-001	3.99999+003	3.28020+003	2.99065+003	6.03613+003 .56509+000
9	4.54670-001	4.98525-001	3.72850-001	4.49999+003	4.23746+003	3.16923+003	7.01004+003 .56509+000
10	5.05189-001	6.10673-001	3.98159-001	4.99999+003	5.19072+003	3.29935+003	7.97220+003 .56509+000
11	5.55708-001	7.21379-001	3.99560-001	5.49998+003	6.13172+003	3.39626+003	8.91820+003 .56509+000
12	6.06226-001	8.30532-001	4.08356-001	5.99998+003	7.05952+003	3.47103+003	9.84903+003 .56508+000
13	6.56745-001	9.38281-001	4.15359-001	6.49998+003	7.97539+003	3.53055+003	1.07668+004 .56508+000
13*	6.85943-001	9.99990-001	4.18796-001	6.76896+003	8.49992+003	3.55977+003	1.12922+004 .56508+000

SUMMARY OF TECHNETIUM IONS ARRIVAL LOCATIONS AND TIMES AT THE OUTFLOW BOUNDRIES

WITH DEPARTURE TIME OF .000YEARS AND AT THAT TIME
THE OUTFLOW RATE IS .13006966+007 CUBIC FEET PER YEARS
AND THE RELATIVE CAVERN HEAD IS 1.0000

PATH NO.	REL. APP. TIME X YEARS	FEET	Y FEET	CUM. FLUX Q/QO	PATH LENGTH FEET
1	7.09939+003	8.49996+003	3.66636+003	5.82124-001	1.10242+004
2	2.60996+003	8.49996+003	1.19431+003	1.82262-001	5.40405+003
3	2.63660+003	8.49999+003	1.39617+003	2.15197-001	5.44850+003
4	2.69242+003	8.49996+003	1.55522+003	2.41123-001	5.55244+003
5	2.76461+003	8.49999+003	1.64711+003	2.56091-001	5.67900+003
6	2.72738+003	8.49997+003	7.76091+002	1.13947-001	5.63973+003
7	2.66218+003	8.49996+003	8.52858+002	1.26493-001	5.52556+003
8	2.62043+003	8.49996+003	9.97939+002	1.50196-001	5.43518+003
9	3.71984+003	8.49993+003	-3.91366+002	9.23118-001	8.26442+003
10	3.73679+003	8.49995+003	9.08907+001	1.92158-003	8.29923+003
11	3.84378+003	8.49995+003	5.55590+002	7.79015-002	8.43904+003
12	4.05101+003	8.49995+003	1.93095+003	3.02275-001	8.72495+003
13	4.23655+003	8.49995+003	2.32218+003	3.65770-001	9.00049+003
14	4.48843+003	8.49995+003	2.66444+003	4.21143-001	9.34066+003
15	4.79952+003	8.49997+003	2.95771+003	4.68443-001	9.73179+003
16	5.20045+003	8.49994+003	3.20748+003	5.06614-001	1.01810+004
17	5.82404+003	8.50000+003	3.42508+003	5.43521-001	1.07400+004
18	6.78696+003	8.49992+003	3.55577+003	5.65083-001	1.12922+004

STEADY FLOW WITH TC-99 EXCHANGE
 DEPARTURE TIME = 0.00 YEARS
 SCALE 1 INCH = 1000 FEET

APPENDIX C

MAINTAINING OR MODIFYING THE COMPUTER PROGRAMS

APPENDIX C

MAINTAINING OR MODIFYING THE COMPUTER PROGRAMS

A synopsis of the overall PATHS program and related routines is presented here. A complete listing of the codes and test cases, on microfiche, is included at the end of this appendix. The following discussion also shows the relationships between the various programs and the corresponding files they generate.

In large measure, the information in this appendix is incidental to what the program user needs to get his work done. For someone who must maintain or modify the PATHS system, however, this overview is essential.

OVERVIEW OF PATHS SYSTEM

What we so far have called PATHS is actually a global name for three related FORTRAN programs. These programs are PATHS, GROUND, and LOCQAR. PATHS and LOCQAR previously were coded in BASIC; now all three are available in ASCII FORTRAN on the Univac 1100/44 time sharing EXEC operating system.

