The far field migration of radionuclides in groundwater through geologic media

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The Far Field Migration of Radionuclides In **Groundwater"** through Geologic Media

By

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DISSERTATION

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Ho**

To my wife Selma, for her love and support.

To my parents, for the way they brought me

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Daniel K. S. Ting

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THE FAR-FIELD MIGRATION OF RADIONUCLIDES IN GROUNDWATER THROUGH GEOLOGIC MEDIA

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Abstract

This work models the radionuclide migration by groundwater flow in geologic media after nuclide release from a high level waste repository. Predictive analytical methods are presented that can be used to assess the performance of a repository site, and which estimate the potential hazard at the biosphere to the general public. The results of the analysis are presented by analytical formulas and a set of computer codes which evaluate these solutions has been developed.

The exact analytical non-recursive solution to the one-

1. Introduction

The viable disposal of high level nuclear waste in repositories located deep in a geologic media will depend among other factors, on the speed of the far field migration of radionuclides in the groundwater through the geologic media. This work intends to model the radionuclide migration in groundwater after their release from the waste package until their discharge into the biosphere.

This modelling produces a predictive method that can be used to assess the performance of a particular combination of waste package and repository site, and estimates the potential hazard to the general public. A set of computer codes based on these methods has been developed. An important aspect throughout this study is the analytical character of the solutions used. When contrasted against numerical schemes used to solve the equivalent problem (Si), the advantages of analytical methods are clearly evidenced. These consist of minimal computing time, the absence of convergence and precision criterias needed and the fact that the dependence on physical parameters of the solution are easier to recognize.

The overall waste disposal problem can be divided into three main parts: the near-field problem, the far-field problem and the pathways to ingestion. In the near-field problem, the design of the package containing the waste form and its

dimensional nuclide transport equation with sorption equilibrium and without solubility limitations is studied. A parametric study showing the influence of the water travel time, the leach time, the time for beginning of leaching and the retardation coefficients on the maximum concentration of every nuclide present in the high level waste is presented by an approximation method. The results indicate that for most of the parameter range considered, I-129 and Ra-226 are the potentially most hazardous nuclides. The hazard due to the leaching of high level waste packages is compared to that of the leaching of an equivalent amount of natural uranium ore.

The analytical non-recursive solution for the migration of radionuclides in two-dimensional groundwater flow is studied next. With neglect of dispersion, the solution to the one-dimensional transport equation is applicable along a streamline of the two-dimensional groundwater flow described by Darcy's law. The potential function driving this flow can be represented either by analytical expressions or by field piezometric measurements. The analysis yields the contaminated region for any member of a chain of arbitrary length and evaluates its concentration in that region. One can also evaluate the discharge rate as well as the cumulative discharge at the biosphere.

The far field migration of radionuclides in groundwater in two candidate repository sites has been studied. These are the

surrounding engineered barriers as well as the definition of the repositories parameters are adressed. The modelling of how the groundwater might reach the waste package, corroding it and releasing radionuclides into surrounding aquifers is studied. The result of the near-field problem should describe how the radionuclides are released into nearby aquifers.

The far-field problem uses the result of the near-field problem as the boundary condition and studies the migration of these radionuclides in groundwater through aquifers until they discharge into the biosphere. This is the problem analyzed in this work.

After these radionuclides are released into the biosphere, which can be a river, a well or any other possible source of fresh water, the actual pathways that the nuclides follow until they are ingested must be determined and the resultant health effects evaluated. The number of health effects caused by the accidental release of radionuclides from the repository will ultimately be the measure of the adequacy of the proposed combination of the waste package and the repository site.

Different investigations are being presently carried to describe the near-field problem (Chambre, Zavoshy in P.3). Simplified models have in the past been proposed to describe the near-field problem (B4,H1) and the so called "decaying band release mode" is adopted as the boundary condition describing the

release of radionuclides from the repository. To avoid the detailed evaluation of the pathways to ingestion and to determine the health effects to the public due to the failure of a repository, the Maximum Permissible Concentration (MPC,10CFR20) was used as a potential hazard index. The radionuclide concentrations at the biosphere are compared to their MPC values.

By using these simplifications for the near-field problem and for the pathways to the ingestion, the entire effort of this work can be concentrated in the modelling of the far-field migration of radionuclides in groundwater through geologic media. The groundwater flow field is described by the Darcy's law in conjuntion with the groundwater mass conservation equation and it is considered to be in steady state. Soil porosity and water density are assumed to be constant. Sorption reactions between nuclides in the groundwater with the solid phase are assumed to be governed by a linear isotherm. In this present study, the effects of hydrodynamic dispersion are assumed to be negligible. This is a conservative assumption since dipersion tends to broad the migration bands reducing the magnitude of the concentrations. Reduction in the arrival time of the band is negligible (H3). Furthermore, any nuclide is allowed to dissolve without solubility limitations, which is also a conservative assumption.

Lester et al (L1), Burkholder et al (B4) solved analytically the radionuclide transport equation for a one-dimensional constant groundwater flow. The solution is

sites of the Waste Isolation Pilot Plant (WIPP) in New Mexico and the Basalt Waste Isolation Project (BWIP) in Hanford, Washington. If an accident occurs after 1000 years, the contamination of nearby rivers due to the discharge of 1-129 and Ra-226 leached out from the waste during a period of 10000 years does not exceed the maximum permissible concentrations.

restricted to actinide chains with three members only. Higashi (H2) solved the same problem using a corrected boundary condition and showed the resultant differences in the solution. Foglia et al (F3) use the superposition principle in the solution to the transport equation with the dispersion term included. Hadermann (H4), Foglia (Hi) propose solutions to the one-dimensional transport equation in a heterogeneous media consisting of several different layers. Chambre (Hi) derived the analytical non-recursive solution to the one dimensional transport equation without dispersion which evaluates the concentration of any member of a chain of arbitrary length. Later on, Chambre (Pi) extends the one-dimensional non recursive solution to describe the migration of radionuclides in two and three dimensional flow fields.

In chapter 2, a review of Chambre*s solution (HI) to the one-dimensional flow is presented and also a computer program (UCBNE25) that has been developed based on this solution is described (Tl). Sample calculations are shown. In chapter 3, an approximate solution to the one-dimensional transport problem is presented. This simplified form of the solution allows one to obtain analytically the extremum of the solution: the time when the maximum concentration occurs at a fixed field position as well as the field position where the maximum concentration occurs at a fixed time. The results are presented in simple tabular form for easy use and they are applicable for chains with up to three members. This analytical method to determine the extremum

avoids time consuming evaluation of complete concentration histories to determine the maximum. A computer program, UCBNE20, based on this method has been developed.

Using this program, a parametric study showing the influence of each parameter (i.e. the water travel time, the leach time, the time for beginning of leaching and the retardation coefficients) on the maximum concentration of every nuclide present in the high level waste has been done. The result indicates that for most of the parameter ranges considered, I-129 and Ra-226 are the potentially most hazardous nuclides. The hazard due to the leaching of high level waste packages is compared to that of the leaching of an equivalent amount of natural uranium ore and also to the mill tailings resulted from processing the ore. Assuming that they have comparable leach rates, we show that the potential hazard due to the leaching of natural uranium ore is always larger than that of an equivalent amount of reprocessed high level waste.

In chapter **4,** the analytical non-recursive solution for the two- dimensional transport equation (Chambre,Pi) is first reviewed. The most important result derived in the solution is that when dispersion is neglected, the solution to the one-dimensional transport equation is applicable along a streamline of the two-dimensional groundwater flow. In this study, the potential function driving the two-dimensional groundwater flow can be represented either by analytical expressions or by field

piezometric measurements.

Analytical representation of groundwater flows is carried out by superimposing an arbitrary number of point sinks and point sources. This superimposition can represent flow fields of arbitrary complexity. On the other hand, a given number of scattered potentiometrie field data can be used to represent the potential level curves by fitting the data with a minimal total curvature spline function (Briggs,Bl). This later method allows the aquifer to have inhomogeneous hydraulic conductivity although isotropic.

Based on the above described methods, a computer program UCBNE21 has been developed and is described in this chapter. This program determines the two-dimensional contaminated region, at any time after the release started, for any member of a chain of arbitrary length and evaluates its concentration in the contaminated region. In addition, if the location of the intersection of the biosphere with the contaminated region is known, UCBNE21 evaluates the discharge rate as well as the cumulative discharge at the biosphere. The program has the capability of using the graphic software to automatically generate graphs of desired output functions.

The far-field migration of radionuclides in groundwater in two candidate repository sites has been studied. These are the sites of the Waste Isolation Pilot Plant (WIPP) in Eddy County,

New Mexico and the Basalt Waste Isolation Project (BWIP) in Hanford, Washington. In both cases, it is shown that contamination of nearby rivers due to the discharge of radionuclides from the aquifers surrounding the assumed locations for the repository sites does not exceed the Maximum Permissible Concentration for any nuclide, in the event of an accident.

Finally, source listings for the programs UCBNE25, UCBNE20 and UCBNE21 as well as their data input descriptions are given in Appendix A, B and C respectively.

2. Migration of Radionuclides in One-Dimensional Groundwater Flows Through Geologic Media

2.1 Introduction

In this section, the modelling of the far field migration of radionuclides in one-dimensional groundwater flow through geologic media is studied. There are two groups of radionuclides in high level wastes that present potential hazard to the biosphere: the long lived fission products (e.g. 1-129,Tc-99,etc.) and the long actinide chains (e.g. Cm-246—*- Pu-242—«• U-238-^- U-234— Th-230-— Ra-226) .

To accurately predict the transport of an actinide, it is necessary to consider its linkage to all its precursors through the decay chain. Previous analytical solutions to the radionuclide transport equation were recursive in nature (L1). Due to the method of solution employed, the solution could be explicitly expressed for chains of up to three members only. Therefore, actual numerical evaluations were limited to three members chains only. However, in either spent fuel or in high level reprocessed waste there exist longer actinide chains and their analysis had to be treated by simplifying assumptions which allowed one to reduce these longer chains into three member chains.

In a previous report, Chambré (H1,section 4.4) presented the analytical non recursive solution to the radionuclide transport equation for one dimensional flows. This solution allows one to evaluate the concentration history of any member o a chain of arbitrary lenght without having to solve for its precursors. Evaluation of this solution requires little computing time.

The solution has been programed into the computer program UCBNE25 and a typical calculation is done and graphical results are presented. The UCBNE25 program uses the graphic display software available at the LBL computer center to automatically generate graphical outputs.

2.2 The radionuclide transport equation and side conditions

The system considered is an one-dimensional single region geologic media where the groundwater velocity is constant. Dispersion effects are assumed to be negligible. The sorption-desorption reactions between radionuclides in the liquid with the solid phase are assumed to be in equilibrium. No solubility limit of any nuclide in the groundwater is considered. Media properties characterizing soil, water and radio-chemistry are treated as isotropic and constant.

Subject to the above assumptions, the conservation equation for the i-th member of a radionuclide chain in the groundwater can be written as follows (Hi,section 2.3).

$$K_i \frac{\partial N_i}{\partial t} + v \frac{\partial N_i}{\partial z} + \lambda_i K_i N_i = \lambda_{i-1} K_{i-1} N_{i-1}, \quad i = 1,2,\ldots, \quad \lambda_0 = 0 \qquad (2.2.1)$$

Here, $N_i(z,t)$ is the concentration of the i-th species in the water, K_j are the retardation coefficients, λ_i the decay constants (1/yr), z the distance from the repository, v the constant groundwater velocity and t the time after the release starts. The initial condition, at any point $z>0$, is expressed by

$$N_i(z,0) = 0 \quad ; \quad z>0 \qquad (2.2.2)$$

The boundary condition can be represented by an arbitrary

release function

$$N_i(0,t) = N_i G_i(t) \qquad t>0 \qquad (z \bullet 2 \ll 3)$$

where

$$NT_1 = M_1.VQT \qquad (2.2.4)$$

Here NV is the initial concentration of the i-th member nuclide when the leaching starts (HI, section 3.2), M|? is the corresponding initial number of atoms at the repository, Q is the total volumetric flow rate across the waste (m^3/yr), T is the duration of the release (yr) and (t) is an arbitrary prescribed release function.

The solid waste form is assumed to be leached in such a way that the boundary condition can be represented by the so called decaying band release model (HI). In this model, every nuclide is assumed to be released during a time period T called the leach time. It can be shown that this model will produce a release function which is expressed by the following relationship (Hi, section 3.2)

$$G_i(0,t) = \sum_{j=1}^{i} B_{ij} \exp(-X_j . t)[h(t)-h(t-T)] \qquad (2.2.5)$$

where h(t) is the step function and B•^ are the Bateman coefficients

$$B_{ij} = \sum_{m=1}^{j} \left[\sum_{r=m}^{i} \frac{1}{\prod_{l=m}^{i} \{X - x.\}} \right] \qquad (2.2.6)$$

2.3 The general non-recursive analytical solution

The solution to Eq. (2.2.1) subject to the side conditions Eq.(2.2.2) and Eq.(2.2.3) has been obtained analytically (Chambre,Hl) and it can be written as

$$N_{i}(\sigma,t) \ll N^{o}_{i} " e^{\lambda_i K_i \sigma} G_{i} (t-K_{i}\sigma) +$$

$$+ \sum_{j=1}^{i-1} A^{(i)}_{j} N^{o}_{j} \; l \; -r \; D^{(j)} \; [g \; (t) \circledR G \bullet (t)] \quad - A_{m} K_{m} \sigma \tag{2.3.1}$$

Here, a is defined as the water travel time

$$a " z/v \tag{2.3.2}$$

and the coefficients are defined as follows

$$A^{(i)}_{j} = \prod_{r=j}^{i-1} A_{r} K_{r} \tag{2.3.3}$$

$$m \quad n. \; (K - K) \tag{2.3.4}$$

$$D^{(j)}_{rm} \quad \prod_{q=j} (A_{qm} - A_{rm}) \tag{2.3.5}$$

$$\lambda_{ij} - \frac{A_i K_i - A_j K_j}{K_i - K_j} \tag{2.3.6}$$

and where

$$g_{rm}(t) = e \qquad h(t-K\ o) \tag{2.3.7}$$

the convolution integral is expressed as

$$g_{rm}(\quad) \quad V^{t-c)} \tag{2.3.8}$$

One should note the non-recursive character of the above solution, which allows one to evaluate the concentration of an arbitrary member of a chain of any length directly, without having to solve for its precursors. Due to the analytical form of the solution, which does not require recursive calculation, this solution presents clear advantages when compared to numerical schemes utilized to solve the partial differential equation system, Eq.(2.2.1).

When the decaying band release boundary condition is used (Eq. (2.2.5)) to express the release function (t) in the convolution integral Eq. (2.3.8) the solution is rewritten as

$$N_1(c,t) = N \cdot \exp(-X.K_1\ c)\ [I B_1 \cdot \exp[\sim\ .\ (t-K\ .\ a)\ )\ ]\ [h\ (t-K_i\ o)\ -h\ (t-T-K\ .$$

$$+ \sum_{j=1}^{i-1} \sum_{k=1}^{j} Q_{rm}^{(j)} B_{jk} \{\exp[-\Delta_{rm}(t-K_m\ o) - \lambda_m K_m\ o]\ [h\ (t-K_m\ o) -$$

$$-\exp\ (-T\ (\ddot{A}_k - i_m)\ )\ h(t-K_m\ o)\ -\exp[-A_k t-\ (X\hat{}\ -X\hat{}\hat{}\ o]\ [h\ (t-K_m O\ -$$

$$-h\ (t-T-K\ \ o)l\ \} \tag{2.3.9}$$

$$\text{Ml} \qquad (K - K \ )^{,} \qquad \sum_{q=j}^{i-1} \frac{rr}{{}^{n}.X_{n}K} \qquad (2.3.10)$$

$$q*r*m$$

The solution when written in the form of Eq. (2.3.9) has the advantage that when two nuclides in the same chain have the same value of the retardation coefficient, Eq, (2.3.9) shows that the concentration N.(z.t) is finite. This is because $Q_{i}^{rm}=0$ when $K_r=K_m$ and the exponential terms containing $A_{r\tilde{m}}$ tend to zero when K_r tends to K . Therefore, with the above manipulations to transform Eq.(2.3.1) into Eq. (2.3.10), the singularity which existed for $K_r = K_m$ is removed.

2.4 Sample calculations with the program UCBNE25

The general non-recursive analytical solution to the nuclide transport equation subject to the decaying band release boundary condition, Eq.(2.3.9) has been programed into the computer with the 1abe1 UCBNE25. A complete listing of the program as well as the description of the input requirements are given in Appendix A.

Here, a sample run of the program is presented. Two important long actinide chains are considered. The chains and their members parameters are shown in Table 2.1. The results in the printouts or in the graphs are given in terms of the concentrations and/or water dilution rates $w\hat{}(z,t)$, (m^3/yr), which is defined by the following expressions

$$w_i(z,t) = Q_{x_i} N_i(z,t) / (MPC)_i \qquad t > 0 \qquad (2.4.1)$$

where MPC stands for Maximum Permissible Concentration (Ci/m) and it is given in 10CFR20. Physically, the water dilution rate represents the. volumetric flow rate needed to dilute the activity discharge rate to drinking water standards (PI). Therefore it is an index of the potential harm to the public health and one can directly compare water dilution rates for different nuclides.Furthermore, if the water dilution rates of all nuclides are added one would obtain the total water dilution rate for all nuclides.

For the sample calculation, the leach time was assumed to be 10^4 years and the time delay for the beginning of leaching is 10^3 years. The time for beginning of leaching represents the durability of the canister and the engineered barriers surrounding the waste form. Figure 2.1 and Figure 2.2 show the concentration history for the chain which ends in Ra-226 (4n+2 chain, the second even actinide chain, see Table 3.11) for several different water travel times z/V (years). Because of the large retardation coefficients and relatively short half-lives, Cm-246 and Pu-242 cannot migrate as far as and U-238 can, decaying much earlier. Since U-238 migrates farther they carry their daughters Th-230 and Ra-226. This long migration capability allied to its high toxicity makes Ra-226 one of the most hazardous nuclides. Furthermore, one can notice that because Cm-246 and Pu-242 half lives are so much smaller than U-238 half life, their decay does not affect the U-238 concentration significantly. For practical purposes, for the assumed set of parameters, the 4n+2 chain can be subdivided into two chains. This simplification is extensively used in Chapter 3. The behaviour of the migration bands of the actinide chains are discussed in detail in Chapter 3.

Figure 2.3, Figure 2.4 and Figure 2.5 show how the concentration of the "Np-237" chain (4n+1 chain, the first odd actinide chain, see Table 3.11) changes with time for several different water travel times z/V. For the same reasons stated as for the previous chain, Cm-245 and Am-241 cannot migrate very

far. Np-237 which has a low retardation coefficient can carry its short lived daughter relatively far.

Since dispersion effects are neglected in this work, the migration bands have well defined time intervals where the concentration is non trivial. This fact can be seen in any of above figures. These time intervals are the contamination times for that particular nuclide at that particular position characterized by z/V. Although the figures showing the results of the sample calculation expressed the concentrations in terms of the water dilution rates, the program UCBNE25 has the option of ploting the concentration curves of the individual nuclides of the chain instead. (See description of the program UCBNE25 in Appendix A).

Table 2.1 Nuclide Parameters for the Sample Calculation

Chain	Cm-246	Pu-242	U-238	U-234	Th-230	Ra-226
T* (yr)	5.5E+3	3.8E+5	4.5E+9	2.5E+5	8.0E+4	1.6E+3
K.** x	3.0E+3	1.0E+4	1.4E+4	1.4E+4	5.0E+4	5.0E+2
MPC ***	4.0E-6	5.0E-6	4.0E-5	3.0E-5	2.OE-6	3.0E-8
**** i	1.9E+0	2.0E-1	4.3E-2	0.0	0.0	0.0

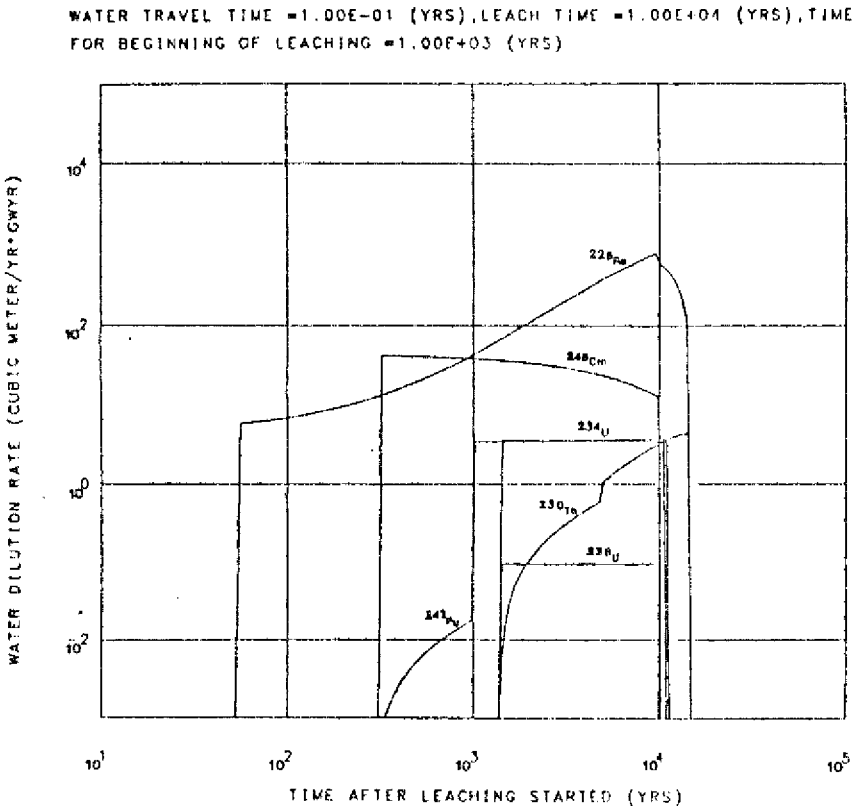
Chain	Cm-245	Am-241	Np-237	U-233	Th-229
T* (yr)	9.3E+3	4.6E+2	2.1E+6	1.6E+5	7.3E+3
V ** 1	3.0E+3	1.0E+4	1.0E+2	1.4E+4	5.0E+4
MPC ***	4.0E-6	4.OE-6	3.OE-6	3.0E-5	5.0E-7
JVJ^ **** i	9.8E+0	4 .5E+3	1.6E+0	0.0	0.0

* T is the leach time, representing the duration of release

** From (LI)

*** From 10 CFR20,(Ci/m^3)

**** From (B2),(Ci/Gwe.yr)



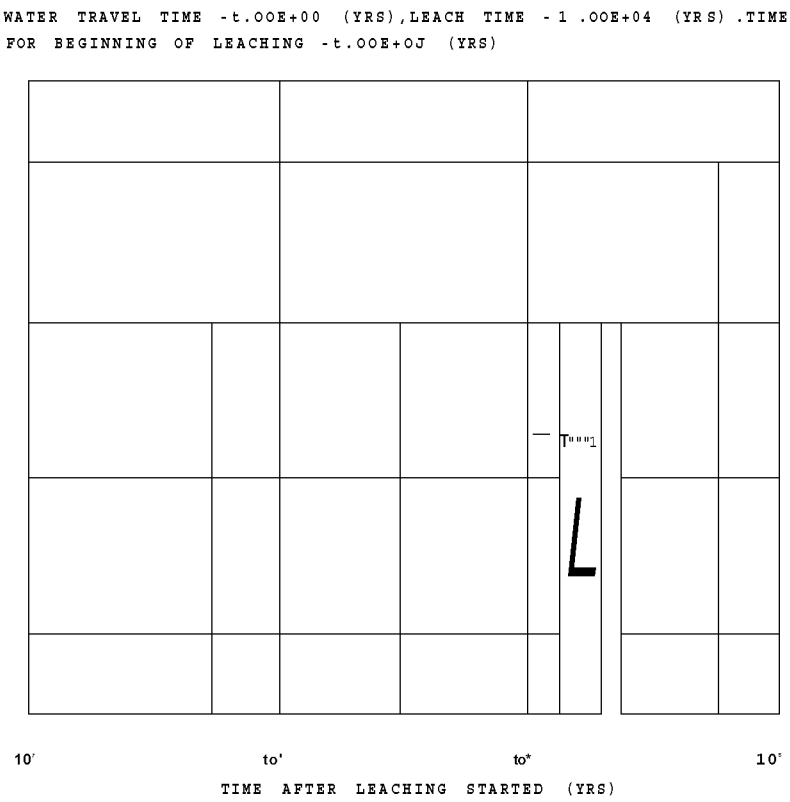
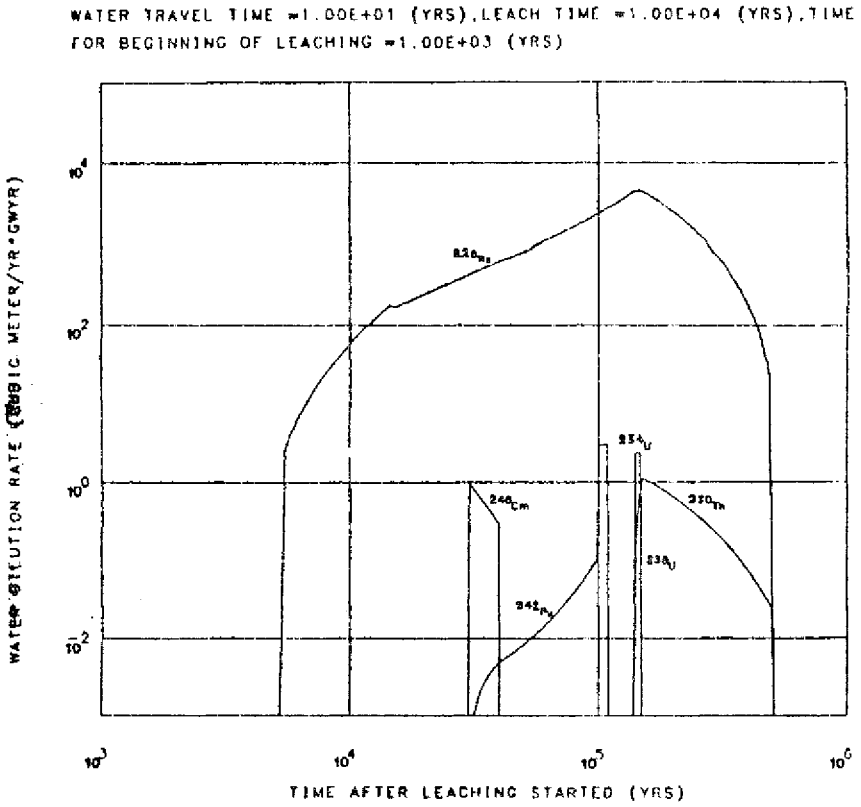


Figure 2.1 Concentration history at water travel times of z/v=0.1 and z/v=1.0 years for the 4n+2 actinide chain.



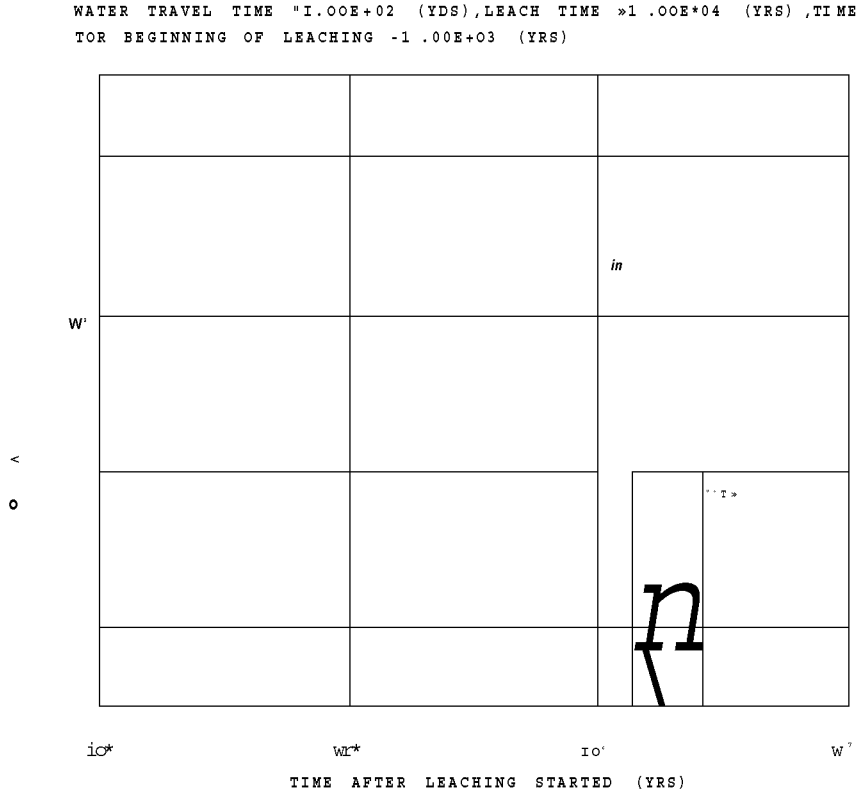
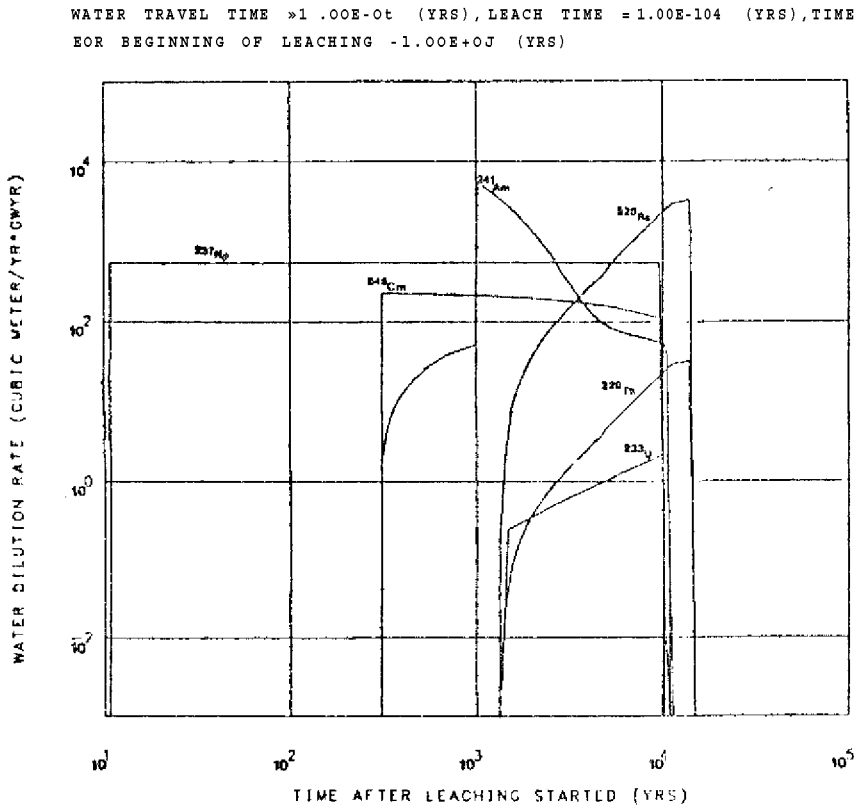


Figure 2.2 Concentration history at water travel times of z/v=10 and z/v=100 years for the 4n+2 actinide chain.



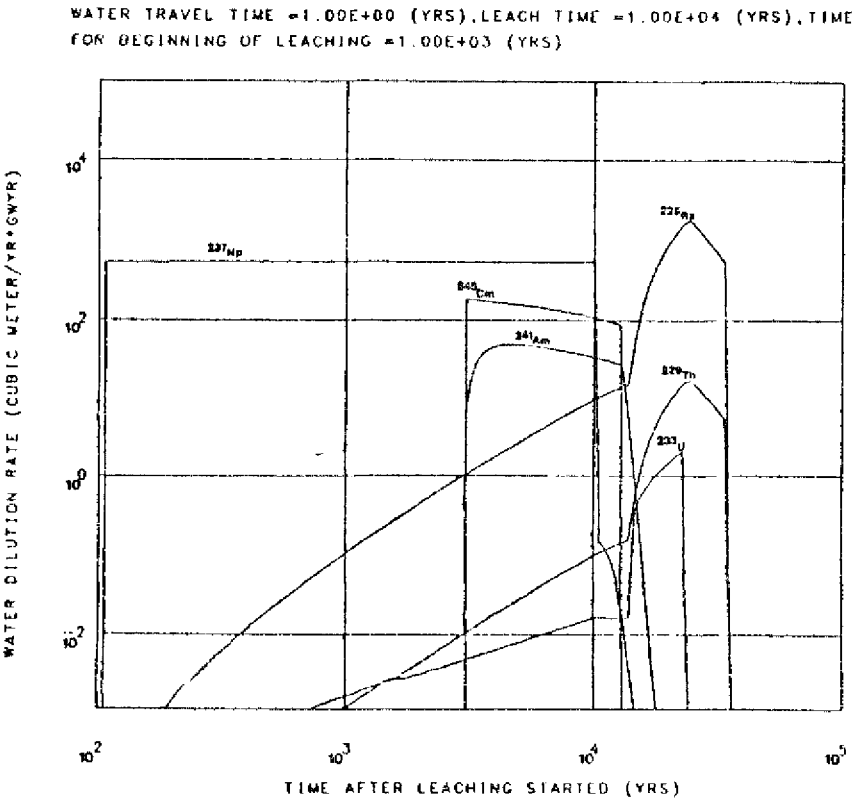
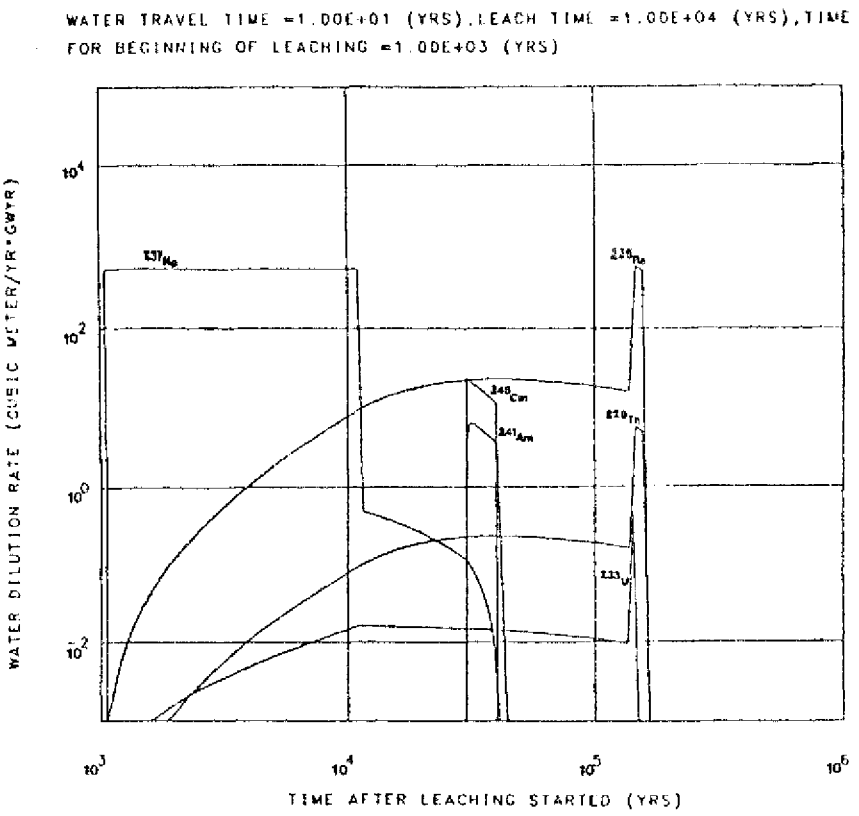


Figure 2.3 Concentration history at water travel times of z/v=0.1 year and z/v=1.0 year for the 4n+1 actinide chain.



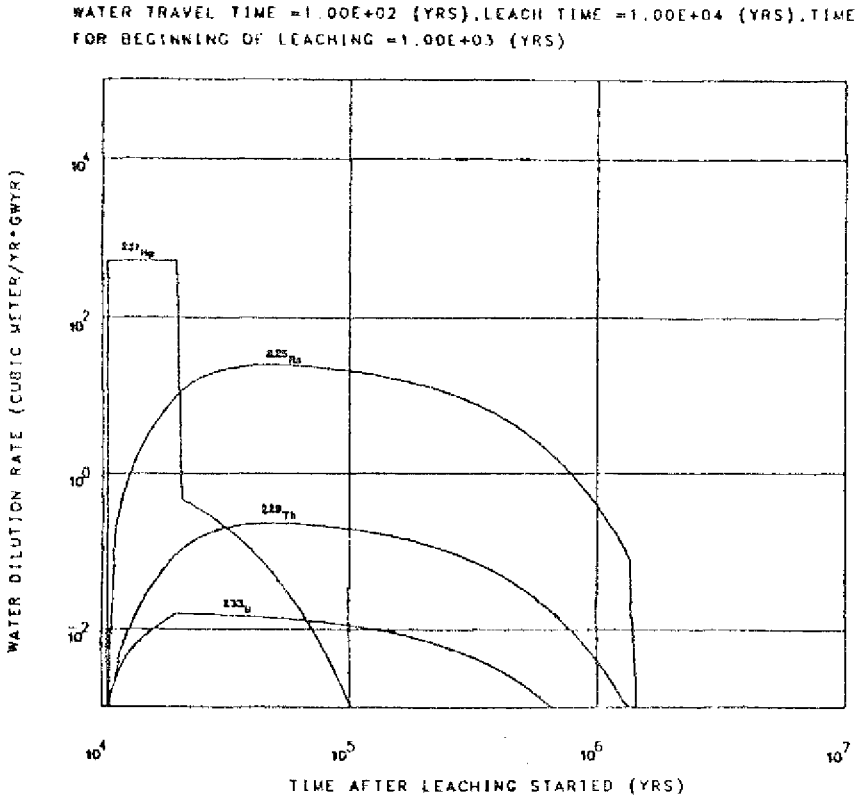
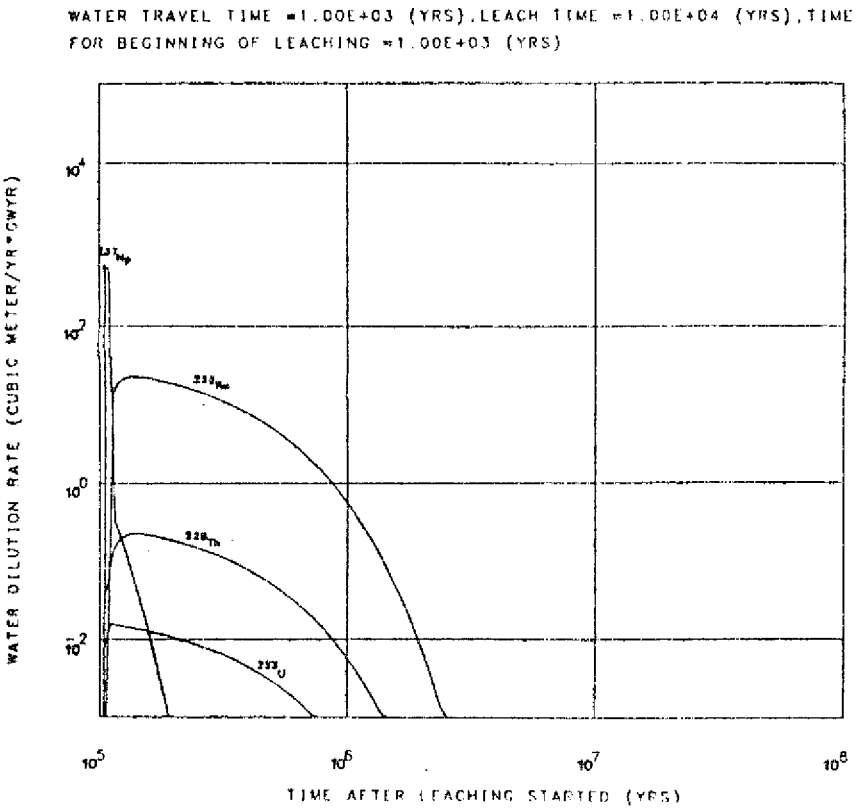


Figure 2.4 Concentration history at water travel times of z/v=10 years and z/v=100 years for the 4n+1 actinide chain.



WATER TRAVEL TIUE -1 .00T»04 (YRS).LEACH TIME -1.00C404 (YRS) .TIME rOR BEGINNING OF LEACHING -1.00E403 (YRS)

TIME AFTER LEACH ING STARTED (YRS)

ure 2.5 Concentration history at water travel times of z/v=1000 years and z/v=10000 years for the 4n+1 actinide chain.

3. Maxima of Release Bands

3.1 Introduction

This research is concerned with the determination of the maxima values of nuclide concentrations which occur during the migration of nuclide chains in geologic media. One is interested in the determination of the position of the maximum concentration of a given nuclide at a fixed time as well as the time at which the maximum is observed at a fixed position in the field. The analysis should be applicable to actinide chains present in high level reprocessed waste and in unreprocessed spent fuels.

Normally, the most direct method for the determination of the maxima concentrations would be to solve the appropriate system of transport equations and then search for the extrema of the solutions. Instead of doing this we present an approximation method which allows us to determine the extrema in concentrations without having to calculate the entire concentration history. The method concentrates entirely on the determination of the extrema: their positions in space at a fixed time and their occurrence at a fixed position.

In this study we are neglecting dipersion effects. The results obtained by using this assumption are more conservative

than those which take dispersion into account. One-dimensional water transport and equilibrium sorption for the nuclides in the water and on the soil is assumed. The soil and water properties as well as the water velocity are considered constants.

The basic idea in the approximation method is that when the leach time is small compared with a radionuclide half-life, the exact solution to a band release boundary condition can be approximated by solutions which have forms similar to those when an impulse release boudary condition is used. The extrema are then easily and directly determined from these approximate solutions and the results have a simple and compact form. The approximation method has been extensively tested for all nuclides which are present in high level unreprocessed wastes by comparing it with available results obtained from the exact solution. The range of values for the leach time for which the approximation is accurate has been determined.

Use of this method avoids time consuming evaluation of the complicated exact solution formulas and it provides a quick insight into the effects of the physical parameters on the extrema. As an additional result, the time interval during which a given position is contaminated (contamination time) and the spatial region that is contaminated at a given time (extend of the contamination region) can be also readily obtained. The method will evaluate with good accuracy the extremum of the exact solutions to a decaying band release (without dispersion) and it

is shown to work provided the leach time is smaller than the half-lives of the nuclides envolved. Most of the waste forms considered have predicted lifetimes which satisfy such a condition.

The effects on the maxima concentration (expressed in terms of peak water dilution rates) due to the variation of a number of parameters values were studied. The parameters were: the water travel time, the leach time, the time for beginning of leaching and the sorption coefficients. Results are presented in tables and graphs.

Finally, to obtain a qualitative comparison of the potential harm to the biosphere caused by the groundwater leaching of the solid waste we evaluated water dilution rates of the leaching of an equivalent amount of natural uranium ore mill tailings generated in producing the fuel needed to generate 1 Gw(e)yr of electricity in a PWR which produced such a solid waste. In addition the water dilution rates of the leaching of an equivalent amount of the ore was also studied.

3.2 The governing equations and the approximate solution

The system considered is a one-dimensional single region where the flowing groundwater velocity and the soil and water properties are constant. The sorption-desorption process is in equilibrium and dispersion effects are negligible. The governing equation for the concentration $N_i(z,t)$ of the i-th member of a radioactive chain is written as (Hi, Eq.4.102)

$$\frac{\partial N_i}{\partial t} + v\frac{\partial N_i}{\partial z} = \lambda_{i-1}N_{i-1} - \lambda_i N_i \qquad i = 1,2,3 \qquad (3.2.1)$$

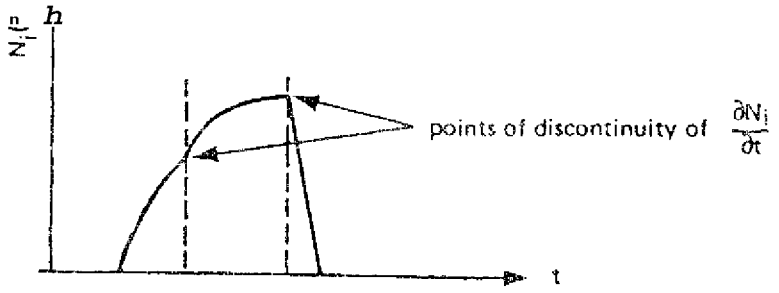
The initial and boundary conditions are expressed as (Hi, Section 3)

$$N_i(z,0) = 0, \text{ for all } z>0 \qquad (3.2.2)$$

$$N_i(0,t) = N_{i-1}^0(t)\,[h(t) - h(t-T)] \qquad (3.2.3)$$

When a decaying band release occurs at the repository, the general release function $N_i^0(t)$ is the Bateman's function, h(t) is the unit step function and T is the leach time (yr), (see Section 2.2). The general solution to the governing equation Eq. (3.2.1) subject to the initial condition Eq. (3.2.2) and the boundary condition Eq.(3.2.3) was developed in the previous report (Chambre, H1), and it is rewritten in Section 2.3, Eq. (2.3.1) through Eq.(2.3.8).

The task of finding the extremum of the general solution Eq. (2.3.1) for an arbitrary i-th member is too complex to be performed analytically. This is caused by the presence of step functions which can result in a discontinuous first order derivative inside the domain where the concentration is non zero. The maximum could eventually be located at that point where the discontinuity occurs but the analytical methods provided by differential calculus would fail to detect it. Such a situation is depicted in the following sketch

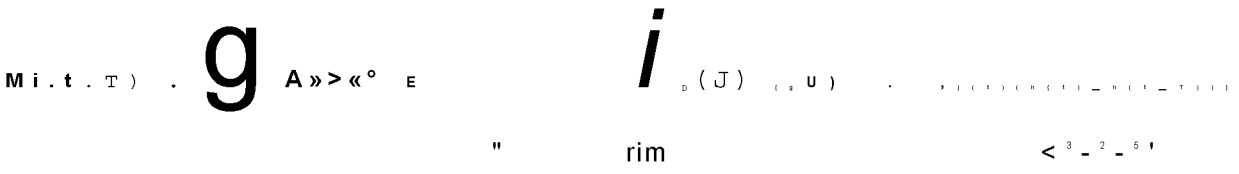


The general solution Eq. (2.3.1) can be seen to be a function of the leach time T as well as z and t, i.e.: N^(z,t,T). Furthermore, one can notice that the solution Eq. (2.3.1) can be rewritten in the following form

$$N_i(z,t,T) = N^{\circ} e^{-\lambda_i t} \left[\theta_1(t-T)\, h(t) - h(t-T) \right] \cdot G_i(z,t,T) \qquad (3.2-4)$$

where the function $G_i(z,t,T)$ is readily identified from Eq.(2.3.1). Since most difficulties in evaluating analytically the extremum resulted from the terms represented by G^(z,t,T), we

will approximate these functions by simpler forms in order to enable us to obtain the solution extremum in compact and closed form. Let us rewrite the function G.(z,t,T)



For small values of the leach time T, T<< 1/A_. , j=l, 2....i, an approximation to the function (z,t,T) is obtained by using an approximation to the law of the mean for continuous functions

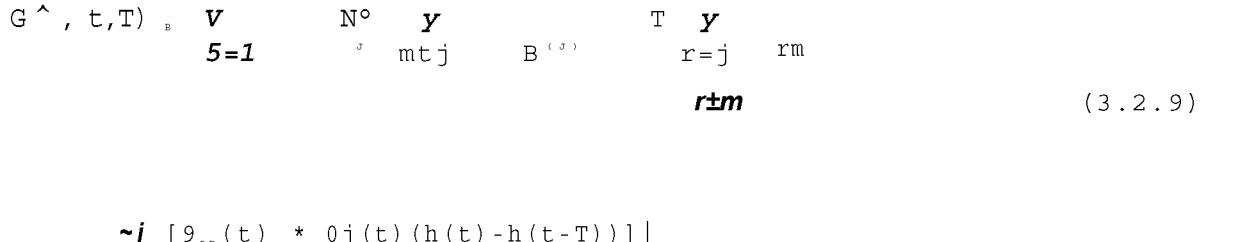
$$G.(z,t,T)=G.(z,t,T=c)+T^{3}-\{G.(z,t,T=c)\},0<c<T \qquad (3.2.6)$$

By setting T=0 in Eq.(3.2.5) one can readily see that G^ (z,t,T=0) =0 and Eq. (3.2.6) is approximated by setting c=0

$$G.(z,t,T) \approx T\,[jL\,G.(z,t.T\ll 0)] \qquad (3.2.7)$$

Eq. (3.2.7) is next used to simplify Eq. (3.2.5). First note that

where $\delta(t)$ is the Dirac's delta function. By using Eq. (3.2.7) in Eq. (3.2.5) one has the following result



The brackleted term is expanded below

$$\frac{\partial}{\partial T}\int g_{rm}(T)\,\delta_j(t-\tau)[h(t-\tau)-h(t-T-T)]\,dT \qquad (3.2.10)$$

by using Eq. (3.2.8) there results

$$\int g_{rm}(\tau)\,\phi_j(t-T)\,\delta(t-T)\,d\tau = \qquad (3.2.10a)$$

by using the integration property of the delta functions, it yields

$$= g_{rm}(t)\,\phi_j(0) = g_{rm}(t)\ , \text{ since } \phi(0) = 1 \qquad (3.2.11)$$

with the help of Eq.(3.2.11) one can rewrite Eq.(3.2.9)

$$G_i(z,t,T) = T\,A\cdot N^{\circ}\ \ldots\ \sum\ \frac{-(x_m/v_m)^2}{m}\ \ldots\ T\,g_{rm}(t) \qquad (3.2.12)$$

The above expression for the function $G_i(z,t,T)$ has the same form as if we had solved Eq.(3.2.1) using the impulse release boundary condition instead of a decaying band release boundary condition. The solution to Eq. (3.2.1),Eq. (3.2.2) and an impulse release boundary condition which can be mathematically represented by (t)=T $\delta(t)$, has been obtained in the previous report Hi, Eq.(5.10), (5.20), (5.21) and (5.22), where they are explicitly written for i=1,2,3. Those equations can be used here to explicitly express the approximate form of the function $G_i(z,t,T)$ for i=1,2,3. Therefore, the concentration of a i-th

member nuclide, Eq.(2.3.1) can be rewritten in its approximate form with the help of Eq. (3.2.12) as

$$N_i(z,t,T) = N^\circ e^{-\lambda_i z} \{L(t - t_i) [h(t - t_{i-1}) - h(t - t_i - T)] + \sum_{m=1}^{i-1} A_m^{(i)} N_m^\circ \sum_{k=1}^{m} V_{mk} \frac{e^{-\lambda_m z} - e^{-\lambda_k z}}{\lambda_k - \lambda_m} D_{mk} T_q (t) \quad (3.2.13)$$

The above general approximate solution for the concentration of an i-th member is specifically rewritten for the first three members of a radionuclide chain. With the help of Eq. (5.20) from reference Hi the solution for the first member is

$$N_1(z,t) = N^\circ \exp(-\lambda_1 t)\, s[v_1 t;\ v_1 (t-T)] \quad (3.2.14)$$

by using Eq. (5.21) from reference Hi, the concentration of the second member is

$$N_2(z,t) = N^\circ \exp\{-\lambda_1 z\}\, S[v_1 t, v_2 (t-T)]\, \hat{}(t) +$$

$$(N^\circ T)\, B_{12} \exp(-\lambda_2 t - \alpha_{21} z)\, S(v_1 t; v_2 t) \quad (3.2.15)$$

Finally, with the help of Eq. (5.22) from HI, one writtes the solution for the third member

$$N_3(z,t) = N°0_3(t)\exp(-\hat{}\ z)S[v_3t;v_3(t-T)] +$$

$$(N°T)\ B_{23}\exp(-\&_{23}t-a_{23}z)\ S(v_2t;v_3t) + \qquad (3.2.16)$$

$$(NJT)\ A\ \exp(-A_{31}t-a_{31}z)\ S(v_1t;v_3t) + \exp\ (-A_{32}t-a_{32}z)S(v_3t;v_2t) +$$

$$+\ \exp\ (-A_{21}t-a_{21}z)\ S\hat{}\ t\hat{}\ t\ )$$

The constants in above equations are defined below

$$\frac{x_i v_i}{v_i - v_j} \qquad (3.2.17)$$

$$\frac{x_i \quad x_j}{v_i \qquad v_j} \qquad x_i v_j - x_j v_i \qquad (3.2.18)$$

$$a_{ij} = a_{ji} = \frac{x_i - x_j}{v_i -} \qquad (3.2.19)$$

$$A = x_1x_2v_3/[v_1(A_2-X_3)' v_2(x_3-x_1) + v_3(x_1x_2)] \qquad (3.2.20)$$

The function S(a(t);b(t)) which is actually a short hand notation for a difference of step functions is defined as follows

$$S[a(t);\ b(t)] = h[a(t) - z] - h[b(t)-z] \qquad (3.2.21)$$

We have therefore obtained an approximate solution which represents the decaying band release problem for small leach times but which has a simpler form than the exact solution. In the next Sections analytical formulas for the **extremum** of this solution are derived.

3.3 Extremum of the solution for the first member

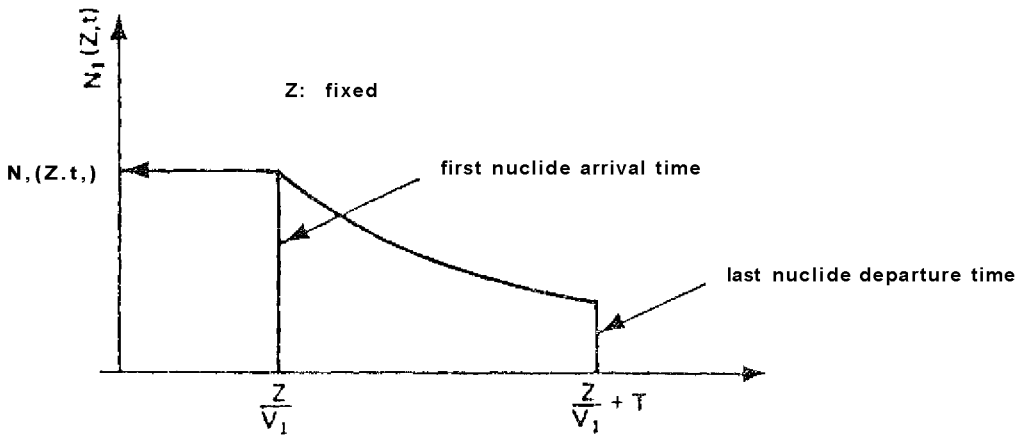
Let us denote the time of the maximum concentration of a given i-th member at a fixed position by t^ and the corresponding concentration by N^(z,t^). Conversely, the position of maximum concentration at a given fixed time t will be denoted by z.. The corresponding concentration will be (z^t) . The solution for the first member is the simplest and reads

$$N_1(z,t)=N^{\circ}\exp(-X\ t)\ \{h(v_1 t-z)-h(v_x(t-T)-z)\} \qquad (3.3.1)$$

One should note that for the first member the approximate solution is equal to the exact solution. The problem can be divided into two parts: the determination of the time of maximum concentration at a given fixed position and the determination of the position of the maximum concentration at a given fixed time.

3.3.1 Determination of the maximum concentration at a given fixed position.

At a fixed position, the solution Eq. (3.3.1) can be visualized by the following sketch



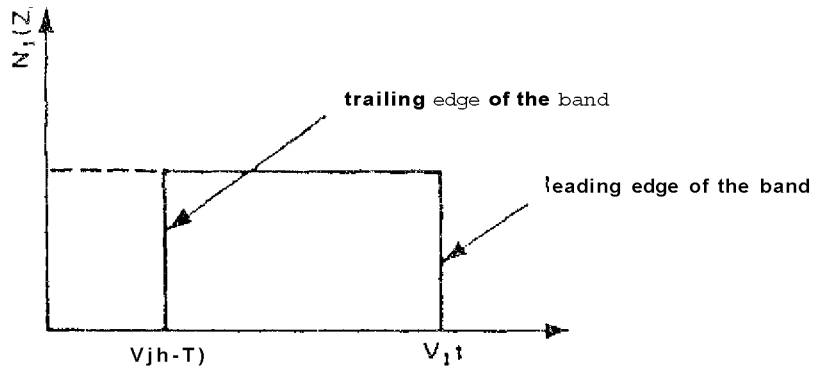
It is apparent that the maximum at a fixed position z occurs at the arrival time of the first nuclide: t^=z/v^ and the corresponding concentration is

$$N_1(z, t_i) = N_1 \exp(-X^/v^)z \qquad (3.3.2)$$

3.3.2 Determination of the position of the maximum concentration at a given fixed time

At a fixed time the concentration is constant with respect to position and the position of maximum could be any value of z

between v^t and v^(t-T). The following sketch illustrates thi case



The maximum concentration is given by the following

$$N_i(z_{1f}t) = N\hat{}\exp(-A_i t) \qquad (3.3.3)$$

but the position of extremum is not unique. It is located at

$$v_i(t-T) < z_i < v_i t \qquad (3.3.4)$$

3.4 Extremum of the solution for the second member

The determination of t2 and can be divided into stages:

1-The second member is not present at the repository initially ($N_2^0=0$).

2-The initial amount of the second member at the repository is significant ($N_2^0 \neq 0$).

3.4.1 The second member is not present initially at the repository

By setting $N_2^0=0$ in Eq.(3.2.15) one has, since $A_{21} = A_{12}$ ($a_{21} = a_{12}$) (this property of interchangeability of the A_{ij} and a_{ij} coefficients subscripts shown in Eq.(3.2.18) and Eq.(3.2.19) will be extensively used throughout this work)

$$N_2(z,t) \quad N_1 T \hat{} - S(v_1 t; v_2 t) \exp(-A \hat{} t \sim a_2, z) \qquad (3.4.1)$$

Note that the coefficient of the exponential term i.e. the brackleted term is always positive. This is because when

$$'l > V^{S('l/'2)} = h('i'-z) - h(v_2 t-z) - 1 \qquad (3.4.2)$$

$$'l < '2 \; {}^{S}C v_1; v_2) = h(Vjt-z) - h(v_2 t-z) = -1$$

The exponential term is a monotonically decreasing or

increasing function of either z or t, depending on the sign of either A_{12} or A_{21} respectively. The determination of the time t_2 of the maximum concentration at a given fixed position z is first studied. At a fixed position z, the concentration of the second member is an exponential function of time. It will be a monotonically increasing or decreasing function of tine depending if A_{Y2} is negative or positive, respectively.

When is positive the concentration $N_2(z,t)$ will decrease monotonically as t increases. Therefore, the maximum will always occur on the "arrival time of the first nuclide" at a fixed position z. When $v < $ the first nuclide arrives at z in a time $t_2 = z/v_2$ and when $v > v_2$ the first nuclide arrives at $t_2 = z/v_1$. Figure 3.1.a and Figure 3.1.b represent schematically such situations.

Conversely, when A_{12} is negative the concentration $N_2(z,t)$ will increase monotonically as t increases. Therefore, the maximum in this case will occur on the "departure time of the last nuclide" from the position z. When $v > v_2$ the last nuclide departs from z at a time $t_2 = z/v_2$ and when $v < v_2$ the last nuclide departs at a time $t_2 = z/v$. Figure 3.1.c and Figure 3.1.d represent schematically these cases. The above four possibilities are summarized in Table 3.1. In this case the maximum at a fixed position z always occurs at a time determined by the velocity of the nuclide which has the smaller product A.K. according to Table 3.1. One can therefore reduce Table 3.1

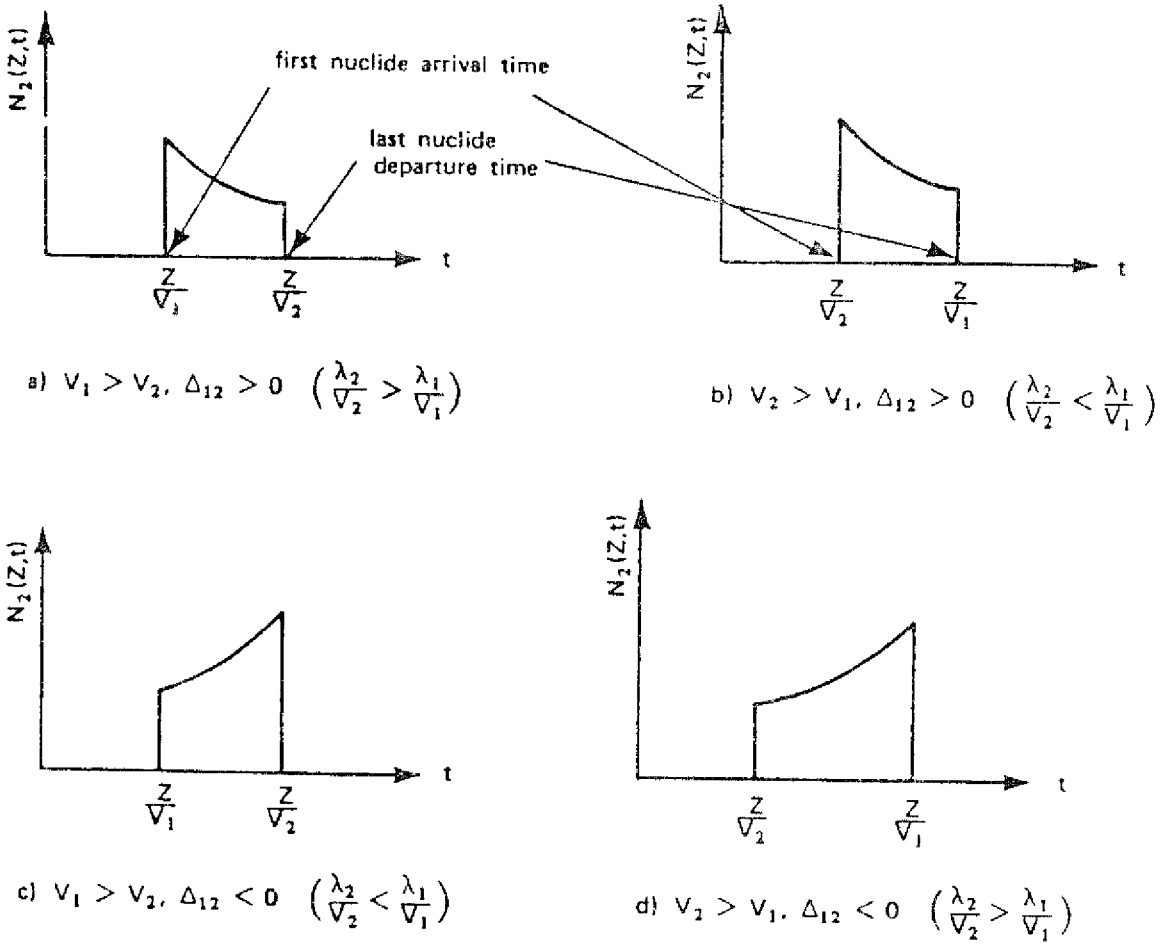


Figure 3.1- Different possibilities for the maximum of a 2nd member at a fixed position when N° = 0.

into the following more compact form shown in Table 3.2. The corresponding concentrations can then be evaluated using t^ from Table 3.2 in Eq.(3.4.1)

Case:		
	$t_2 = \hat{}\ (x_2K_2 > XjKj)$	
$K_2 < Kj$		

Table 3.1-Different possibilities of the time to attain maximum concentration for second member at a fixed position

0

x jKj y x	
	$t, = -K,$ $2 \quad v \quad 1$

Table 3.2- Time of maximum concentration for the second member when $N_2 = 0$ .at a fixed position.

Next, the determination of the position of the maximum concentration at a given fixed time is studied. One sees from Eq. (3.4.1) with a fixed time t, that when a^ is positive the concentration $N_2(z,t)$ will decrease monotonically as z increases. Therefore, the maximum wi11 always occur at the "trailing edge" of the migration band. When $v\hat{}> v_2$ the trailing edge is determined by $z_2 = v_2 t$ and when $v_2 > v\hat{}$, the trailing edge is at $z_2 = v\hat{}t$. These situations are represented schematically by Figure 3.2.a and Figure 3.2.b.

Conversely, when $a\hat{}_2$ is negative the concentration $N_2(z,t)$ will increase monotonically as z increases. Thus, the maximum will always occur on the leading edge of the band. In this case, when $v_1 > v_2$ the leading edcre is $z_2 = v_1 t$ and when $v_1 < v_2$, it is $z_2 = v_2 t$. Thus, the maximum will always occur on the leading edge of the migration band. Figure 3.2.c and Figure 3.2.d represent schematically these cases. The four possibilities for the location of the maxima, z_2 at a fixed time t are summarized in Table 3.3 below.

	$a_{tr} = \frac{x_1 - x_2}{v_1 - v_2} > 0$	$\gg 12 \bullet 7j - v_2 < 0$
$v_1 > v_2$	$2\hat{} = V\hat{}t \ (x_j > x_r)$	$1_r = Vjt \ (x_r > x_j)$
$v_1 < v_2$	$2_2 = Vjt(x_2 > x_j)$	$2_2 = V_2 t \ (x_j > x_2)$

Table 3.3 Different possibilities of the position to attain a maximum concentration for a second member ($N\hat{}=0$).

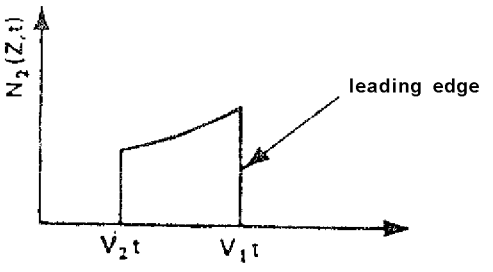
Vit

a) Vj > Vj, a,, > 0 (X, > X,

z

V,t

b) V, > V,. or,, > 0 (A, > A,]



2

c) V, > V,. a , < 0 (A, > A,

V,t V,t

d) V, > V,, a,, < 0 (X, < X,

Figure 3.2 Different possibilities for the maximum of a 2nd member at a fixed time when N° = 0.

In this case one notices that the maxima always occurs at the location determined by the velocity of the nuclide with the smaller decay constant, regardless of which nuclide travels faster. Therefore, one can conclude that at a fixed time, the position of the maximum is determined by the decay constant of the nuclides. Hence, one can further simplify Table 3.3 into Table 3.4. The corresponding concentration can then be evaluated using Eq. (3.4.1)

$x_2 > x_x$	$x_2 < X_j$
$z_2 = Vjt$	$^2 2 = v$

Table 3.4 Position of the maximum concentration for the second member at a fixed time when $N_2^0 = 0$.

The determination of the extremum for the second member is now illustrated with a numerical example. Consider for instance the following chain

Cm-246 — Pu-242 —^—~

4.8E+3 yr 2.9E+5 yr

For the purpose of illustration let us adopt the following values: 1^=3000 and K_2=10G000. The time of maximum concentration at a fixed z can be readily read from Table 3.2 by using the condition $\lambda_1 > A_2 K_2$, and it is $t_2 = z/v_2$. The corresponding concentration is

$$N_2(z,t) = (N_1 T) B_{12} \exp(-\lambda_2 v_2 z) \qquad (3.4.2a)$$

Similarly, the position of maximum concentration at a fixed time t can be obtained from Table 3.4 by using the condition $X > A$, and it is $Z_2 = v_2 t$. Hence, the maximum concentration at a fixed time t is

$$N_2(z_2,t) = (N^{\wedge} T) B \exp(-X_2 t) \qquad (3.4.2b)$$

Consider a position z=1000 meters away from the repository, a time t=1000 years after the leaching started, a water velocity of v=10 m/yr and a leach time T=103 years. Then, at the position z=1000 meters the maximum concentration occurs at a time t =10^ years and it has a magnitude of $N_2(z,t)/N^{\wedge}=0.01$. Conversely, after t=1000 years, the maximum concentration occurs at a position [illegible] meter from the repository with a concentration [illegible].

Besides the determination of the extremum of the solution, another features of the approximate solution can be deduced, namely: the contamination region at a fixed time and the contamination time interval at a fixed position. Let us denote by the region which is contaminated by the i-th nuclide at a given time. For the second member, from Eq. (3.4.1) one notices that the solution is non trivial in the region defined by

$$= v_f t - v_s t \qquad (3.4.6)$$
$$2$$

Here v.pt is the front edge of the band and v is the fastest nuclide velocity, v^t is the trailing edge of the band and v is the slowest nuclide velocity.
s

On the other hand, the contamination time interval which is the time interval in which there are i-th member nuclides present at a given position z, it is denoted by 6.. For the second member, from Eq.(3.4.1) one concludes that

$$9 = z/v - z/v \qquad (3.4.7)$$
1 s r

where z/v_r is the first nuclide arrival time at a given position z and z/v_s is the last nuclide departure time. The effect of a large difference in nuclides velocities is a large contamination time interval and contaminated region (see Eq.(3.4.6) and Eq.(3.4.7)), but the corresponding maxima concentrations are reduced since they are inversely proportional (see Eq.(3.4.1)).

With the data from the previous example, the contaminated region at a given time t would be

$$R_2 = (v^ - v^)t \sim 2.33 \times 10^{-4} vt \quad \text{(meters)}$$

while the contamination time at a given position z would be

$$62 = z/v_r - z/v^ = 7.00 \times 10^{3} (z/v) \quad \text{(years)}$$

where v is the groundwater speed

Suppose we are interested again in a time t=1000 years, z=1000 meters and v=10 m/yr, the contamination time interval 02=7.OE+5 years while the contaminated region is $R\hat{}=2.3$ meters. Therefore, at a position 1000 meters away from the repository, Pu-242 will be present during 7»OE+5 years and after 1000 years of the beginning of leaching, the Pu-242 migration band has only spread to a extension of 2.3 meters.

3.4.2 The second member has non zero initial concentration at the repository

In this case, N *0 and Eq. (3.2.15) contains both terms

$$N_2(z,t) = N_2^0 \exp\left(-\frac{\lambda_2 z}{v_2}\right) S[v_2 t; v_2(t-T)]\ \phi_2(t) + N_1^0 \frac{T\lambda_1 v_2}{v_1 - v_2} \exp(-\Delta_{21} t - \alpha_{21} z)\ S(v_1 t, v_2 t) \qquad (3.4.8)$$

The added term represents those second members nuclides initially emitted at the repository and it has the same form as the first member solution Eq.(3.2.14). The second term represents the decay of the first member nuclides which were emitted at the repository generating daughter nuclides. Evaluation of the extremum of each of these individual terms has been done in past sections.

Eq.(3.4.8) can be seen as a superposition of two functions represented by each one of the terms described above. Let us consider a fixed position z, the first term is non trivial in the time interval $z/v_2, z/v_2+T$ and $\$_2(t)$ is an exponential function of A_2, A_1. But since we have assumed $T << 1/A_j$, $j=1,2$, the exponential decay during this time interval T is negligible and we can assume this term as being a band of constant magnitude. Hence, one can set $\$_2(t)=1$ in Eq. (3.4.8).

The different configurations that Eq. (3.4.8) can take, depending on the relative magnitude of the nuclide velocities, are illustrated in Figure 3.3. When no daughters are present initially at the repository ($N_2=0$), the extremum is always located at one of the boundaries of either the contaminated time interval in the case of a fixed position or the contaminated region in the case of a fixed time. However, when $N \neq 0$, one can see in Figure 3.3 that one might have a interior maximum, i.e. when the time of maximum t_2 occurs inside the contamination time interval. In this case, the extremum cannot be determined based solely on the monotonic character of the functions envolved.

The dotted lines in Figure 3.3 represent the case when the first term contribution is smaller than the second term contribution. For the cases "b" and "c" the time of maxima is clearly $to=z/v_2$. However, in the cases "a" and "d", one must evaluate $N(z,t=z/v\hat{})$ and $N_2(z,t=z/v_2)$ using Eq. (3.4.8) to decide whether the extremum occurs at z/v-, or $z/v_{\text{„}}$. Taking the ratio of

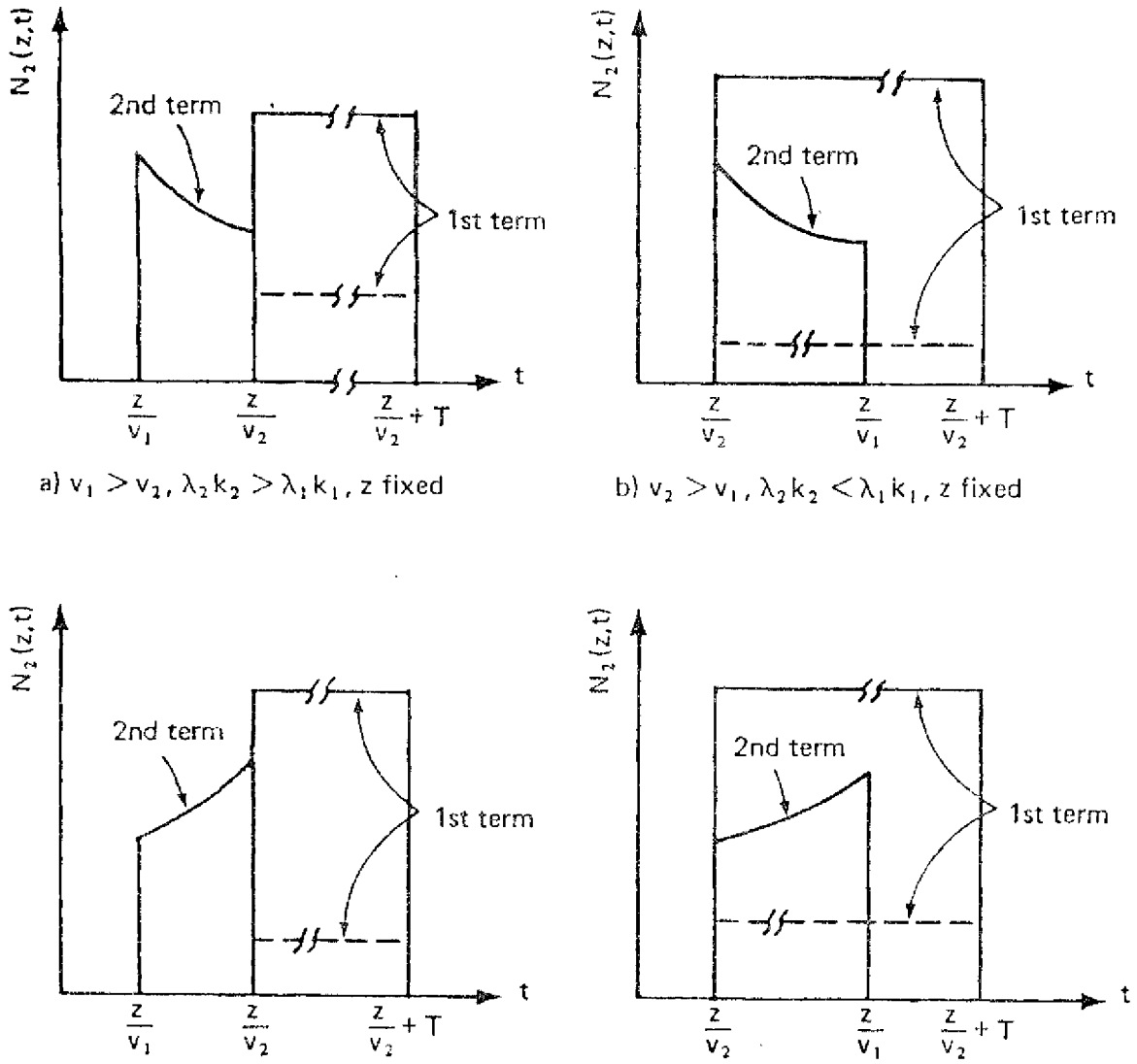


Figure 3.3 Possible configurations for the concentration $N_2(z,t)$ at a fixed position z ($N_2 \neq 0$).

above concentrations calculated by using Eq. (3.4.8) and denoting it by R one has

$$R = \frac{N_2(z,t = v_2)}{N_2(2,t = J-)} \qquad \frac{N2 + \hat{} \; l^B12l}{(NJT) \; , b_{12l}} \exp \qquad (3.4.9)$$

therefore, when R> 1 the concentration N_2 (z, ***t=z/^2)*** is the largest and t =z/V but when R <1 the concentration N (z, t-z/v-^) is the largest and in this case t2=z/V^. The coefficient B-^ is inside a modulus sign because the product B times the function S(vjt;v_2t) is always positive as it is shown in Eq. (3.4.2).

Consider first the case when R>1. For the cases "a" and "d" ^2K2>1K1 and if oae solves Eq. (3.4.9) results

$$z > \frac{\ln \; N° \; . \; (NjT)|B_{12l}}{u^{(H?T»}l^B12|} \qquad \text{yields:} \quad t_2 « \frac{}{1} \qquad (3.4.10)$$

Similarly, for the case when R<1, when Eq.(3.4.9) is solved for z one obtains

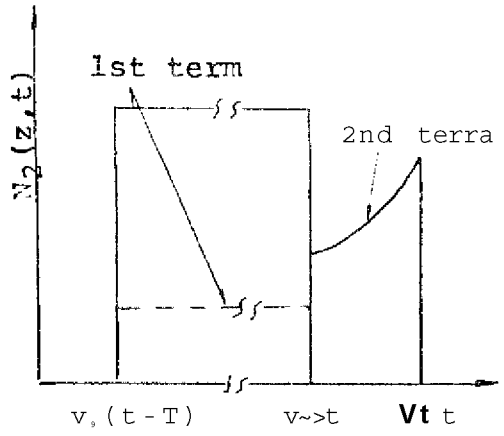
$$z < \frac{\ln \; N2 + \; 1^B12[}{\hat{} \; _\circ \; D \; , B_{12} \; ,} \qquad \text{yields:} \quad t_\circ = \qquad (3.4.11)$$

Denoting the quantity on the right hand side of Eq. (3.4.10) and Eq. (3.4.11) by W

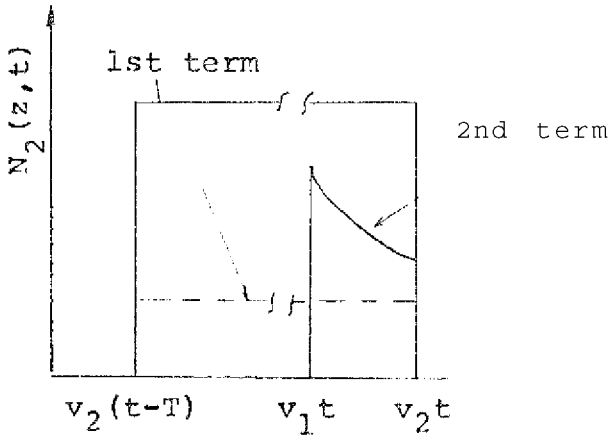
The following Table 3.5 summarizes the time for the maxima concentration of the second member at a fixed position when its initial concentration is non zero.

Table 3.5 The time when the maximum concentration of the second member occurs at a fixed position when the initial daughter concentration is non zero (N^0) .

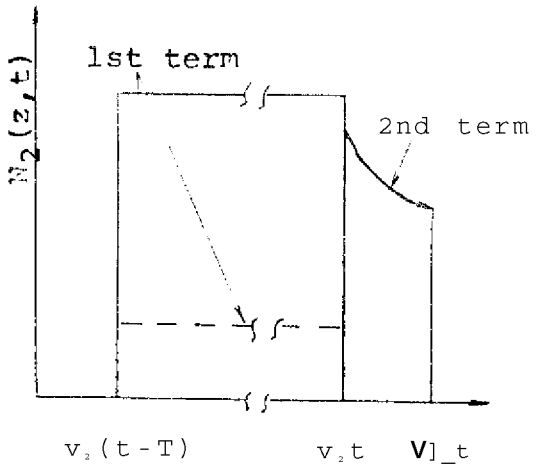
Next, the case of the extremum for the second member at a fixed time is studied. Figure 3.4 shows the different configurations that the second member concentration Eq. (3.4.8) can take, depending on the relative magnitude of the nuclide velocities. For a given fixed time, the cases "b" and "d" show clearly that the extremum occurs at z=v„t. This is because when the two terms are added, the largest value of the concentration will always occur at z->=v t.



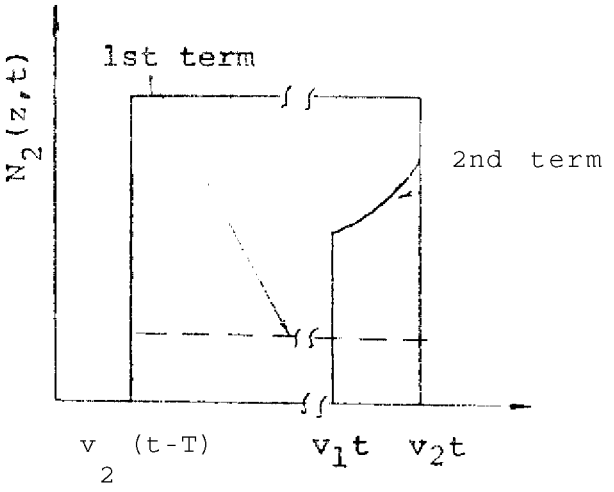
a) $v > v_2$, $x_2 > X$-j, t fixed



b) $v_2 > v_1$, $a_2 < >_{11}$, t fixed



c) $v_1 > v_2$, $A_2 < \hat{}_1$, t fixed



d) $v_2 > v_1$, $> ._2 > x_1$, t fixed

Figure 3.4 Possible configurations for the concentration of the second member $N_2(z,t)$ at a fixed time (N_2 #0)

For the cases "a" and "c" one must compute the concentrations at the points z=v^t and z=v^t where the extremum may occur and compare them to decide which one is actually the maximum. By using Eq. (3.4.8) one evaluates the concentrations at z=v-j t and z=v_t and denoting their ratio by R' results

$$R' = \frac{N_2(z=v_2t,t)}{N_2(z\hat{}v-\hat{}t)} \qquad N_2 + TNj\,B_{12} \qquad \exp(X\hat{}-X_2)t \qquad (3.4.13)$$

When R'>i/the concentration at z-v$_2$t is the largest and the maximum occurs at z~=v t. The time t is solved in Eq.(3.4.13) 2 when the condition R>1 is satisfied (i.e. the maximum occurs at z=v$_2$t)

$$t < \sim \frac{\ln \; {}^{\prime\prime}2 \; {}^{\prime} \; ({}^{\prime\prime}\mathbf{I}^{\tau})\,!^{\beta}121}{L({}^{\prime\prime}\ddot{\imath}o^{\tau}> \; !^{\beta}i;} \qquad (3.4.14)$$

Conversely, when R<1, the concentration at z=v^t is the largest and the extremum occurs at z^-v^t. Solving Eq.(3.4.13) for the time t when the condition R<1 is satisfied results

$$t > - \frac{\ln \; N^{\circ\,\prime} \; (NjT)}{(NJT)_{12}} \qquad (3.4.15)$$
$$(^{\times}\mathbf{I} - {}^{\times}2)$$

The different possible cases for the extremum of the 0 concentration of the second member when N_2*0 at a fixed time shown in Figure 3.4 and Eq. (3.4.14) and Eq. (3.4.15) are summarized in Table 3.6 below

	t < W	t > w'
$x_1 > x_2$	$z_2 = V$	
$x_1 < x_2$	$z_2 = v_2 t$	$t_2 = v_x t$

In (N?T; '12!

, $w's$ - J_{12l}

where $x_1 \sim x_2$

Table 3.6 The position of the maximum concentration for the second member at a fixed time when N ^ 0.

When the second member is initially present at the repository, the contamination time and the contaminated region can be determined according to Eq.(3.4.8). They are summarized in Table 3.7 below (see Appendix D for the derivations). One should notice that when the initial amount of the second member is negligible Tables 3.5 and 3.6 reduce to Tables 3.2 and 3.4 respectively. This is because W and W» are null when $N_2^0=0$ and the conditions z>W and t>W' are always satisfied.

Cases	Contarni nation time	Contaminated region
$v_1 > v_2$	$\bullet^{*}-(\sqrt{ii})^{*T}$	$R_2 - v_1 t \sim v_2 \hat{} \sim T \hat{}$
$v_1 < v_2$	$9_2 = \frac{}{v_1 v_2} - \text{if} - \frac{}{v_1 v_2} > T$	$R_2 = (v_2 - v_1)t \text{ if } (v_2 - v_1)t > v_2 T$
	$e_0 = T \text{if} \frac{}{v_j} - \frac{}{v_2} < T$	$R_2 - v_2 T \hat{} f \hat{} v_2 \sim v_1 \hat{} * v_2 T$

Table 3.7 Contamination time and contamination region for the 2 member when N° + 0.

3.5 Extremum of the solution for the third member

This problem is again subdivided into two stages:

1-The initial amount of the third member present at the repository is zero ($N_3^0 = 0$).

2-The initial amount of the third member is significant at the repository, ($N^0 \neq 0$).

3.5.1 The initial amount of the third member at the repository is zero

By setting $N^0 = 0$ in Eq.(3.2.16) the solution for this case reads

$$N_3(z,t) = T(B_{23}N^0 - AN^0)\exp(-\lambda t - \ldots\ i)\ S(v_2 t;\ v_3 t) +$$

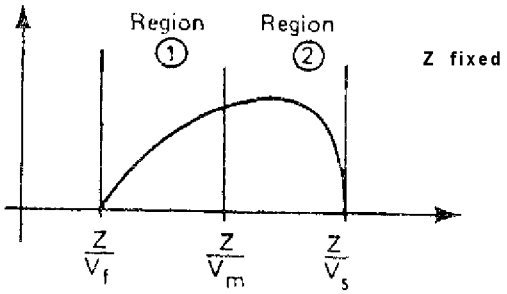
$$N_j TA \exp(-\lambda_{13} t - a_{13} z)\ S(v_1 t; v_3 t) \qquad (3.5.1)$$

$$-N^c_x TA \exp(-\lambda_{12} t - \mathbf{a}\hat{} z)\ s(\mathbf{vjt};\ \mathbf{V}_3 t)$$

Depending on the relative magnitudes of the nuclide velocities, the functions $S(v^0 t; v^0 t)$ can assume the values of -1 ,0 or +1. Therefore, for each one of the six possible different combinations of the three nuclide velocities, different signed terms in Eq. (3.5.1) will arise. The task of determining the extremum of the Eq. (3.5.1) is indeed expanded to the task of

determining the extremum of six different functions, depending on the relative magnitude of the nuclide velocities.

In order to determine the time of the maximum concentration at a fixed position, the following procedure is adopted. For a particular set of nuclide velocities, v_s, v_m, v_f, where subscript s stand for slowest, m for medium and f for fastest, the solution can be sketched as follows



The form of the solution for the concentration of a third member Eq.(3.5.1) does not permit two nuclides in the same chain to have the same velocity. The terms represented by B_{ij} (see Eq. (3.2.17)) have a singularity when $v_i = v_j$. Since the three nuclides have necessarily different velocities, at a fixed position *z*, the migration band boundaries z/v_s, z/v_m and z/v_f have different values. Two different regions are thus defined: region 1 where $z/v_f < t < z/v_m$ and region 2 where $z/v_m < t < z/v_s$.

Consider for instance the case where $v_1 > v_2 > v_3$ (f=1, m=2, s=3). Therefore, in region 1 $z/v_1 < t < z/v_2 < z/v_3$ and in region 2 $z/v_1 < z/v_2 < t < z/v_3$. Recalling the definition of the functions $S(v_i t; v_j) = h(v_i t - z) - h(v_j t - z)$ one can evaluate the value

of these functions in Eq.(3.5.1) in each region.

In region 1

$$S(v_2t;v_3t)=h(v_2t-z)-h(v\hat{}t-z)=0-0=0$$

$$S(v_3t;v_3t)=h(v_xt-z)-h(v_3t-z)=1-0=1$$

$$S(v_1t;v_2t)=h(v-\hat{}-z)-h(v_2t-z)=1-0=1$$

In region 2

$$S(v_2t;v_3t)=h(v_2t-z)-h(\mathbf{V}gt-z)=1-0=1$$

$$S(v_1t;v_3t)=h(\mathbf{V}jt-zJ-h(v_3t-z)=1-0=1$$

$$S(v\hat{}t;v2t)=h(v_1t-z)-h(v_2t-z)=1-1=0$$

The solution Eq.(3.5.1) takes different form in each of these regions, because the functions $S(v\hat{}t;\mathbf{v}jt)$ assumes different values in each region for the same set of nuclide velocities. Let us summarize in Table 3.8 the values of the functions $S(v\text{-}t;v_jt)$ in each region and for the six possible combinations of the nuclide velocities, (see Eq. (3.2.21)).