PATHS is an interactive program that prompts the user to enter all information necessary to create a coded file. The file is a run stream that can be batched to execute GROUND. This batch program performs the lion's share of the calculations. GROUND calculates the fluid travel time along each flow path, the coordinates of each path, and the distance traveled. In addition, calculations are saved that make it possible to generate CalComp plots showing the flow paths graphically. GROUND also writes a file summarizing the fluid arrival calculations. This may be viewed from the terminal after GROUND finishes execution, thereby giving the user a capsulized view of results before the run is printed and delivered. GROUND also generates a binary data file. This file feeds LOCQAR, which can be executed after the completion of GROUND.

Like PATHS, LOCQAR is interactive, but solicits very little data before calculated results of outflow location and rates are printed.

Pictorially, the flow through the system is as follows:

PROGRAMS

LOCQAR

LOCQAR is the simplest of the three programs. It is a short (325-cards) program that reads the binary data file created by GROUND and then interacts with the user for more information, asking about ten questions. (See Appendix B for an example of usage.) Only the last 100 lines of code are used to process data and print out the results via the terminal. LOCQAR uses only one subroutine, SEEBIT, which interprets information from the terminal.

Currently LOCQAR is maintained as source, relocatable, and absolute under the file and element name NELSON*LOCQAR.RUN.

PATHS

PATHS is relatively long (1440 cards), because it is an interactive code. Operationally, it is simple and straightforward, flowing linearly through the code, asking the user questions, slowly building up a reservoir of data to create a job stream for the GROUND program.

By using CALL FACSF, PATHS creates internally an SDF file catalogued under the user's project ID and the file name GRND_. GRND has appended the job number entered by the user. This file is opened, closed, and freed by PATHS. It is also batched for execution if the user desires.

PATHS has several subroutines, all but two of which are trivial, only writing out information helpful to the user. The two non-trivial subroutines are SEEBIT and BLANKS, used to read information from the terminal. Currently PATHS is maintained as source, relocatable, and absolute under the file and element name NELSON*PATHS.RUN.

Data Entered

The following detailed input sequence has been prepared to show the procedure for using PATHS to collect draft input data.

The PATHS input sequence list includes all of the variables that the program requires, in the order each is requested. It also shows explicitly the program flow and how various input variables are skipped from entry based on the responses to the questions. While probably too detailed for most terminal work, it is useful in maintaining or modifying the interactive PATHS program.

Detailed Input Data Sequence List

(CONTROL CARD INFORMATION)

1. _____ = ACCT Enter your account number.
2. _____ = USERID Enter your user ID.
3. _____ = PROJ Enter your project ID.
4. _____ = ADDRES Enter your name/address.
5. _____ = PASSWD Enter your password.

(DATA FOR PROGRAM GROUND)

6. _____ = $D_0 = D_0$ is the stratum thickness.
 7. _____ = R is the distance to the boundary. (Units consistent with D_0).
 8. _____ Standard distance or T termination of pathline. (Yes or No)
 If Yes:
 9. _____ = XMAX is the terminating abscissa value.
 If No:
 9. _____ = TMAX is entered if desired; the maximum travel time for flow paths.
 10. _____ = $R_0 = r_0$ is the cavern radius. (Units consistent with D_0 .)
 11. _____ = $H_0 = H_0$ is the head in the cavern. (Units consistent with D_0 .)
 12. _____ = $K_0 = K_0$ is the stratum hydraulic conductivity. (Units consistent with D_0 . Whatever time units are involved in hydraulic conductivity sets the units for the travel time.)
 13. _____ = P is the effective stratum porosity.
 14. _____ S or T steady or transient cases.
 15. _____ = U_0 is the initial uniform gradient.
- If STEADY case skip to 22
16. _____ = U_M is a later gradient value. (See Figure 1.)

If no STEADY case skip to 21

17. _____ = TM

is the time parameter of the gradient equation in time units of K_0 .

18. _____ = A

19. _____ = B

20. _____ = C

Parameters used in the calculation of the uniform gradient.

21. _____ Enter S, E or C (serpin, exponential or cyclic) for computing variation in the cavern head. (See Figures 1 and 2.)

If E skip to 32. If C skip to 28.

22. _____ = HI

is the initial value of the cavern head in units of H_0 .

23. _____ = HM

Maximum value of the head in units of H_0 .

If HI is equal to HM skip to 32.

24. _____ = TN

is a time parameter. Units consistent with TM for the variation of the uniform gradient U.