In the case of the solution for the second member concentration discussed in last section, the functions were always monotonically decreasing or increasing inside the domain of definition and the extremum was located at the boundaries of the domain of definition. However, for the third member solution, the first partial derivative of the concentration with respect to time may vanish inside one of the two regions defined above. In this case, one might have a interior maximum and this possibility must be investigated,

		Region 1			Region *2*		
Case	W ᵛ s	S(v₂t;v₃t)	S(v₁t;v₃t)	S(v₁t;v₂t)	S(v₂t;v₃t)	S(Vjt;v₃0	S(v₁t;v₂t)
1	W ᵛ 3	0	1	1	1	1	0
2	W ᵛ i	-1	-1	0	0	-1	-1
3	W ᵛ 2	0	1	1	-1	0	1
4	2 3 I	1	0	-1	0	-1	-1
5	v,>v,>v„	-1	-1	0	-1	0	1
6	ᵛ2 ᵛ1 ᵛ3	1	0	-1	1	1	0

Table 3.8: Values for the functions S(v.t;v.t) =h(v.t-z)-h(v•t-z)

The procedure adopted to evaluate the time of maximum for each of the six cases will be to evaluate the individual maximum of the concentration for each region and then to compare them in order to decide which one is actually the true extremum of the solution in both regions. The first of the six cases listed in Table 3.8 will be studied in detailed. For the case 1, where v^> region is studied individually. In region 1, from Eq.(3.2.16) and Table 3.8 the concentration distribution in this region is given by

$$\frac{N}{N_1}(z,t) = TA\exp(-A_{13}t - o_{13}z) - TA\exp(-A\hat{}t - a_{11}z) \qquad (3.5.2)$$

and it is non trivial for a given z>0 in the time interval: $z/v\hat{}< t<z/v_2$ which is the domain of definition of Eq. (3.5.2). The partial derivative with respect to time of Eq.(3.5.2) is

$$\frac{1}{TN_1}\frac{^{3N}3}{o\ 3T} \sim (^{2>t)} - ^{AA}12^{exp(-A}13^{t} \sim {}^{H}13^{z)} - AA_{13}\exp(-A_{12}t - a_{12}z) \qquad (3.5.3)$$

The function described by Eq. (3.5.2) can have, if any, only one extremum in its domain of definition because Eq.(3.5.3) can have only one zero, if any, in its domain of definition (region 1). The zero of Eq. (3.5.3), if it exists, occurs at

$$t_{3} = \frac{^{1}}{A_{21} - A_{31}}\ ^{A}21 \qquad (3.5.4)$$

By evaluating Eq.(3.5.3) at the beginning of its domain of

definition t=z/v^ one has

$$1 \quad {}^{3N}3 \qquad z \qquad {}^{x}] \tag{3.5.5}$$

furthermore, one can show that

$$A(A_{21}-A_{31}) = -V P_{v} - \longrightarrow 0 \tag{3.5.6a}$$

hence,

$$-r\hat{}\,(z,t=-) > 0 \text{ for any } 2 > 0.$$

Therefore, Eq.(3.5.2) is initially increasing and if the zero of Eq. (3.5.3) lies inside the domain of definition the extremum will be a maximum, i.e., if $z/v\hat{} < t_3$(Eq. (3.5.4)) $< z/v_2$, t3 will be a point of maximum. On the other hand, if t^ given by Eq. (3.5.4) does not exist or it lies outside the domain of definition, the function Eq.(3.5.2) is monotonically increasing in its domain of definition and the maximum will occur at the end of the region 1, i.e. $t,=z/v,$. The inequality resulting from t lying inside the domain of definition can be expressed in terms of the position z by using Eq. (3.5.4)

$$1 \quad {}^{A}21\sim{}^{A}31 \qquad {}^{In}\,'13 \qquad (a\,21^{-ot}\,31)^{s} \tag{3.5.6}$$

The same derivation is repeated for the second region. From Eq. (3.2.6) and vising Table 3.8 the concentration

distribution in this region is given by

$$U,t) = T(\frac{M2B23}{N} - A) \exp(-A_{23}t - a_{23}2) + TA \exp(-i\hat{}t - a\hat{}z) \qquad (3.5.7)$$

and it is non trivial for a given z> 0 in the interval $z/v_2<t<z/v_3$ which is the domain of definition of Eq. (3.5.7). The partial derivative with respect to time of Eq.(3.5.7) is

$$\begin{array}{l} 1\ {}^{S}M3 \qquad I \qquad {}^{B}23M2\backslash \\ -\ -_{3T}-(z,t) \ =(T\ A\ -\ -)\ A_{23}\ \exp(-A_{23}t-_{a,3}z: \\ {}^{N}| \qquad\qquad\qquad {}^{N}1 \\ \quad TAAj_3\ \exp(\sim A_{13}t-aj_3z) \end{array} \qquad (3.5.8)$$

Again, the function described by Eq.(3.5.7) can have, if any, only one extremum in its domain of definition. This is because Eq.(3.5.8) can have, if any, only one zero in its domain of definition. The zero of Eq. (3.5.8) , if any, occurs at

$$\begin{array}{l} {}^{6}32{}^{A}31 \end{array} \quad In \quad \frac{A - B_{23M2/M1\ A32}}{'13} \ -\ (a_{23}\sim a_{13})_2 \qquad (3.5.9)$$

Let us evaluate Eq.(3.5.8) at the end of the domain, $t=z/v_3$

$$\begin{array}{l} \pm\_\_\_\_\pm \\ {}_{N}O\ at \end{array} \quad \begin{array}{l} (z\ \mathbf{t}\ -\ -)\ -\ T\ A(A_{23}-A_d)\ -\ {}^{M}2{}^{B}23{}^{A}23 \\ \mathbf{U\ .\ t\ -} \qquad\qquad \mathbf{-\ T} \end{array} \quad \begin{array}{l} exp \\ \bullet \end{array} \quad \begin{array}{l} (\_\ \_\ _z) \\ {}^{V}3 \end{array} \quad \mathbf{-\ If} \qquad (3.5.10)$$

Two possibilities results from Eq. (3.5.10)

jATip^f < 1 yields ^ (z . t . f - X O (3.5.12)

Suppose given by Eq. (3.5.9) exists and it is interior, i.e,

$$z/v_2 < t_3(\text{Eq.3.5.9}) < z/v_3 \qquad (3.5.13)$$

Then, when Eq. (3.5.11) is true, if the partial derivative Eq. (3.5.10) is positive t^ is necessarily a point of minimum, while if the inverse occurs t^ given by Eq. (3.5.9) is a point of maximum. On the other hand, if t_3 given by Eq. (3.5.9) does not exist or it is outside the domain of definition, the function Eq. (3.5.7) is monotonically increasing if the derivative evaluated in Eq.(3.5.10) is positive and the extremum occurs at $t_3 = z/v_3$. Conversely, $N_3(z, t)$ is monotonically decreasing if the derivative in Eq. (3.5.10) is negative and there results the extremum on $t_3 = z/v_2$. The inequality Eq.(3.5.13) can be rewritten by using Eq. (3.5.9) to express this condition in terms of the position z

$$\frac{2}{v_2} < \frac{1}{a_{32} - a_{31}} < \frac{}{3} \qquad (3.5.14)$$

After having determined the time of the maximum in each region, one substitute these values of time back into the corresponding Eq. (3.5.2) and Eq. (3.5.7) to evaluate the maxima concentrations in each region. By comparing these concentrations one can finally decide about the actual maximum for both regions.

Above procedure will yield the extremum for the third member concentration for the first case of the Table 3.8 at a fixed position. This derivation is repeated for the other five cases listed in Table 3.8 and a general form of the extremum can be obtained and it is summarized in Table 3.9. As before, a given case is denoted by: v p v > v . where the subscripts indicate
f m s

f=fastest nuclide velocity, f=1, 2, 3.

m=intermediate nuclide velocity, m=1, 2, 3.

s=slowest nuclide velocity, s=1, 2, 3.

(For example, the case 1 in Table 3.8 would be f=1, m=2, s=3).

3.5.2 Extremum of the solution for the third member when its initial amount at the repository is non zero

In this case, the complete solution Eq. (3.5.1) is required

$$N_3(z,t) = N_3 \exp(-\hat{} -) \; S[v_3 t; v_3(t-T)] \; \hat{}(t) + \tag{3.5.15}$$

$$N°TB_{23} - N°TA) \exp(\sim°23^{t} \sim^{a}23^{z}\hat{} \; \hat{}(v\hat{}t; v\hat{}t) +$$

$$\hat{}TA \exp(-A_{3,1}t - a_3 j2) \; S(v\hat{}t; v_3 t) + N°TA \exp(-A\hat{}t - a\hat{}z) \; S(v\hat{}t, v\hat{}t$$

The second term which is inside the bracklet was analyzed in the previous section and its extremum can be determined by using Table 3.9. When N^*0, a new term (first term on the right

Region 1

Condition: / 77 i −fs . . − 1 7 (Ma, mf − fs)

Satisfied

ln(mf) − (σ − σ)2 / *fs / mf fs

Note:

Cases l, 3: M . 1

Cases 2,4: M =1 − Nj A

Cases 5, 6: M (N, A)

w ¿1 " ^ ^ 7 7 Nf

Not Satisfied

Cases 1,3: t^

Cases 2,4: if:

W, > 1: t, « — l — 3 v.

W1 < 1: t3 − — v.

Cases 5, 6; if:

W. <-l: t, − — 1 − 3 v.

W, > −1 : t3 " v

Region 2

Condition: — v < — fs — ms fs < ′ 2 — S

Satisfied

1" Ma !ü (°ms − fs)2 / fs / Vs − fs

Note:

Cases 2, 4: M − 1

Cases 1, 3: H − 1 (N0 23 / N?A)

Cases 5, 6: H

23 23

Not Satisfied

Cases 2,4: t^

Cases 1,3: if

W2 > l: t3 .f−

W0 < 1: − — 2 3 vm

Cases 5, 6; if:

W2 <-l: t3 . L .

W2 > −1 : t3 . −

Table 3 .9 Summary of the determination of the extremum for the 3 member (N^ = 0)

hand side) is superimposed. Recalling the assumption of small leach time, i.e., T<< 1/ Xj, j=1,2,3,and by realizing that this added term is non trivial in the interval ($z/v_3, z/v_3+T$) of duration T, one can neglect changes in the Bateman's functions and take $ (t) =1. Therefore, the first term can be seen as a band of duration T and constant magnitude.

Depending on the relative magnitude of the nuclide velocities, different configurations result from the superimposition of the two terms. Consider for example Figure 3.4. In case "a"of Figure 3.4 the two terms are non trivial in independent time domains and one can evaluate the extremum of the second term (using Table 3.9) and the extremum of the first term (using Eq.(3.3.2)5 separately. The largest concentration will define the true maximum for both terms.

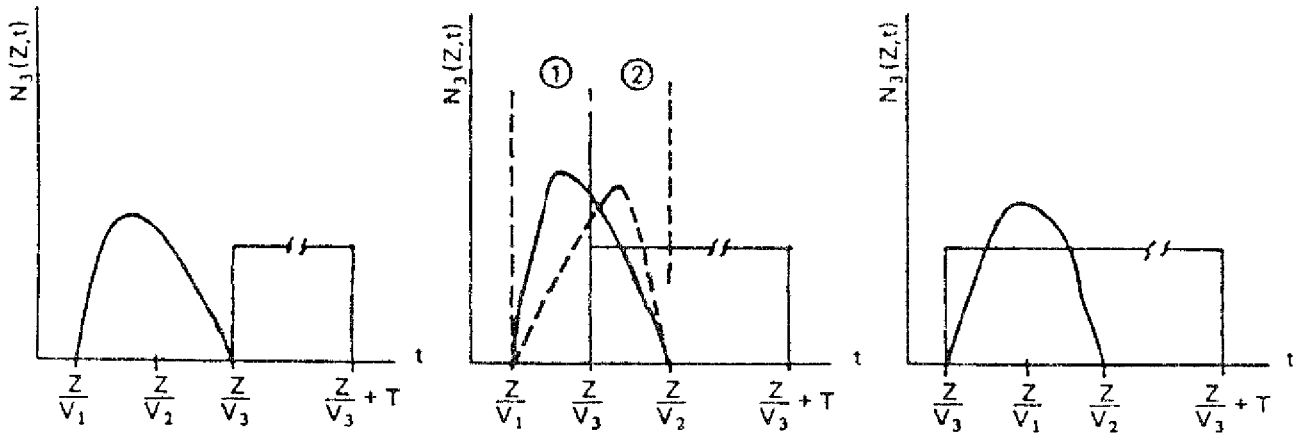


Figure 3.4 Possible configurations of the solution for the 3rd member when N° f 0.

In case "b" of Figure 3.4 we have two possibilities:when the extremum of the second term occurs in region 1 and when it occurs in region 2 (dotted line). In either case, one can decide about the true maximum by evaluating the concentration Eq. (3.5.15) at $t=z/v_3$ which is the point of extrema for the first term and comparing to the concentration Eq. (3.5.1) at the point of extrema for the second term alone obtained by using Table 3.9 and taking $N°=0$ in Eq. (3.5.15). Again, the larger of them will define the true maximum.

In case "c" of Figure 3.4 the extremum occurs clearly at the point of extremum of the second term but the magnitude is larger by the addition of the first term. Above examples does not exhaust all possibilities, since we might have a sufficiently large z so that z/v^+T lies inside the domain of the second term. But in any case, it can be shown that the following steps will yield the time of maximum t^ at a fixed position z

1-Evaluate (^ z, $t=z/v_3$) using Eq. (3.5.15) with both terms.

2-Use Table 3.9 to obtain $t_{\overline{3}}$ for the second term alone.

3-Evaluate $N_3(z,1_3)$ with 1_3 obtained in step 2 above.

4-Compare (z, $t=z/v_3$) from step 1 and N^(z, 1_3) from step 3.

5-If concentration from step 1 is larger than that from step 3 then t-^z/v^

6-If the opposite is true then t_3 is obtained from step 2.

Two cases can be distiguished in the determination of the

contamination time and in the contaminated region for the third member,

a-When the third member is not present at the repository initially the contamination time $\underset{3}{6}$ as well as the contaminated region can be readily obtained from Eq.(3.5.1) and Table 3.8. They can be expressed by

$$0_3 = z/v_s - z/v_r \qquad (3.5.18)$$

$$R_3 = (v_f - v_s)t \qquad (3.5.13)$$

b-When the third member has non zero initial concentration at the repository, using Eq.(3.5.15) and Table 3.8 one can construct the following Table 3.10. The derivations are shown in Appendix D.

Case:				

Table 3.10: Contamination time and contaminated region for the 3 member (N^0).

3.6 Example of the utilization of the method and comparison with the exact solution results

To verify the validity of the approximation and to determine the range in leach time for which this approximate solution is accurate in representing the exact solution to a decaying band release the results of the approximate solution with those of the exact solutions are compared. These comparisons are done for different leach times. Comparisons for the first member solutions are not necessary since the exact and approximate solutions have the same form. We studied the U-234 and the Np-237 chains. First consider the following three member chain

	U-234	Th-230	Ra-226	
K_1	1.4E+4	5.0E+4	5.0E+2	
X_i	2.8E-6	9.0E-6	4.3E-4	(1/yr)

Let us consider the water velocity as being v=110 m/yr. The case of no initial daughters at the repository is first studied. In this case, v^> v^> v^. The extremum for the second member Th-230 can be readily obtained from Table 3.2 with the condition $A_2K_2>A\hat{}I\backslash\hat{}$„ The time when the maximum occurs at a fixed position is $t_2=z/v\hat{}$ and corresponding concentration will be, by using Eq.(3.4.1)

$$(z,t,)=(N?T)\hat{}\exp(-)\,z \qquad (3.6.1)$$
$$(v_{\cdot}v_{2})$$

consequently,the contamination time is

$$6 = z / v_2 - z / v_1 \qquad (3.6.2)$$

The time of maxima for the third member at a fixed position can be obtained from Table 3.9. In this present chain f=3, m=1 and s=2. Thus, according to Table 3.8 we are in case 5. The coefficients and cu_. are first evaluated.

	i=3,j=2	i=1,j=3	i=1,j=2	
à	4.75E-6	-1.29E-5	1.14E-5	(1/yr)
	1.92E-3	2.01E-3	-1.11E-3	(1/m)

In the column titled region 1 in Table 3.9 we first check the condition for the existence of interior maximum. Since $N_2=0$ and $B_{23}=0$; hence M=1 and $W_J=0$. Therefore, $\ln(M A_{ra} / A_{fs}) = \ln(A^{\wedge\wedge} / A_{32})$. But since $A^{\wedge} / A^{\wedge} < 0$, the condition for interior maximum cannot be satisfied. Under the column "not satisfied", for the case 5 and with Wj=0, the time of maximum is read out: $t_J = z/v_m = z/v_1$ for the region 1.

Similarly, the condition for existence of interior maximum in region 2 is first checked: $\ln(M A^{\wedge} / A_t J = \ln($ $A_{32}{}^{\wedge=0} * {}^{87} *$ And again the condition for interior maximum is not satisfied, for case 5 and with $W_2=0$ the time of maximum is read from Table 3.9 and it is $t_J = z/v_m = z/v_1$. Since the time of maximum in both region is the same one concludes that $t_3 = z/v_1$. The corresponding maximum concentration is

$$\frac{(z,tJ}{\text{N}1} = TA\exp\left(\frac{A_{32}}{\text{v}1}a_{32}\right)z - TA\exp(-X_1/v_1)z \qquad (3.6.3)$$

and the contaminated time will be given by

$$\mathbf{e}_3 = d/v_2 - 1/v_3)z \qquad (3.6.4)$$

The above results agree well with the exact solution presented by Higashi (H2) for leach time values up to 3.OE+4 years. (see Figure 3,5a and Figure 3.5b). A more detailed study has been conducted to determine upper bounds for the error as one increases the leach time for larger values at the end of this section.

In Figure 3.5a the maximum dimensionless Ra-226 concentration ($N_3(z,t_3)/N^{\wedge}$) is plotted for each fixed position z. There are no initial daughters present at the repository and the leach time is 3500 years. For this value of leach time the agreement was complete.

Figure 3.5b is a similar plot but for a leach time value of 35000 years„ Although this value of leach time is larger than the Ra-226 half life, the approximate solution deviation from the exact solution is smaller than 10%. This is because the Ra-226 concentration is controlled by the decay of U-234 whose half life is much larger than the leach time used.

In Figure 3.6a the calculation was the same as in Figure 3.5a but this time the daughters were initially in transient equilibrium. For this leach time (3500 years) the agreement was complete. In Figure 3.6b a leach time of 35000 years was used which is about an order of magnitude larger than the Ra-226 half-life. Although this fact violates the basic assumption the comparison with exact solution shows that the error is larger only for distances smaller than 10 meters where the decay of the initial Ra-226 nuclides is important. For distances larger than 10 meters where the concentration of Ra-226 is controlled by the decay of U-234 the error is smaller than 10%.

A second important three member decay chain starts with Np-237

	Np-237	U-233	Th-229	
T_H	2.1E+6	1.6E+5	7.3E+3	(years)
K_i	1.0E+4	1.4E+4	5.0E+4	

The retardation coefficients used were taken arbitrarily for the purpose of this illustration. The same calculation done for the U-234 chain are repeated here. Let us first determine the extremum of the solution for the second member. From Table 3.2 and with the condition $\lambda_2 K_2 > \lambda_1 K_1$ we read the time of maximum at a fixed z: $t_2 = z/v_1$ and the corresponding maximum concentration will be

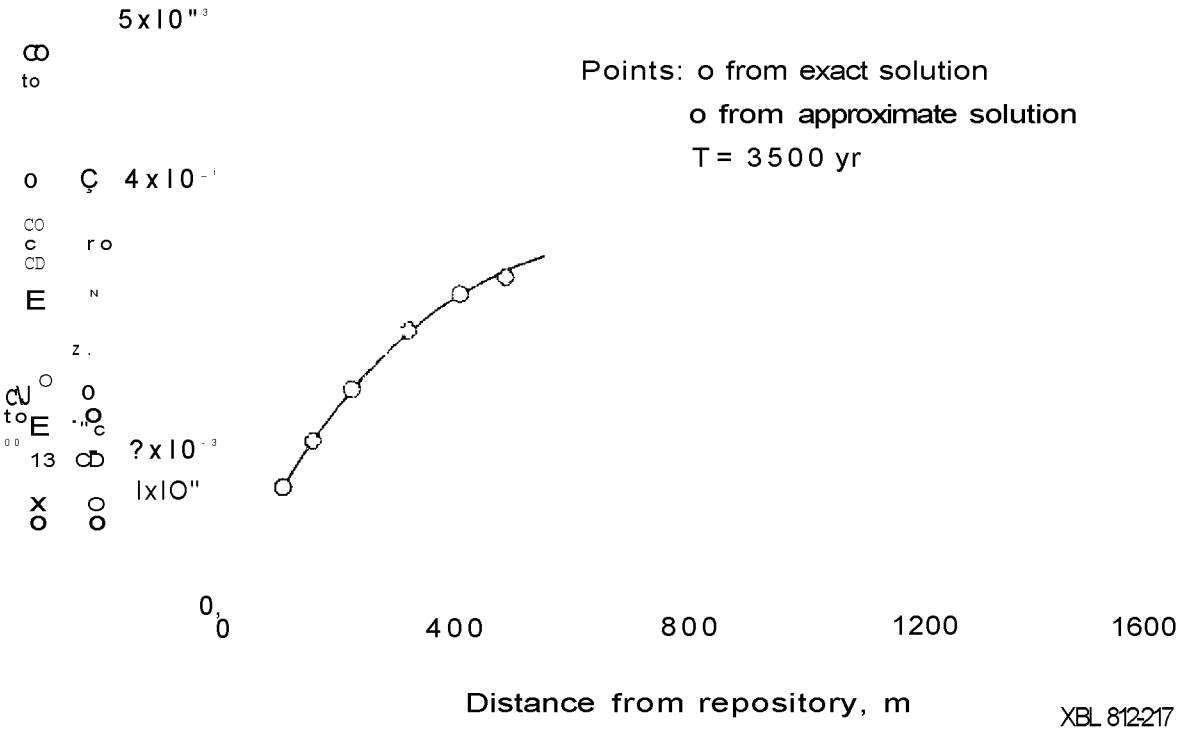


Figure 3.5a Maxima concentrations of " Ra at different fixed positions No initial daughters (N° = N° = 0). No dispersion. T = 3500 years.

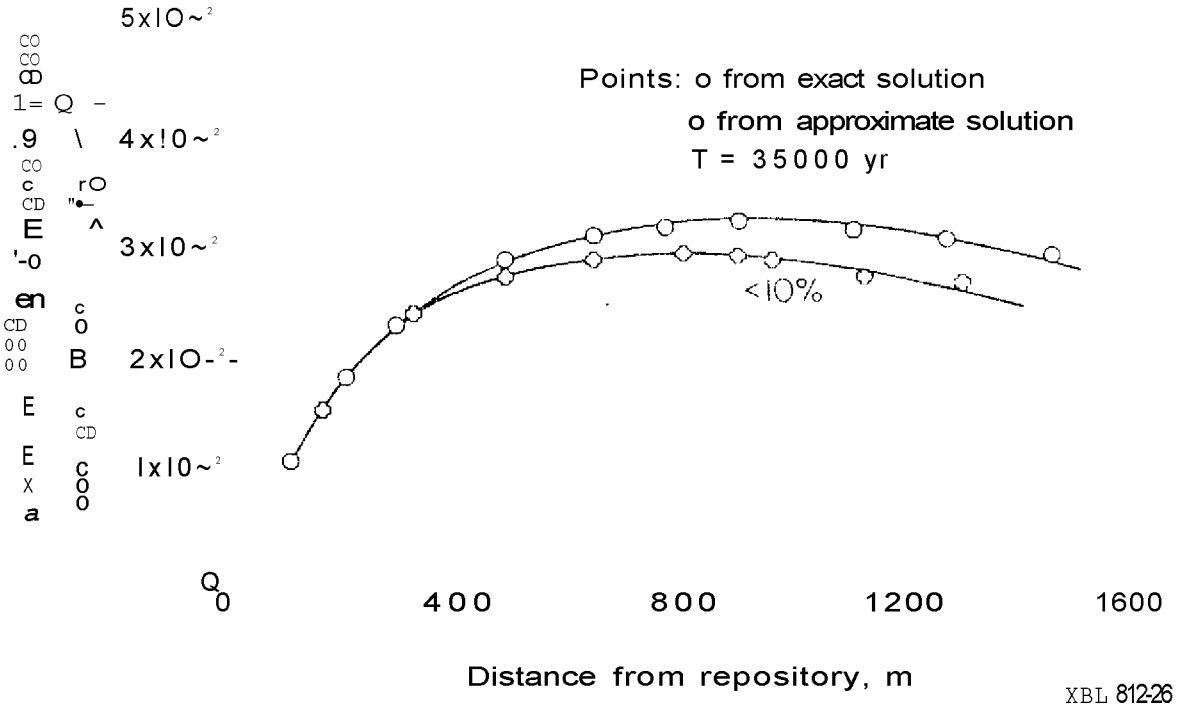


Figure 3.5b Maxima concentrations of ^{226}Ra at different fixed positions No initial daughters (N^ "° No dispersion. T = 35000 years.

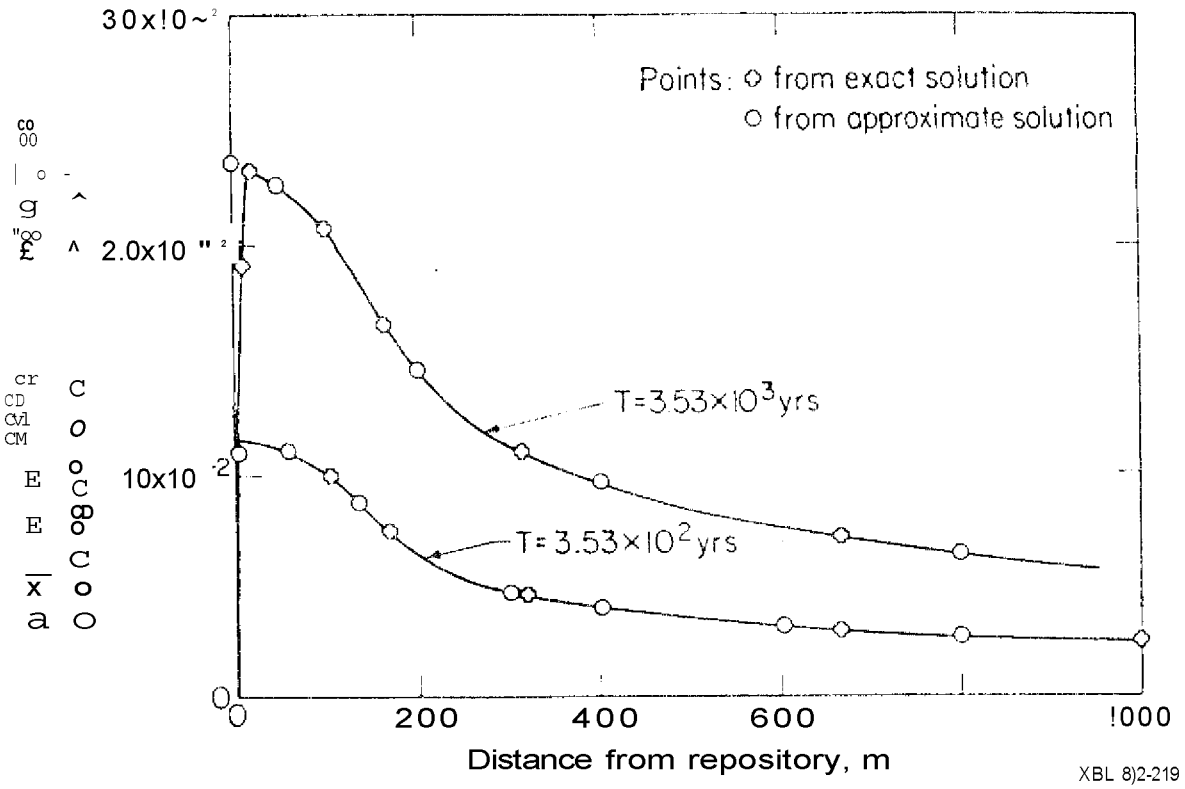


Figure 3 .6a Maxima concentrations of ^{226}Ra at different fixed positions Initial transient equilibrium. No dispersion. T = 3500 years.

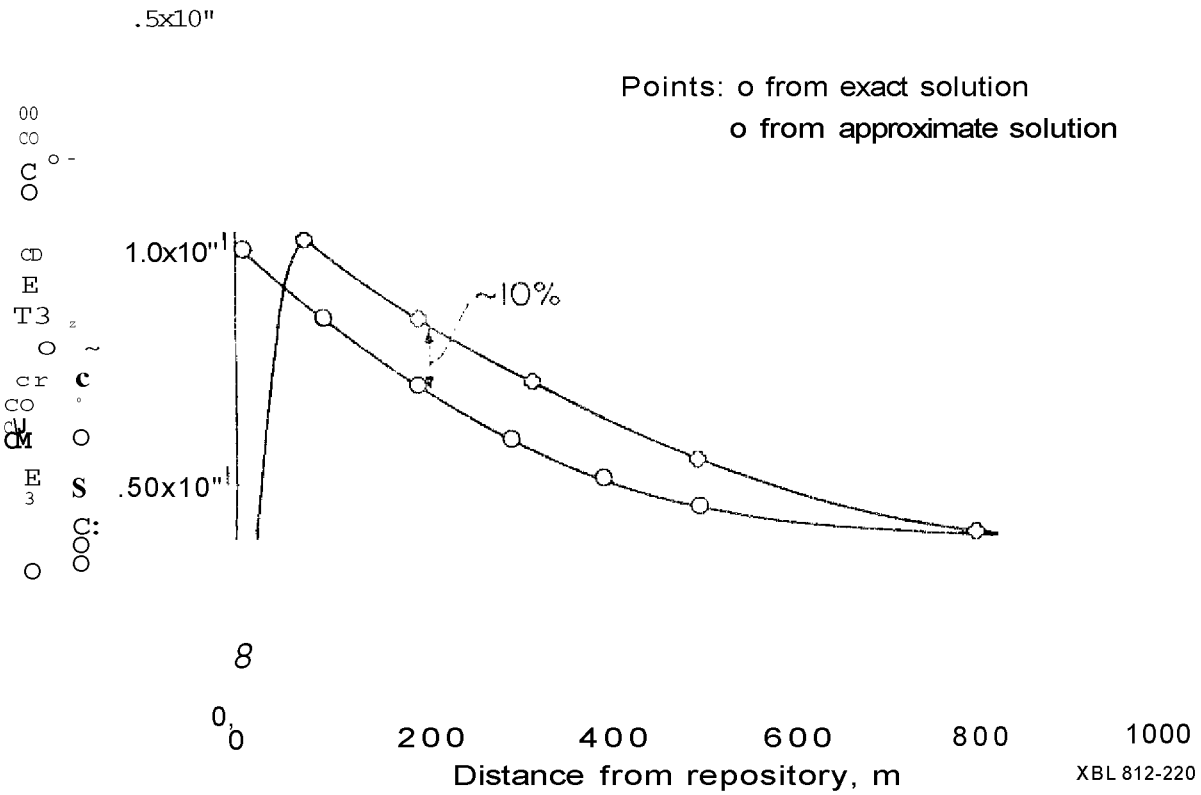


Figure 3 -6b Maxima concentrations of ^{226}Ra at different fixed positions. Initial transient equilibrium. No dispersion. T = 35000 years.

$$N_2(z,t_2) \ll 1 - i - i - e^{v1\ 7} \qquad (3.6.5)$$

The time of maximum for the third member at a fixed position can be determined from Table 3.9. The nuclide velocities are ordered in such a way that we have a case 5. The coefficients A_{ij} and a_{ij} are first evaluated

	i=3,j=2	i=3,j=1	i=1,j=2	
A_{ij}	-4.56E-5	-9.38E-5	1.45E-5	(1/yr)
a_{ij}	6.37E-3	8.55E-3	-1.20E-3	(1/m)

Consider first the case of no initial daughters. Under the column titled "Region 1" in Table 3.9 the condition for the existence of interior maximum is first checked. Since $N_2 \neq 0$ and $B_3 = 0$ hence M=1 and $W_1 = 0$, thus: $\ln(M A_{mf} A_{fs}) = \ln(A_{13}/A_{32}) = 0.721$. The condition for interior maximum cannot be satisfied for positive z. Under the column not satisfied, for a case 5, one reads the time for the maximum: $t_{max} = z/v = z/v_1$.

Similarly, for region 2 the condition for interior maximum cannot be satisfied and from Table 3.9 the time of maximum is obtained: $t_{max} = z/v_2$. Since the maximum concentration in either region occurs at the common boundary $t_{max} = z/v_2$, the maximum concentration for both region is the same and can be expressed by

$$N^*(z,t^*) = TA \exp\left(-\frac{A_{23}}{}z - a_0 z\right) - \exp\left(-\frac{}{v_1} z\right) \qquad (3.6.6)$$

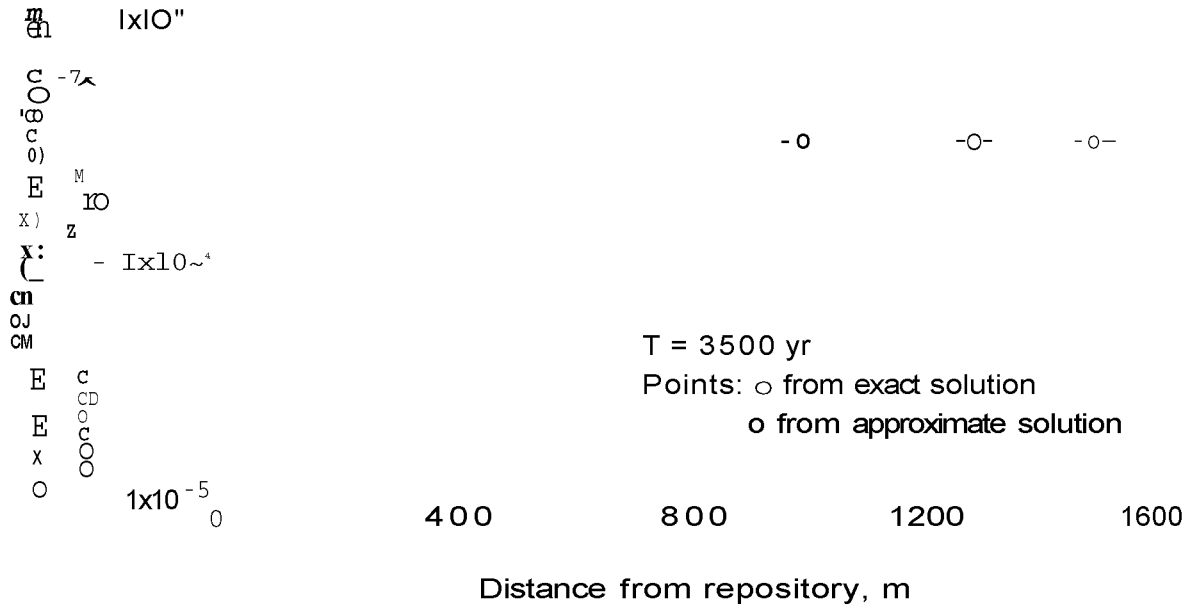
Figure 3.7a and Figure 3.7b show the case of zero initial daughters concentration for leach times of 3500 and 35000 years respectively. Also for this chain, the agreement between the exact and approximate solution is quite good for leach times smaller than 35000 years. Finally, in Figure 3.8a and Figure 3.8b the comparisons are made for the case when the initial daughter concentrations are in transient equilibrium. The curves for the case of a leach time of 3500 years still show good agreement but the curves for the case of a leach time of 35000 years show a small deviation.

Additional comparisons between maxima concentrations obtained by evaluating the exact solutions formulas (reference Hi) and by using the approximate method developed in this work are summarized next. Deviations of the values obtained by the approximate method from those of the exact solution are expressed in terms of percent error which is defined as:

$$e\,(\%) = ((\text{exact} - \text{approximate})/\text{exact}) * 100 \qquad (3.6.7)$$

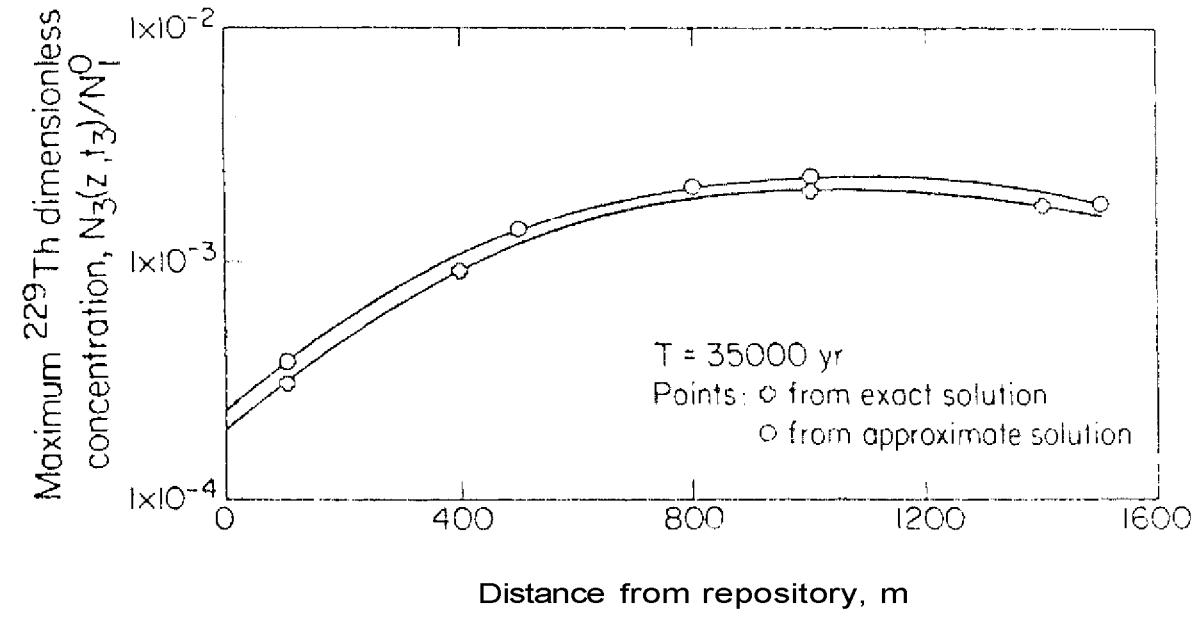
Here, the two chains analyzed previously in this section are studied again but using instead the initial concentrations and retardation coefficients listed in Table 3.14a.

Tables 3.10a through Table 3.10d show the percent error in the maxima concentrations calculations of Ra-226, Th-229, Th-230 and U-233 respectively, at different values of the ratio



X6L 812-221

Figure 3 .7a Maxima concentrations of 1h at different fixed positions No initial daughters (N° = N° = 0). No dispersion. T = 3500 years.



XBL 812-222

Figure 3 .7b Maxima concentrations of Th at different fixed positions. No initial daughters (N° = N° = 0). No dispersion. T - 35000 years.

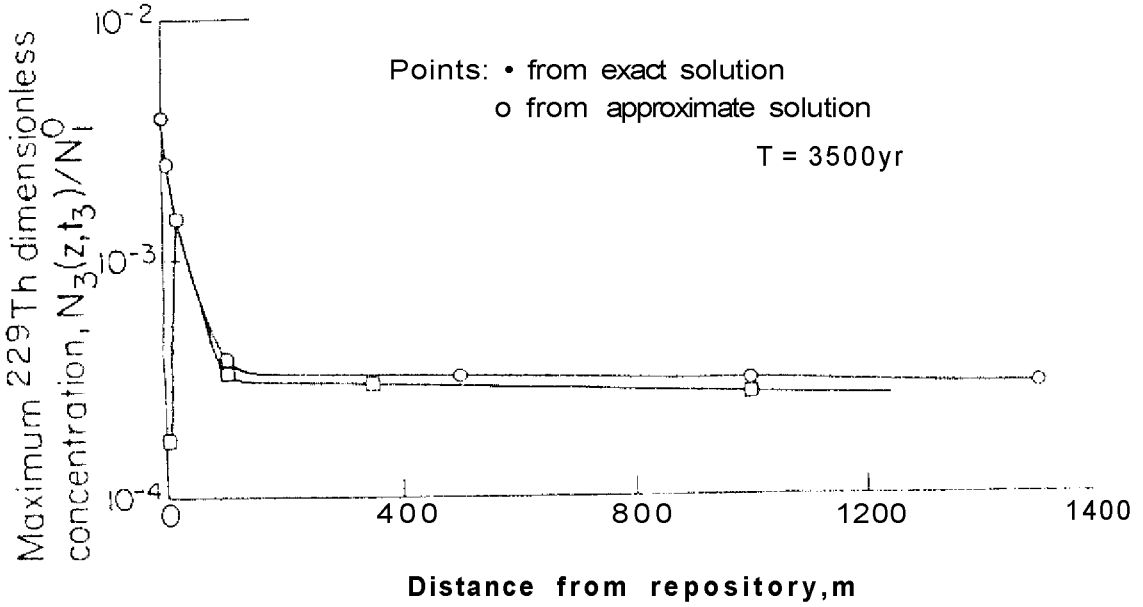


Figure 3.8a Maxima concentrations of ^{229}Th at different fixed positions Initial transient equilibrium. No dispersion. T = 3500 years.

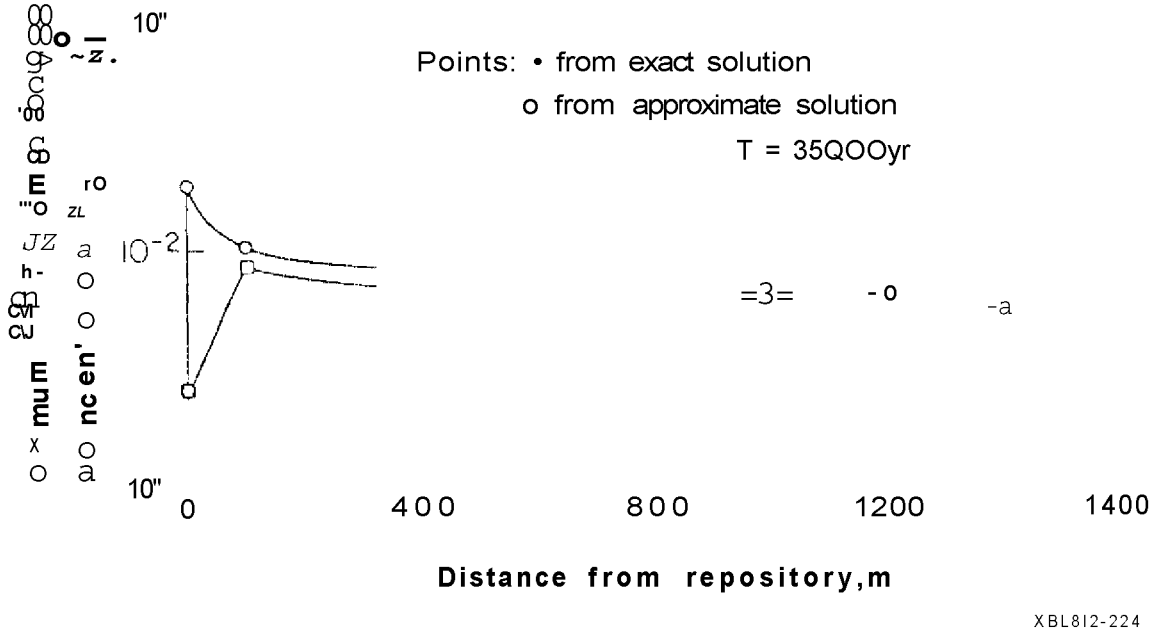


Figure 3.8b Maxima concentrations of Th at different fixed positions. Initial transient equilibrium. No dispersion. T = 35000 years.

distance/water velocity (z/V,water travel time) and for different leach times.

All four tables show that for leach times smaller than **1000** years where the condition $T<<T^{\wedge}$ is satisfied, the error is negligible for all values of z/V. For leach times between 1000 and 10000 years the error is greater than 10% only for water travel times smaller than 1 year. Since groundwater velocities are expected to be smaller than 10 m/yr, for leach times of the order of 10000 years the approximate method is applicable for path lenghts z greater than 10 meters which in general is the range of interest for far field migration studies.

Finally, for leach times of the order of 10^{5} years or larger, the error becomes unacceptable for any value of water travel time. In view of above results, the condition $T<<T^{\wedge}$, can be relaxed and the vality of the method can be extended to leach time of the order of 10000 years provided the water travel time is larger than one year.

z/v(yr)	T(yr): 10	10^{2}	10^{1}	10^{4}	5 10^{0}
	0	8.0	10.0	49.0	24.0
10^{-1}	0	1.0	3.0	38.0	98.0
10^{0}	0	0	0.2	11.0	42.0
10^{1}	0	0	0	3.0	39.0
10^{2}	0	0	0	3.0	43.0
10^{3}	0	0	0	3.0	40.0
10^{4}	-	-	-	-	50.0

Table 3.10a: Percent error of the approximate method in the evaluation of the maxima concentrations of $^{?2fi}$Ra

z/v(yr;	T(yr) 10	10'	10'	10	10'
10^{-2}	0	7.0	55.0	85,	95.0
10"	0	7.0	42.0	75	93.0
10^{0}	0	5.0	18.0	50.	82.0
10^{1}	0	4.0	9.0	19	82.0
10^{2}	0	0	0	1	14.0
10^{3}	0	0	0	1	10.0
10^{4}	0		0	1	10.0

Table 3.10b: Percent error of the approximate method in the evaluation of the maxima concentrations of ^{229}Th

z/v(yr)	T(yr) 10	10^	10³	10⁴	5
10""	0	7.0	19.0	52 0	33 0
10-¹	0	5.0	9.0	41 0	30 0
10°	0	0	5.2	22 0	2 0
10¹	0	0	1.0	8 0	94 0
10²	0	0	1.0	6 0	96 0
10³	0	0	1.0	6 0	124 0
10⁴	-	-	-	-	-

Table 3.10c: Percent error of the approximate methoa in the evaluation of the maxima concentrations of Th

z/v(yr)	T(yr) 10	10'	10'	10	10'
10"	0	7.0	30.0	81 .0	99.0
10"	0	6.0	22.0	72.0	99.0
10°	0	0	9.0	55.0	99.0
10¹	0	0	5.0	23.0	98.0
	0	0	1.0	2.0	27.0
i0-	0	0	1.0	2.0	33.0
10⁴	0		1.0	2.0	23.0

Table 3 .10d: Percent error of the approximate method in the evaluation of the maxima concentrations of U

3.7 Analysis of the effects of variation in parameters values on the maxima concentrations

In this section we apply the method developed in previous sections to analyse the effects on the maximum concentration caused by variations in the values of the parameters. The main advantage of this present method is that it avoids the need of detailed evaluation of the complete solution and the subsequent search for the extremum. One can use this method to analytically evaluate directly the extremum, saving therefore considerably computing time.

Although this can be done with the help of a pocket calculator, when a large number of cases is to be evaluated as in the case of a parametric analysis, it is very useful to program this method into the computer so that one can evaluate the extremum of any number of nuclides and for any number of sets of parameters all at once. A computer program called UCBNE20 was developed which uses this method in evaluating the potential hazard at the biosphere resultant from the release of radionuclides present in the waste packages. A complete listing and description of data input requirements are given in Appendix B.