25. _____ = D

26. _____ = E

27. _____ = F

Parameter used in serpin option to calculate H. Skip to 32.

28. _____ = HMC

is the mean cavern head.

29. _____ = HAC

is the amplitude of the cyclic head.

30. _____ = TOC

is the beginning time of the cyclic flow from the cavern.

31. _____ = TMC

is the ending time of the cyclic flow from the cavern.

32. _____ Are there additional wells or caverns? (Yes or No)

If no skip to 48.

33. _____ = J = j

is the number of wells.

34. _____ = XWELL = x_j

is the x coordinate of the well.

35. _____ = YWELL = y_j

is the y coordinate of the well.

36. _____ = ROWELL

is the stopping radius of the well.

If steady case skip to 38

37. _____ Is well serpin or cyclic? (S or C)

If cyclic skip to 44

38. _____ = QI is the initial flow rate of well (see Figure 2).

39. _____ = QM is the maximum flow rate of well.

40. _____ = TNWELL = TN_j is time parameter in calculating well flow rate

41. _____ = DWELL = DW_j Parameters used by the serpin

42. _____ = EWELL = EW_j } option to calculate the well flow

43. _____ = FWELL = FW_j } rate.

Return to 34 until all wells have been read.

After all wells have been read skip to 48.

44. _____ = QQ_j is the mean inflow (+) or outflow (-) rate of the well.

45. _____ = QA_j is the amplitude about the mean inflow (+) or outflow (-) of the well.

46. _____ = TOWELL is the beginning time of the cyclic flow of the well.

47. _____ = TMWELL is the ending time of the cyclic flow of the well.

Return to 34 until all wells have been read.

After all wells have been read continue at 48.

48. _____ = VS Max 12 character unit label of DO's length.

49. _____ = WS Max 12 character time units of K0.

50. _____ = THETA0 = θ_0 the angle in degree around the cavern well to the starting point for the first pathline.

51. _____ = THETAM = θ_M the maximum angle in degrees to the lost pathline starting point along the cavern wall.

52. _____ = NTHETA = $N\theta$ the number of equally spaced pathlines desired along the cavern wall that will be generated beginning with THETA and ending with THETAM.

If THETA0 is not equal to THETAM skip to 58.

53. _____ Are the initial path lengths zero? (Yes or No)

54. _____ Enter x coordinate of the pathline starting point.

55. _____ Enter y coordinate of the pathline starting point.

If initial path lengths are zero skip 56 and 57.

56. _____ Enter L-path length in units of D0.

57. _____ Enter starting TIME in units the same as time units of K0.

Return to 54 until NTHETA have been read, then skip to 59.

58. _____ = KEHETA is the number of pathlines that will be generated between THETAM and 179.99 (+)⁰.

59. _____ = T0 = t_0 is the departure time in units of K0 of first fluid fluid particles leaving the cavern for which calculations will be made.

If steady case skip to 63.

60. _____ = TF = t_f is the departure time in units of K0 of final fluid particles leaving the cavern for which calculations will be made.

61. _____ = NT is the number of equally spaced departure times beginning with T0 and ending with TF that will be calculated.

If T0 is not equal to TF skip to 63.

62. _____ = T Enter all NT time increments from the terminal.

Repeat 62 until all NT have been read.

63. _____ Is there an ion exchange delay? (Yes or No)

If no skip to 67.

64. _____ = CHEM is the chemical name of the ion (12 character name max.)

65. _____ = KD = K_d is the equilibrium distribution coefficient

66. _____ = $BD = B_d$ is the bulk density of the porous material in units consistent with KD.
67. _____ = DELTA is the time increment used in computing flow along a given path. (Program PATH aids in providing range for proper selection.)
68. _____ Enter the number of steps to be used for integration over the delta increment (six usually suffices).
69. _____ = ITLIM is the number of iterations (5000 is the upper limit).
70. _____ = NPRINT is the value N such that every Nth time increment is printed. (Program PATH aids in this selection).
71. _____ = EPSLN is the near zero convergence for finding R.
72. _____ Are plots desired? (Yes or No).

If no skip to 77.

73. _____ Are 30-inch-high plots desired? (If not 11 inch high plots result.)
74. _____ = XCENTER The (x, y coordinates in inches of the cavern
75. _____ = YCENTER center to be plotted from (0,0) lower
76. _____ = SCALE } left corner of the plot window.
- is the scale factor in units/inch to be used in the plot.
77. _____ Is detailed computer printout desired? (Yes or No)
78. _____ Enter the job run number. (Digits from 1 to 9)
79. _____ Is the job to be submitted? (Yes or No)

(Note: The job stream created is saved as the runstream PROJ*GRND_. Where PROJ is the project ID (item number 2) and is the job run number (item number 78). PROJ*GRND_ is available for modification through EDITOR for job submittal also.)

GROUND

The GROUND program calculates flow pathlines and arrival times. It is a program of about 1150 cards. Apart from the output data GROUND generates on each path of flow, it creates a summary file BQ3VH_ of path data, a binary file for LOCQAR called LOCQ_, and CalComp plots. (NOTE: The dash_ is for the appended number, the number of the run set in the PATHS program.)

GROUND begins by reading the data created by PATHS. It then prints this data read, identifying it for the user. Next the variables read in are scaled and the beginning time loop is started. If the run is a steady case, only one starting time for the flow paths calculated is used. However, for transient cases, the program loops back to pick up the next starting time flow paths are to be calculated for. Execution continues like this until the final starting time is reached that flow paths are to be calculated for.

With the beginning of each pathline to be calculated, initializing is done, including the initializing for setting up the x and y arrays for plotting the paths. Depending on cavern behavior or type of flow subroutines HM, SERPIN or CYCLE will be called to calculate exponential, serpin or cyclic flow. Next, the possible influence of wells on the flow is introduced. A call to subroutine RKDE is made, which in turn calls function DYWELL to obtain the incremental numerical solution through a modified Runge-Kutta technique (Gill, 1951). This process is continued for each pathline until the terminating distance (XMAX) or terminating time (TMAX) is reached.

As each pathline is calculated, every NPRINT (see item 70 of PATHS input data sequence list) interval of data is printed; i.e., the (x, y) coordinates of the point plus the time and distance traveled. At the end of the pathline, the final line is printed and also saved for the summary print out of final locations and times for all path lines are calculated. Also if plots are desired, a call is made to subroutine WRIT at the end of each pathline calculated to have it plotted. Then a new pathline is begun and cycled through as before until the final pathline is processed. With the final pathline calculated, GROUND comes to conclusion, unless it is a transient case in which the entire execution of pathline flow begins again, but with a new starting time.

Apart from the subroutines already mentioned, program GROUND calls subroutine BOX to encase the plots generated. Subroutines SIMP and NEWTON remain a part of the code but they are not used. They are maintained for possible use later.

Currently program GROUND is maintained as source, relocatable, and absolute under file and element name NELSON*GROUND.RUN . Because GROUND calls the CalComp routines in plotting, it is necessary to include this library of routines when creating the relocatable and absolute files, namely:

```
@ MAP , IS , NELSON*GROUND.RUN
IN  NELSON*GROUND.RUN
LIB  CALCOMP*LIB.
END
```

Variable Names

Because GROUND reads the variables originally solicited from the user by the program PATHS, a flow diagram of how they are read follows. Also, because GROUND frequently renames these variables, this flow diagram should be compared with the variable list in Appendix B under the discussion "Using EDITOR". As an example, note that the variables for row 9 of PATHS are respectively: R, R, HO, KO while GROUND names them respectively: S, RMAX, HO, EKO. The lines in this flow diagram are numbered to correspond to their counterpart in Appendix B.

VARIABLES READ BY GROUND

8. TITLE
9. S,RMAX,HO,EKO
10. RO,ROS,TP,UO
11. RM,P,TM
12. PATH,AAKD,BBD
13. CHEM,PROJ,VH3,IPROJ
14. AST,BST,CST,KTHETA
15. THETAO,THETAM,TO,NTHETA
16. TF,TIMEX,EPSLN,ITLIM
17. DELTA,NT,STEP,NT
18. XMAX,XC,YC,ISK
19. SC,DST,EST,FST
20. GST,OST,XTEST,YSTOP1
21. HMEAN,HAMP,TOCYC,TMCYC
22. PARAMA,NWELL,P1

23. ROWELL(I),XWELL(J)
24. YWELL(I),TNWELL(I)
25. QI(I),QM(I),DWELL(I)
26. EWELL(I),FWELL(I),Q(I),QQ(I)
27. TOWELL(I),TMWELL(I)
28. WELLOP(I)