According to the assumptions made in the development of the method, UCBNE20 will be restricted to the following:

1. One dimensional systems.

2. Constant water velocities, soil and water properties.

3. Negligible dispersion effects.

4. Leach times smaller than nuclide half lives.

5. Maximum chain size is three members.

If above conditions are met, UCBNE20 will evaluate the following quantities for a given i-th member of a chain:

1. Time of maximum at a fixed position, $t^{\wedge}$

2. The coreespondent maximum concentration.

3. The correspondent maximum water dilution rate.

4. The contamination time for that position.

In order to apply this method for any nuclide, it is necessary first to reduce the long actinide chains into three members or less chains by suitable simplifications.

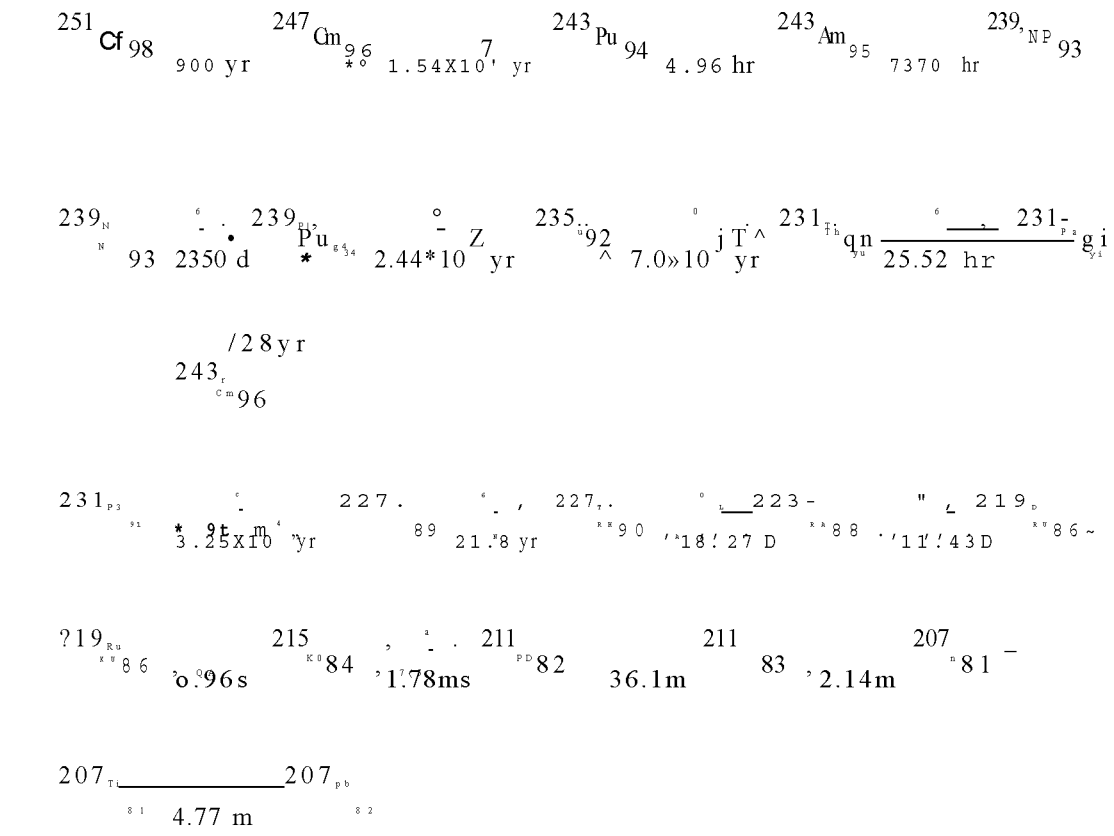
3.7.1 Reduction of actinide chains

The actinide chains present in high level wastes have more than three members and cannot be treated by the method above. But because some elements have very short half lives while some others have very long half lives, these chains can be broken into shorter chains.

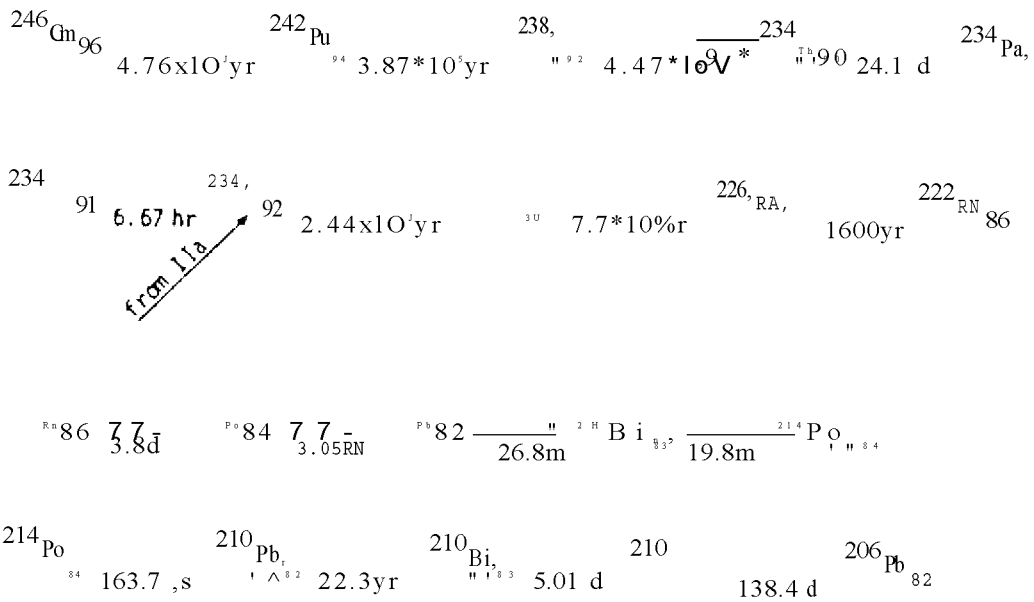
There are four distinct complete actinide chains present in high level wastes. They are shown in Table 3.11 below. In order to reduce these chains into smaller chains, the following factors

Table **3 .11:** Actin**ides Chains Present in PWR** Spent Fuel **and** Reprocessed Waste.

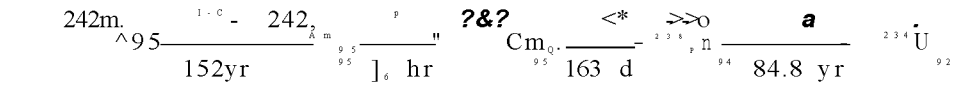
I) The 4n+3 chain:



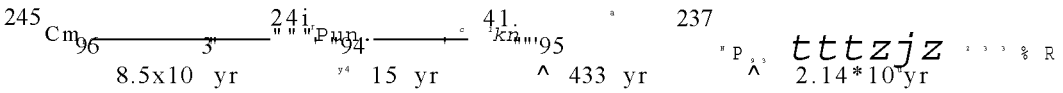
11) The 4n+2 chain:

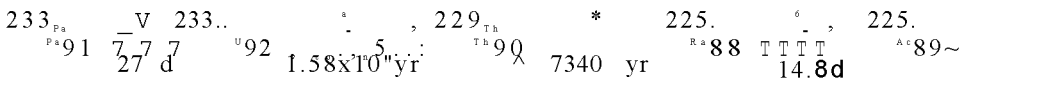


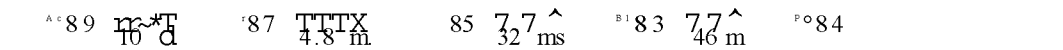
Ha): Branch of 4n+2 chain



III) The 4n+1 chain:







IV) The 4n chain:

232 U 92

must be taken into account:

a)Whether the waste is unreprocessed or reprocessed;which type of reactor has generated it;when the leaching starts after the burial. These factors determine basically the initial amount of a given nuclide.

b)The relative magnitude of the retardation coefficients and the half lives of a precursor and its daughters. (See discussion about secular equilibrium for migrating chains in HI,section **4.5).**

For this present study, we will consider the initial amount of actinides in the waste as being that of the reprocessed HLW from spent fuels of a PWR and the range of time for beginning of leaching is below 10^5 years. With these assumptions we have defined the nuclides activities that are initially present in the repository.

In addition, we assume that the sorption equilibrium contants of the actinides do not differ more than four orders of magnitude from each other. With above assumptions the following simplifications can be made:

1. A very short-lived nuclide can be considered as being in secular equilibrium with its long-lived precursor, i.e.$X\hat{}K\hat{}N\hat{}=X\hat{}$

According to reference (Hi), the necessary condition to have secular equilibrium is that $X_i.K_i >> X_{i-1}.K_{i-1}$.Since we have assumed that the retardation coefficients do not differ more than four orders of magnitude from each other, the half life of the

daughter must be at least four orders of magnitude smaller.

2. On the other hand, if a nuclide has a much shorter half life than its precursors one can assume that every short lived precursor initially present in the waste has decayed by the time that the waste dissolution begins. The initial concentration of this long-lived nuclide should include those nuclides of the precursors which have already decayed.

With these two assumptions, each one of the four chains can be broken into the following smaller chains: (The nuclide in parentheses are in secular equilibrium with its precursor).

The first chain 1, (4n+3 chain) can be subdivided into the following chains

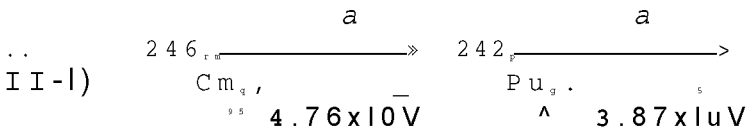
1-1) $^{251}_{98}Cf \xrightarrow{\alpha} {}^{247}_{96}Cm$ 900 yr

$^{247}_{96}Cm$ 1.57×10^{7} yr $^{243}_{95}Am$ 7370 yr $^{239}_{94}Pu$ 2.44×10^{4} yr

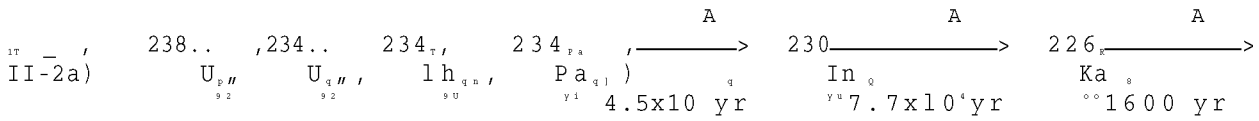
(assume that all ^{243}Cm has decayed to ^{239}Pu)

1-3) $^{235}U \xrightarrow{(^{231}Th)} {}^{231}Pa \xrightarrow{(^{227}Ac)}$ ^{235}U 7.0×10^{8} yr $^{231}_{91}Pa$ $^{227}_{89}Ac$ 3.25×10^{4} yr

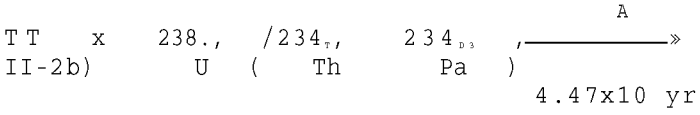
Subsequent elements are in secular equilibrium with Pa-231. The next chain II, (4n+2 chain) can be subdivided into the following chains

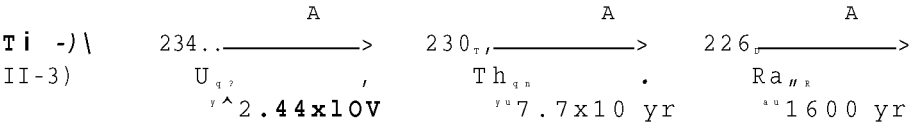


If the times of interest are of the order of the $^{234}U_{92}$ half-life or longer one should consider the following chain:



On the other hand, if the time scale is smaller than $^{234}Ug^{\wedge}$ half-life the following chains should be considered instead of (II-2a):





In this later case, if the dissolution begins after hundreds of years or more one can assume that every nuclide in the branch Ila of the 4n+2 chain has decayed to form U-234 nuclides. But sometimes we are interested in the effects of fuel dissolution beginning at the time the waste is emplaced, and at other times we are interested in what happens if dissolution does not begin for hundreds of years or more. The decay of the initial Pu-238,Am-242m and Cm-242 in the waste to form U-234 is important. In waste from fuel reprocessed a few months after discharge, Cm-242 is the most important source of U-234 (B2).

This and the less important sources Pu-238 and Am-242m would have to be considered as members of the chain if the dissolution were assumed to occur immediately and if we were interested in the contamination of groundwater quite near the repository. In any of above cases, all remaining nuclides are in secular equilibrium with Ra-226.

In chain III, (4n+1 chain), one can neglect the first element Cm-245 because of the low quantities initially present in the reprocessed waste. On the other hand, there is a large amount of Pu-241. For practical purposes, the chain beginning with the decay of Pu-241, to form Am-241 and Np-237 is quite important. If waste dissolution were to begin at the time waste is put into a repository, the existing inventory of Pu-241 in unreprocessed spent fuel is important, even after a delay time of 10 years from reactor discharge to emplacement in a repository. If waste dissolution were not to begin for a hundred years or so, from a practical point of view Am-241 becomes the first member, i.e., the half life for the effective decay of the parent of Am-241 is only 13 years instead of 8500 years. If waste dissolution begins hundreds of years or more after emplacement the chain III (4n+1 chain) can be reduced to the following chain

$$^{237}_{93}Np \xrightarrow[2.14\times10^{6}\ \text{yrs}]{} {}^{233}_{91}Pa \xrightarrow[1.58\times10^{5}\ \text{yr}]{} {}^{233}_{92}U \longrightarrow {}^{229}_{90}Th \longrightarrow {}^{}_{}U\ 7340\ \text{yr}$$

Where the initial amount of Np-237 should include the decay of Pu-241 and Am-241. All other subsequent nuclides are in secular

equilibrium with Th-229. Finally, chain IV (4n chain) can be reduced to the following chain

$$^{240}_{94}Q_A \xrightarrow{6540\ yr} {}^{236}_{92}Q? \xrightarrow{7} {}^{232}_{90}qn \xrightarrow{1.4\times10^{10}\ yr}$$

U-232 can be neglected, and all other subsequent nuclides are in secular equilibrium with Th-232).

3.7.2 Evaluation of peak water dilution rate

To estimate the potential hazard to the biosphere we use the Maximum Permissible Concentration (MPC) according to 10CFR part 20, Appendix B. These are the nuclide concentrations in water which will result in the maximum allowable dose for an average individual who has all his daily water intake from such a source. The water dilution rate is the volumetric flow rate of a aquifer or surface water into which the migrating radionuclides discharge such that the concentration of any nuclide will not be above the MPC concentrations. Therefore, the peak water dilution rate is calculated as follows

$$w_1 = Q \; X_x . N_{\cdot 1}(z,t_i)/(MPC)_I \qquad (3.7.1)$$

Where Q is the volumetric groundwater flowrate (m^3/yr) across the waste and $(MPC)_i$ has units of (Ci/m^3) and they are listed in Table 3.14a).

3,7.3 The reference case and the range of variation of the parameters

The reference case is defined by the following set of parameters:

1. The time lapsed between the emplacement and the beginning of the waste dissolution is denoted by t_g and is taken to be 1000 years. This parameter represents the expected lifetime of the protective barriers. t_g does not show up directly in the solutions but its variation leads to changes in the initial inventories of each nuclide present in the waste when the leaching starts. The nuclide inventories present in the waste at t_g=1000 years are listed in Table 3.14a and they were obtained from reference (B2). These inventories are from the reprocessed waste of spent fuels of a PWR after generating 1 Gw(e)yr of electricity with a load factor of 80%, a thermal efficiency of 34% and a burnup of 30.4 MwD/kg. These spent fuels are reprocessed after 150 days cooling period and 0.5% of the Pu and U are lost to the waste. The time elapsed between discharge and emplacement in the repository is assumed to be negligible.

2. The duration of the release (leach time) is denoted by T_4 and is taken to be 10^4 years. This number represents the expected lifetime of a proposed waste form. It is assumed that the waste matrix dissolves at a constant rate over time T and all

contained radionulides dissolve when the matrix dissolves.

3. The position downstream where the contaminated water streamline meets the aquifer is called the path lenght. It is denoted by z and for the reference case it will be 1000 meters.

4. The reference velocity of the water flowing past the repository will be v=10 m/yr. The reference water travel time will therefore be z/V=100 years.

5. The sorption retardation coefficient is denoted by K^. The reference set of values is given in Table 3.14a, obtained from (B2).

The procedure adopted here to analyse the effects of the variation of the parameters values on the peak water dilution rate is to keep all parameters fixed at the reference values with the exception of one of them which is varied. This is done in turn for each one of the relevant parameters. Each parameter is varied in the range given by Table 3.12 below. The analysis of the variation of the retardation coefficient for nuclides which are first members of a chain can be studied by the results of the variation in water velocity. This is because they are both related to the same parameter V^=V/K^. For three member chains the following cases shown in Table 3.13 were calculated.

In each one of the six cases described in Table 3.13 one of

		Min imum	Max imum
Time of beginning of leaching		1 yr	10^{5} yr
Leach time	T	10 yr	50,000 yr
Water travel time	z/v	10^{-3} yr	10^{8} yr
Equilibrium constant		10^{2}	10«

Table 3.12 Range of variation of the parameters

	Cases :	K_L	K_2	K_3
1	$K_2 > k_2 > K_\wedge$	10^{2}	Varied	10^{4}
2	$K_\wedge > K_2 > K_2$	10^{4}	Varied	10^{2}
3	$K_2 > K_2 > K_J$	10^{2}	10^{4}	Varied
4	$K_1 > K_3 > K_2$	10^{4}	$10_{?}$	Varied
5	$K_2 > K_J > K_2$	Varied	10^{4}	10^{2}
6	$K_3 > K_1 > K_2$	Varied	2	10^{4}

Table 3.13 Variation of equilibrium constants values for three-member chain analysis.

the retardation coefficient is kept fixed at the lower limit (100), the other at the upper limit (10^4), while the third is varied inside the range (100-10000). The calculations are done for every one of the six possible combinations described in Table 3.13. With these six cases we cover the possible different combinations of retardation coefficient for three member chains. Consider for instance case 1. When K_2 approaches K^=100, case 1 tends to case 6 and if K_2 approaches K_3=10000, case 1 in this case tends to case 3. By analyzing these six cases one can predict qualitatively the behaviour of the solution for a three member chain for any different combination of sorption coefficients.

3.7.4 Results of the calculations

Table 3.14a and Table 3.14b show the results of the calculations for the reference case. In Table 3.14a the nuclide parameters are listed. The column titled "member" indicates whether the element is considered a first, second or third member in a chain. A number 4 indicates that the nuclide is in secular equilibrium with the nearest long lived precursor.

The last column which is titled "Attenuation factor" is the product X^K^,(1/yr). Table 3.14b actually shows the results of the calculation. The number under the column "1-st" is the identification number of the first precursor of that nuclide (if

any) in the chain, and the number under column "2-nd" is the identification number of the second precursor. Let us identify the results in each column with the nomenclature used in past sections

"TIME OF PEAK (YR)"=t_i

"MAXIMUM N/N "=N.(z,t.)/N?

"WAT.DIL.(m^3/yr.Gw(e)yr)"=w_i

"CONTAM.TIME (YR)"=

For the reference case, the largest peak water dilution rate is that of 1-129 which is a volatile fission product. Although it has been recovered separately it is assumed to be also present in the dissolving waste material. In addition, it is also assumed that 1-129 has a dissolution leach time equal to that of the reprocessing high level waste. Similar assumptions are made about H-3 and C-14.

Because of its unit retardation coefficient, 1-129 peak is the first to arrive at the reference water travel time. Following 1-129, the next important contributor is the actinide Np-237 which has high toxicity and initial activity. Ra-226 produced by the decay of the U-234 originally present at the repository presents also significant peak water dilution rate at this reference water travel time because of its low MPC value. Ra-226 has the smallest MPC value followed by 1-129. In addition to 1-129, the fission products Tc-99, Sn-126, Se-79 and Zr-93 also present significant peak water dilution rates.

Table 3.14a Sample Output - Nuclide Parameters for the Reference Case. (The Nuclide Parameters are Listed Below) Time for Beginning of Leaching is 1.00E+03(YR)

NUMBER	NUCLIDE	MEMBER	HALF-LIFE (YR)	SORPTION CONST.	MPC (CI/M**3)	INITIAL ACTIVITY(CI)	ATTENUATION FACTOR (1/YR)
1	H-3	1	1.20E+01	1.00E+00	3.00E-03	1.58E-21	5.78E-02
2	C-14	1	5.60E+03	1.00E+01	8.00E-04	1.15E+01	1.24E-03
3	SE-79	1	6.50E+04	1.00E+02	3.00E-04	1.09E+01	1.07E-03
4	SR-90	1	2.80E+01	1.00E+02	3.00E-07	3.74E-05	2.48E+00
5	ZR-93	1	9.50E+05	1.00E+04	8.00E-04	5.2OE+01	7.29E-03
6	NB-93M	1	1.40E+01	l.OOE+04	4.00E-04	1.59E-21	4.95E+02
7	TC-99	1	2.10E+05	1.00E+00	2.00E-04	3.89E+02	3.30E-06
8	RU-106	1	1.00E+00	1.00E+01	1.00E-05	1.00-200	6.93E+00
9	CO-113	1	1.40E+01	l.OOE+04	3.00E-05	4.13E-19	4.95E+02
10	SM-126	1	1.00E+05	1.OOE+03	2.00E-05	1.49E+01	6.93E-03
11	SB-125	1	2.70E+00	1.00E+02	1.00E-04	7.13-107	2.57E+01
12	1-129	1	1.70E+07	1.00E+00	6.00E-08	1.OOE+OO	4.08E-08
13	CS-134	1	2.00E+00	1.00E+03	2.00E-05	1.91-144	3.47E+02
14	CS-135	1	3.00E+06	1.00E+03	1.00E-04	7.80E+00	2.31E-04
15	CS-137	1	3.00E+01	1.00E+03	2.00E-05	2.69E-04	2.31E+01
16	CE-144	1	7.80E-01	2.20E+03	l.OOE-05	1.oo-2oo	1.95E+03
17	PM-147	1	4.40E+00	2.50E+03	2.00E-04	1.07E-62	3.94E+02
18	SM-151	1	8.70E+01	2.50E+03	4.00E-04	1.18E+01	1.99E+01
19	EU-152	1	1.30E+01	2.50E+03	6.00E-05	2.33E-21	1.33E+02
20	EU-154	1	1.60E+01	2.50E+03	2.00E-05	2.94E-14	1.08E+02
21	EU-155	1	1.80E+00	2.50E+03	2.00E-04	1.06-162	9.62E+02
22	RA-225	4	4.10E-02	5.00E+02	5.00E-07	2.86E-03	8.45E+03
23	RA-226	3	1.60E+03	5.00E+02	3.00E-08	3.25E-03	2.17E-01
24	TH-228	4	1.90E+00	5.00E+04	7.00E-06	2.45E-02	1.82E+04
25	TH-229	3	7.30E+03	5.00E+04	5.00E-07	2.86E-03	4.75E+00
26	TH-230	2	8.00E+04	5.00E+04	2.00E-06	1.72E-02	4.33E-01
27	U-233	2	1.60E+05	1.40E+04	3.00E-05	6.22E-02	6.06E-02
28	U-234	1	2.50E+05	1.40E+04	3.00E-05	I.99E+00	3.88E-02
29	U-235	1	7.10E+08	1.40E+04	3.00E-05	7.60E-03	1.37E-05
30	U-238	1	4.50E+09	1.40E+04	4.00E-05	4.50E-02	2.16E-06
31	NP-237	1	2.10E+06	1.00E+02	3.00E-06	1.44E+01	3.30E-05
32	PU-238	2	8.60E+01	1.00E+04	5.00E-06	2.84E+00	8.06E+01
33	PU-239		2.40E+04	1.00E+04	5.00E-06	5.58E+01	2.S9E-01

Table 3.14a (Continued)

NUMBER	NUCLIDE	MEMBER	HALF-LIFE (YR)	SORPTION CONST.	MPC (CI/M**3)	INITIAL ACTIVITY(CI)	ATTENUATION FACTOR (1/YR)
34	PU-240	2	6.60E+03	1.OOE+04	5.00E-06	2.45E+02	1.05E+00
35	PU-241	4	10.3E+01	1.OOE+04	2.00E-04	9.10E+00	5.33E+02
36	PU-242	2	3.80E+05	1.OOE+04	5.00E-06	1.93E-01	1.82E-02
37	AM-241	2	4.60E+02	1.10E+04	4.00E-06	1.91E+04	1.66E+01
38	AM-42M	1	1.50E+02	1.10E+04	4.00E-06	1.18E+00	5.08E+01
39	AM-243	1	7.90E+03	1.10E+04	4.00E-06	4.40E+02	9.65E-01
40	CM-242	4	4.50E-01	3.00E+03	2.00E-05	1.18E+00	4.62E+03
41	CM-243	1	3.20E+01	3.00E+03	5.00E-06	3.54E-08	6.50E+01
42	CM-244	1	1.80E+01	3.00E+03	7.00E-06	1.41E-12	1.16E+02
43	CM-245	1	9.30E+03	3.00E+03	4.00E-06	9.10E+00	2.24E-01
44	CM-246	1	5.50E+03	3.00E+03	4.00E-06	1.63E+00	3.78E-01

a) 1,2,3; indicate first, second or third member of a chain respectively; 4 indicates secular equilibrium with the nearest long lived precursor

b) Sorption constants are the overall equilibrium constant, i.e., the ratio of the amount in water and solid to the amount in water (see B3)

c) MPC are the maximum permissible concentrations in water (see B2)

d) Nuclide activities in waste, 10^3 yrs after emplacement. High level reprocessing waste from 7Gwe produced in a LWR (see B2)

e) Attenuation factors are the products of decay constants and sorption constants.

Table 3.14b Sample output, results for the reference case using UCBNE20

LEACH TIME (YR)	PATH LENGTH(M)	WATER VELOCITY (M/YR)
1.0000E+04	1.0000E+02	1.0000E+00

No.	NUCLIDE	MEMBER	1ST	2ND	TIME OF PEAK (YR)	MAXIMUM N/NO	WAT. OIL. (M**3/ GW*YR**2)	CONTAM. TIME (YR)	PERCENTAGE
1	H-3	1	0	0	1.00E+02	3.10E-03	1.63E-25	l.OOE+04	.000
2	C-14	1	0	0	1.00E+03	8.84E-01	1.27E+00	1.00E+04	.047
3	SE-79	1	0	0	l.OOE+04	8.99E-01	3.26E+00	l.OOE+04	.121
4	RB-90	1	0	0	l.OOE+04	3.25-108	4.06-110	l.OOE+04	.000
5	ZR-93	1	0	0	1.00E+06	4.82E-01	3.13E+00	l.OOE+04	.116
6	NB-93M	1	0	0	1.00E+06	0.	0.	l.OOE+04	0.
7	TC-99	'	0	0	1.00E+02	1.00E+00	1.94E+02	1.00E+04	7.195
8	RU-106	1	0	0	1.00E+03	0.	0.	l.OOE+04	0.
9	CD-113	1	0	0	1.00E+06	0.	0.	l.OOE+04	0.
10	SM-126	1	0	0	1.00E+05	5.00E-01	3.72E+01	l.OOE+04	1.379
11	SB-125	1	0	0	l.OOE+04	0.	0.	l.OOE+04	0.
12	1-129	1	0	0	1.00E+02	1.00E+00	1.67E+03	l.OOE+04	61.715
13	CS-134	1	0	0	1.00E+05	0.	0.	l.OOE+04	0.
14	CS-135	1	0	0	1.00E+05	9.77E-01	7.62E+00	l.OOE+04	.282
15	CS-137	1	0	0	1.00E+05	0.	0.	l.OOE+04	0.
16	CF-144	1	0	0	2.20E+05	0.	0.	l.OOE+04	0.
17	PM-147	1	0	0	2.50E+05	0.	0.	l.OOE+04	0.
18	SM-151	'	0	0	2.50E+05	0.	0.	l.OOE+04	0.
19	EU-152	1	0	0	2.50E+05	0.	0.	l.OOE+04	0.
20	EU-154	1	0	0	2.50E+05	0.	0.	1.00E+04	0.
21	EU-155	1	0	0	2.50E+05	0.	0.	l.OOE+04	0.
22	RA-225	4	25	0	4.40E+04	3.77E-01	2.16E+01	4.99E+06	.008
23	RA-226	3	26	28	1.40E+06	2.96E-04	3.07E+02	4.95E+06	11.381
24	TH-228	4	34	0	1.00E+06	2.51E-467	8.78E-43	1.00E+06	.000
25	TH-229	3	27	31	4.40E+04	2.61E-07	2.16E-01	4.99E+06	.008
26	TH-230	2	28	0	1.40E+06	2.22E-04	6.93E-02	5.00E+06	.003
27	U-233	2	31	0	l.OOE+04	2.44E-05	1.54E-02	1.40E+06	.001
28	U-234	1	0	0	1.40E+06	2.06E-02	1.37E-01	l.OOE+04	.005
29	U-235	1	0	0	1.40E+06	9.99E-01	2.53E-02	l.OOE+04	.001
30	U-238	1	0	0	1.40E+06	1.00E+00	1.12E-01	l.OOE+04	.004
31	NP-237	1	0	0	l.OOE+04	9.97E-01	4.78E+02	1.00E+04	17.710

Table 3.14b (continued)

LEACH TIME (YR)	PATH LENGTH(M)	WATER VELOCITY (M/YR)
1.0000E+04	1.0000E+02	1.0000E+00

No.	NUCLIDE	MEMBER	1ST	2ND	TIME OF PEAK (YR)	MAXIMUM N/NO	WAT. DIL. (M**3/ GW*YR**2)	CONTAM. TIME (YR)	PERCENTAC
32	PU-238	2	38	0	1.10E+06	0.	0.	1.00E+06	0.
33	PU-239	2	39	0	1.00E+06	2.89E-12	8.37E-09	1.00E+06	.000
34	PU-240	2	42	0	1.00E+06	1.60E-29	1.23E-42	1.00E+06	.000
35	PU-241	4	43	0	3.00E+05	1.96E-10	8.90E-10	l.OOE+04	.000
36	PU-242	2	44	0	1.00E+06	1.37E+00	6.65E-01	1.00E+06	.025
37	AM-241	2	43	0	3.00E+05	5.47E-11	2.51E-07	1.10E+06	.000
38	AM-42M	1	0	0	1.10E+06	0.	0.	l.OOE+04	0.
39	AM-243	1	0	0	1.10E+06	1.24E-42	1.36E-38	l.OOE+04	.000
40	CM-242	4	38	0	1.10E+06	0.	0.	l.OOE+04	0.
41	CM-243	1	0	0	3.00E+05	0.	0.	l.OOE+04	0.
42	CM-244	1	0	0	3.00E+05	0.	0.	l.OOE+04	0.
43	CM-245	1	0	0	3.00E+05	1.96E-10	4.45E-08	l.OOE+04	.000
44	CM-246	1	0	0	3.00E+05	3.83E-17	1.15E-15	l.OOE+04	.000

Identification number (first column) of the first precursor;

Identification number of the 2nd precursor

Time of maximum concentration at the given path length

Maximum dimensionless concentration:; N-j (z , t-j)/N-j

Correspondent maximum water dilution rate (see Eq. (2.7.68))

Time interval that this nuclide is present at the given path length

Percentage of the sum of all peak water dilution rates (in Column 8) for all nuclides.

The variation of peak water dilution rate $w^{\wedge}$ with water travel time is shown in Figure 3.9. For water travel times smaller than 10 years, Am-241 and Pu-239 produce the largest peak water dilution rates. Their peaks die out quickly for larger water travel times. Ra-226 water dilution rate builds up from the decay of U-234 and reaches the largest value at a water travel time of about 100 years. Between 10 and 1000 years, Ra-226 is the largest contributor. For water travel times larger than 1000 years only those nuclides with small attenuation factor will be present. This is the case of 1-129 which has the smallest attenuation factor of them all being the last to die out at about 10^{8} years. Allied to its high toxicity, 1-129 is one of the most important nuclides to be contained. Besides 1-129, at large water travel times, Np-237 and Tc-99 also present significant water dilution rates. They roll off at about $10^{\wedge}$ years. With the exception of 1-129, Np-237 and Tc-99 all other significant radionuclides have peak water dilution rate curves which roll-off quickly before water travel time of 1000 years.

The variation of the time for peak $t^{\wedge}$ with water travel time is shown in Figure 3.10. The linear variation is expected for the first and second members of chains according to the results of the method developed in preceding sections. For third member nuclides Ra-225 (Th-229) and Ra-226 we see that their times for peak are interior to the time domain only for very short water travel times (less than 0.1 year). For larger times

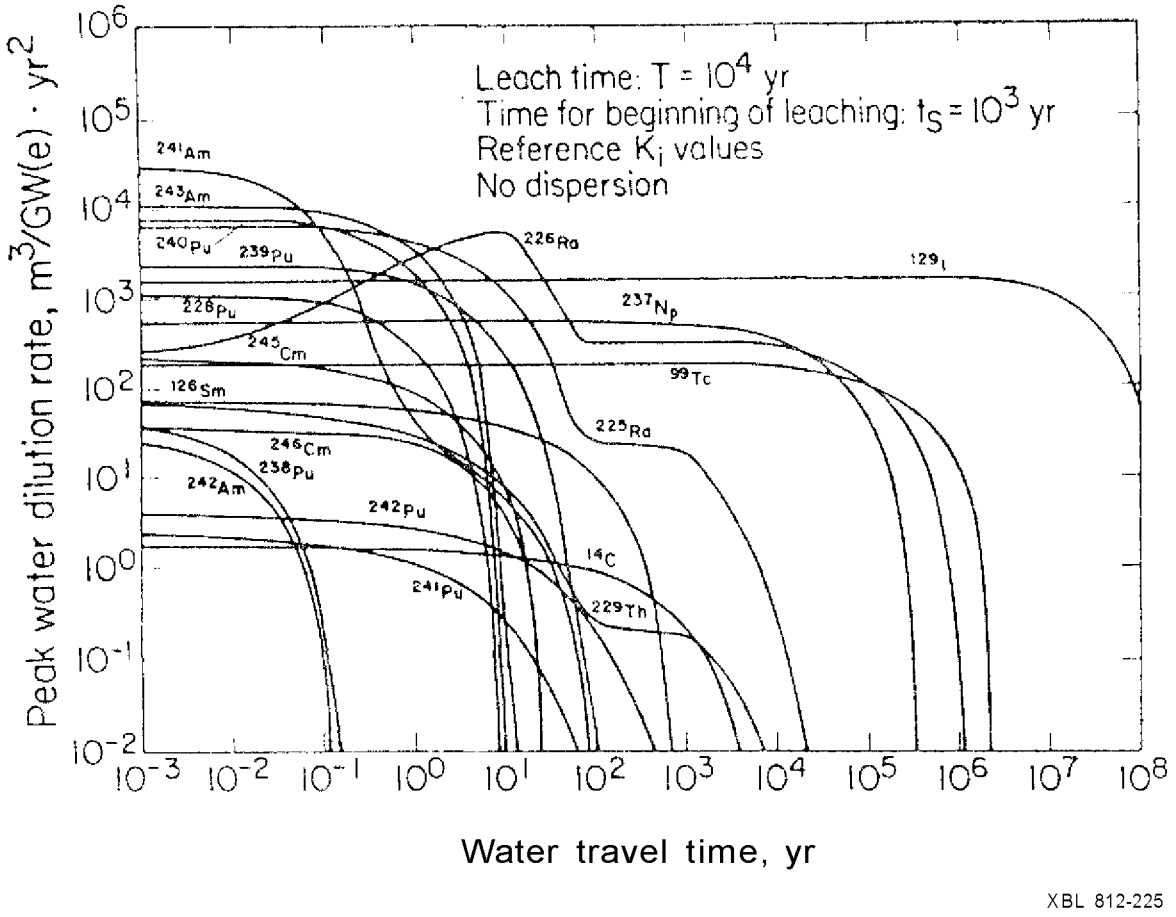


Figure 3.9 Variation of peak water dilution rate with water travel time for reprocessed PWR high level waste.

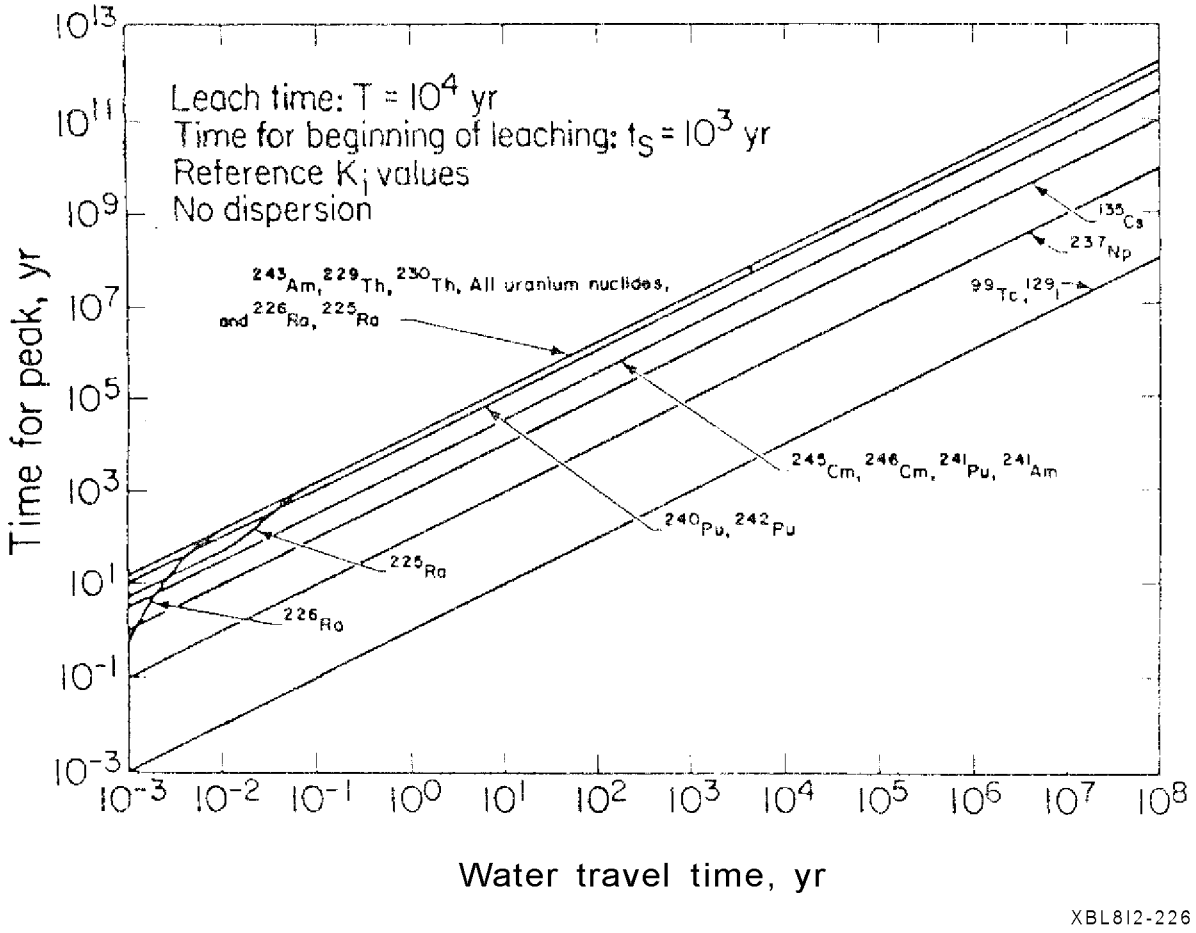


Figure 3.10 Variation of time for peak with water travel time for reprocessed PWR high level waste.

their peaks travel on the U-234 and U-233 characteristics respectively.

At a fixed water travel time the first peaks to arrive are those of 1-129 and Tc-99 which travel with the water front velocity because of their assumed unit retardation coefficient. One hundred years later the Np-237 peak reaches that position followed by Cs-135 peak 10 years later. Only after about 10 years later all other nuclides peaks start to arrive. The nuclides Ra-226, Pu-240, Pu-239, Am-241 and Am243 take a much longer time (10^4 years) to reach a given position than do 1-129 and Tc-99. If these nuclides (1-129, Tc-99, Ra-226 (U-238) and Np-237) could be contained, the range of water travel time of concern would be reduced to 1000 years, because all other nuclides with significant peak water dilution rates have already decayed to negligible values of water dilution rates before water travel times of 1000 years.

Figure 3.11 shows the variation of peak water dilution rate with leach time T for a fixed water travel time. For all first member nuclides for each order of magnitude increase in leach time we have an order of magnitude decrease in its peak water dilution rate. However, for the third members Th-229 (Ra-225) and Ra-226 changes in leach time have no effect on their peak water dilution rates. Therefore, changes in waste forms will not affect the magnitude of the peak water dilution rates of Ra-226 and Ra-225 (Th-229). Another important result which is not shown

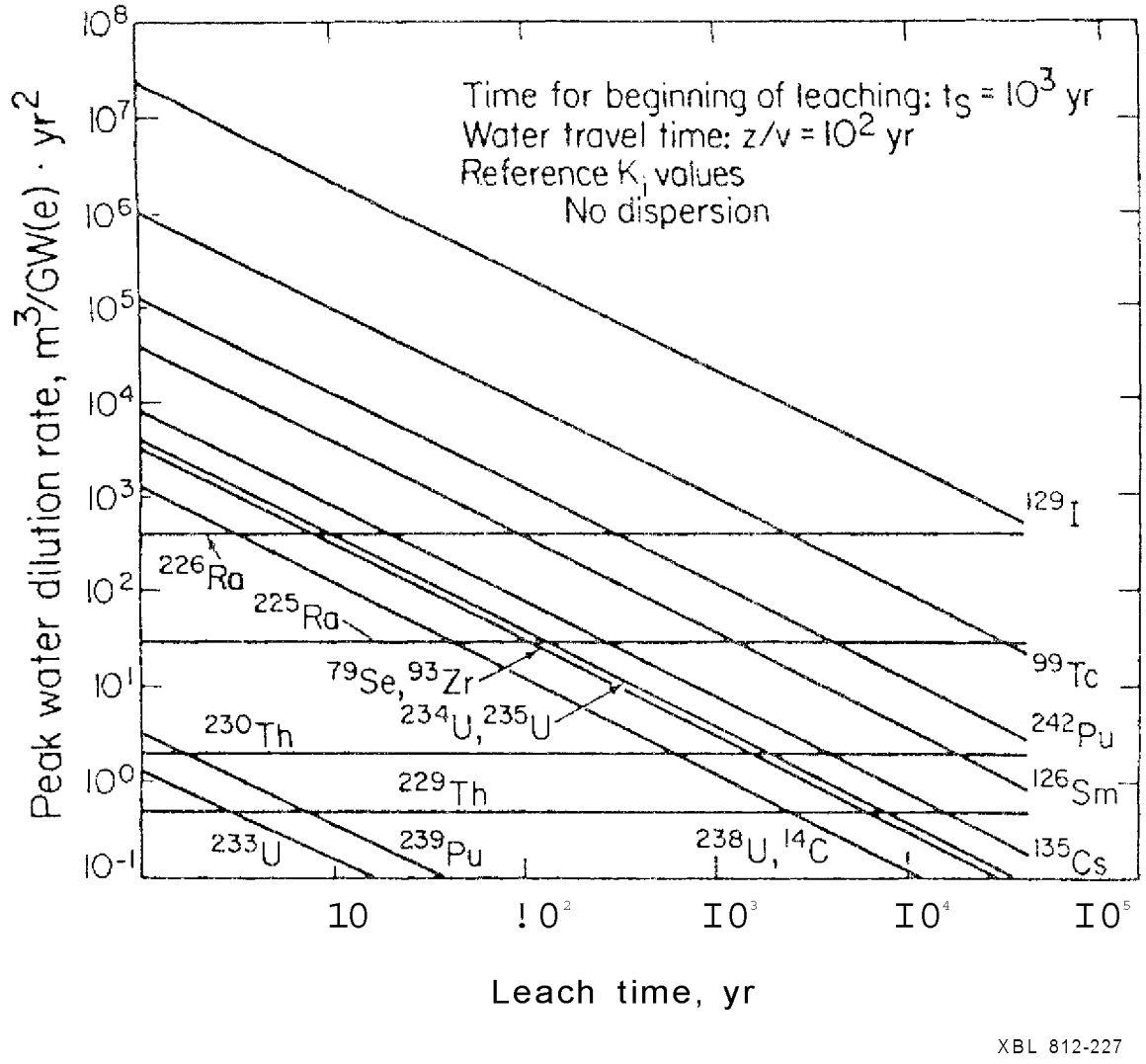


Figure 3.11 Variation of peak water dilution rate with leach time for reprocessed PWR high level waste.

graphically but it is implicit in the method is that the time for peak of any nuclide is independent of the leach time.

The effect of variation of the time for beginning of leaching on the peak water dilution rate is minimal as one can see in Figure 3.12. A delay in starting the dissolution can eliminate the shorter lived fission product like H-3, C-14, Sr-90 and Cs-137. When leaching begins as early as one year after emplacement the actinides Pu-241, Pu-238 and Cm-242 have not decayed to their long lived daughters yet and they will be present in the groundwater. But at the assumed reference water travel time of Figure 3.12, they have already decayed before they can migrate such a distance. All other important nuclides have half lives larger than 10^5 years. The initial inventory will not be changed significantly by the presence of engineered barriers. Although these barriers will not affect the magnitude of the peak water dilution rates they will delay the time when these peaks occur.

The variation of peak water dilution rate of the third members Ra-225 and Ra-226 with the value of the retardation coefficient are shown in Figure 3.13 through Figure 3.18. Each figure shows each one of the six cases described in Table 3.13. The half lives of the radionuclides in the U-234 chain are ordered in the same way as the half lives of the nuclides in the Np-237 chain are ordered. When the equilibrium coefficient of correspondent nuclides in each chain are equal, the behaviour of

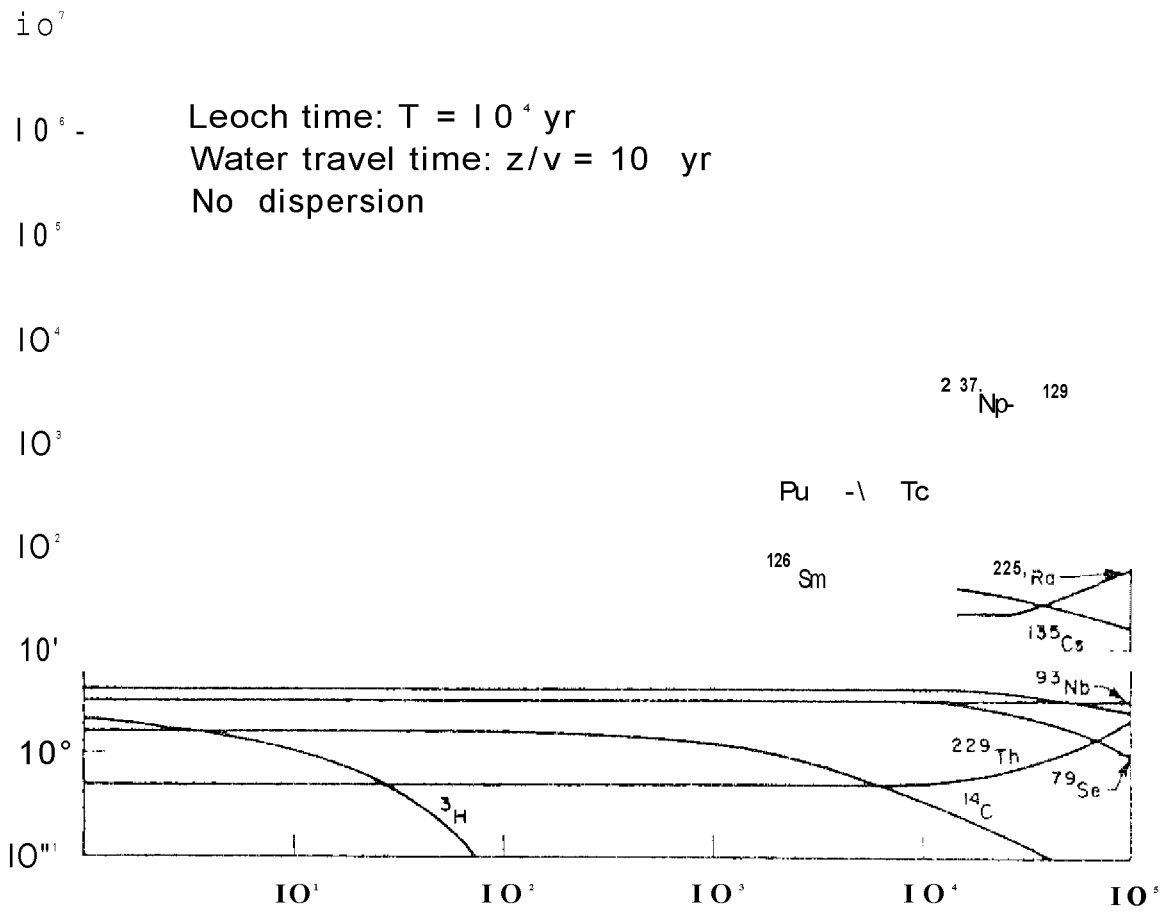


Figure 3 .12 Variation of peak water di1ution rate with the time for beginning of leaching for reprocessed PWR high level waste.

the solutions is expected to be also the same. In the figures for each one of the six cases, the above mentioned fact is confirmed. The variation of the peak water dilution rates with water travel time for each case shows its own characteristic behaviour differing from case to case in each of the six cases.

Figure 3.13 shows the. case 1 where K^ > K^ > K^. The curves for Ra-226 show same behaviour as the curves for Th-229 differing only in the magnitude of the peak water dilution rates. In case 1 the value of and were fixed at 10^4 and 10^2, respectively and K_2 was varied between those extremes. For all values of K_2 taken, the peak water dilution rate is approximately constant for water travel times of up to 100 and decaying monotonically thereafter. When K_2 value tends to 100, case 1 is approaching case 6. This fact can be confirmed by looking at the curves representing the case 6 (Figure 3.18) where K> K . > K~ and J 1 2 comparing to the curves in case 1 when K_2 is smallest. In case 1 as well as in case 6, no increase in peak water dilution rate with increased water travel time is observed.

Figure 3.14 shows case 2 where > K_2 > . In this case, an increase in peak water dilution rate with water travel time is observed. As K_2 is reduced to values close to 100 we are departing from case 2 and entering the case 4 where no increase is observed for any value of which is being varied. On the other hand, when K_2 approaches 10', case 2 tends to case 5 whose curves also show an increase in peak water dilution rate with

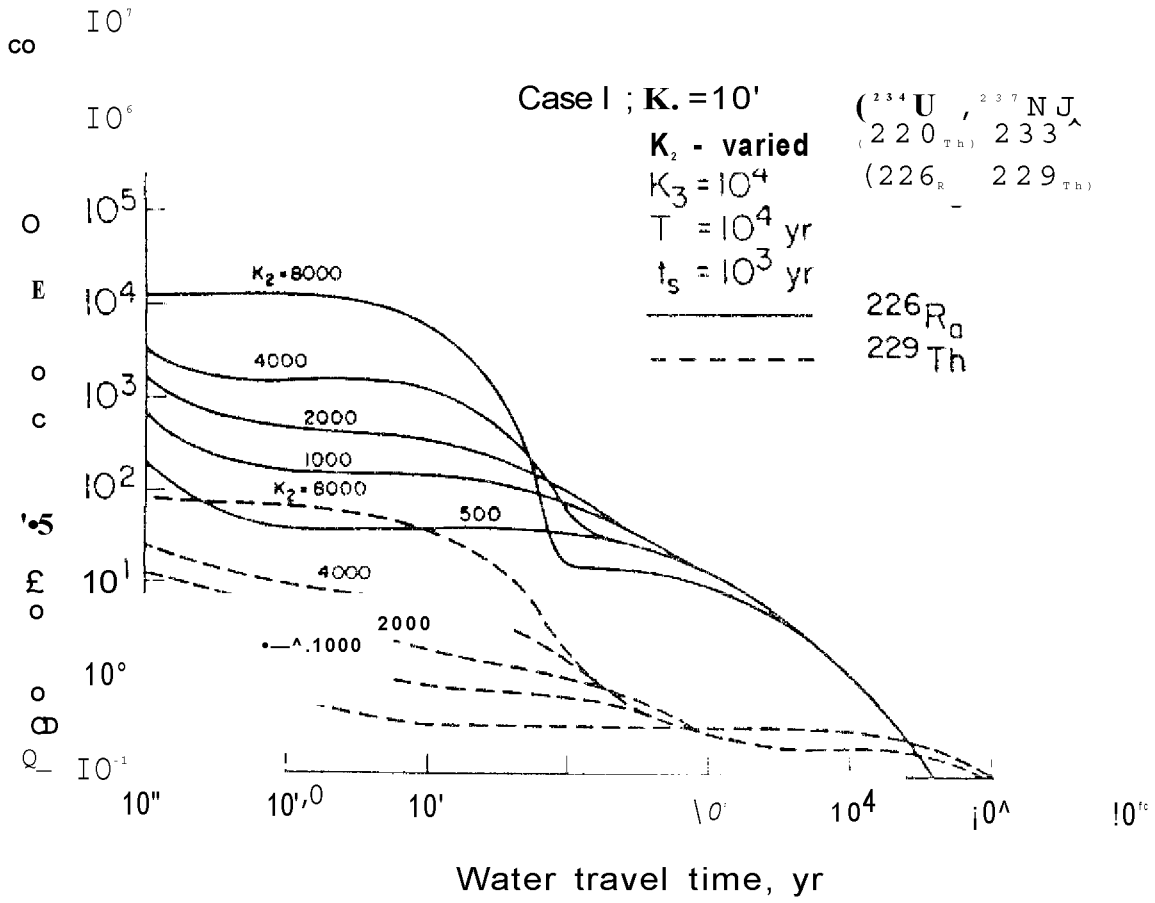


Figure 3-13 Variation of peak water dilution rate of third members ^{229}Th, ^{226}Ra ... in, *Ra* with the sorption coefficient and with water travel time for reprocessed PWR high level waste.

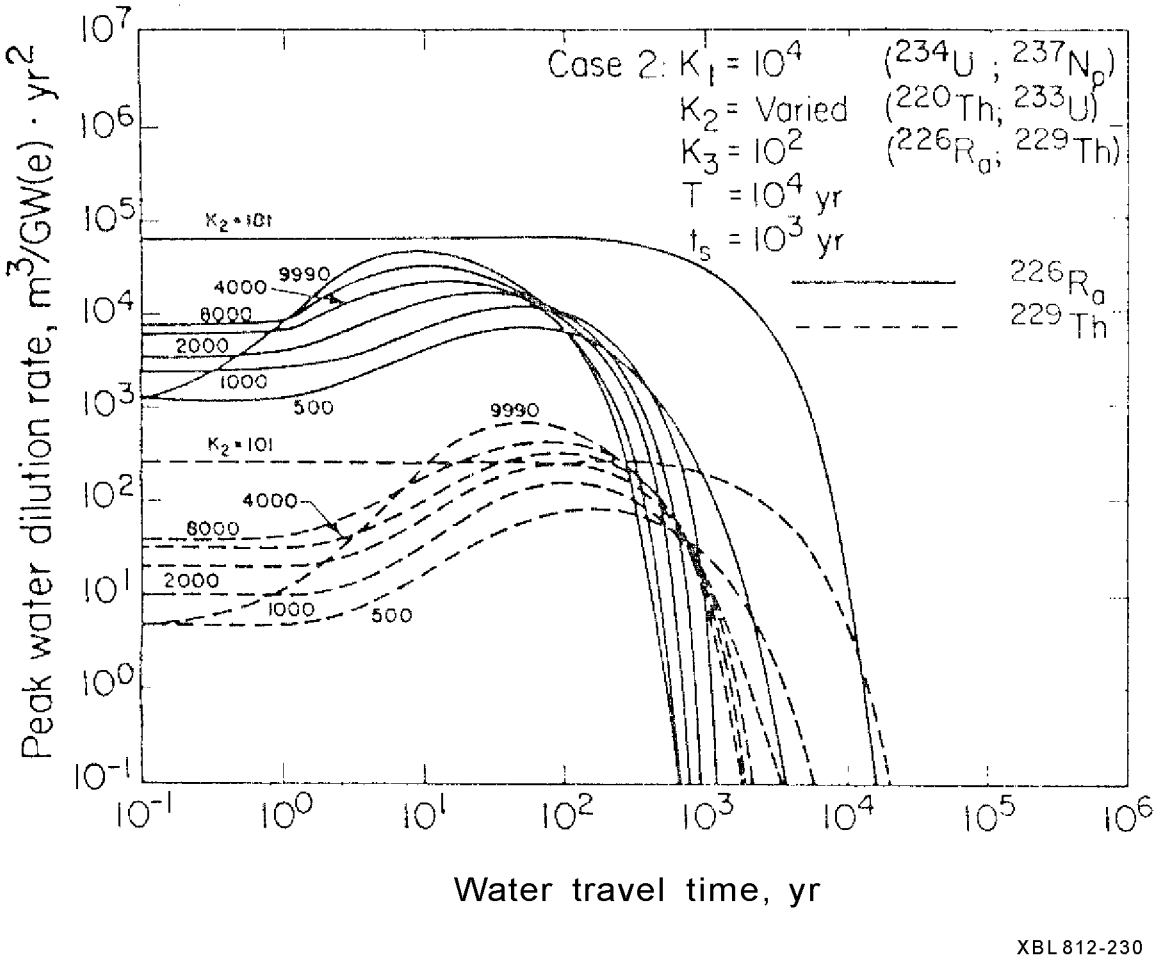


Figure 3.14 Variation of peak water dilution rate of third members ^{229}Th, ^{226}Ra with the sorption coefficient and with water travel time for reprocessed PWR hi-gh level waste.

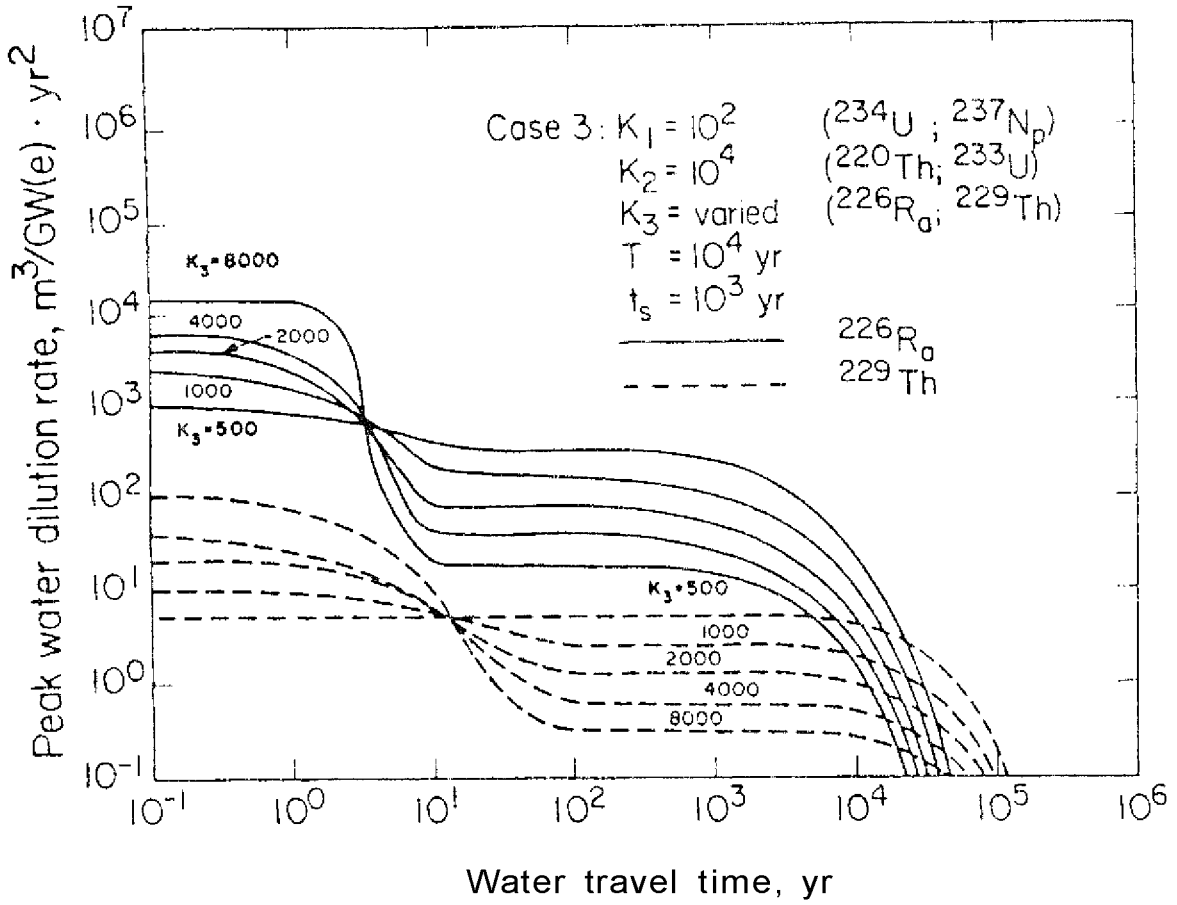


Figure 3.15 Variation of peak water dilution rate of third members ^{229}Th, ^{226}Ra with the sorption coefficient and with water travel time for reprocessed PWR high level waste

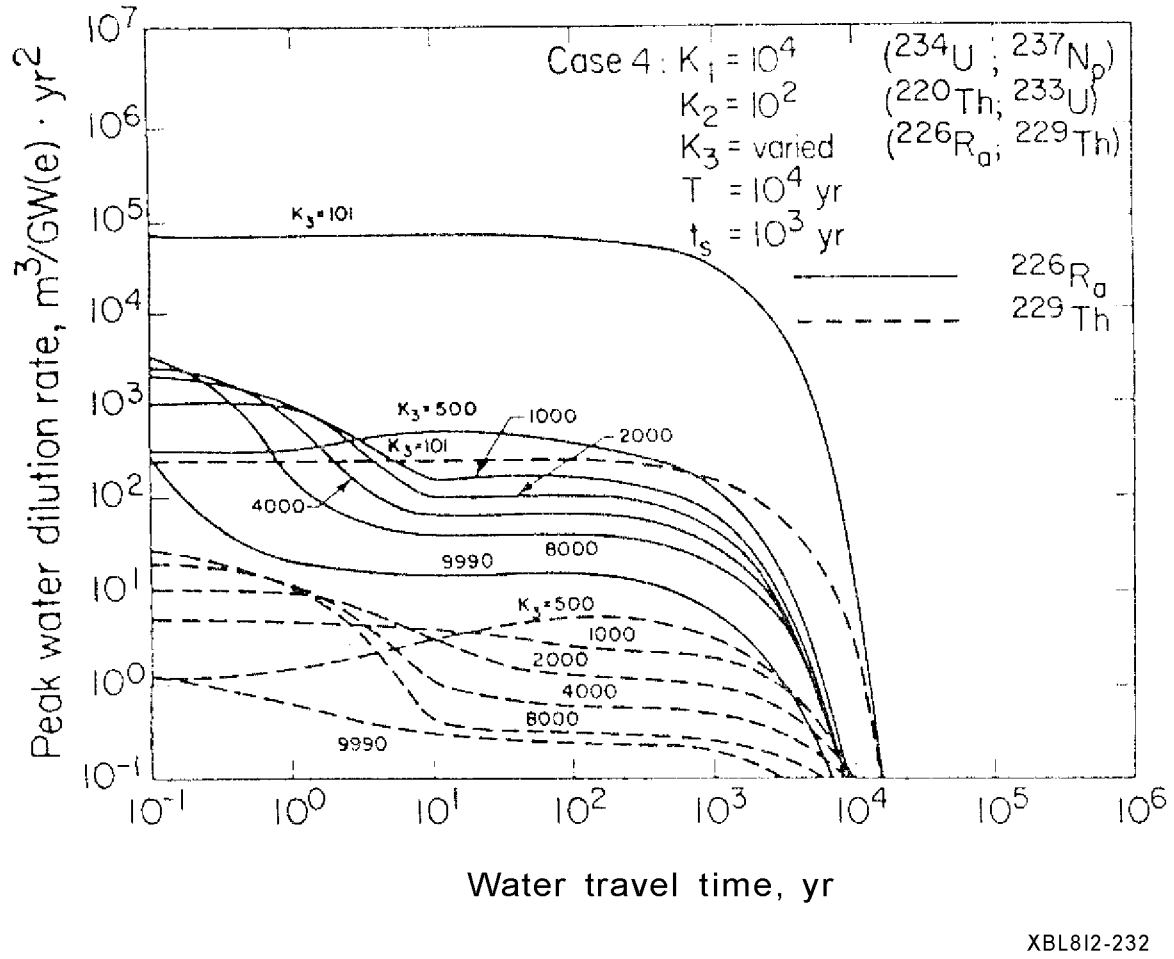


Figure 3.16 Variation of peak water dilution rate of third members ^{229}Th, ^{226}Ra with the sorption coefficient and with water travel time for reprocessed PWR high level waste.

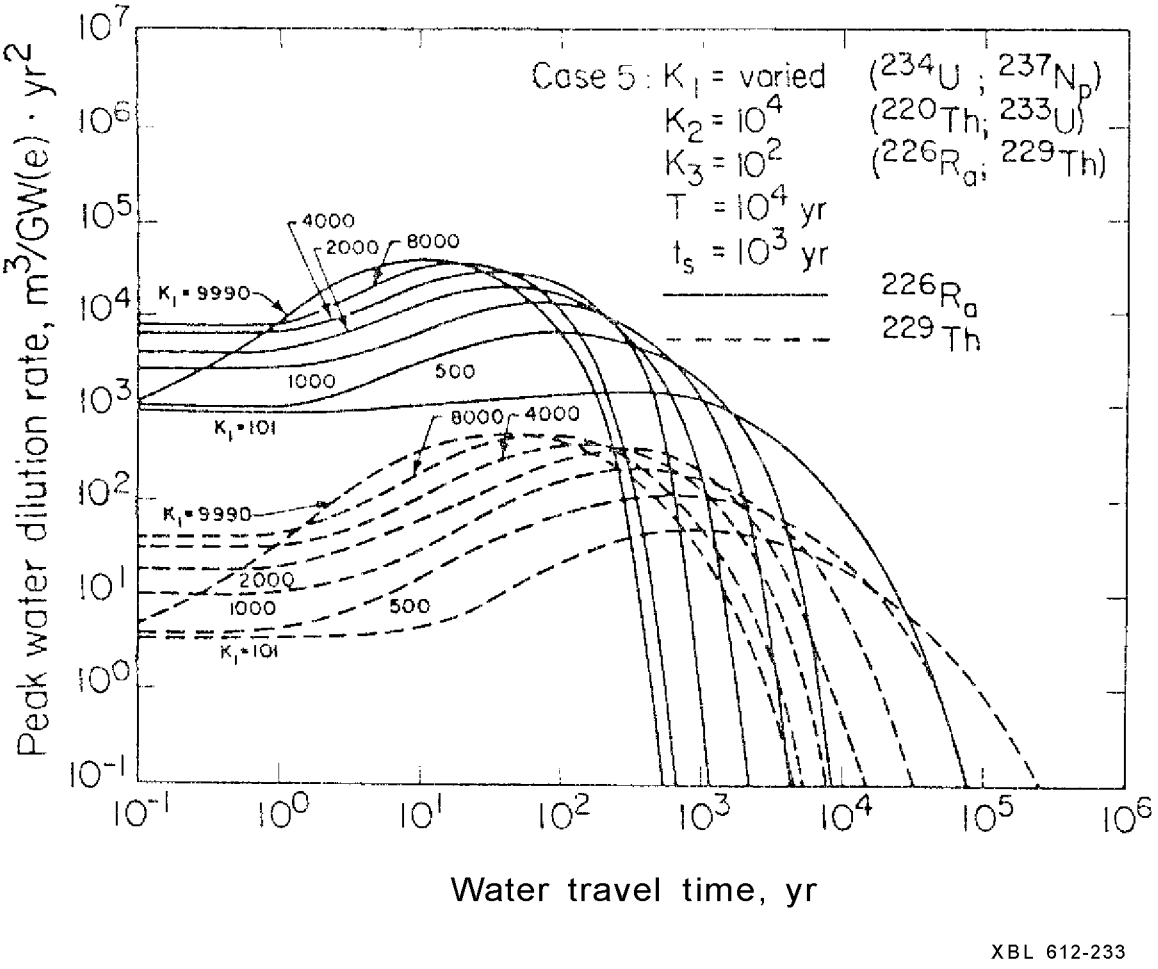


Figure 3.17 Variation of peak water dilution rate of third members ^{229}Th, ^{226}Ra with the sorption coefficient and with water travel time for reprocessed PWR high level waste

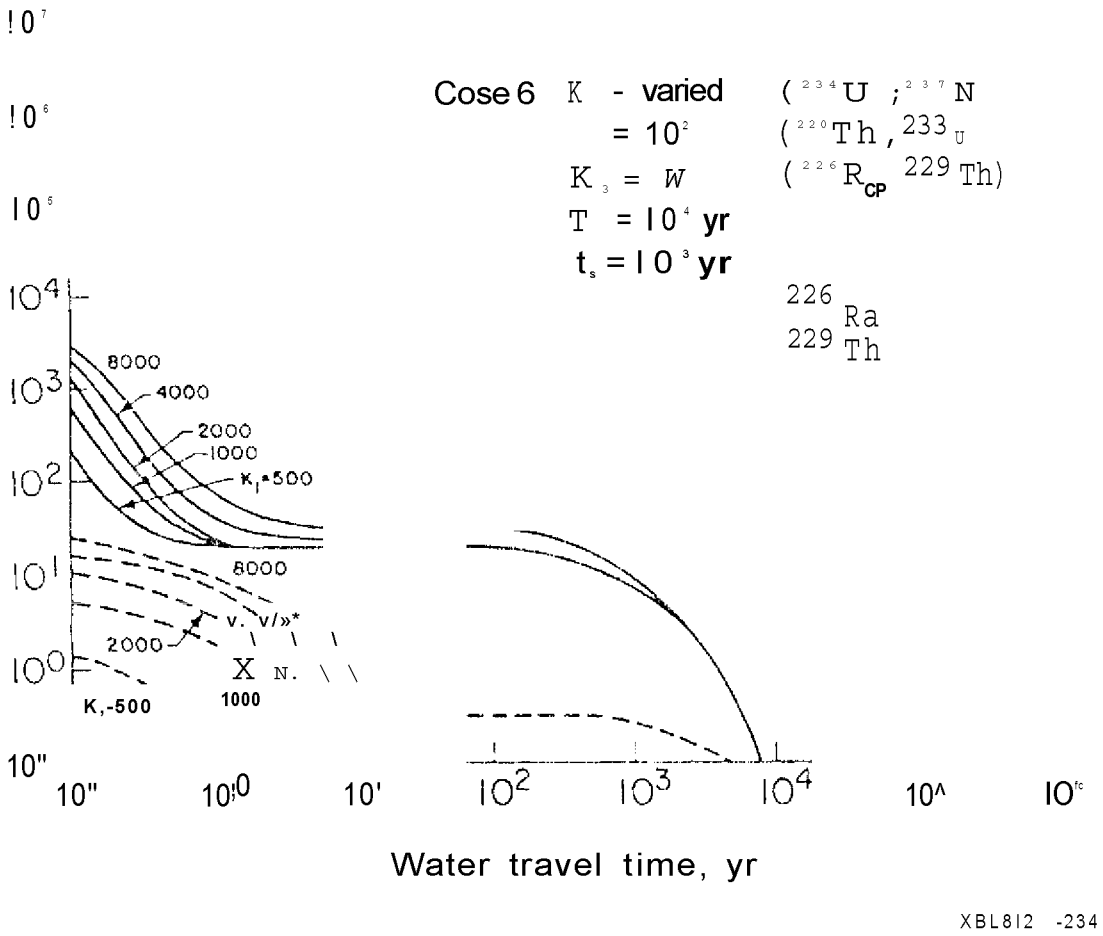


Figure 3 .18 Variation of peak water dilution rate of third members ^{229}Th, ^{226}Ra with the sorption coefficient and with water travel time for reprocessed PWR high level waste.

time. Case 2 and case 5 are the only cases where these build up and subsequent roll off in peak water dilution rate occur. These two cases have the common fact that has a smaller value than K and K_2. In all other cases, the peak water dilution rate decreases monotonically with water travel time.

3.7.5 Leaching of natural uranium ore and ore mill tailings

The nuclide inventories of the reprocessed high level waste used in the reference case is the result of the generation of 1 Gw(e)yr of electricity by a PWR. They operate at 33% thermal efficiency, 80% load factor and with a burnup of 30.4 MwD/kg. Such an electrical generation requires the total amount of 30.3 Mg of UO_2 fuel enriched to 3.3% U-235. To evaluate the amount of natural uranium ore required to produce this amount of fuel let us consider a gaseous diffusion enrichment plant with a depleted uranium stream with 0.0036 atom fraction of U-235. By a simple mass balance in both the total number of atoms and in U-235 atoms, one conclude that it is required 250 Mg of natural uranium ore. The eventual losses during fabrication are 1%, in conversion to hexafluoride is 0.5% and in milling and concentration is 5% (B2). The total activity of the uranium present in such ore will be 82 Ci of U-238 and 1.7 Ci of U-235.

When the uranium ore is processed, it is milled and

purified to remove the non-uranium rock. The non-uranium radioactive decay daughters, e.g. Th-230 and Ra-226 are also separated and are left with the piles of mill tailings. Suppose these piles of mill tailings are buried in such a way that a equivalent initiating event which started the leaching of the high level reprocessed waste canisters also happens for the piles of mill tailings. One can assume that the leach rate of the mill tailings is the same as the reference value adopted for HLW, i.e. 10000 years.

Since the ore body is expected to be where it has been for periods longer than 10^5 years, the initial activities of all daughters are in transient equilibrium with U-238. Also, for the purpose of this illustration, one can assume that U-238 and U-234 are in solution with the same chemical form (thus, with the same retardation coefficient) which allows us to consider U-234 as in secular equilibrium with U-238 because the intermediates Th-234 and Pa-234 have very short half-lives.

The peak water dilution rates resulting from the leaching of such piles of mill tailings are calculated and shown in Figure 3.19. The peak water dilution rate for Ra-226 from the mill tailings as well as the envelope of the peak water dilution rates of all nuclides present in a reprocessed HLW (Figure 3.9) are plotted against water travel time. Ra-226 peak water dilution rate due to the dissolution of the mill tailings is larger than the envelope of the peaks due to the leaching of the high level

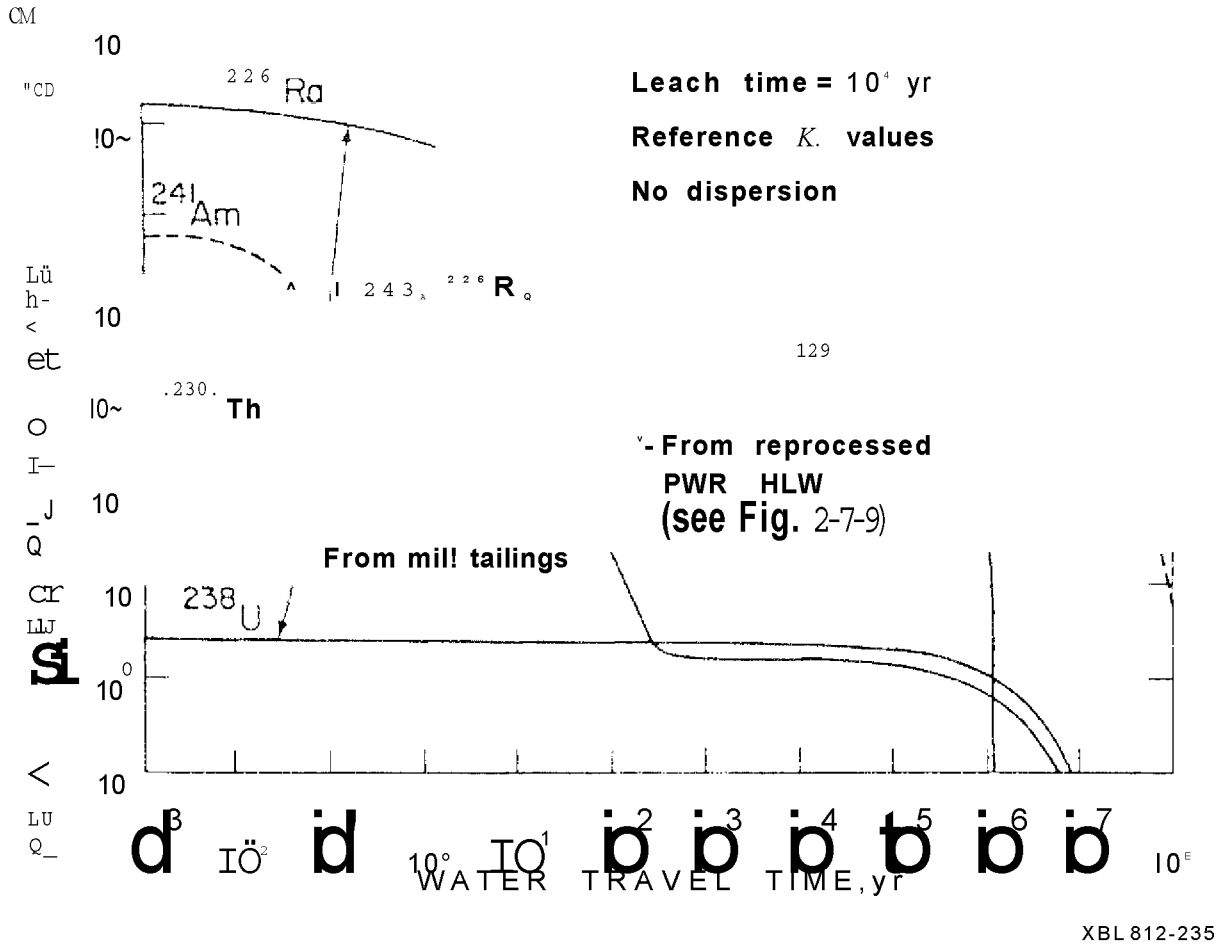


Figure 3.19 Variation of peak water dilution rate from natural uranium ore mill tailings with water travel time.

waste canisters. After water travel time of 10^6 years Ra-226 peak water dilution rate roll off rapidly because its precursor has already decayed.However, for water travel times larger than 10^9, HLW curve still shows the contribution of 1-129 although three orders of magnitude smaller than that of Ra-226 resulting from mill tailing leaching.

The same calculation done for the leaching of the mill tailings is repeated for the equivalent amount of natural uranium ore. In this case all the uranium will be present, not only 5% as in the case of mill tailings. One assume again that the same scenario adopted for the high level waste is valid for the uranium ore. Figure 3.20 shows the peak water dilution rate of Ra-226 due to the leaching of the uranium ore compared to the envelope of the peak water dilution rates of all nuclides present in the HLW. Again, the peak water dilution rate for Ra-226 in the ore is always larger than the envelope of the HLW nuclides indicating that for this set of retardation coefficients, the leaching of the equivalent amount of natural uranium ore used to produce the amount of waste considered is potentially more hazardous than the high level waste itself.

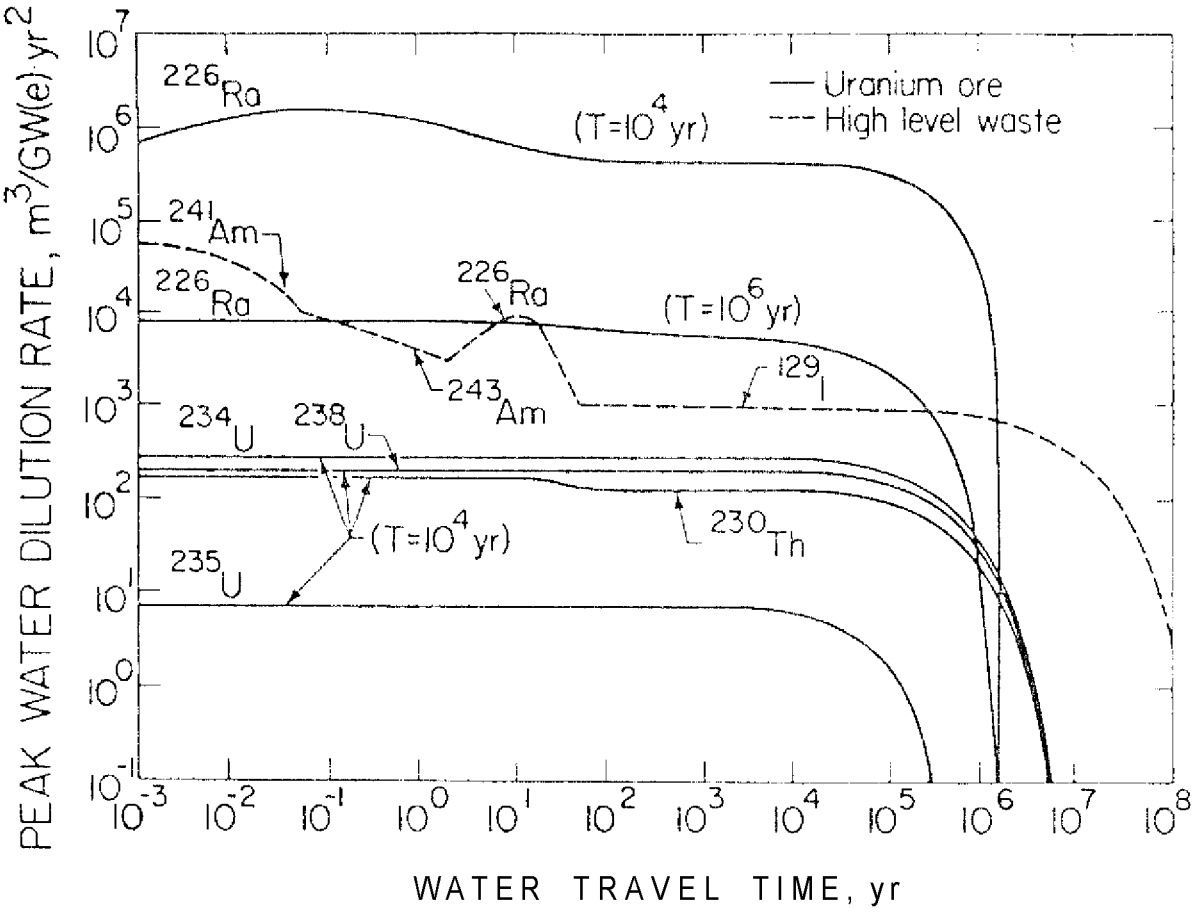


Figure 3.20 Variation of peak water dilution rate with water travel time, from leaching of natural uranium ore.

4. Migration of Radionuclides in Two-Dimensional Groundwater Flows Through Geologic Media

4.1 Introduction

This research is concerned with the prediction of radionuclide concentrations in aquifers in which a stationary two-dimensional groundwater flow is established. Repositories will be located in rock formations with no significant water content. However, abnormal events can occur which can cause radionuclide release from the waste package. These nuclides can eventually reach a nearby aquifer discharging into a fresh-water source.

Both migration of long actinide chains and long lived fission products in two-dimensional geological media as well as their discharges into the biosphere is modelled in this work. The theory on which this modelling is based upon was developed and presented in a previous report (Chambre,P1). This method provides a more realistic way than a one-dimensional model to assess the potential hazard to the biosphere posed by the accidental release of radionuclides from a high-level waste repository.

Analytical solutions to the radionuclide transport equation existent to date have been restricted to one-dimensional

groundwater flows. When two-dimensional flow fields needed to be considered, numerical schemes had to be invoked. Besides the capability of analyzing two-dimensional flow fields, the analytical non-recursive character of the present solution to the transport equation allows one to evaluate the concentration of an arbitrary member of a chain of any length without having to solve for its precursors. The evaluation of this solution requires little computing time.

In this present study, the two-dimensional groundwater flow is in steady state and dispersion effects are neglected. Adsorption reactions between nuclides in the water with the geologic media are assumed to be in equilibrium and there is no solubility limit of the nuclides in the groundwater.

The most important result derived in the theory is that when dispersion is negligible, the solution to the one-dimensional radionuclide transport equation is applicable along a streamline of the two-dimensional potential flow (Darcy's flow). The problem is then divided into two parts, namely: the determination of the hydrological flow net (i.e. the potential lines and the streamlines of the flow) and the evaluation of the radionuclide concentrations along the streamlines which passed by the source line in the aquifer being thereby contaminated. The discharge rate into the biosphere is also obtained.

The groundwater flow field can be represented either by

analytical expressions or by (scattered) field measurements of the groundwater potentials. The analytical representation is affected by superimposing an arbitrary number of point sinks and point sources. This superimposition can represent flow fields of arbitrary complexity. On the other hand, a given number of scattered potentiometric field data can be used to represent the flow net by fitting the data with a minimal total curvature spline function (B1). The above two methods can be combined to analyze the effects of injection and pumping wells in existing aquifers.

Once the potentiometric surface is determined and values for the hydraulic conductivity at the site obtained, the streamlines and the water travel time function (see Eq.(4.2.10)) can be obtained by the method of characteristics. The next step is to apply the solution of the one dimensional nuclide transport equation along a streamline. Finally, if the location of the intersection of the biosphere with the contaminated streamlines is known one can evaluate the discharge rate into the biosphere.

The above described steps are performed by the computer program (UCBNE21). Due to the semi-analytical character of this program, the computing time is much smaller than finite-difference schemes used to solve the equivalent problem. A complete listing of the program is given in Appendix C. The program has the capability of using the LBL Computer Center plotting software to automatically generate graphs.

As an application of the utilization of this computer program we studied the far field migration of radionuclides for two candidate repository sites. These are the Waste Isolation Pilot Plant **(WIPP)** in Eddy County, **New** Mexico and the Basalt Waste Isolation Project (BWIP) in Hanford, Washington. Hydrological data available for both sites are reviewed and the contaminated regions for the most important nuclides as well as the nuclide discharge rates, are estimated by applying this two dimensional analytical theory for radionuclide transport.

4.2 Theoretical Background

The theoretical developments leading to the solution of the radionuclide transport equation in a two-dimensional geological media are presented in a previous report (Chambré, PI.) . In this section we summarize the important steps shown in that work and we also emphasize the important results needed in the present work.

4.2.1 The governing equations

The two-dimensional hydrological groundwater flow is time independent, incompressible and it is a Darcy-type flow. Dispersion effects are neglected and sorption reactions are assumed to be in equilibrium. No solubility limits are considered, but by suitably defining the boundary condition one should be able to apply the present solution with solubility limit of the first member. Water density and soil porosity are considered constants.

Subject to above assumptions, the conservation equation for the nuclide concentration in water (x,y,t) for the i-th member of a chain is given by (PI,Eq.(5.1.1))

$$K_i \frac{\partial N_i}{\partial t} + \hat{V} \cdot (\hat{v} N_i) = K_{i-1} \lambda_{i-1} N_{i-1} - K_i \lambda_i N_i \qquad i=1,2,\ldots \qquad (4.2.1)$$

Here K_i are the retardation coefficients, v is the groundwater velocity (m/yr),*i are the decay constants (1/yr). In view of the incompressibility assumption the groundwater velocity satisfies the following conservation of mass relation

$$V \cdot v = 0 \qquad (4.2.2)$$

where the groundwater velocity is given by Darcy's law

$$v = -kV\langle\} \quad ; \quad k = k'/e \qquad (4.2.3)$$

Here k' is the hydraulic conductivity of the soil (m/yr), c is the porosity and $\langle p$ is the hydraulic head (m). Although k is the hydraulic conductivity divided by the porosity, we will refer to k as being the hydraulic conductivity. Substituting Eg. (4.2.3) into Eq. (4.2.1) and using Eq. (4.2.2) the transport equation is rewritten as

$$\frac{\partial N_i}{\partial t} - \nabla \cdot \left(\langle H \langle \frac{\partial N_i}{\partial x} \right) \frac{\partial}{\partial x} + \frac{\partial}{\partial y} \left(\frac{\partial N_i}{\partial y} \right) + A_i K_i N_i = A_{i-1} K_{i-1} N_{i-1} \qquad (4.2.4)$$

$$i = 1,2 \ldots \quad A_0 = 0$$

Let us denote by R the region of interest and by P any point inside R (see Figure 4.1). The radionuclides are assumed to be released along a line source S in R and a point on S will be called Q. With the above notation,the initial condition (Pi,Eq. (5.1.4)) and the boundary condition (Pi,Eq. (5.1.5)) can be expressed by the following relationships

$$N_1(P,0) = 0 \quad ; \quad P * Q \quad ; \quad P \in R \qquad (4.2.5)$$

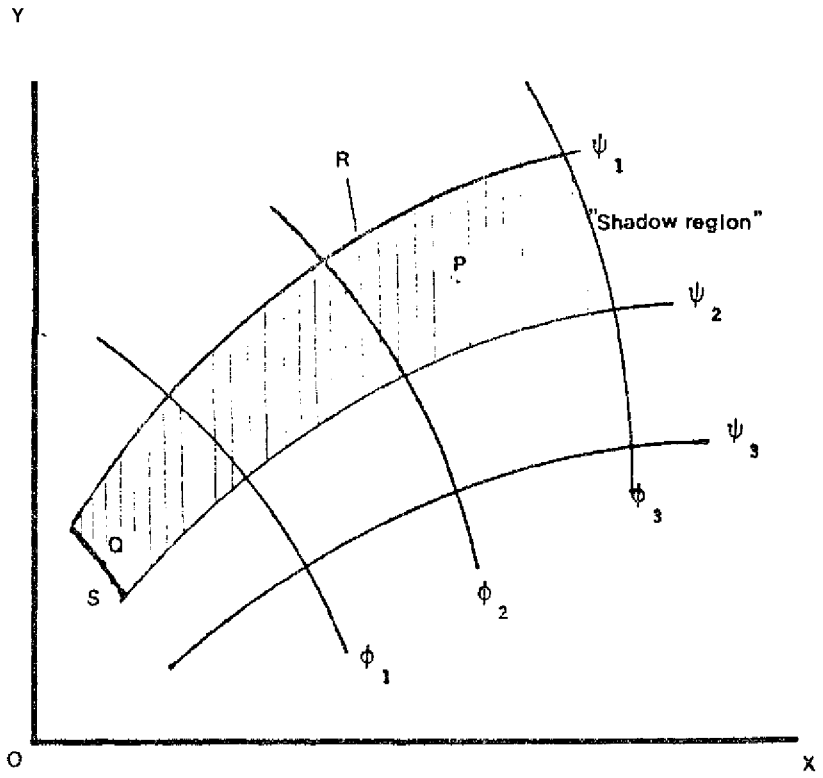


Figure 4.1 Pictorial view of the system being studied: R is the region of interest, P is any point inside R, S is the the source line, Q is a point on the source line are the streamlines and ϕj are potential lines.

$$N_i(0,t) = N^{\circ}G_i(Q,t) \quad ; \quad QcS, \quad t>0 \qquad (4.2.6)$$

$$G_i(P,t) = 0 \quad ; \quad t<0, \quad PeRUS \qquad (4.2.7)$$

where $G^{\wedge}(Q,t)$ is an arbitrary release function which describes the time dependent dissolution and release of the waste into the aquifer. is the initial concentration of the i-th nuclide.Eq.**(4.2.2)** and Eq.**(4**.2.3) describe the groundwater flow field while Eq. **(4**.2.**4)**,Eq. **(4.2**.6) and Eq. **(4**.2.7) govern the radionuclide transport through the geologic media.