Loops
NWELL times
(Skips these if
NWELL equals zero)

35. JLEN
36. JTIM
37. CASE

a

PROGRAM LISTINGS AND OUTPUT FOR TEST CASES

The complete listings of the PATHS, GROUND and LOCQAR program are provided on microfiche. The first test case is the "Example Transient Case (Two Wells)" described in the body of the report and illustrated in Appendix B. Most of the output of the first test case was also shown in Appendix B though some of the detail printout was omitted. The complete output listing is provided on microfiche below. The second test case is the "Steady Flow with Tc-99 Exchange" illustrated in Appendix B. The complete listing of the output for test case 2 is also included in the microfiche envelope.

APPENDIX D

DEFINITIONS OF TERMS

APPENDIX D
DEFINITIONS OF TERMS

		<u>Units</u>
A	is a parameter in the $W(t')$ and $U(t')$ time-dependent functions (see Figure 1).	T
B	is a parameter in the $W(t')$ and $U(t')$ time-dependent function (see Figure 1).	None
B_d	is the bulk density of the porous material.	FT^2/L^4
C	is a parameter in the $W(t')$ and $U(t')$ time-dependent function (see Figure 1).	T^2
C'	is the contaminant concentration in the flowing ground-water.	FT^2/L^4
C^0	is the dimensionless contaminant concentration (see Equation A-45).	None
C_1	is a constant in the dimensionless potential function.	None
C_0	is the initial concentration in the pond or cavern.	FT^2/L^4
C'_0	is a constant to be determined in the potential function.	FL/F
D=DWELL	is a parameter in the $H(t')$ time-dependent function (see Figure 1).	T
DW_j	is a time parameter in the flow rate, $Q_j(t')$, for the jth well (see Figure 1).	T
D_0	is the stratum thickness (see Table 1).	L
E=EWELL	is a parameter in the $W(t')$ time-dependent function (see Figure 1).	None
EW_j	is a time parameter in the flow rate, $Q_j(t')$, for the jth well (see Figure 1).	None
F=FWELL	is a parameter in the $H(t')$ time-dependent function (see Figure 1).	T^2

		<u>Units</u>
$F(t)$	indicates a function of time, t .	None
FW_j	is a time parameter in the flow rate, $Q_j(t')$, for the j th well (see Figure 1).	T^2
H	is the dimensionless head at any time, t , in the cavern or pond.	None
H'	is the time-dependent energy head in the cavern or pond.	FL/F
H_0	is the initial or steady head in the cavern (see Equation A-2).	FL/F
HI	is a parameter in the time-dependent cavern head equation (see Figure 1).	FL/F
TN_j	is a time parameter in the flow rate, $Q(t')$, function for the j th well (see Figure 1).	T
$TOWELL_j$	is the initial time parameter in the cyclic flow rate, $Q(t')$, function for the j th well (see Figure 2).	T
$TMWELL_j$	is the later cyclic time parameter in the flow rate, $Q(t')$, for the j th well (see Figure 2).	T
$TNWELL_j$	is a computer-used name equivalent to TN_j .	T
U	is the time-dependent uniform gradient strength.	L/L
UO	is a parameter in the time-dependent uniform gradient function (see Figure 1).	L/L
UM	is a parameter in the time-dependent uniform gradient function (see Figure 1).	L/L
$W(t')$	is the general serpin equation form of time dependence (see Figure 1 or Equation A-18).	
W_T	is the contaminant outflow rate (see Equation 17).	F/T
$XMAX$	is the stopping distance for pathlines in the positive x coordinate direction (see sketch in Table 1).	L
$XCENTER$	is the x -coordinate in inches for the origin $x'=0$, $y'=0$ for plots (see Table 1).	L

	Units
$XWELL_j = x'_j$ is the x-coordinate location of the center of the jth well.	L
YCENTER is the y-coordinate in inches for the origin $x=0$, $y=0$ for the automatic machine plots (see Table 1).	L
$YWELL_j = y'_j$ is the y-coordinate location of the center of the jth well.	L
J=N is the total number of wells.	None
HM is a parameter in the time-dependent cavern head equation (see Figure 1).	None
K is the ratio of the exchangeable ion travel time to that of the fluid (see Equation 13).	None
K_d is the equilibrium exchange distribution coefficient (see Equations 13, A-48).	$FT^2/4L$
K_o is the hydraulic conductivity.	$L^3/TL^2 \left(\frac{L}{L} \right)$
$K\theta = K\theta_{\theta}$ is the number of pathlines that will be generated between θM and $179.99 (+)^{\circ}$ originating on the cavern wall.	None
L denotes length units.	L
M_o is the pond or cavern source strength.	L
$M_j = \frac{Q_j}{D_o K_o}$ is the well strength of the jth well.	L
N=J is the total number of wells in the flow system.	None
NT is the number of equally spaced departure times beginning with t_o and ending with t_f that will be calculated (see Table 1).	None
$N\theta$ is the number of equally spaced pathlines along the cavern wall that will be generated beginning with θO and ending with θM .	None
P is the effective porosity.	None
Q is the leakage rate from the cavern (see Equation A-40).	L^3/T

		<u>Units</u>
Q_i	is the cumulative flow rate (see Equation A-43).	L^3/T
Q_j	is the volume inflow or outflow rate of the jth well.	L^3/T
QI_j	is the initial inflow (+) or outflow (-) rate for the serpin well option (see Equation A-18 and Table A-1).	L^3/T
QM_j	is the maximum inflow (+) or outflow (-) rate for the serpin well option (see Equation A-18 and Table A-1).	L^3/T
QQ_j	is the mean inflow (+) or outflow (-) rate for the cyclic option of time dependence for well flow (see Equation A-19 and Table A-2).	L^3/T
QA_j	is the amplitude of the cyclic well inflow (+) or outflow (-) rate (see Equation A-19 and Table A-2).	L^3/T
Q_o	is a constant leakage rate from the cavern used as a scaling value (see Equation 9).	L^3/T
Q'	is the leakage rate from the cavern (see Equation A-20).	L^3/T
R	is the distance (radial) to the groundwater outflow area, or the remote boundary. It also is used in scaling (see Equation A-2).	L
$ROWELL_j$	is the numerical stopping radius around the jth well (see Table 1).	L
$SCALE$	is the scale used in the automatic plots (see Table 1).	$L/inch$
T	denotes the arrival time and also time units.	T
$TMAX$	is the stopping time along the pathlines (see Table 1).	T
TM	is a time parameter in the $U(t')$ function (see Figure 1).	T
TN	is a time parameter in the $H(t')$ function (see Figure 1).	
g	is the gravitational scalar.	L/T^2

		<u>Units</u>
j	as a subscript denotes the variable applies to the jth well.	None
ln	is the natural logarithm to the base e.	None
p	is the fluid pressure.	F/L^2
q'	is the unit fluid outflow rate across the boundary; i.e., into the river.	$L^3/T/L$
$q = \frac{R}{D_o K_o H_o} q'$	is the dimensionless fluid flow rate across the boundary.	None
r	is the dimensionless radial coordinate variable in cylindrical coordinates.	None
r'	is the radial variable in cylindrical coordinates.	L
r' _o	is the effective cavern radius.	L
r _o	is the dimensionless effective cavity radius.	None
s	is the location along the outflow boundary; i.e., along the river (see Equation 17).	L
t	is the dimensionless time variable (see Equation A-2).	None
t'	is the time variable.	
t _o	is the departure time of the first fluid particles leaving the cavern wall or from the other specified locations.	None
t' _o	is the departure time of the fluid particles from a given location.	T
w _o	is a parameter in the serpin equation (see Figure 1 or Equation A-18).	None
w _{oc}	is a parameter in the cyclic equation (see Figure 2 or Equation A-19).	None
w _m	is a parameter in the serpin equation (see Figure 1 or Equation A-18).	None