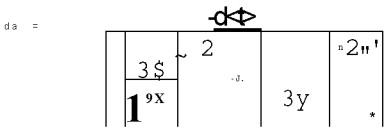
4.2.2 Two-dimensional groundwater flow fields and the water travel time function

Two-dimensional groundwater flows are representable by potential flows and one can define the streamfunction of the flow $\$(x,y)$ by the following (Pl,Eq. (5.2.2))

$$\frac{3I|I}{3*} = -k\frac{3<\}>}{3y} \qquad (4.2.8)$$

$$\frac{3^{\wedge}}{3y} = k\frac{3<(>}{3x} \qquad (4.2.9)$$

The water travel time function o(x,y), (yr), is defined along a fixed streamline by the following equation (Pl,Eq. (5.2.7))



for $\psi(x,y)$ = constant (4.2.10)

Physically, $\sigma(x,y)$ represents the time an elementary volume of water, initially at a position (x_0, y_0), takes to reach a given position (x,y) downstream travelling along the streamline which passes through these two points. By using the orthogonality condition between the streamfunction $\psi(x,y)$ and the potential function $\phi(x,y)$ in addition to the definition of the water travel time function $\sigma(x,y)$, the conservation equation for the i-th member of a radioactive chain Eq.(4.2.4) can be reduced to the following greatly simplified form (Pl,Eq. (5.2.6))

3N. 3N.

Eq. (4.2.11) is valid along a streamline where $\psi(x,y) = c$. The concentration along this streamline is now a function of only two variables, i.e. $N_i = N_i(\sigma(x,y), t)$. We will now change the notation $\sigma(x,y)$ showing explicitly the dependence on (x,y) along a streamline by simply writing a. Therefore, the concentration of the i-th member will be denoted by $N_i(a,t)$.

Thus the two-dimensional problem of evaluating (x,y,t) can be reduced to a one-dimensional problem of evaluating (o,t) along a streamline provided one knows how the water travel time varies along that streamline. In the next section we will show how this problem can be solved by making use of the previously

derived analytical solution for the one-dimensional problem (Chambre,Hi,section 4.4).

4.2.3 The solution of the two-dimensional transport equation

From the definition of the water travel time function *o* Eq.(4.2.10) one can realize that lines of constant potential are parallel to lines of constant water travel time along a streamline (i.e. ,when d$=0 implies d o=0 in Eq. (4 . 2 .10) when d'|' = 0 .

This parallelism is mathematically expressed as

$$(kv^{**}) \bullet (V\,c) = -1 \quad ; \quad *Mx,y) = c \qquad (4.2.12)$$

The side conditions that o(x,y) must satisfy are (Pl,Eq. (5.3.3) and Eq. (5.3.4)),see Figure 4.1.

$$a(Q) = 0 \quad ; \quad QcS \qquad (4.2.13)$$

$$a(P) > 0 \quad ; \quad \text{P is a point in the shadow region (see Figure 4.1)} \qquad (4.2.14)$$

The initial and boundary conditions for the radionuclide concentrations along a streamline can be restated as (Pl,Eq. (5.3.8))

$$\mathbf{N}_i(P,0) = N_i(a,0) = 0 \quad ; \quad o > 0 \qquad (4.2.15)$$

$$N_i(Q,t) = 1\hat{}(0,0 = N_i G_i(0,t) \quad ; \quad t>0, \quad o=0 \tag{4.2.16}$$

Let us define $G_i(t)=G_i(0,t)$. Fiquro 4.1 illustrates the system being studied. Only those streamlines which cross the source line S will be contaminated. In the case of Figure 4.1 all the streamlines contained between the lines and $\backslash h_2$ form the region which can contain radionuclides since there is no dispersion. This region downstream from the repository will be called the "shadow region". Therefore, the shadow region is the specific region of interest where the calculations are going to be performed.

For a given streamline crossing the line source S at. a point Q one must solve Eq. (4.2.11) subject to the initial condition Eq. (4.2.15) and the boundary condition Eq. (4.2.16). The radionuclide concentrations are now expressed as a function of the time t started after the beginning of the release and of the water travel time o counted from the time when the water leaves the source line S.

Mathematically, this problem can be made equivalent to its one-dimensional counterpart with a constant water velocity. Replacing (z/v) in the governing equation Eq. (2.2.1) for the equivalent one-dimensional problem by o , one obtains the governing equation for the two-dimensional problem valid along a streamline of the flow i.e. Eq.(4.2.11). Therefore, the solution for the one- dimensional case Nj_(z/v,t) can be used to express

the radionuclide concentration along a streamline $N_i(o,t)$ once we replace z/V by cr . The solution to the one-dimensional radionuclide transport equation with constant water velocity was developed in a previous report (Chambre,Hl). Here the solution is rewritten

$$N_i(Kt) = N^{\circ} \; ; \; {}^{A}i^{K}i^{\circ} \quad (t - K_{i0}) \; f$$

$$\cdot \; - A K o \; \cdot \; c \qquad (4.2.17)$$

$$j=1 \quad J \quad m=i \quad 7^{\wedge} \quad r=j \quad \text{™} \quad 1\ 8\ \text{™}\ U\ J \quad 3 \quad JJ$$

$$r?\%$$

The coefficients are defined as follows

(4.2.18)

$$A_{l}^{P} = \sum_{r=j}^{n} A_r^K r$$

(4.2.19)

$$m \qquad \sum_{r=j}^{n} (K_r - K_m)$$

(4.2.20)

$$D_{rm}^{Cj)} \qquad \sum_{q=j}^{n} (A_{qm} - A_{rm}^{N})$$

(4.2.21)

$$A_{il}^{-} = \sqrt{\frac{A.K. - \grave{A}.K.}{K. - K.}}$$

The function g (t) is defined by the following expression

$$g_{rnr}(t) = e^{-A_r (t-K_a)} h(t-K_m\sigma) \qquad (4.2.22)$$

The symbol * represents the convolution integral of the function in the brackleted term

$$g_{rm}(t) \circledast G_j(t) = \int_0^t g_{rm}(\zeta)\, G_j(t-\zeta)\, d\zeta \qquad (4.2.23)$$

Repositories will be located in rock formations with no significant quantities of water,and release of radionuclides from the waste package and consequent contamination of surrounding aquifers will occur in case of an abnormal event. The proposed scenario (D1,R2) for the accidental release of radionuclides from the repository assumes that a fracture is formed which connects the repository to a surrounding aquifer. The water flowing through this fracture leaches out radionuclides from the waste package and carries them to the aquifer. Although the transport of radionuclides through this fracture takes actually some time,in this study we assume this time to be negligible. In other words,the repository is assumed to be placed directly in the aquifer being considered. This is a conservative assumption. Therefore,the source line S described in Figure 4.1 will indeed represent the repository.

A commonly used release mode of radionuclides from the repository is the so called decaying band release. This model states that every nuclide is released with the same constant

release rate during a period called leach time T (yr). Mathematically this release mode is expressed by the following (HI)

$$G_i(t) = \sum_{j=1}^{i} B_{ij} \exp(-\lambda_i t)\,[h(t)-h(t-T)] \qquad (4.2.24)$$

where B_{ij} are the Bateman coefficients. The initial concentration N_i^0 is given by the following expression (Hi, section 3.2)

$$N_i^0 = \frac{M_i^0}{QT} \qquad (4.2.24a)$$

here M_i^0 is the total activity of the i-th nuclide when the leaching started, Q is the total groundwater flowrate in the aquifer through the waste (m^3/yr) and T is the leach time (yr). In this present work we adopted the above model and the solution Eq. (4.2.17) is rewritten after substituting Eq. (4.2.24) and evaluating the convolution integral

$$N_i(o,t) = N_i^0 \exp(-\lambda_i K_i 0)\left[\sum_{i=1}^{i} B_{ii} \exp(-\lambda_i (t-K_i 0))\right] f h(t-K_i a) - h(t-T-K_i$$

$$+ \sum_{j=1}^{i-1} \sum_{m=j}^{i} \sum_{\substack{r=j \\ r\neq m}}^{i} \sum_{k=1}^{j} Q_{rm}^{(j)} B_{jk} \{\exp[-\Delta_{rm}(t-K_m \sigma) - \lambda_m K_m \sigma]\,[h(t-K_m \sigma) - \qquad (4.2.26)$$

$$-\exp(-T^{\wedge}-A^{\wedge}))\,h(t-K_m 0) - \exp[-\lambda_k t \sim (\lambda_m-\lambda_k)\ 0]\,[h(t-^{\wedge}a) -$$

$$-h(t-T-K\ 0)]\ )$$

where the new coefficient is defined by

i-1

q ^) . ———— r m ———— q=3 g q

rm (\v\v À r K r + w H tVq 'V' VVm K q " K r > ^ r K r ^^q 5 J

q=j

q*r#m

(4.2.27)

An important feature of this later form of the solution is that it allows the possibility of two or more nuclides in the same chain to have the same retardation coefficient value. The singularity caused by equal values that the previous solution contained is thus removed.

If the boundary condition along every point on the source line S has the same value,this will cause the concentration along a line of constant water travel time (isochronous lines) to be also constant (see Eq. (4.2.26)). Hence,the isochronous lines and the iso-concentration lines coincide with each other although each function has different values on these lines.

Therefore,to completely describe the concentration history one must obtain the groundwater flow net (i.e.the streamlines of the flow) and how e(x,y) varies along each streamline. When o(x,y) is substituted into Eq. (4.2.26),it will yield the concentration of the i-th member in the groundwater.

In the next Section 4.3 a superposition of an arbitrary number of point sinks and point sources is used to represent some

complex groundwater flows. An analytical expression for the Potentiometrie surface is derived and we show how to determine the streamlines,the water travel time function and the radionuclide concentrations. In Section 4.4 ,a set of (scattered) Potentiometrie field data for a groundwater aquifer is used to construct the Potentiometrie surface. This is done by fitting the data with a minimal total curvature spline surface.

4.3 Two-Dimensional Groundwater Flows Represented by an Analytical Expression

Many groundwater flows can be adequately simulated by the superposition of an arbitrary number of point sinks and point sources in an uniform flow. In addition, when such an analytical potential function is superimposed onto the potentiometrie surface of an actual aquifer (see next Section 4.4) one can analyze the effects of injection and/or pumping wells.

4.3.1 The analytical solution for a point sink-point source flow field

Before studying the general case of an arbitrary number of point sinks and sources, let us first consider an injection well and a pumping well located at a distance 2a apart in an infinite homogeneous isotropic medium. The hydraulic head is given by the expression (PI,Section 5.4)

$$(x,y) = \frac{Q}{keD_{0}.2T!} \ln \bullet /(x-a)^{x} - y^{2} - \% \quad (4.3.1)$$

$$. (x+a)^{2} - y'$$

Where Q is the volumetric flow rate (m^3/yr) of either the source or the sink. D_{0} is the aquifer thickness (m) and $_{e}$ is the porosity of the geologic media. Here the hydraulic conductivity k (m/yr) is taken as being constant. The corresponding stream function is given by the following relationship

$$f(x,y) = \frac{Q}{gDq2tt}\arctan\left(\frac{y}{x-a}\right) - \arctan\left(\frac{y}{x+a}\right) \qquad (4.3.2)$$

To obtain the water travel time function for this flow field one substitutes Eq. (4.3.1) into Eq. (^.2 .10). One then integrates the resultant expression along a streamline (i.e. holding \\> constant) starting from a curve of constant potential on which one assumes the source to be located, up to a line of constant potential * downstream. Along the initial constant potential line ◁ , o=0. In the previous report (Chambre, PI) this integration was performed and the resultant expression is

$$o(x,y) = \frac{a^{2E}D_n 2^{Tr}}{(1-c^2)}\left(\frac{1}{c+\cosh *}\sinh\langle J\rangle - \frac{2c}{(l-c^2)^{\wedge}}, \tan^{-1}\left|\left(\frac{1-c}{1+c}\right)^{2}\tanh\left(\frac{x}{2}\right)(-)\right|\right)^{2}_{*\,i} \qquad (4.3.3)$$

where $_{\circ}eD_{\circ}2rr/Q$; $\langle t\rangle_2 - 4 > eD_{\circ}2tt/Q$

if $c = \cos(\hat{}eD_{\circ}2Tr/Q) = \pm 1$ and (4.3.4)

$$o(x,y) = \frac{Ea^{2}Dq2\pi}{Q}\left\{-\tanh(x/2) - \frac{1}{6}\tanh^{3}(x/2)\right\}^{2}_{\bullet}, \qquad (4.3.5)$$

if c * ±1

Let us first define the dimensionless hydraulic head * by the following

$$* = *kD_{\circ}e27r/Q \qquad (4.3.5a)$$

and the dimensionless stream function by

$$Y = \hat{D}_{-}e2ir/Q \qquad (4.3.5b)$$

and finally, the dimensionless water travel time function by

$$I = oQ/a^{2}eD_{0}2\hat{i}r \qquad (4.3.5c)$$

Eq. (4.3.5a), Eq. (4.3.5b) and Eq. (4.3.5c) are plotted in Figure 4.2. The streamlines are circular segments centered along the dimensionless ordinate axis (y/a) and the potential lines are circles with centers on the dimensionless abaissas (x/a). The lines of constant water travel time are shown by the dotted curves.

To evaluate the concentration of a given member of a radioactive chain at a given time t after the leaching started one simply substitutes Eq. (4.3.3) or Eq. (4.3.5) into the general non-recursive solution Eq. (4.2.26). Clearly, the isochronous lines will also be the iso-concentration lines. This completely analytical solution will be used as a benchmark example for comparisons with the results from the semi-analytical methods used in next Section 4.3.2 where completely analytical solutions are difficult to obtain.

A point sink-point source configuration can be used in practice to experimentally determine aquifer parameters like the hydraulic conductivity k and radionuclide migration parameters

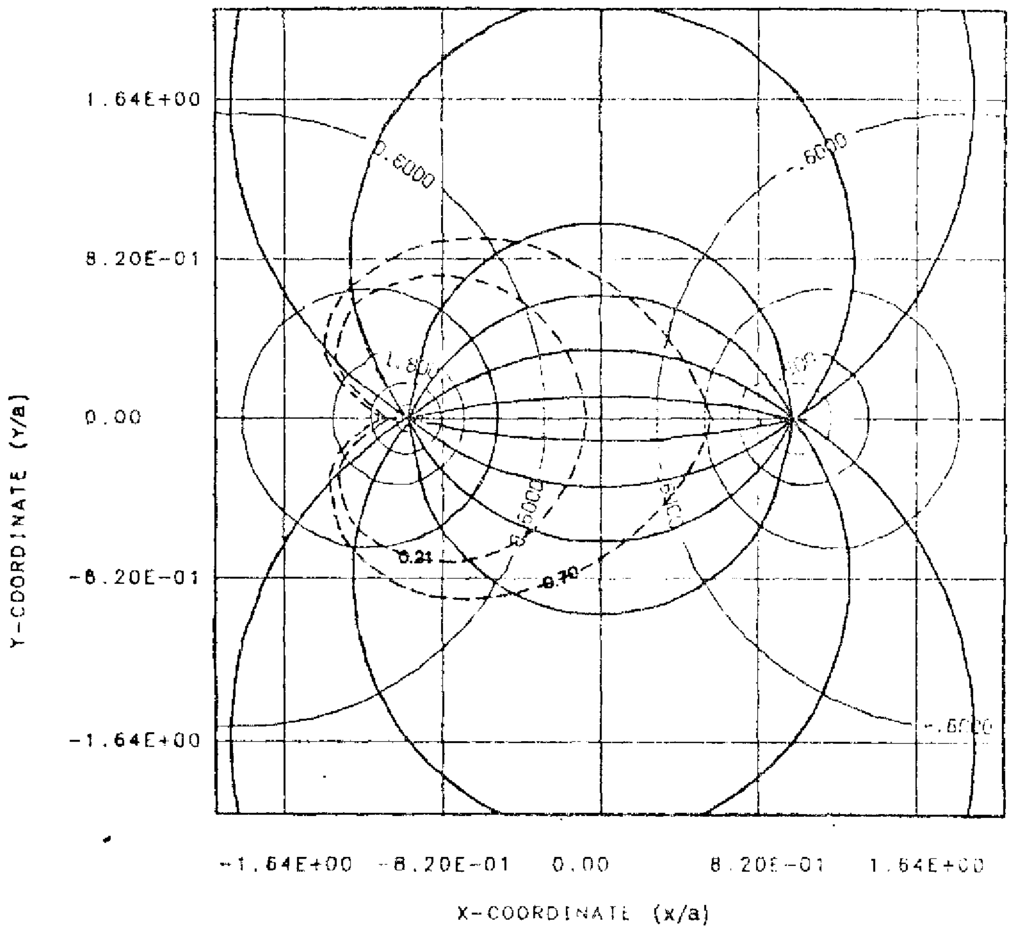


Figure 4.2 Potential lines and streamlines for the point source and point sink flow.Dotted lines indicate isochronous lines (which also are the iso-concentration lines).

like the retardation coefficient . For this illustration, let us assume that the hydrological parameters are known and one is interested in experimentally determine the retardation coefficient of a nuclide.

In order to use the solution to the two-dimensional nuclide concentration Eq. (4.2.26) one must simulate a decaying band release Eq. (4.2.24) at the injection well (the point source). This is done by preparing an initial inventory (Ci) for each member of the chain. These nuclides are injected at a rate M?/T into the we11, of volumetric flow rate Q (m^3/yr), during a period of time T (yr). For a choosen medium, the transmissivity (i.e. the product kD^ (m /yr) is known. The retardation coefficients of the precursors are also assumed to be known. The parameters Q and T are selected to provide reasonable water travel times at the pumping well (point sink) so that the arrival time of the first nuclide is not too long. By monitoring the concentration history at the pumping well and comparing with the analytical solution one can determine the retardation coefficient for the i-th member of the chain.

For the purpose of this illustration, let us consider a geologic medium with the following parameters: 0^=10 meters and k=5 m/yr, the injection well flow rate is 0=7000 m^3/yr and the duration of the release is T=0.3 years. Furthermore, one curie of pure Ra-226 is released at a constant rate of 1/0.3 Ci/yr into the injected water. The injection we11 and the pumping well are

separated by a distance 2a=60 meters.

The first nuclide arrives at the pumping well at a time given by

$$= K_{mxn} \cdot o_{mm} \qquad (4.3.5d)$$

where K_{mm} is the smallest retardation coefficient of all nuclides in the chain. if the nuclide has no precursors, K_{mm} is its own retardation coefficient. a_{min} is the smallest water travel time to the pumping well of all the contaminated streamlines.

The last nuclide arrives at the pumping well at a time given by

$$t_d = K_{max} o_{max} + T \qquad (4.3.5e)$$

where K_{max} is the largest retardation coefficient of all nuclides in the chain, if the nuclide has no precursors, K_{max} is its own retardation coefficient. a_{max} is the longest of all water travel time to the pumping well for any of the contaminated streamlines.

One can conclude that the duration of release will be given by

$$t_d - t_a = K_{max} o_{max} - K_{mm} o_{mm} + T \qquad (4.3.5f)$$

Figure 4.2a and Figure 4.2b show the location of the Ra-226 contaminated region (dotted area) for two different times after the experiment started. For these figures, the assumed retardation coefficient is 10. Figure 4.2c shows the Ra-226 discharge rate history Eq. (4.4.20) at the pumping well for different values of the retardation coefficient. Figure 4.2d show the Ra-226 cumulative discharge history Eq. (4.4.21) at the pumping well for the same retardation coefficients of Figure 4.2c. By plotting the actual measured Ra-226 cumulative discharge and/or the discharge rate history on Figure 4.2c and/or Figure 4.2d one can extrapolate an experimental value for the Ra-226 retardation coefficient in that geologic media.

4.3.2 Superposition of an arbitrary number of point sinks and point sources on an uniform flow field

When Darcy's law Eq. (4.2.3) with constant hydraulic conductivity k is combined with the conservation of mass Eq. (4.2.2) there results

The linear character of the above governing equation for the groundwater potential allows one to superimpose different

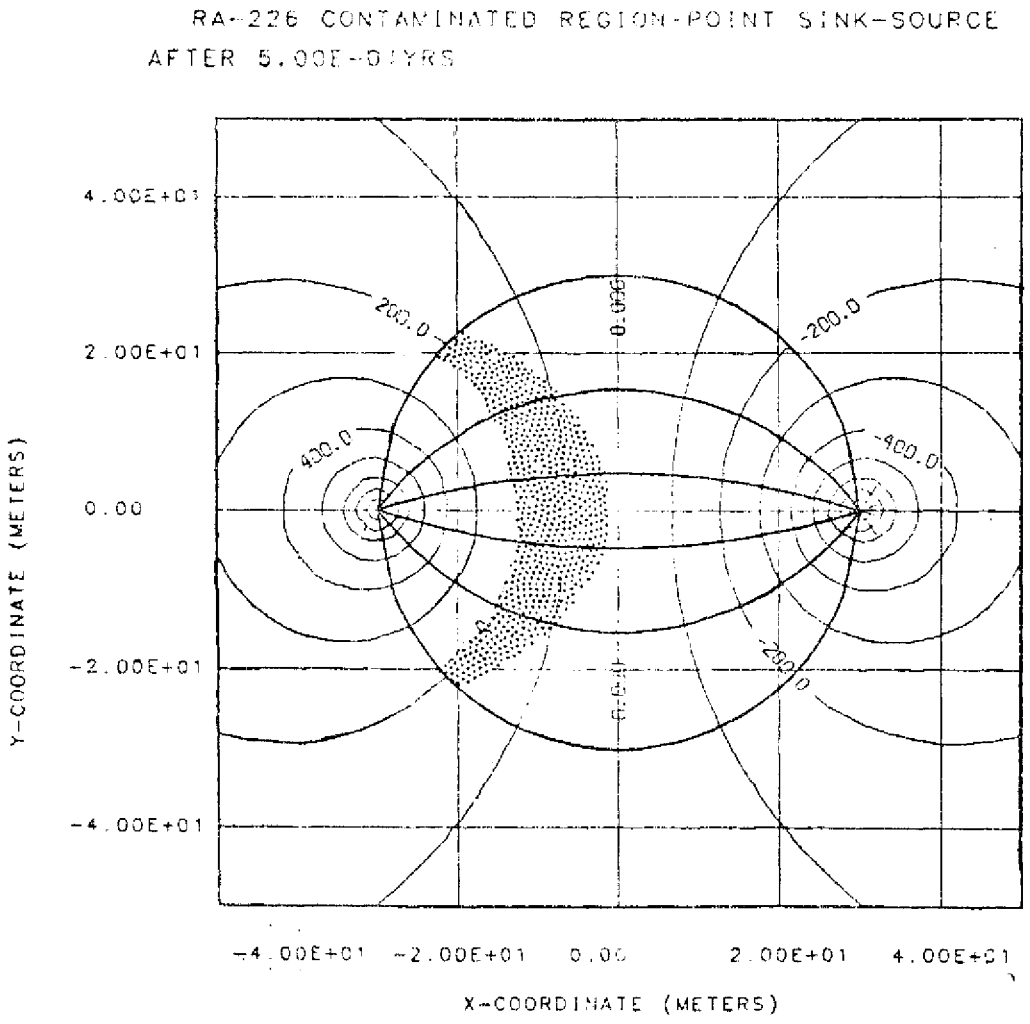


Figure 4.2a Ra-226 contaminated r*»<fion after 0.5 years in the point sink and point source experiment with an injection anale of (-**V2** to **V2**) at the injection pump.The flow rate is 7000 m**V**yr.Potentials are in meters above MSL.

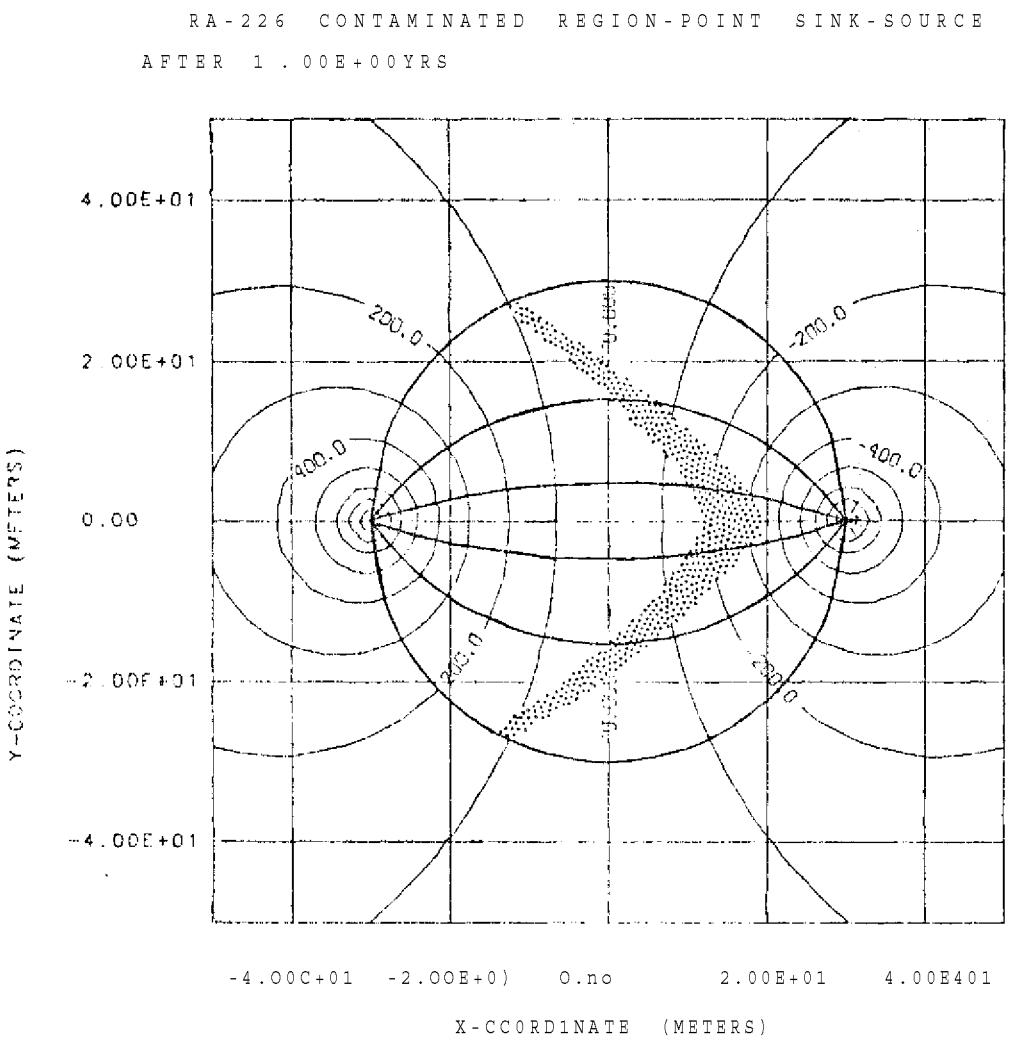
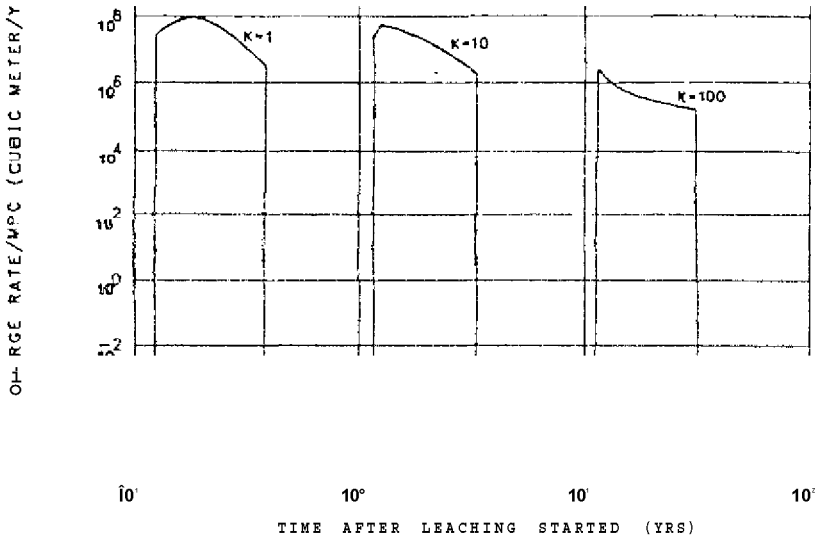


Figure 4,2b Ra~226 contaminated region after 1 year in the point sink and point source experiment with an injection angle of (-V2.to T/2) at the injection well.The flow rate is 7000 m/yr.Potentials are in meters above MSL.

RA-226 DISCHARGE RATE HISTORY AT PUMPING WELL



RA-226 CUMULATIVE DISCHARGE HISTORY AT PUMPING WELL

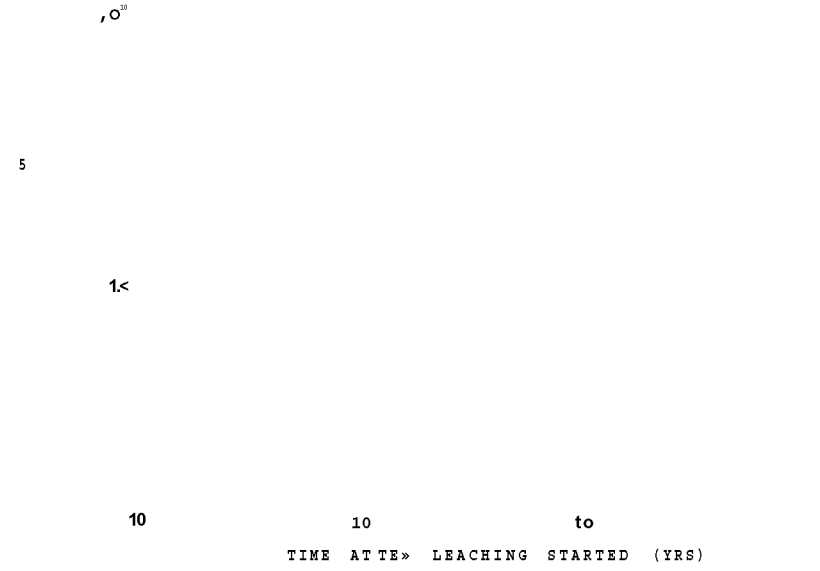


Figure 4.2c and 4.2d Ra-226 water dilution rate (discharge rate/ MPC) and Ra-226 water dilution volume (cumulative discharge/MPC) at the pumping well for retardation coefficients of 1,10 and 100.

potential fields to obtain a composite configuration. A single point source or point sink located at a position (x_j, y_j) produces a potential field given by (L2)

$$\Phi(x,y) = \frac{-Q}{} \ln[(x-x_j)^2 + (y-y_j)^2]^{1/5} \qquad (4.3.7)$$

3

where Q_j is the volumetric flow rate (m^3/yr) and when $Q_j > 0$, Eq. (4.3.7) represents the hydraulic head of a point source, while when $Q_j < 0$, it will represent the hydraulic head of a point sink. The uniform flow in the x-direction yields a hydraulic head given by

$$\Phi(x,y) = -v_x x A \qquad (4.3.8)$$

Superimposing the hydraulic heads due to N distinct point sources or point sinks with an uniform flow will generate the following hydraulic head and stream functions

$$\Phi(x,y) = \frac{v_x}{k} x - \frac{N}{j=1} \frac{Q_j}{2\pi k e D_o} \ln[(x-x_j)^2 + (y-y_j)^2] \qquad (4.3.9)$$

$$\Psi(x,y) = -v_x y - \sum_{j=1}^{N} \frac{Q_j}{2\pi e D_o} [\arctan(\frac{y-y_j}{x-x_j})] \qquad (4.3.10)$$

The velocities in the x and y directions will be respectively be given by

$$v_x = -k\frac{\partial \Phi}{\partial x} = v_0 + \sum_{j=1}^{N} \frac{Q_j}{2\pi D_0} \frac{x - x_j}{(x-x_j)^2 + (y-y_j)^2} \qquad (4.3.11)$$

$$v_y = -k\frac{\partial \Phi}{\partial y} = \sum_{j=1}^{N} \frac{Q_j}{2\pi D_0} \frac{y - y_j}{(x-x_j)^2 + (y-y_j)^2} \qquad (4.3.12)$$

Although in the last section it was possible to analytically obtain the water travel time function for the case of a single point sink and a single point source, the integration of Eq. (4.2.10), when Eq. (4.3.9) is used instead, becomes difficult to be performed analytically. We will resort to the use of the method of characteristics in conjunction with a Runge-Kutta numerical integration scheme to obtain the water travel time function. First recall the parallelism condition between the potential lines and the isochronous lines, Eq. (4.2.12)

$$\left(k\frac{\partial \Phi}{\partial x}\right)\frac{\partial \tau}{\partial x} + \left(k\frac{\partial \Phi}{\partial y}\right)\frac{\partial \tau}{\partial y} = -1 \quad ; \quad d\tau = 0 \qquad (4.3.13)$$

which is a first order partial differential equation (hyperbolic equation) for the variable τ, since the partial derivatives of the hydraulic head multiplied by the constant hydraulic conductivity k are known (Eq. (4.3.11.) and (4.3.12)). The method of characteristics consists in determining a direction at each point of the (x,y) plane along which the integration of Eq. (4.3.13) transforms to an integration problem of an ordinary differential equation (CI).

Consider first the definition of total derivative of the water travel time function

$$d\sigma = \frac{\partial \sigma}{\partial x}dx + \frac{\partial \sigma}{\partial y}dy \qquad (4.3.13a)$$

Eliminating the partial derivative of σ with respect to x from Eq.(4.3.13) and (4.3.13a) results

$$(v_x\, d\sigma + dx) + (v_y\, dx - v_x\, dy)\frac{\partial c}{\partial y} = 0 \qquad (4.3.13b)$$

This equation is independent of $\frac{\partial a}{\partial x}$ because $\frac{\partial a}{\partial x}$ and v_y are functions of x,y only and do not depend on $\frac{\partial \sigma}{\partial x}$. The equation can also be made independent of $\frac{\partial \sigma}{\partial y}$ by choosing points on a curve C in such a way that the following relationship is satisfied

$$v_y\, dx - v_x\, dy = 0 \qquad (4.3.13c)$$

With this choice Eq. (4.3.13b) yields

$$v_x\, d\sigma + dx = 0 \qquad (4.3.13d)$$

Eq. (4.3.13c) is a differential equation for the curve C which is called the characteristic equation of the partial differential equation Eq. (4.3.13) and Eq. (4.3.13d) is an ordinary differential equation for the solution *a* along the curve C. The solution of the partial differential equation for σ, Eq. (4.3.13)

can thus be obtained by the simultaneous solution of two ordinary differential equations. These equations can be restated as follows

$$\frac{dx}{v_x} = \frac{dy}{v_y} = \frac{do}{-1} \qquad (4.3.14)$$

The simultaneous integration of Eq. (4.3.13c) and Eq. (4.3.13d) starting from a point $(x^{\wedge}, y_{\circ})$ on the initial source line S up to a point (x,y) downstream will yield the value of the water travel time at that point (x,y). The partial derivatives of the potential function being given by Eq. (4.3.11) and Eq. (4.3.12), the above integration can be carried out by using the Runge-Kutta integration method.

Let us first demonstrate that the characteristics of the above differential equation Eq. f4.3.13) coincide with the streamlines of the flow. Along a streamline where $d^{\wedge} - 0$, and by using the definition of total derivatives one has

$$di[- = \frac{3t|/}{3x}dx + \frac{3iJ>}{3y}dy = 0 \qquad (4.3.16)$$

By using the relationships Eq. (4.2.8) and Eq. (4.2.9) which define the streamlines one has

$$\frac{3<f>}{3x}dx + \frac{3\,\text{◄J}}{3y}dy = 0 \qquad (4.3.17)$$

which yields

$$\frac{dx}{v_x} \quad \frac{dy}{v_y} \qquad (4.3.17a)$$

Therefore, Eq. (4.3.17) defines a streamline and it has the same form as the characteristic equation for the water travel time function Eq. (4.3.13c). This result will be of practical importance for us since both the water travel time function and the radionuclide concentration being evaluated along the same curves facilitates the calculations.

One chooses along the source line S a given point $(x^{\wedge}, y_q)$ where $o(^{*}0/Yg)^{\cdot}0\bullet$ After defining a new abcissa $x^{\wedge}x^{\wedge}+nAx$ one integrates Eq. (4.3.14) from x_0 to x_n to obtain the new ordinate y_n corresponding to the position $(^{*}_{n}, Y_n)$ along the streamline which passes through $(x_{\varrho}, y^{\wedge})$. Simultaneous integration of Eq. (4.3.15) will yield the value of $c(x_n, y_n)$. Substitution of this $a(x^n, y^n)$ into the solution for the radionuclide concentration Eq. (4.2.26) will yield $N_i(x_n, y_n, t)$ on that streamline. This can be repeated for any arbitrary number of points (y_{-n}, Y_r) on that same streamline by choosing adequate values for Ax and n. Once that streamline has been analyzed one can start from another point $x_0, y_n)$ on the source line S and repeat this procedure for this new streamline. By starting from enough points along the source line one can cover the entire "shadow region".

To assess the accuracy of this method we use it to solve

the pair point source and point sink problem and we compared the solution to the exact solution presented in the last section Eq. (4.3.3). The difference between the exact solution for the water travel time and the approximate solution is expressed in terms of percent error defined as

$$e(\%) = \frac{\hat{}\ \circ_{exact} \quad \mathbf{approximate}\ \hat{}}{a_{exact}} \qquad (4.3.18)$$

Table 4.1a show the result of the calculations for the different streamlines shown in Figure 4.2, characterized by the angle of the initial point on the source line. Since the system is symmetric with respect to the **x** axis, only the results for half of the streamlines are reported. The first column is the dimensionless x coordinate (x/a) and the second column **is** the corresponding dimensionless y coordinate (y/a) for that streamline. The third column is the dimensionless hydraulic head as defined in Eq. (4.3.5a), the fourth column is the dimensionless streamfunction Eq. (4.3.5b) and as one expected it is constant along this streamline. The fifth and sixth column are the exact and approximate values of the dimensionless water travel time function as defined by Eq.(4.3.5c), respectively. Finally, the last column is the percent error Eq.(4.3.18) and one can see that the agreement is quite complete.

Streamlines coordinates for the point sink and point source flow with the corresponding values of the dimensionless potentials,streamfunctions,water travel times and the error percentage of the semi analytical water travel time calculations.

CHARACTERIS X-CCORDIN	IC NO. 1 RI Y-CUCRD IN	SI TORY AN3L =-9. CCE+ 01 POTENT IAL	STREAMFUN.	EXACT TIME	APRQX TIME	ERROR PERCNT
-9. 0O0E-01	- 4. 401E- 01	1 .463E+00	-1 .575 E+00	1 .019E-01	1.019E-01	7. 59 6E- 05
-8.000E-01	-6.042E-31	1. 393E+ 03	- 1. 575E+ 03	2. 02 7E-01	2.327E-31	7,442E-05
-7.CC0E-C1	~ -7.134E-01	8.6 32F-01	"-1.575E+00"	""3.C33e-01	3. 033E-O1	5. 096E-05
-6. G00E-01	- 8. C42E-C1	6.900E-0L	-1 .575E+00	4 .039 E-0 1	4.03'>E-01	3.842E- 05
-5 .0 CO E-0 1	-8 .702E-J1	5.469E-01	- 1. 575E+03	5. 344E-01	5. 044E-01	3.080E-05
-4. CCOE-OL	-9.2 07 E-Cl	4 .2 IB E-01	-1 .575E+00	6.049E-01	6. 049E-01	2. 569E- 05
-3.0C0E-C1	- 9.582E- C1	3. C82E-C1	-1 .575E+03	7 . 053 E-01	7 .0 538-01	2 .204E-05
-2 .003 E-3 1	-9 .e43E-3 1	2 .019E- 01	- 1.575E+30	8. G58E-01	8. C53E-C1	I .929E-C5
-9. 9^9E~02	-9. 9 92 E-01	9.990E-02	-1 .575E+00	9 .0 62E-01	9.062E-01	1.716E- 05
7 .963B-06	- 1.CC4E+C0	- 7.9 3CE- 06	- 1. 5 75 E + 00	1.307E+30	1 .007 E+0 0	1 .54 5 E-05
1 .0C0E-01	-9 .992 E-0 1	-9 .992E-G2	- 1 .575E + C0	1.10 7E + 0 0	1. IC7E + 00	1.4Q5E-05
2. 000E-01	-9. P4GE-G1	-2 .019E-01	-1 .575 E+30	1 .207E+0 0	1.207E+00	1. 290E- 05
3.000E-CI	-9 .5 8 2E-Ji	- 3.082E- 01	- 1. 575E+03	1 .3 08E + 00	1.3 08 E + DD	1 . 192E-35
CGOE-01	-9 .207 E-31	-4 .2 18E-0 1	- 1.575E+00	1.4C8E+00	I. 408E + 00	1. 110E-05
5. OCOE-01	- 8. 7 02E-C1	-5 . 469E-0T	-1.575E+00"	1 .509 E+00 ~	1.509 E+00	1.044E-G5
b .OCOE-0 1	-8 .042E-01	- 6. 9COE-01	- 1. 575E-+Q3	1.609E+00	1.539E+30	1.032E-35
7.CC0F-01	-7.184E-01	-6 .6 32E-0 I	- 1 .5 75 E + C0	1.710E+00	1. 7 10E + 0 0	1. 032E-05
8.C00E-01	-6 . 042E-01	- 1. 093E + CO	-1 . 5 75 t+00	1.811 E+00	1 .8 1 1E+00	1.565E-05
9.OCOE-01	-4 .4 HE - 0 1	- 1.464E + 00	- 1. 575E +00	1.911E+03	1.9L1E+33	1.441E-C4
1.CCOE+CO	-5 .S01E-C3	-5. .878E+00	4 .7 08 E+0 0	2 .0 13E+00	2. 013E +00	9. 102E-04

4.4 Aquifers Potentiometrie Surfaces Represented by-Interpolation of Field-Measured Piezometric Data

4.4.1 Introduction

Hydrogeological studies of a proposed site for a high level waste repository usually provide an approximate description of the aquifer geometry with geologic maps and some distributed piezometric head observations collected during field tests accumulated over the past. In addition, limited data on hydraulic conductivities are also supplied.

The most common utilization of these data in the determination of the potentiometrie surface of the aquifer as well as its parameters is the so called "model calibration" (L3,N3). This is done by solving the groundwater mass conservation equation Eq.(4.4.1) subject to suitable boundary conditions and some initial guesses for the aquifer parameters. The resultant solution *(x,y) is then compared to the field data. By using assumed weighting functions new guesses for the aquifer parameters are obtained. This procedure is repeated until a satisfactory agreement is obtained between the calculated and measured potential function. The governing equation in the absence of sources and sinks is

$$\frac{\partial}{\partial x}\left\{K\frac{\partial \phi}{\partial x}\right\} + \frac{\partial}{\partial y}\left\{K\frac{\partial \phi}{\partial y}\right\} = 0 \qquad (4.4.1)$$

The above method presents some disadvantage since uniqueness cannot he guaranteed because infinite number of combinations of hydraulic head and hydraulic conductivity can be solutions to Eq.(4.4.1) and local parameters values can be calculated by traditional methods only under the assumption of homogeneity {e.g. pumping tests based on the Theis equation (Fl)). These measured parameters will only represent local behavior of the aquifer failing to represent the inhomogeneous character of the aquifer on a regional scale (S3).

4.4.2 Determination of the potentiometric surface

In our present study we use the measured piezometric data to fit a potential function. Once the potential function is determined one can solve Eq. (4.4.1) for the hydraulic conductivity k. This problem is known as the "inverse problem" (Fl).

The problem of interpolating a smooth two dimensional function to a finite number of data points was treated by Briggs (Bl). He optimizes a third order spline fit in two dimensions by minimizing the total curvature (also called the Gauss curvature) of the function. It is shown (Bl) that this condition requires the desired function to satisfy the following biharmonic equation

$$+ 2 \frac{\partial^{8}\{\}}{\partial x^{2}\partial y^{2}} + \qquad = 4_{n} \tag{4.4.2}$$

Here $ are given piezometric data points at the discrete points (x_n, y_n), n=1,2,....M. Eq. (4.4.2) is the equation which describes the displacement of a thin elastic sheet in two dimensions under the influence of point forces. The desired function must satisfy constraining values ϕ_n within the region of interest. Numerical solution to Eq. (4.4.2) when written as a set of algebraic equation by expressing the derivatives with finite differences yields the desired function $\phi(x,y)$. This method has been programed into the Surface Gridding Library (SGL) and implemented at the LBL computer center (S2).

Therefore, by specifying a given number of values for the potential function at different points inside the region of interest one can construct the potentiometrie surface by using the SGL computer program. Once the potential function is known, the next step is to solve the inverse problem, i.e. to determine the hydraulic conductivity k.

4.4.3 Solution to the inverse problem

Different solutions have been proposed to the inverse problem. Among those, Emsellem and Marsily (E1) propose a modified form of the Cauchy*s problem, Frind and Pinder (F2) propose a Galerkin's scheme solution, Nelson (N2) makes use of the energy dissipation method while Sagar (S3) solves algebraically the finite difference form of the Eq. (4.4.1).