		<u>Units</u>
Q_i	is the cumulative flow rate (see Equation A-43).	L^3/T
Q_j	is the volume inflow or outflow rate of the jth well.	L^3/T
QI_j	is the initial inflow (+) or outflow (-) rate for the serpin well option (see Equation A-18 and Table A-1).	L^3/T
QM_j	is the maximum inflow (+) or outflow (-) rate for the serpin well option (see Equation A-18 and Table A-1).	L^3/T
QQ_j	is the mean inflow (+) or outflow (-) rate for the cyclic option of time dependence for well flow (see Equation A-19 and Table A-2).	L^3/T
QA_j	is the amplitude of the cyclic well inflow (+) or outflow (-) rate (see Equation A-19 and Table A-2).	L^3/T
Q_o	is a constant leakage rate from the cavern used as a scaling value (see Equation 9).	L^3/T
Q'	is the leakage rate from the cavern (see Equation A-20).	L^3/T
R	is the distance (radial) to the groundwater outflow area, or the remote boundary. It also is used in scaling (see Equation A-2).	L
$ROWELL_j$	is the numerical stopping radius around the jth well (see Table 1).	L
$SCALE$	is the scale used in the automatic plots (see Table 1).	L/inch
T	denotes the arrival time and also time units.	T
$TMAX$	is the stopping time along the pathlines (see Table 1).	T
TM	is a time parameter in the $U(t')$ function (see Figure 1).	T
TN	is a time parameter in the $H(t')$ function (see Figure 1).	
g	is the gravitational scalar.	L/T^2

		<u>Units</u>
j	as a subscript denotes the variable applies to the jth well.	None
ln	is the natural logarithm to the base e.	None
p	is the fluid pressure.	F/L^2
q'	is the unit fluid outflow rate across the boundary; i.e., into the river.	$L^3/T/L$
$q = \frac{R}{D_o K_o H_o} q'$	is the dimensionless fluid flow rate across the boundary.	None
r	is the dimensionless radial coordinate variable in cylindrical coordinates.	None
r'	is the radial variable in cylindrical coordinates.	L
r' _o	is the effective cavern radius.	L
r _o	is the dimensionless effective cavity radius.	None
s	is the location along the outflow boundary; i.e., along the river (see Equation 17).	L
t	is the dimensionless time variable (see Equation A-2).	None
t'	is the time variable.	
t _o	is the departure time of the first fluid particles leaving the cavern wall or from the other specified locations.	None
t' _o	is the departure time of the fluid particles from a given location.	T
w _o	is a parameter in the serpin equation (see Figure 1 or Equation A-18).	None
w _{oc}	is a parameter in the cyclic equation (see Figure 2 or Equation A-19).	None
w _m	is a parameter in the serpin equation (see Figure 1 or Equation A-18).	None

		<u>Units</u>
w_{mc}	is a parameter in the cyclic equation (see Figure 2 or Equation A-19).	None
x' and y'	are the Cartesian coordinates.	L
x and y	are the dimensionless Cartesian coordinates (see Equation A-2).	None
x_j and y_j	are the coordinates of the center of the j th well.	None
x_0 and y_0	are the dimensionless coordinates defining the cylindrical cavern wall (see Equations 5 and 6).	None
ρ	is the fluid mass density.	FT^2/L^4
θ	is the angular coordinate variable in cylindrical coordinates. (The x-coordinate axis is along $\theta = 0$).	Degrees
θ_j	is the angular coordinate of the center of the j th well (see Figure A-1).	Degrees
$\theta_0 = \text{THETA}_0$	is the angle around the cavern wall to the starting point of the first pathline generated (see Table 1).	Degrees
$\theta_M = \text{THETA}_M$	is the maximum angle around the cavern wall to the starting point of the last regularly spaced pathline generated (see Table 1).	Degrees
$\phi' = \frac{p}{\rho g} + z$		
	is the dimensional potential energy in the stratum.	LF/F
ϕ	is the dimensionless potential head (see Equations A-2 and A-17).	None
∇	is the del operator; i.e., $\frac{\partial}{\partial x} \hat{i} + \frac{\partial}{\partial y} \hat{j}$	None
∇'	is the dimensionless del operator; i.e., $\frac{\partial}{\partial x'} \hat{i} + \frac{\partial}{\partial y'} \hat{j}$	1/L
$\underline{u}$	is the dimensionless macroscopic pore velocity vector (see Equation A-27).	None
$\underline{u}'$	is the macroscopic pore velocity vector (see Equation A-25).	L/T

		<u>Units</u>
u_x	is the dimensionless velocity component in the x-coordinate direction.	None
u_y	is the dimensionless component in the y-coordinate direction.	None
ψ	is stream function (see Equation A-34).	None
ψ_0	is the steady scaling source strength (see Equation A-42).	None
ψ_s	is the cumulative outflow from the circular source (see Equation A-37).	None