These solutions require either complex numerical schemes or assumptions which might bias the orioinal data.

In this present, work the method of characteristics is used to solve the Cauchy's problem. Consider Eq. (4.4.1) where <f>(x,y) is known. Eq.4.4.1 can be rewritten as a first order differential equation (hyperbolic equation) in the unknown variable k (x,y)

$$m(x,y)\frac{9k}{3x} + n(x,y)\frac{9k}{3y} = -k \qquad (4.4.4)$$

where m (x, y) and n(x,y) are known functions given by the following

$$m(x,y) = \frac{3\$/3x}{V^{c}<\}>}; \quad n(x,y) = \frac{94>/3y}{V^{c}cf>} \qquad (4.4.5)$$

It can be shown (CI) that integration of Eq. (4.4.4) in the region of interest R is possible when boundary conditions for k(x,y) are prescribed along a line S cutting every streamline of the flow in the region R i.e. when a value of k is known on every streamline of the region R. Since the potential function <Mx,y) has already been evaluated by SCI,, the streamline which are independent of the values of k (see Eq.(4.3.17a)) can be determined by using the method of characteristics as described in Section 4.3,2. So defined the problem of finding the hydraulic conductivity can be solved by the method of characteristics and possess an unique solution (CI). Since the governing equation

for the hydraulic conductivity has the same form (hyperbolic equation) as the governing equation for the water travel time function Eq. (4.3.13), the derivation of the characteristic equation Eq.(4.3.13a) through Eq.(4.3.14) for the water travel time is applicable for the hydraulic conductivity provided one changes v_x by $m(x,y)$ and v_y by $n(x,y)$. Therefore, from Eq. (4.3.14) one can obtain the characteristic equations of Eq. (4.4.4)

$$\frac{dx}{m(x,y)} = \frac{dy}{n(x,y)} = \frac{dk}{-k} \qquad (4.4.6)$$

Rewriting separately the differential equations

$$\frac{dy}{dx} = \frac{n(x,y)}{m(x,y)} \qquad (4.4.7)$$

$$\frac{dk}{dx} = \frac{-kV^2\langle f\rangle}{3\langle\}\rangle/3x} \qquad (4.4.8)$$

Comparing Eq. (4.4.7) with Eq. (4.3.17a) one concludes that the characteristic curves of Eq. (4.4.4) are indeed the streamlines of the flow. The region R of interest is the "shadow region" of the repository. The *shadow region" is formed by the streamlines which pass through the source line represented by a curve S. In order to integrate Eq. (4.4.8) one needs therefore to specify values for the hydraulic conductivity k along the source line S.

To evaluate the water travel time function let us first recall Eq. (4.3.13)

$$v_x \frac{\partial o}{\partial x} + v_y \frac{\partial o}{\partial y} = -1 \quad ; \quad \text{dip} = 0 \tag{4.4.9}$$

The characteristic equations are rewritten from Eq. (4.3.13c) and Eq. (4.3.13d)

$$\frac{dy}{dx} = \frac{v_y}{v_x} \tag{4.4.10}$$

$$\frac{do}{dx} = \frac{-1}{v_x} \tag{4.4.11}$$

Utilization of this method presents an additional practical advantage since the solution to the transport equation Eq. (4.2.27) applies along a streamline of the flow and one must integrate Eq. (4.4.7) anyway. At the same time integration to obtain the water travel time and the hydraulic conductivity can also be carried out.Eq. (4.4.7), Eg. (4.4.8) and Eq. (4.4.11) are to be integrated simultaneously in this order.

One starts from a point $(x_\circ, Y_q)$ on the repository curve S where the initial value for the hydraulic conductivity $k(x_\circ, y)$ is assumed to be known and the water travel time is $a(x\hat{}, y\hat{}) = 0$. Defining a new abcissa $x = x + nAx, n=1,2...N$ and Ax is arbritrarily choosen one integrates first Eq. (4.4.7) to obtain y corresponding to the abcissa $x\hat{}$ on the same streamline.

Simultaneous integration of Eq. (4.4.8) and Eq. (4.4.11) will yield

$k(x_n, y_n)$ and $o(x_n, y_n)$"

After repeating this integration for all abaissas $x_n, n=1,2$ **N** one will have defined that particular streamline of the shadow region. At the same time the values of the water travel time and hydraulic conductivity have also been determined at the same points along this streamline. Substitution of (x,y) into Eq. (4.2.27) will yield the value of the radionuclide concentration along this streamline.

By choosing different points (x_o, y_o) on the source line S and repeating the above described calculation one can cover the entire "shadow region". This method calculates therefore the two-dimensional distribution of the i-th member of a radionuclide chain of arbitrary length in a stationary two-dimensiona1 groundwater flow through an inhomogeneous isotropic geologic medium.

The integrations are carried out numerically using a Runge-Kutta scheme. The partial derivatives of the potential function are expressed in finite central difference form

$$\left(\frac{\partial f}{\partial x}\right)_{n} \qquad \frac{\Phi_{n+1} - \Phi_{n-1}}{2\Delta x} \tag{4.4.12}$$

$$\left(\frac{\partial *}{\partial y}\right)_{j} \qquad \frac{\Phi_{j+1} - \Phi_{j-1}}{2\Delta y} \tag{4.4.13}$$

And the Laplacian operator is approximated by

$$\frac{(\phi_{n+1,j} - 2(f)_{n,j} + \phi}{Ax^2} + \frac{(\phi_{n,j+1} \quad 2\phi_{n,j}}{Ay^2} \qquad \text{Hl2} \quad (1.4.14)$$

One must keep in mind that this method assumes the measured piezometric data in the region of interest as well as the measured hydraulic conductivity along the repository curve as being reliable. By using this data this method provides a way of modelling actual groundwater flows through aquifers.

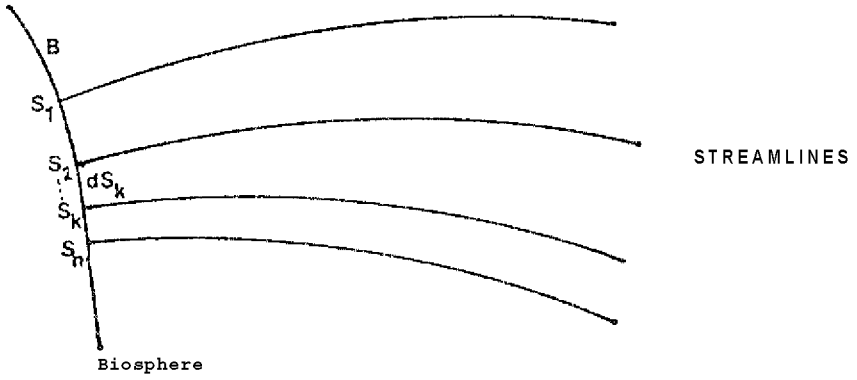
If hydraulic conductivity data are provided in the shadow region one can compared them with the calculated value. Assuming that these data are reliable, in case of desagreement between the calculated data and the field data one can justify these differences by considering them as the result of localized sinks or sources which were not considered in the governing equation Eq. (4.4.4).

4.4.4 Evaluation of radionuclide discharge rates into the biosphere and cumulative discharge in the biosphere

Having determined $N_i(x,y,t)$ provided us with a quantitative picture of the migration of that particular nuclide through the geologic media after being released from the repository. However, one measure of the potential hazard to the general public can be obtained by evaluating the cumulative, amount of

curies of individual nuclides actually discharged into a potential source of fresh water,taking into account decay after discharge.

Let us denote by q^(t) the discharge rate (Ci/yr) of the i-th member of a radionuclide chain into the biosphere at a time t after the chain was released from the source line. Consider the intersection of the *shadow region" streamlines with the biosphere which is represented by a curve B. This curve is subdivided into n subcurves of arc with length ds^ as shown in the following sketch



Let the water velocity at a point s_k be $v(s_k)$,(m/yr), the aquifer thickness be $h(s_k)$,(m) and the nuclide concentration $N_1(S_y,t)$. The discharge rate through an element ds is given by

$$dq_i = v(s_k)h(s_k)N_i(s_k,t)ds_k \qquad (4.4.15)$$

To obtain the discharge rate for all the contaminated streamlines that reach the biosphere one integrates Eq (.4.4.15) along the entire curve B

$$q_i(t) = \int_{s_1}^{s} v(s_k)\, h(s_k)\, N_i \{ o(s_k, t)\, ds \qquad (4.4.16)$$

The concentration $N_i\{o(s),t\}$ is readily evaluated by using Eq. (4.2.26). The water velocity is obtained by the following expression

$$v(s_k) = [v_x^2 + v_M^2]^{h} \qquad (4.4.17)$$

However, the aquifer thickness at the biosphere $h(s_1)$ is generally not known. To avoid this problem we make use of the fact that the volumetric flow rate between two streamlines is constant throughout the field. Since the product $v(s)h(s)ds$ is the volumetric flow rate between the streamlines passing through two points along the curve B, this is equal to the volumetric flow rate at the source line between corresponding streamlines. Aquifer thickness at the repository is generally better known than in the far field because more extensive geological studies are carried near the repository site than in the far field. This allows one to evaluate the volumetrie flow rate between those streamlines.

The integral in Eq.(4.4.16) is readily evaluated by a proper numerical scheme (Romberg method,D3) once the integrand is determined for a number of points along the curve B.

The cumulative discharge of a i-th member of a radionuclide

chain. Q_i (t). (Ci) is obtained by integrating the discharge rate $q_i(t)$ from the first nuclide arrival time up to a time t afterwards. The integral is multiplied by the Bateman function to account for the decay of the members of the chain after they are discharged. The radionuclides are assumed to remain stationary in a reservoir after their discharge.

$$Q_i(t) = \int_{t_a}^{t} q_i(T) \prod_{j=1}^{i} B_{j-1,j} \exp(-\lambda_j (t-x))\,dx \qquad (4.4.18)$$

The first nuclide arrival time t_a ,(yr) is an important quantity in assessing the potential hazard of a particular radionuclide. It can be evaluated by the following formula

$$t_a = c_{min} K_{m,m} \qquad (4.4.19)$$

Here, $o_{m,m}$,(yr) is the smallest value of the water travel time on the biosphere curve and K_{min} is the smallest retardation coefficient of all the precursors in the chain. If the chain has only one member, $K_{i,i}$ will be its own retardation coefficient.

In order to be able to compare the potential hazard due to the discharge of different radionuclides into the biosphere one can use the water dilution rate $w_i(t)$, (m^3/yr) as defined in (Pi,Section 2.7). The water dilution rate is obtained by dividing the discharge rate by the Maximum Permissible Concentration, MPC given in (Ci/m^3) by 10CFR20. Thus

$$W_i(t) = q_i(t)/MPC_i \qquad (4.4.20)$$

This ratio is the necessary water flow rate in the biosphere so that it will dilute the discharge rate of that nuclide to drinking water standards. This calculation provides an additional advantage since one can add these required flow rates for every nuclide to obtain an overall hazard index for all nuclides present in the repository.

Similarly, if one divides the cumulative discharge $Q^{\wedge}(t)$ by the MPC of that i-th member one obtains the total amount of water that is needed at the biosphere to dilute the cumulative amount of that nuclide to drinking water standards. This quantity is called water dilution volume (PI,Section 2.7) and is expressed as follows

$$W_i(t) = Q_i(t)/MPC_i \qquad (4.4.21)$$

Finally, the total water dilution rate is the sum of all water dilution rates of individual nuclides

$$w(t) = \sum_{i=1}^{M} w_i(t) \qquad (4.4.22)$$

In the same way, the total water dilution volume is given

by

$$w(t) \quad \sum_{i=1}^{M} w_i(t) \qquad (4.4.23)$$

where M is the total number of nuclides having been discharged into the biosphere at that time t.

4.5 Description of the Computer Code UCBNE21

A computer program labeled UCBNE21 has been developed to perform the calculations described in the previous sections. To give added flexibility the program was subdivided into four subprograms which can be run individually. This is a convenient feature since the concentrations and discharge rate calculations are independent from the hydrological calculations. Once the hydrological calculations for a particular aquifer is done there is no need to repeat it for every nuclide concentration calculation. A complete source listing of the programs is given in Appendix C. The following diagram shows the interelationship between the four subprograms

HYDRO

(hydrological calculations)

<f> (x,y), (x,y), k(x,y), o(x,y)

(print and record on tape)

t

PL0TMAC	P0T3D	DCHARGE
(concentration calculations)	(three dimensional plotting of <f>(x,y))	(discharge rate and cumulative discharge)
Listing+plot	Plot	Listing+plot

The subprogram HYDRO evaluates the potential function on every grid point inside the region of interest. Then it determines a number of streamlines in the "shadow region" of the repository by specifying a number of coordinates for each streamline. On each of these coordinates, the hydraulic conductivity and the water travel time are calculated. Finally it prints out a listing of the coordinates of each streamline with the corresponding values of potential function,hydraulic conductivity and water travel time. These results are saved into tape for posterior use. Description of the data input requirements is given in Appendix C. The structure of the program HYDRO is shown in Figure 4.4. One should notice the possibility of merging the potentials resulting from the analytical representation with those from fitting field data.

The subprogram PLOTMAC reads in data on the radionuclide chain such as decay constants, retardation coefficient, activities at the time of burial, and maximum permissible concentration for each member of the chain. In addition one must specify the migration parameters such as the delay time for the beginning of leaching, the leach time and the time after the leaching started when the calculations are to be performed. Complete description of data input is given in Appendix C. PLOTMAC reads in the shadow region streamlines coordinates and the corresponding water travel times from the tape file produced by HYDRO. By evaluating Eq. (4.2.27) it determines the concentration of each member of the chain on each coordinate of

Figure 4.4 Structure of the program HYDRO

Define region of interest,repository location,Cauchy data on hydraulic conductivity and grid sizes.

Define the number of point sinks and point sources, their location,their strenght and if needed a uniform flow field

Read in measured piezometric data

Evaluate analytical potential function Eq. (4.2.26) on every grid point.

Evaluate measured potential function using the Surface Oridding Library

I

Superimpose the analytical potential with the measured potential,if desired.

Evaluate V_x, Vy and V^2 using Eq. (4.4.12),Eq. (4.4.13) and Eq. (4.4.14)

Numerical integration of Eq. (4.4.7),Eq. (4.4.8) and Eq. (4.4.11)

Print and store on tape

<Mx,y), if (x,y), k(x,y), c(x,y)

each streamline in the shadow region. A printed output is produced and it also uses the graphic software available at the LBL computer center to produce plots. Each nuclide contaminated region is shown in a plot with the contour map of the potential function, the streamlines of the shadow region, the contaminated region and the biosphere curve B as described in Section 4.4.4 (see for example Figure 4.15).

The program POT3D reads the potential function calculated by HYDRO from the tape file and using the graphical software produces a three dimensional view of the potentiometric surface in the aquifer being studied.(see for example Figure 4.11).

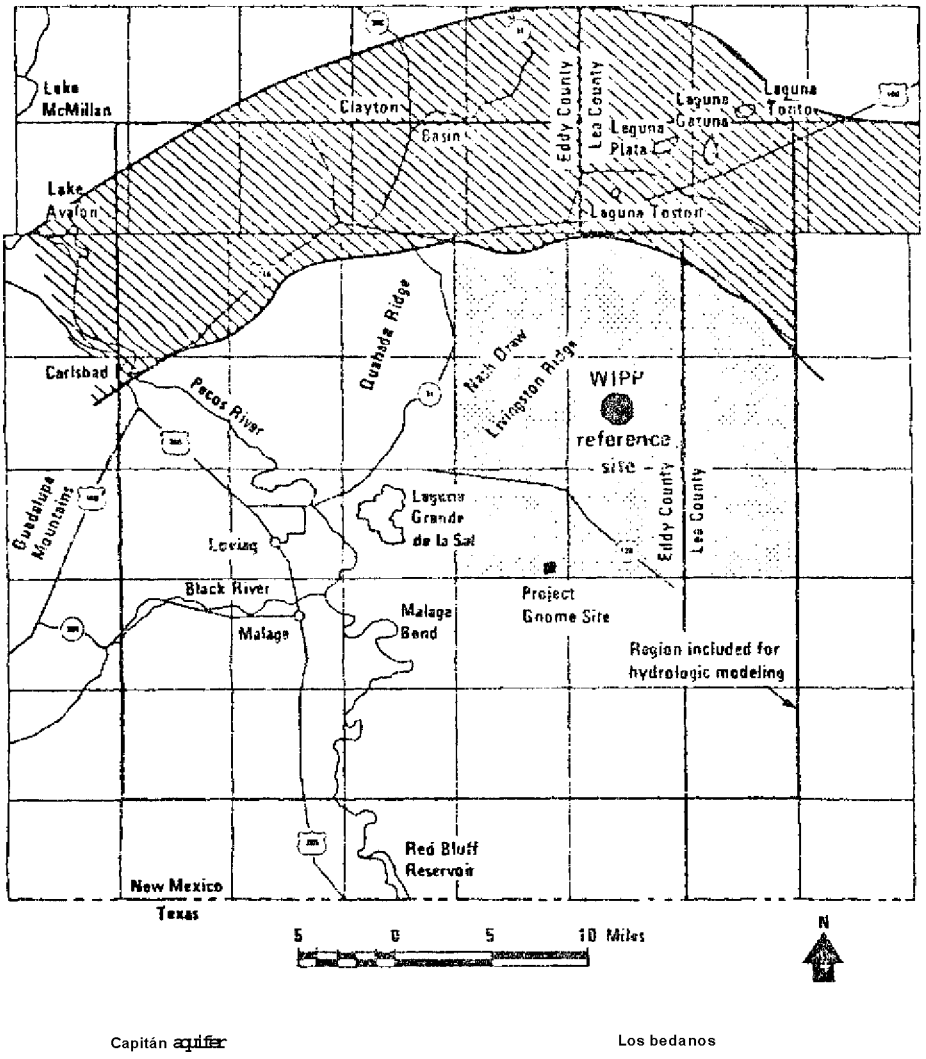
The program DCHARGE evaluates the discharge rate and the cumulative discharge at the biosphere. The calculation is performed for the entire time span of interest (i.e. from the first nuclide arrival time until the last nuclide departure time). Both printed output as well as plots for the discharge rate (expressed as water dilution rate) and cumulative discharge (expressed as water dilution volume) are produced (see for example Figure 4.21). The structure of the subprogram DCHARGE is given in Figure C.1 in Appendix C.

4.6 Modelling of the Far Field Radionuclide Migration at the Reference Site of the Waste Isolation Pilot Plant (WIPP) in Eddy County, New Mexico

4.6.1 Review and interpretation of existent hydrological data

Hydrological data used in this work were obtained primarily from the Department of Energy report:Waste Isolation Pilot Plant (D1) which summarizes the data reviewed by several authors. Among these are Mercer and Orr (M1),Register (R1) and others. In this report we present a brief summary of the available information and the reader should refer to aboves references for more detailed descriptions of the hydrology in the region of the WIPP site.

A map of the modelled region is shown in Figure 4.5. A geologic cross section of the site area looking northwest is presented in Figure 4.6. As it is described in (D1): "The Santa Rosa Sandstone is a moderately permeable formation containing relatively fresh water. However, the low permeability of the Dewey Lake Red Beds prevents significant seepage of water from the Santa Rosa Sandstone to the Rustler Formation below. Two thin aquifers, the Magenta and the Culebra are contained in the Rustler Formation, which is predominantly composed of impervious anhydrite, polyhalites and gypsum. The WIPP reference repository



Capitán aquifer

Los bedanos

Figure 4.5 Hydrologie raodelling région for the WIPP site (Dl)

Figure 4.6 Geologic cross section of the WIPP site area (Dl)

will be in the Salado Formation. The Castile Formation, composed of very pure halite and anhydrite, contains no water-bearing strata. Beneath it lies the Delaware Mountain Group, approximately 3000 ft thick which contains aquifers",

In addition, there is a brine aquifer which contains substantial quantity of water and it is found in the subsurface above the Salado formation in the region of the W1PP site. Register (R1) gives the following description: "The brine aquifer which occurs along the top of the Salado and the base of the Rustler and underlies Nash Draw extends to the Pecos River in the vicinity of Malaga Bend. The aquifer is apparently replenished from precipitation and brine discharge that penetrates the overlying units through fractures and solution zones, then moves southward along the top of the salt and increases in salt concentration until it discharges into the Pecos River at Malaga Bend. The calculated discharge from the brine aquifer is about 200 gal/min".

There are two potential pathways for the radionuclides to reach the biosphere after they are released from the repository. The aquifers contained in the Rustler formation overlying the Salado formation flow southwestward and discharge into Pecos River in the vicinity of Malaga Bend. On the other hand, underlying the repository site we have the Delaware Mountain Group aquifers which, contrary to Rustler aquifers, flow northward, discharging into the Capitan aquifer which is a source of fresh-water.

Two sets of hydraulic potentials representing the Rustler aquifer are given in (D1). In Figure 4.7 a contour map of the measured hydraulic potential for the Rustler aquifer is shown while in Figure 4.8 the calculated hydraulic potential (using model calibration) is shown. Calculations will be done using both set of hydraulic potentials and comparisons will be drawn.

In the same way, two sets of hydraulic potentials for the underlying Delaware Mountain Group aquifers are presented (D1). Figure 4.9 is the mapping of the raw data while Figure 4.10 is the calculated set of hydraulic potential. Data on measured aquifer parameters in the region are not extensively available and the reported values are distributed over a large range of values making the choice of a representative value difficult (C5,D1). However, hydraulic conductivity at the repository site can be estimated (R1). A summary of the hydrological data at the site used in this work is given in Table 4.1

Table 4.1 Summary of hydrological data at the repository site (D1,R1)

	Rustler aquifer	Delaware aquifer
Thickness (m)	65	900
Hydraulic conductivity (m/yr)	A range from 0.1 to 1400;used value=11.	0.3
Porosity	0.10	0.16

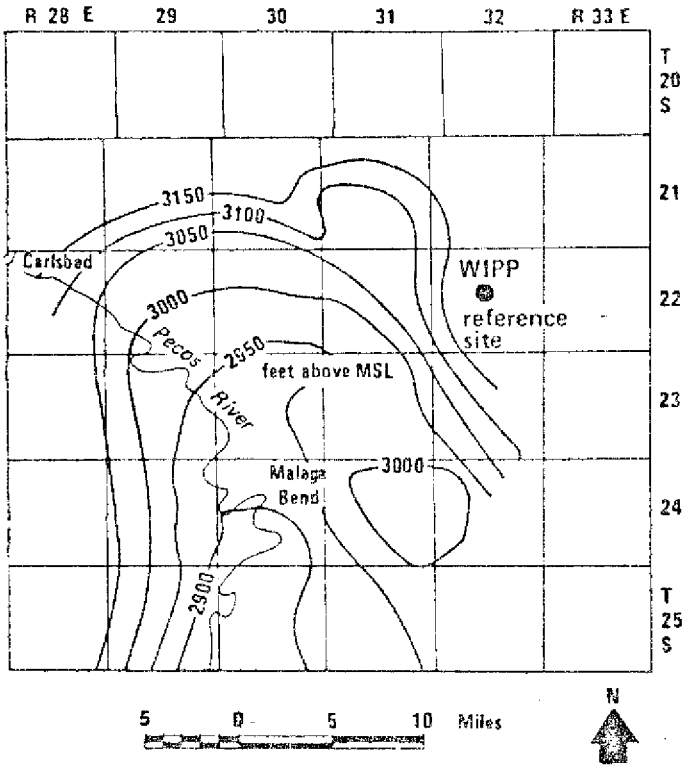


Figure 4.7 Measured hydraulic potential data for the Rustler aquifer (feet above MSL), from (D1)

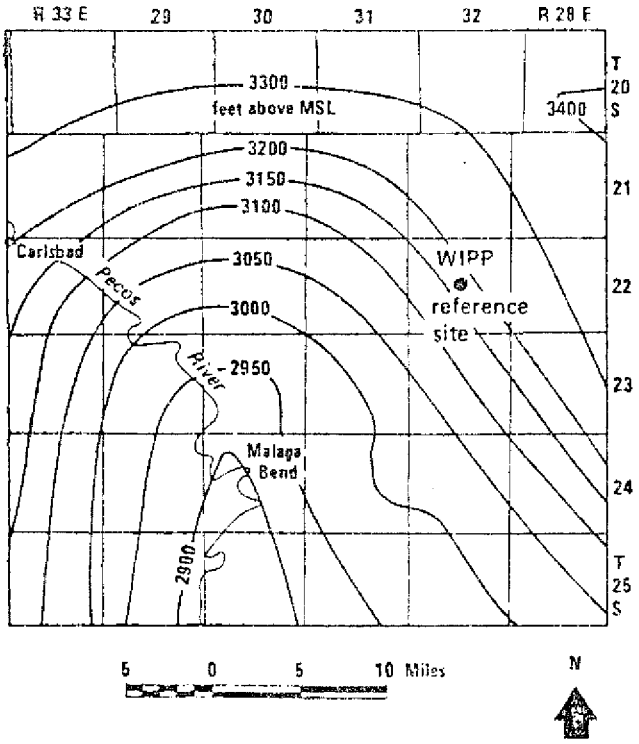


Figure 4.8 Calculated hydraulic potential data for the Rustler aquifer (feet above MSL),from (D1)

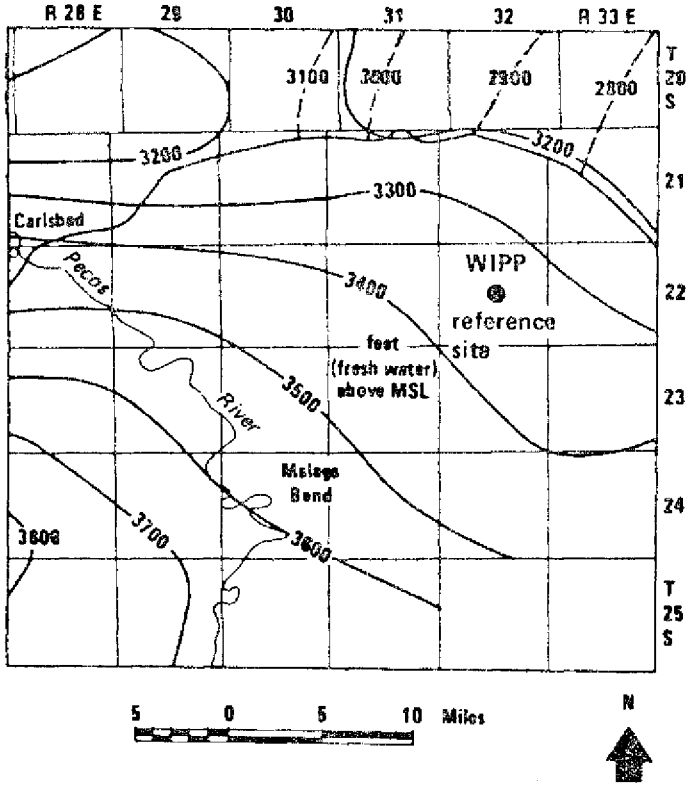


Figure 4.9 Measured hydraulic potential data for the Delaware aquifer (feet above MSL),from Dl

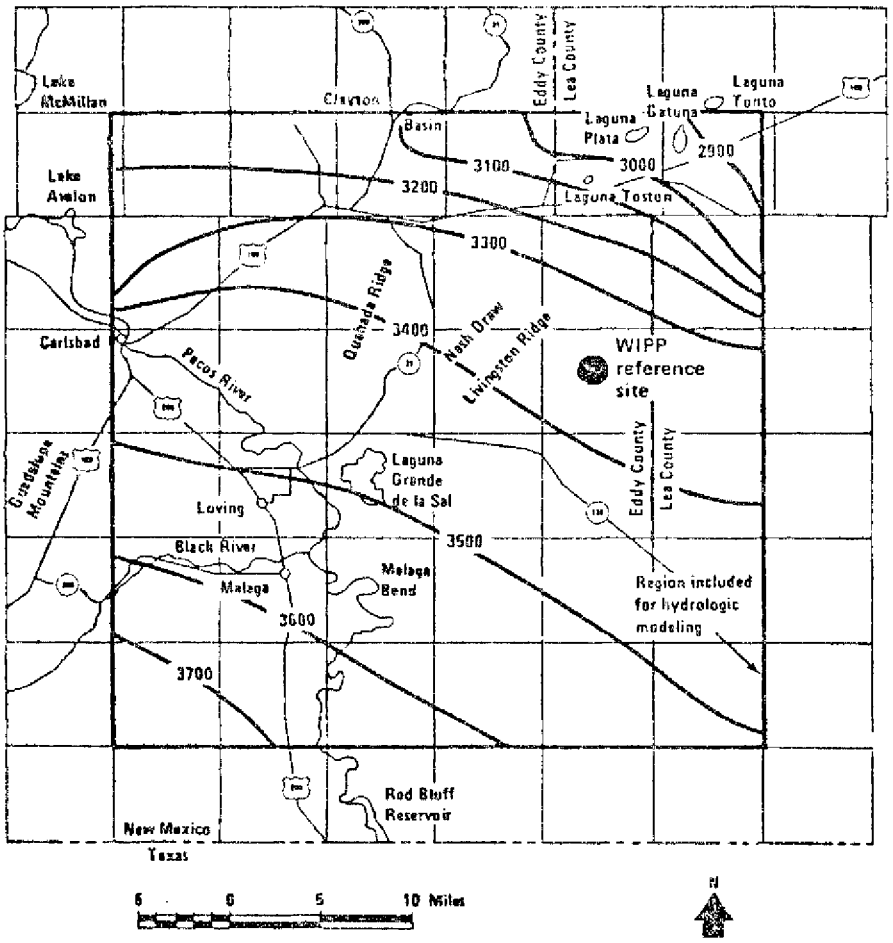


Figure 4.10 Calculated hydaulic potential data for the Delaware Mountain Group aquifer (feet above MSL),from (Dl)

The Salado formation (see Figure 4.6) where the repository will be located and the underlying Castile formation are essentially impermeable and contain no water. In this present analysis we postulate that any radionuclide accidentally released from the waste package due to any abnormal event is transferred through an open fracture to either the overlying aquifers in the Rustler formation or to the underlying Delaware Mountain Group aquifers.

Although the transport of radionuclides in groundwater through these fractures might take some time, we assume this time to be negligible when compared to the transport time in the aquifer itself (typical values are ten years compared to 10000 years,E2). Therefore, conceptually, the model assumes the repository is located in the aquifer being studied. This is a conservative assumption because, if the travel time in the fracture was to be considered, the arrival time of the first nuclide would be larger and also,the concentrations would be smaller.

In assessing the safety characteristic of the site, the Rustler formation aquifers are of primary importance because the hydraulic head in the Delaware aquifer being larger than that of the Rustler aquifer produces an upward driving gradient. In addition, thermally induced convective flows makes the. downward seepage of groundwater unlikely to occur. However, we calculated the migration of radionuclides in both aquifers for the sake of completeness.

4.6.2 Determination of the contaminated regions and radionuclide discharge rates for the WIPP site

The method described in the previous Section 4.4 to predict radionuclide concentrations in a two-dimensional groundwater flow, which is implemented into the computer code UCBNE21 described in Section 4.5, is used in this section. The contaminated regions of the most hazardous nuclides (e.g. I-129,Ra-226) for different times after the leaching started are determined.

The important result derived from these calculations are the time of contaminant arrival to the biosphere and the location of arrival. In addition, once the location and time of contaminant arrival are known, one can evaluate the discharge rate as well as the cumulative discharge into the biosphere. These quantities present a quantitative measure of the efficiency of the repository as we11 as of the geologic media as barriers for the radionuclide migration (N2).

All the long lived fission products and the four long actinide chains (Pi) are considered in this calculation, although only the results for the most hazardous ones wi11 be reported. Several nuclides can be discarded as potentially hazardous because they either have a small half life (with no long lived precursors), a large retardation coefficient, small toxicity, small initial activity or a combination of these possibilities.

To rank the potential hazard of each nuclide due to its discharge into the biosphere let us consider the following group of parameters

$$10T_{1/2} \quad \text{and} \quad 0.001M_i^0/(MPC)_i \qquad (4.6.1)$$

Physically, the first group of parameters (see Eq. (4.4.19)) represents the water travel time if the nuclides were to arrive at the biosphere after 10 half lives. Therefore, if the calculated water travel time at the biosphere is equal to or larger than the first parameter in Eq. (4.6.1), the concentration of that nuclide has already decayed to a fraction $\exp(-\lambda t)=\exp(-(\ln 2)*10)=.001$.

This leads us to the meaning of the second group of parameters. M_i^0 are the initial activities of each nuclide at the time of burial and therefore $M_i^0/(MPC)_i$ represents the volume of water required to dilute that activity to drinking water standards. Hence, the second parameter in Eq.(4.6.1) is the water volume required to dilute the activity present after ten half lives, which was arbritarily choosen to yield 0.1% of the original activity. For shorter lived actinides (e.g. Ra-226) we consider the parameters of its controlling precursor (e.g. U-234 for times scales of the order of 10^5 years or U-238 for longer time scales) and one assumes Ra-226 to be in secular equilibrium with either U-234 or U-238 because the time scale is large enough. Therefore, the potential hazard a nuclide poses to the

biosphere can be measured by the first group of parameters (10T, ^^min^ ' ^i-^^ represents the migration characteristic of that nuclide and by the second group of parameter (0.OOlM^/MPC^) which represents the toxicity and the total amount of that nuclide initially present.By considering the product of the two group of parameters one can obtain an overall hazard index which can be used to compare different radionuclides in order to rank them.

$$I_i = (101Y/K_{mi}) \ln(0.001M_i/MPC_i) \qquad (4.6.2)$$

The long lived fission products parameters are listed in Table 4.2 and the actinide chains parameters in Table 4.3. By comparing the product of the two parameters in Eq. (4.6.1) one can rank all nuclides as far as potential hazard to the public goes. This ranking is shown in Table 4.4. Ra-226 is ranked first because its controlling parent, U-238, requires a water travel time of about 10^9 years to decay ten half lives. The next ranked nuclide is 1-129 which, due to its retardation coefficient of unity, requires a water travel time of 10^8 years to decay ten half lives. As our calculation will show, the next ranked nuclides Tc-99, U-234, etc. contribute very little to the total discharge rate (expressed in terms of total water dilution rate, Eq. (4.4.22)).

Table 4.2 Long Lived Fission Products Parameters for WIPP site

Nuclide	$T_{1/2}$ (yr)	K_i [a]	$(MPC)_i$ (Ci/m³) [b]	M_i (Ci/GwYr) [c]	$10T_{1/2}/K_i$ (yr)	$.001M_i/MPC_i$ (m³/GwYr)
H-3	1.2E+1	1.0E+0	3.0E-3	1.9E+4	1.2E+2	6.3E+3
C-14	5.6E+3	1.0E+1	8.0E-4	1.3E+1	5.6E+3	1.6E+1
Se-79	6.5E+4	6.0E+2	3.0E-4	1.1E+1	1.1E+3	3.6E+1
Sr-90	2.8E+1	1.0E+0	3.0E-7	2.1E+6	2.8E+2	7.0E+8
Zr-93	9.5E+5	**1.0E+4**	8.0E-4	5.2E+1	9.5E+2	6.4E+1
Nb-93m	1.4E+1	**1.0E+4**	4.0E-4	5.0E+0	1.4E-2	1.2E+1
Tc-99	2.1E+5	1.0E+0	2.0E-4	3.9E+2	2.1E+6	1.9E+3
Ru-106	1.0E+0	1.0E+1	1.0E-5	1.1E+7	1.0E+0	1.1E+9
Cd-113m	1.4E+1	**1.0E+4**	3.0E-5	1.3E+3	1.4E-3	4.5E+4
Sn-126	1.0E+5	1.0E+3	2.0E-5	1.5E+1	1.0E+3	7.4E+2
Sb-125	2.7E+1	1.0E+2	1.0E-4	2.1E+5	2.7E+0	2.1E+6
1-129	1.7E+7	1.0E+0	6.0E-8	1.0E+0	1.7E+8	1.7E+4
Cs-137	3.0E+1	4.1E+2	2.0E-5	2.9E+6	7.3E-1	1.5E+8
Cs-135	3.0E+6	4.1E+2	1.0E-4	7.8E+0	7.3E+4	7.8E+1
Ce-144	7.8E-1	1.2E+4	1.0E-5	2.1E+7	6.5E-4	2.1E+9
Pm-147	4.4E+0	2.5E+3	2.0E-4	2.6E+6	1.8E-2	1.3E+7
Sm-151	8.7E+1	2.5E+3	4.0E-4	3.4E+4	3.5E-1	8.5E+4
Eu-152	1.3E+1	2.5E+3	6.0E-5	3.3E+2	5.1E-1	5.5E+3
Eu-154	1.6E+1	2.5E+3	2.0E-5	1.9E+5	6.4E-2	9.4E+6
Eu-155	1.8E+0	2.5E+3	2.0E-4	1.7E+5	7.2E-3	8.7E+5

a/: From reference -(D1),(C2).
b/: From 10CFR20, Appendix B and (P2).
c/: For reprocessed high level waste, LLfR, 10 years decay, 0.5% U and Pu loss into the waste,(B2).

Table 4.3 Actinide Chains Parameters for The WIPP site.

Nuclide	K_i (yr)	(MPC) [J?/] (Ci/m^3)	M (Ci/GwYr)	$10T_{1/2}$ (yr)	$.001M_i/MPC$ (m^3/GwYr)
Ra-225	4.1E-2	6.8E+2	5.0E-7	1.1E+3	8.7E+5
Ra-226***	1.6E+3	6.8E+2	3.0E-8	8.9E+4	1.5E+3
Ra-226****[a]	6.6E+3	6.8E+2	3.0E-8	1.6E+9	5.5E+1
Th-228	1.9E+0	5.9E+4	7.0E-6	1.1E+0	8.9E+4
Th-229	7.3E+3	5.9E+4	5.0E-7	1.1E+3	1.2E+4
Th-230***	8.0E+4	5.9E+4	2.0E-6	8.9E+4	3.2E-1
Th-230****	8.0E+4	5.9E+4	2.0E-6	1.6E+9	8.4E-3
U-233	1.6E+5	2.8E+1	3.0E-5	1.1E+3	2.0E+2
U-234	2.5E+5	2.8E+1	3.0E-5	1.2E+0*	8.9E+4	3.8E+1
U-235	7.1E+8	2.8E+1	3.0E-5	2.3E-3	2.5E+8	7.7E-2
U-238	4.5E+9	2.8E+1	4.0E-5	4.3E-2	1.6E+9	1.0E+0
Np-237	2.1E+6	1.9E+4	3.0E-6.	1.5E+1**	1.1E+3	5.2E+3
Pu-238	8.6E+1	5.7E+4	[r].0E-6	5.1E+2	1.5E-2	1.0E+5
Pu-239	2.4E+4	5.7E+4	5.0E-6	4.4E+1	4.2E+0	8.8E+3
Pu-240	6.6E-3	5.7E+4	5.0E-6	2.7E+2	1.1E-0	5.3E+4
Pu-241	1.3E+1	5.7E+4	2.0E-4	1.4E+4	3.1E+1	7.0E+4
Pu-242	3.8E+5	5.7E+4	5.0E-6	1.9E-1	6.6E+1	3.8E+1
Am-241	4.6E+2	1.0E+4	4.0E-6	4.9E+3	4.6E-1	1.2E+6
Am-242m	1.5E+2	1.0E+4	4.0E-6	1.2E+2	1.5E-1	2.9E+4
Am-243	7.9E+3	1.0E+4	4.0E-6	4.8E+2	7.9E+0	1.2E+5
Cm-242	4.5E-1	3.0E+3	2.0E-5	4,4E+5	1.5E-1	2.2E+7
Cm-243	3.2E+1	3.0E+3	5.0E-6	9.0E+1	1.0E-1	1.8E+4
Cm-244	1.8E+1	3.0E+3	7.0E-6	7.4E+4	5.9E-2	1.0E+7
Cm-245	9.3E+3	3.0E+3	4.0E-6	9.8E+0	3.1E+1	2.4E+3
Cm-246	5.5E+3	3.0E+3	4.0E-6	1.9E+0	1.8E+1	4.8E+2

*Includes the decay of Pu-238,Am-242m and Cm-242.
**Includes the decay of Pu-241 and Am-241.
***Based on U-234 value
****Based on U-238 value
[a]/:From reference (D1), (C2).
[o]/:From 10CFR20,Appendix B and (P2).
[c]/:For reprocessed high level waste,LWR,10 years decay,0.5% U and Pu loss into the waste, (B2). Am-242m is in the metastable form.

Table 4.4 Potential Hazardous Nuclide Ranking for the WIPP site

Ranking	Nuclide	lOT^/Kj^	1\
1	Ra-226	1.6E+9*	6.5E+9
2	1-129	1.7E+8	1.7E+9
3	Tc-99	2.1E+6	1.6E+7
4	11-234	8.9E+4	3.2E+5
5	Cs-135	7.3E+4	3.2E+5
6	Se-179	1.1E+3	2.3E+4

*Ra-226 is assumed to be in secular equilibrium with U-238. Thus values of half-life and retardation coefficients for U-238 are used

The calculated (Dl,using model calibration as described in Section 4.4.1) Potentiometrie data shown in Figure 4.8 is represented in a three dimensional plot in Figure 4.11. The projection of the Pecos River flow pattern onto the Potentiometrie surface is also shown. The shape of the surface clearly indicates that the general direction of flow is southward. The presence of a "valley" in the Potentiometrie surface will cause the streamlines to converge in that region. Such valleys are caused either by a strong sink, as in the case of a river, or by a region of high hydraulic conductivity, as in the case of fracture zones. In the case of the Rustler aquifer with the calculated Potentiometrie data it seems that the valley in the Potentiometrie surface near Malaga Bend is caused by the both the river and a large value of the hydraulic conductivity.

The three dimensional representation of the Potentiometrie surface obtained from the raw data exhibited in Figure 4.8 is

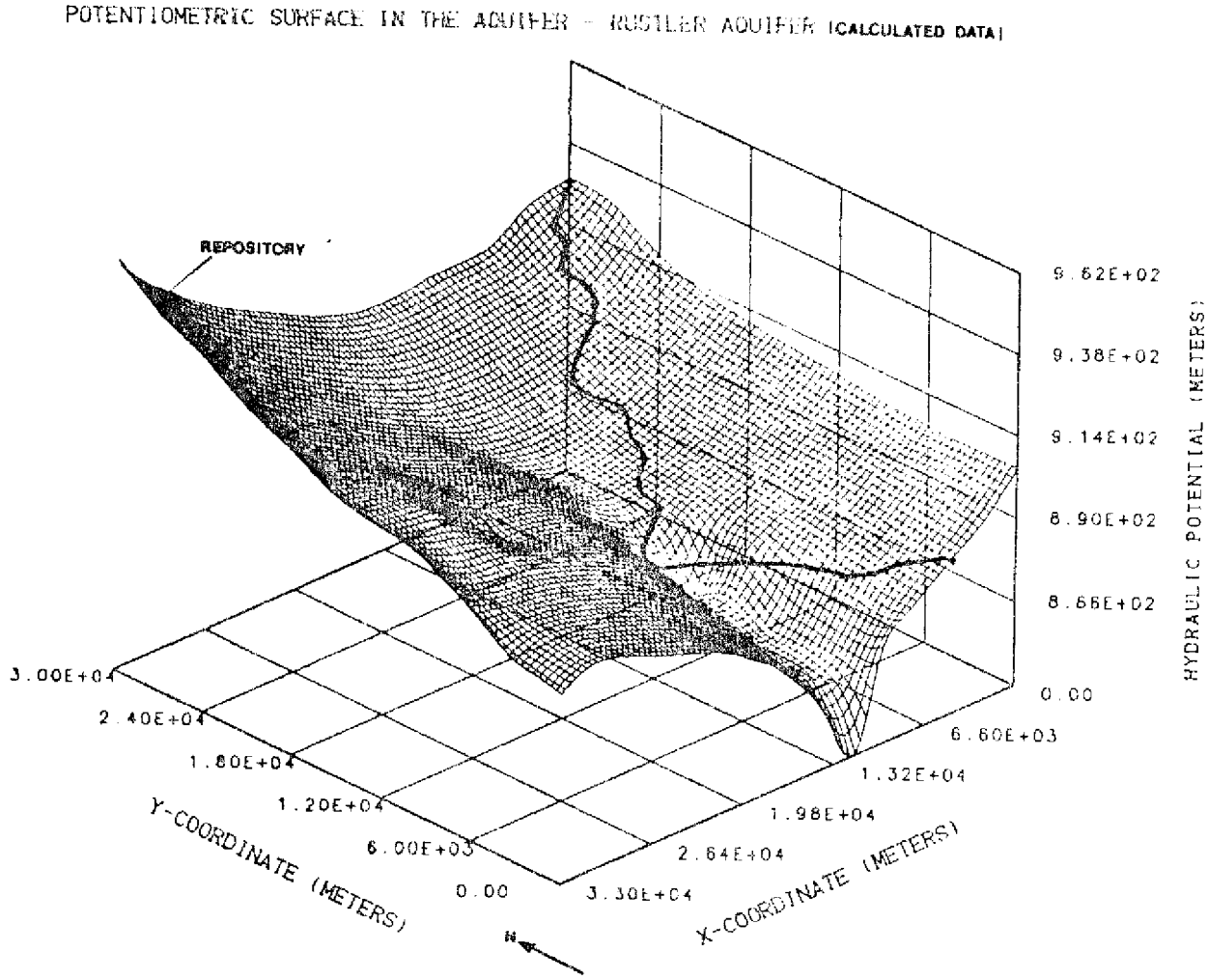


Figure 4.11 The Potentiometrie surface (calculated data) in Rustler aquifer with the projection of Pecos River onto the surface

shown in Figure 4.11a. The same general trend observed in the calculated potential is seen here. However, the "valley" begins in a region located about 10 km to the north. The streamlines of the flow coming from the repository will tend to converge in the "valley" north of Malaga Bend, away from the river. After the streamlines are bunched they will move towards Pecos River.

Hydrological calculations for the determination of the contaminated streamlines, hydraulic conductivities and water travel times were performed by the computer program HYDRO for both sets of potentiometric data. The entire shadow region is covered by five streamlines in each case. The water travel time to reach the biosphere (Pecos River) for each streamline for each set of the potentiometric data is shown in Table 4.5.

Table 4.5 Water Arrival time at the Biosphere for the WIPP site

Streamline no. a/	Water arrival time (years) Rustler Aquifer (calculated data)	Rustler Aquifer (raw data)	Delaware Aquifer (raw data)
1	2.23E+4	2.17E+4	1.68E+6
2	3.15E+4	9.73E+3	6.24E+G
3	4.65E+4	1.82E+4	1.80E+6
4	4.24E+4	3.33E+5	1.40E+6
5	4.11E+4	3.50E+5	3.46E+6

a/ See streamline number in Figure 4.12 and Figure 4.19

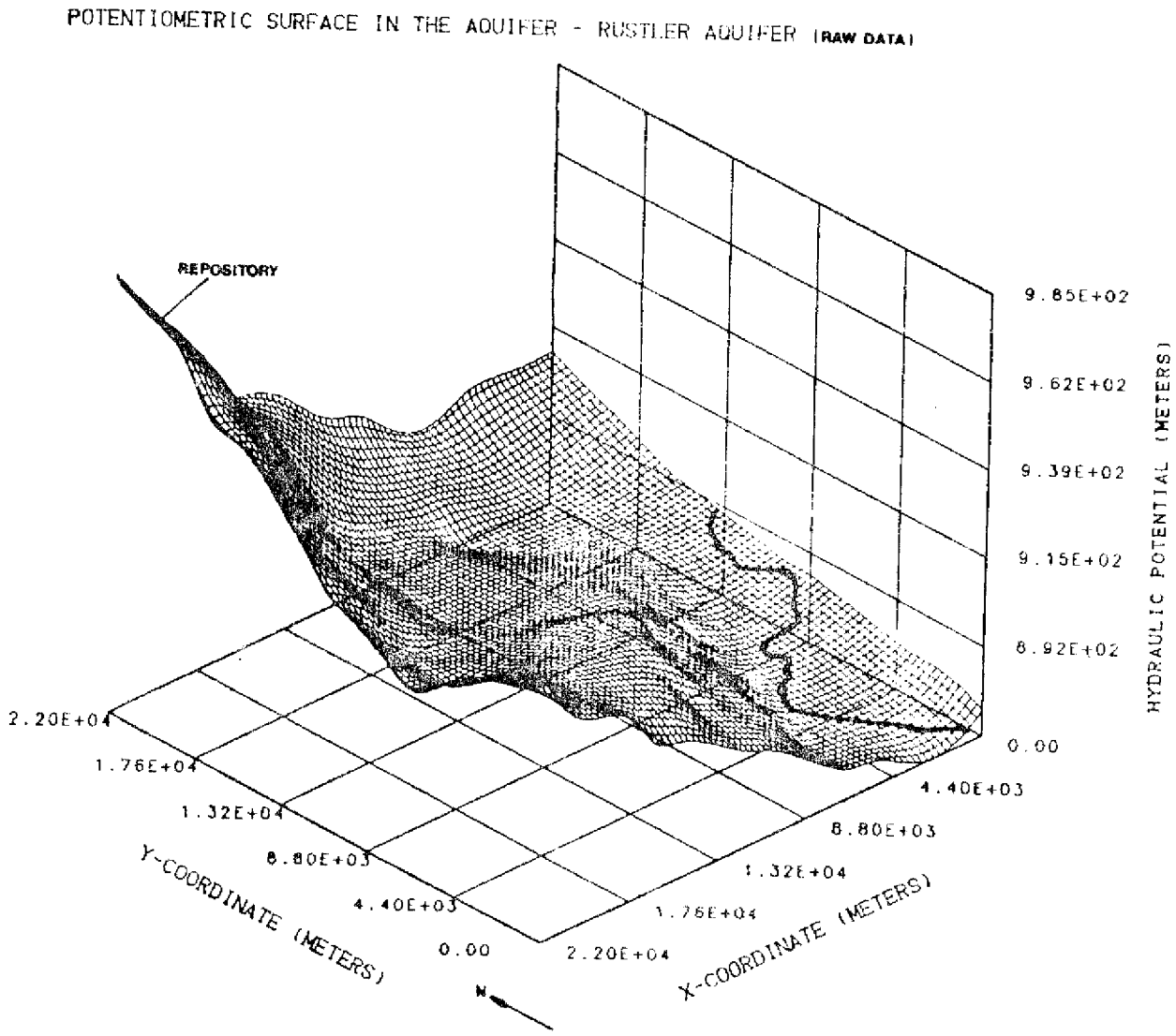


Figure 4.11a Potentiometrie surface (raw data) in Rustler aquifer with the projection of Pecos River onto the surface.

For the calculated (D1) potentiometric data set the shortest water travel time to the biosphere is 2.23E+4 years, while for the raw data set the shortest water travel time to the biosphere is 9.73E+3 years. From these values one can conclude that only the first five ranked nuclides in Table 4.4 will reach the Pecos River after migrating through Rustier aquifer. All other nuclides will be retarded and they will have decayed before reaching the Pecos River.

Figure 4.12 and Figure 4.13 show the 1-129 contaminated region at 10^1, 10^4 and 10^5 years after the leaching started indicated by the dotted areas. The lines of constant potential are labelled with their values expressed in meters above mean sea level. Only the streamlines of the repository shadow region are shown. For these figures the calculated potential data were used. As was expected, the 1-129 will discharge into Pecos River near Malaga Bend. According to Figure 4.13, after 10^5 years almost all 1-129 have already been discharged into Pecos River.

Figure 4.14 and Figure 4.15 show the Ra-226 contaminated region in the WIPP site region. After about 10^6 years Ra-226 starts discharging into the river while the trailing edge of its migration band is still near the repository site, because of the large retardation coefficient for Th-230.

Figure 4.16 shows the water dilution rate of 1-129 in the Pecos River for the calculated set of potentiometric data. Three

values of leach time were used for comparisons (10^4, 10^5 and 10^6). Increasing the value of the leach time by an order of magnitude decreases the water dilution rate by approximately one order of magnitude for 1—129.» The first nuclide arrival time is about 2.0E+4 years for 1-129.

Similarly, Figure 4.17 shows the water dilution rate and water dilution volume for Ra-226 discharging into Pecos River from Rustler aquifer with the calculated set of potentiometrie data. The peak water dilution rate and the peak water dilution volume are three orders of magnitude smaller than for 1-129.And the first arrival time for Ra-226 is 8. OE+5 years.

The calculations were repeated for the other nuclides ranked in Table 4.4 but their contribution to the total water dilution rate were negligible when compared to 1-129 and Ra-226 contributions. Therefore, the total water dilution rate before 8.OE+5 years is due primarily to 1-129 and after that time Ra-226 becomes the major contributor but with a peak value three orders of magnitude smaller. In addition to these quantitative considerations one should notice that the location of discharge for the contaminated streamlines into the Pecos River is practically localized.

Comparable calculations were repeated for the Rustler aquifer, but in this case with the raw set of piezometric data. Figure 4.18 show the 1-129 contaminated region after 10^3 and 10^4

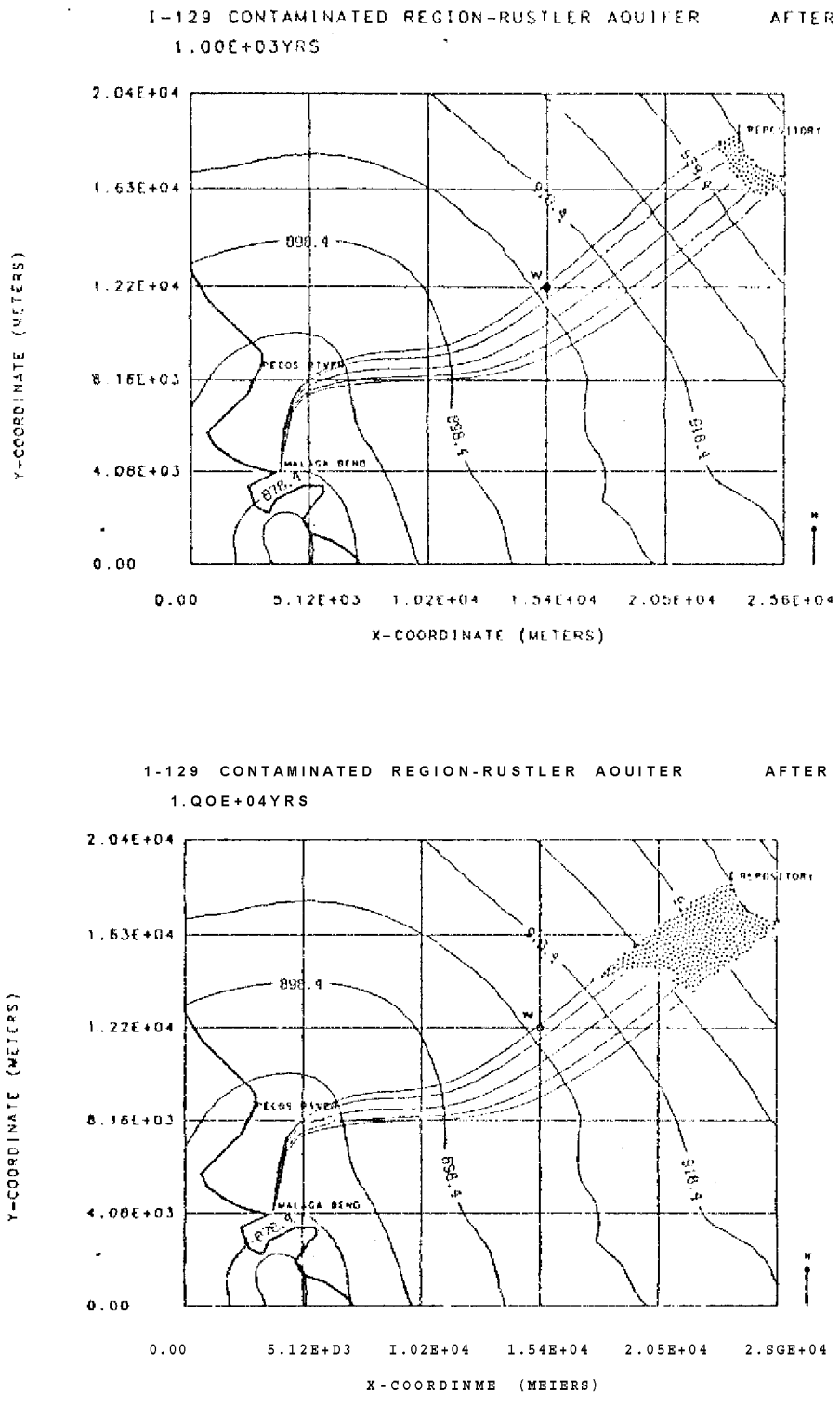


Figure 4.12 1-129 contaminated region in Rustler aquifer (calculated data) after ID3 ..ri in ' years. Potentials are in meters above MSL.

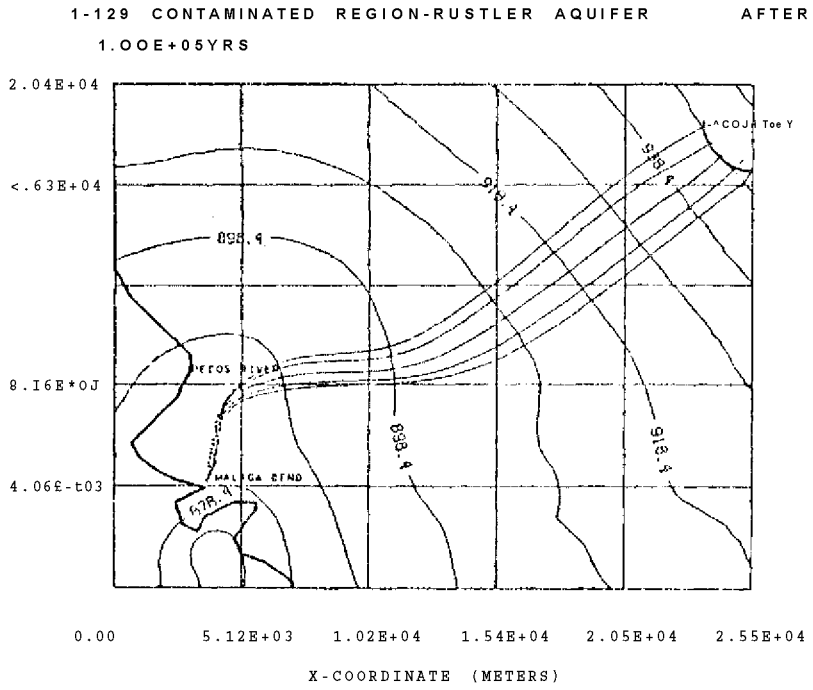
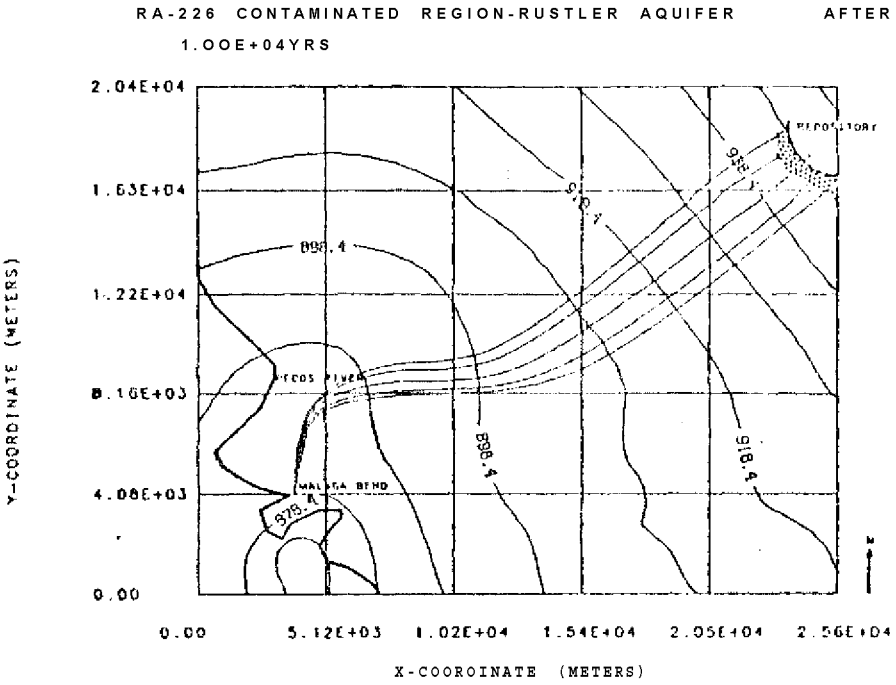


Figure 4.13 1-129 contaminated region in Rustler aquifer (calculated data) after 10° years. Potentials are in meters above MSL.



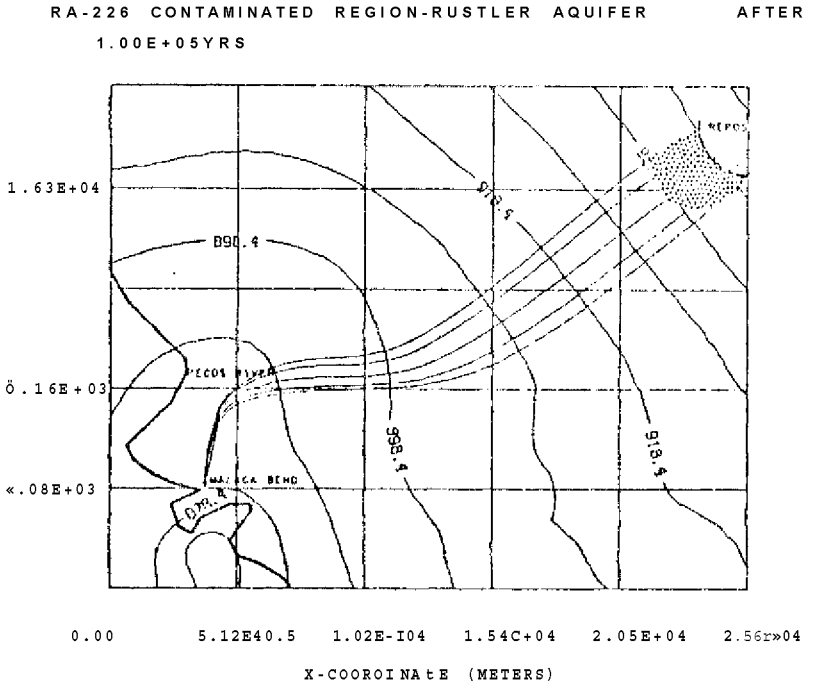
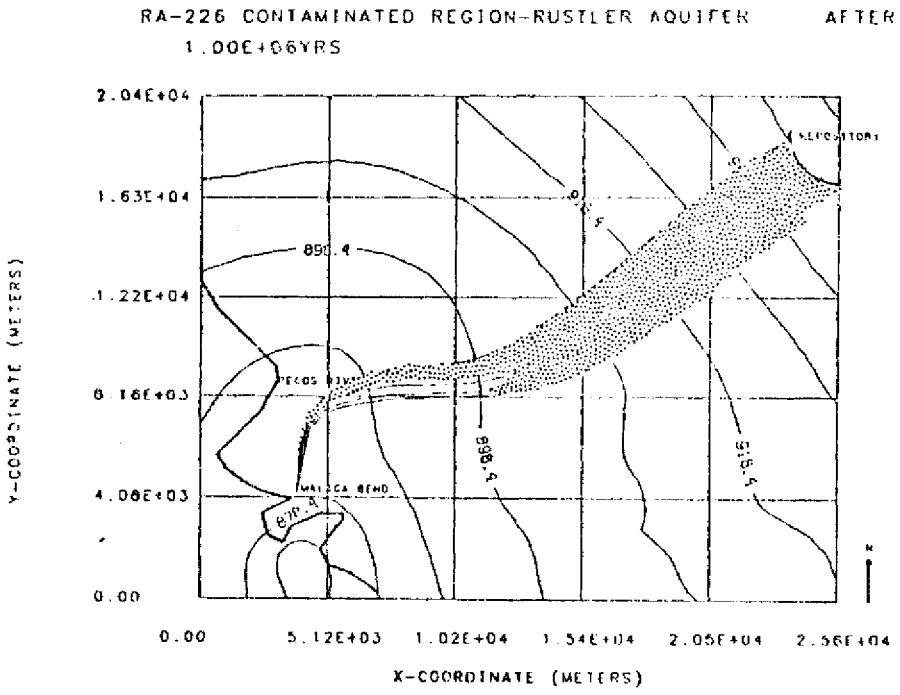


Figure 4.14 Ra-226 contaminated region in Rustler aqui (calculated data) after 1^ and 10^ years. Potentials are in meters above MSL.



Fiaure 4.15 Ra-226 contaminated region in Rustler aquifer (calculated data) after 10* years.

Potentials are in meters above MSL.

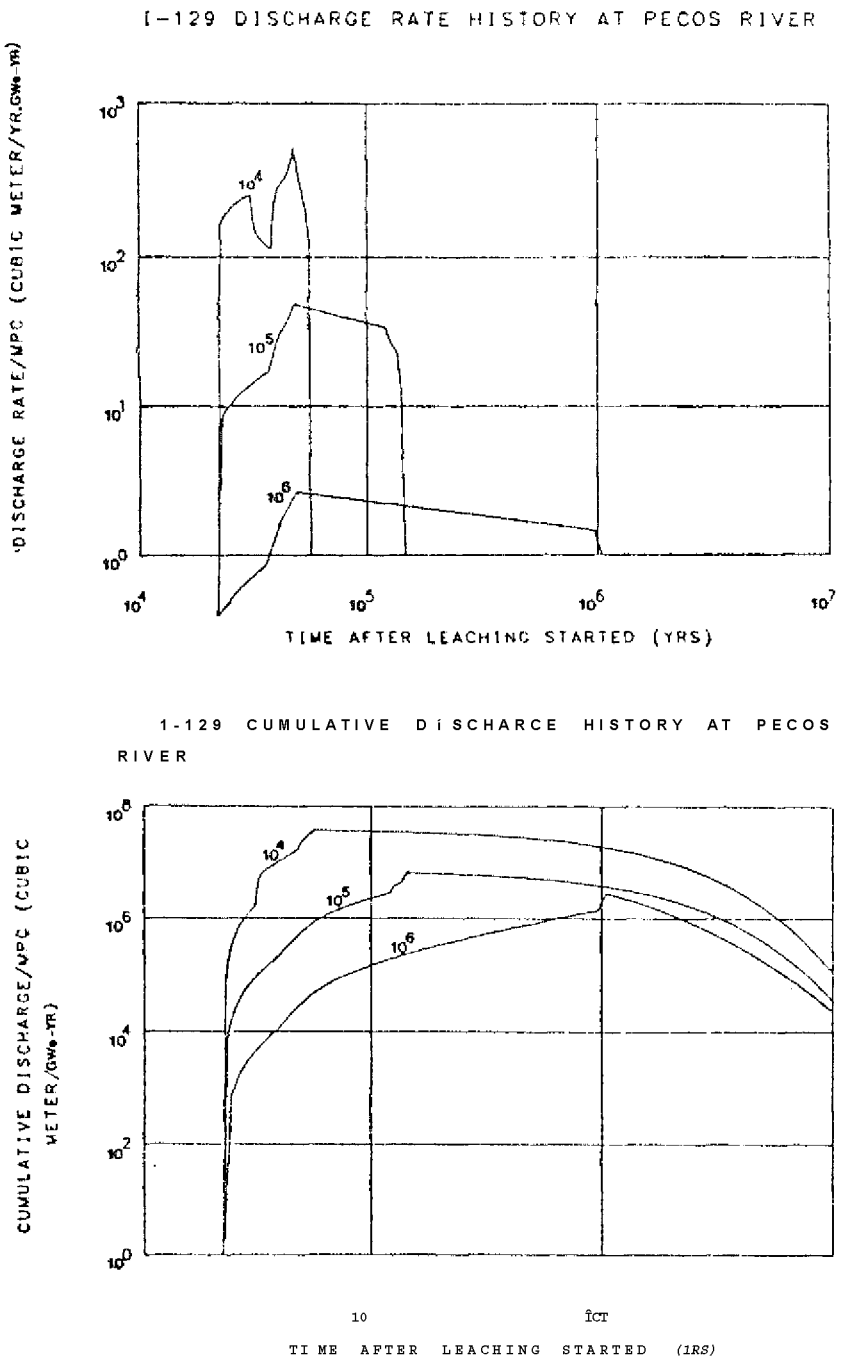


Figure 4.16 1-129 discharge rate/MPC (water dilution rate) and cumulative discharge (water dilution volume) at Pecos River discharging from Rustler aquifer (calculated data) for leach times of 10^4, 10^5 and 10^6 years

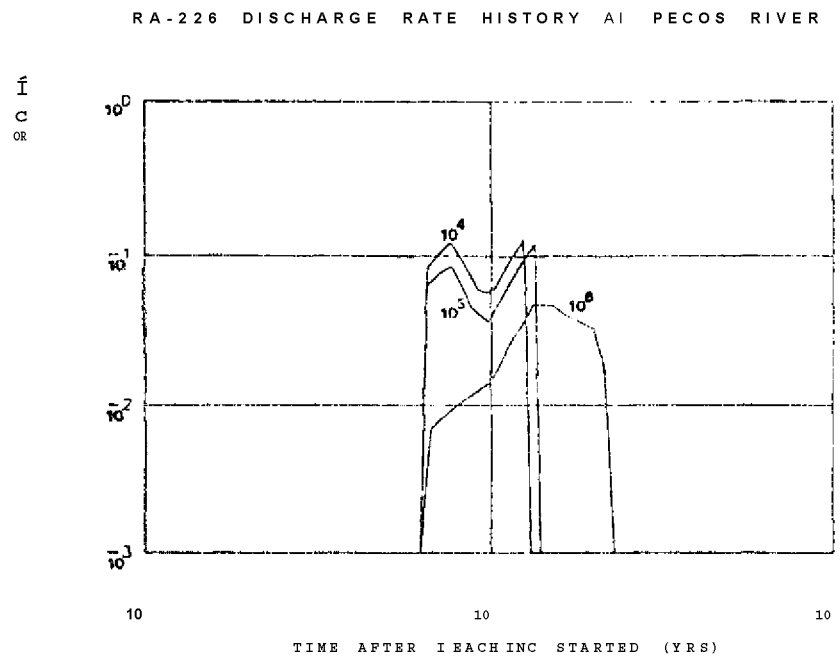


Figure 4.17 Ra-226 discharge rate/MPC (water dilution rate) and cumulative discharge/MPC (water dilution volume) at Pecos River discharging from Rustler aquifer (calculated data) for leach times of 10^,10^ and 10 years

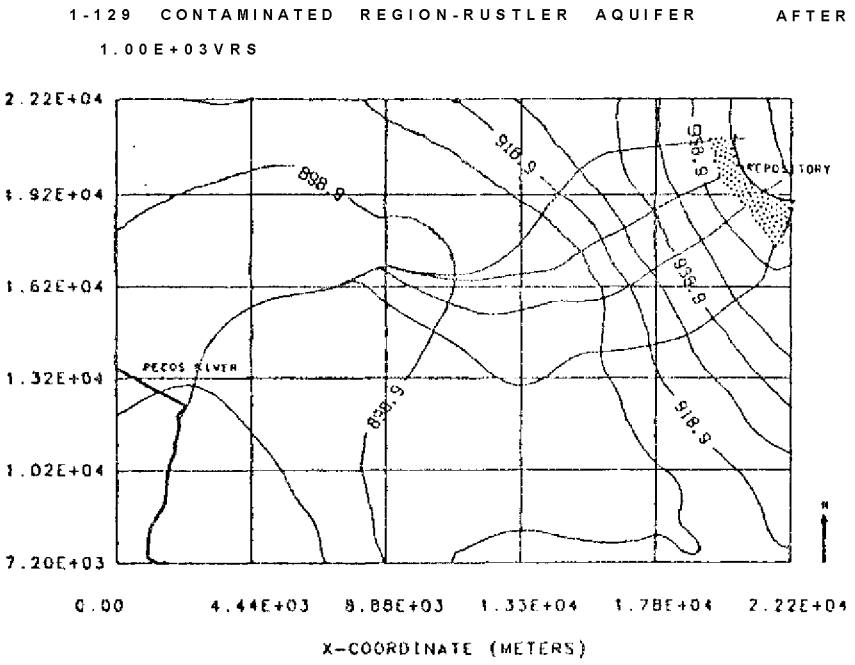
years from the beginning of leaching. Compared to the figures for the calculated potential data case one notices that the confluence of streamlines occurs earlier and the discharge into Pecos River is farther north of the Malaga Bend. After 10^5 years 1-129 has been totally discharged from the Rustler aquifer.

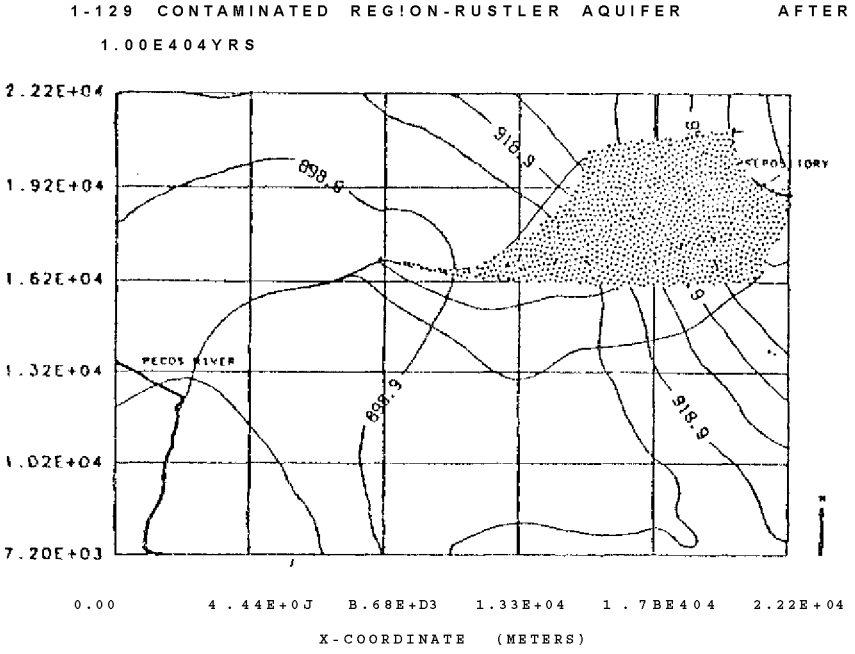
Figure 4.19 and Figure 4.20 show the contaminated region for Ra-226 in Rustler aquifer with the raw set of data for 10^7 thru 10 years. Figure 4.21 shows the 1-129 water dilution rate and water dilution volume, respectively, while Figure 4.22 show the water dilution rate and water dilution volume of Ra-226.

For this case, using the raw set of data, the first 1-129 reaches Pecos River after 10^4 years and Ra-226 after 4.0E+5 years instead of 3.0E+4 years and 9.0E+5 years for the calculated set of potentials. The magnitude of the water dilution rate are comparable to those obtained in the calculated set. of data case.

During the period between 1937 and 1975 the maximum recorded Pecos River flow rate at Malaga Bend was 1.1E+11 m^3/yr while the lowest was 4.5E+6 m^{-i}/yr. In the same period the average river flow rate was 1.7E+8 m^3/yr.

These Pecos River flow rates at the Malaga Bend are compared to the maximum total water dilution rate of 500 m^3/yr for radionuclides discharging into Pecos River at any time. This maximum occurs for 1-129, using the calculated potential and a





18 1-129 contaminated region in Rustler aquifer (raw data) after 10-3 and 1 JQA years. Potentials are in meters above MSL.

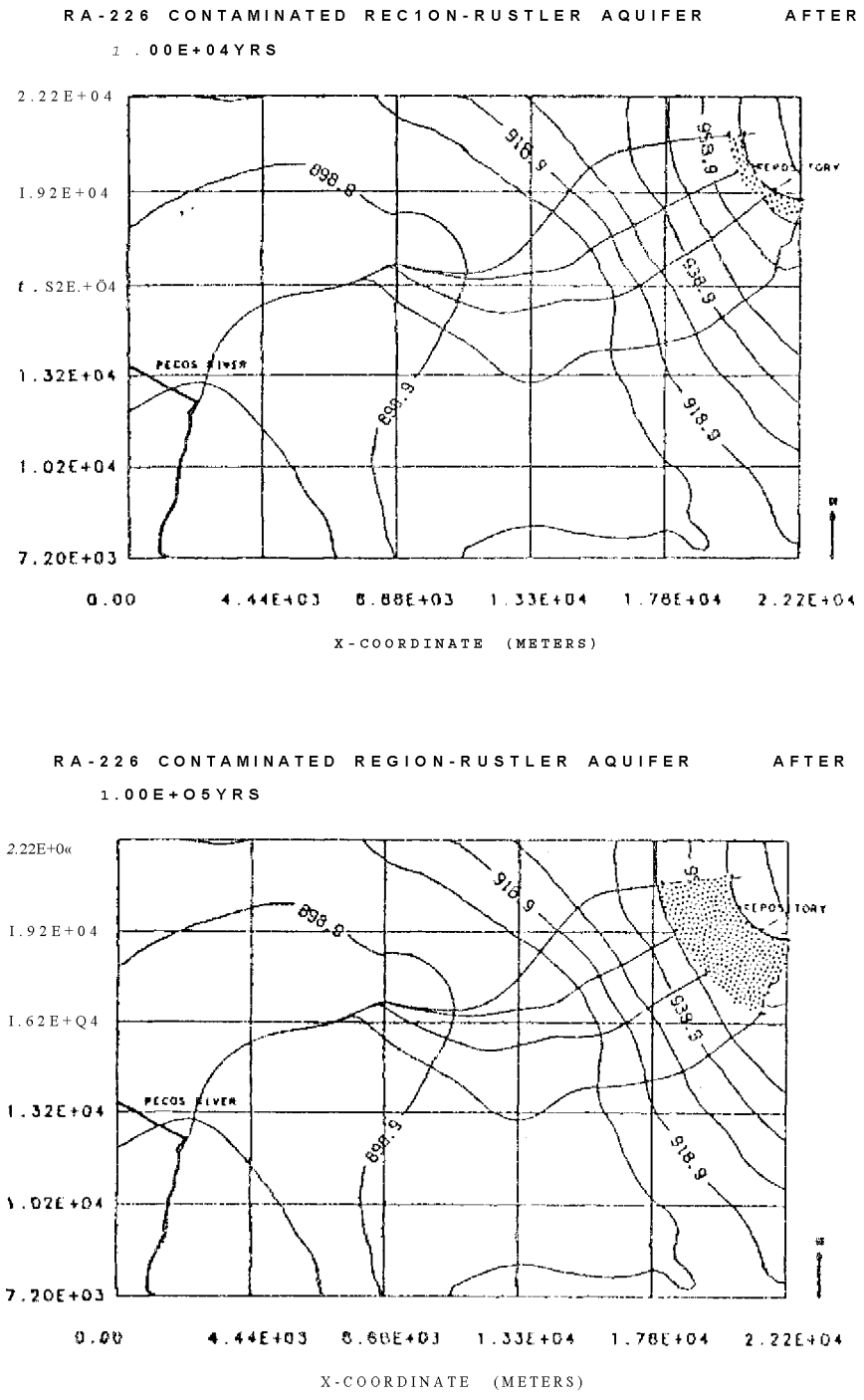
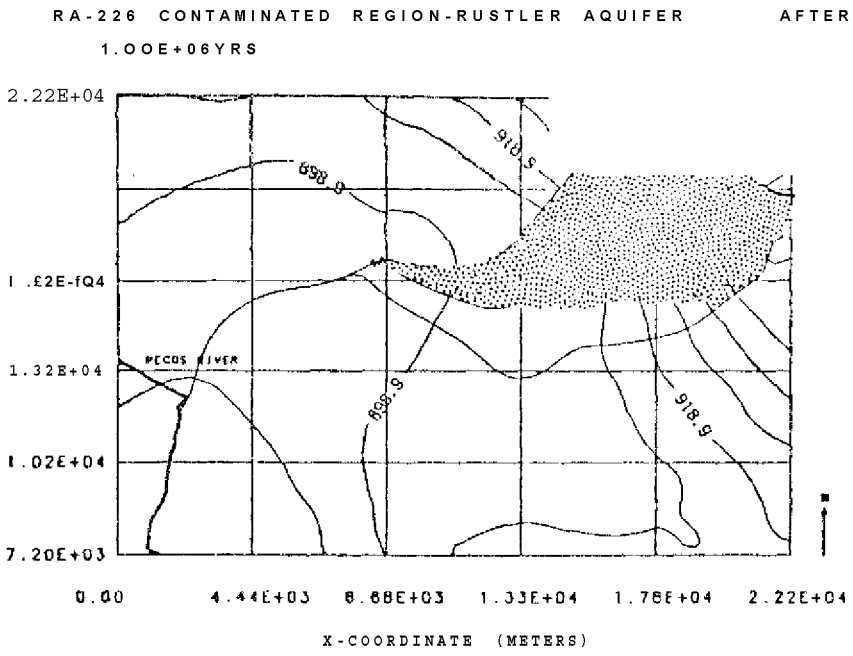


Figure 4.19 Ra-226 contaminated region in Rustler aquifer (raw data) after 10^ and 10^ years. Potentials are in meters above MSL.)



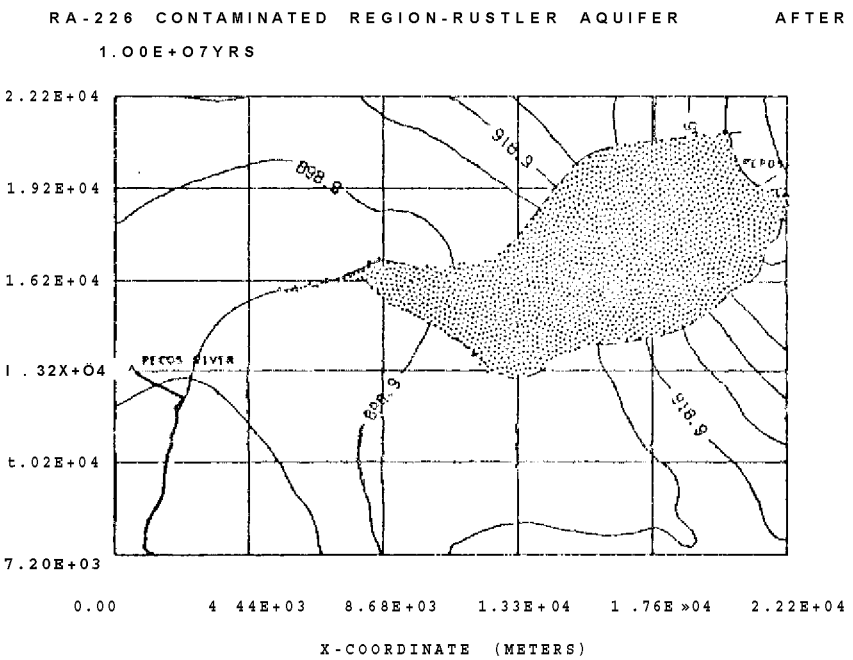
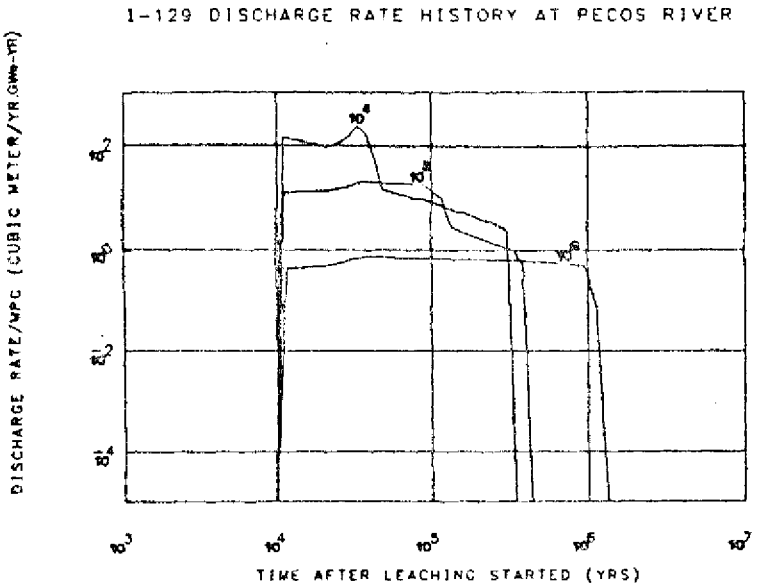
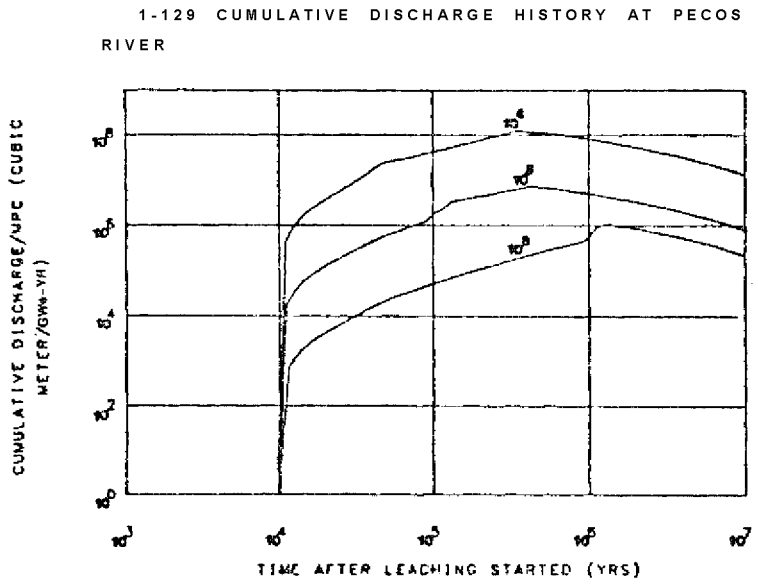


Figure 4.20 Ra-22.6 contaminated region in Rustler aquifer (raw data) after 10^6 and 10^7 rears. Potentials are niven in meters above MSL.





Fiaure 4.21 1-129 discharge rate/MPC (water dilution rate) and cumulative discharge/MPC (water dilution volume) at Pecos River discharging from Rustler aquifer (raw data) for leach times of 10^4, 10^5 and 10^6 years

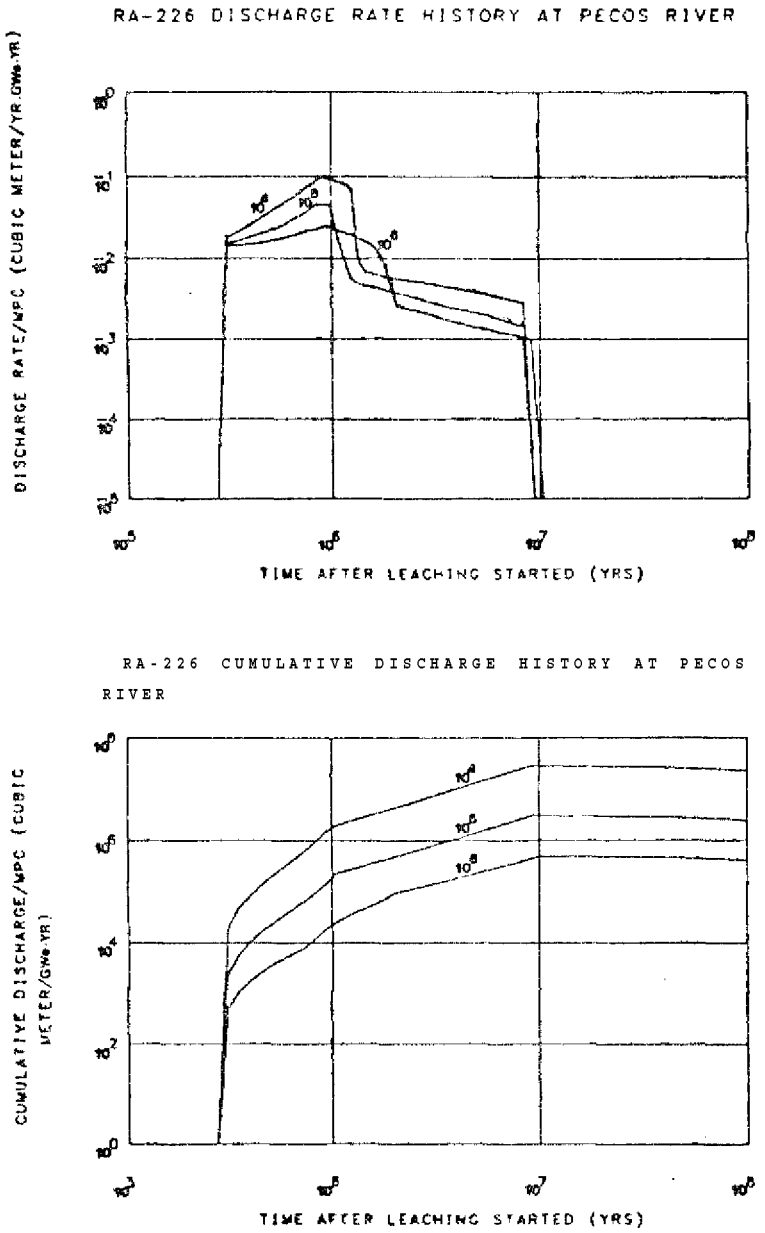


Figure 4.22 Ra-226 discharge rate/MPC (water dilution rate) and cumulative discharge/MPC (water dilution volume) at Pecos river discharging from Rustler aquifer (raw data) for leach times of 10^{4}, 10^{5} and 10^{6} years

leach time of 10 years. One concludes that when Pecos River is flowing at its minimum capacity it is still larger by a factor of 1000. Taking into account the fact that the amount of waste considered in the calculations is the result of production of one Gw(e)yr by a LWR, the Pecos River minimum flow rate would be sufficient to dilute to MFC levels the contamination caused by the reprocessed high leve1 waste of 330 LWR's operating during their 30 years lifetime at full capacity.

At the WIPP site the downward seepage of contaminated groundwater into the underlying Delaware Mountain Group aquifers will be very unlikely. This is because the temperature gradient caused by the decay heat in the waste packages wi11 produce an upward driving force due to density gradients. In addition, even after sufficient time for the heat generation to be significantly reduced, the hydraulic potential in the Delaware aquifer, being larger than in the Rustler aquifer, will cause the flow through any connection between them to be upwards.

Even if the Delaware aquifer were to be contaminated, the potential hazard due to the discharge of radionuclides into the Capitan aquifer situated about 30 km to the north would be small because the water travel times in this aquifer are large. Nevertheless calculations were performed for this case based on calculated (Dl) set of hydraulic heads.

Figure 4.23 shows the potentiometrie surface in the

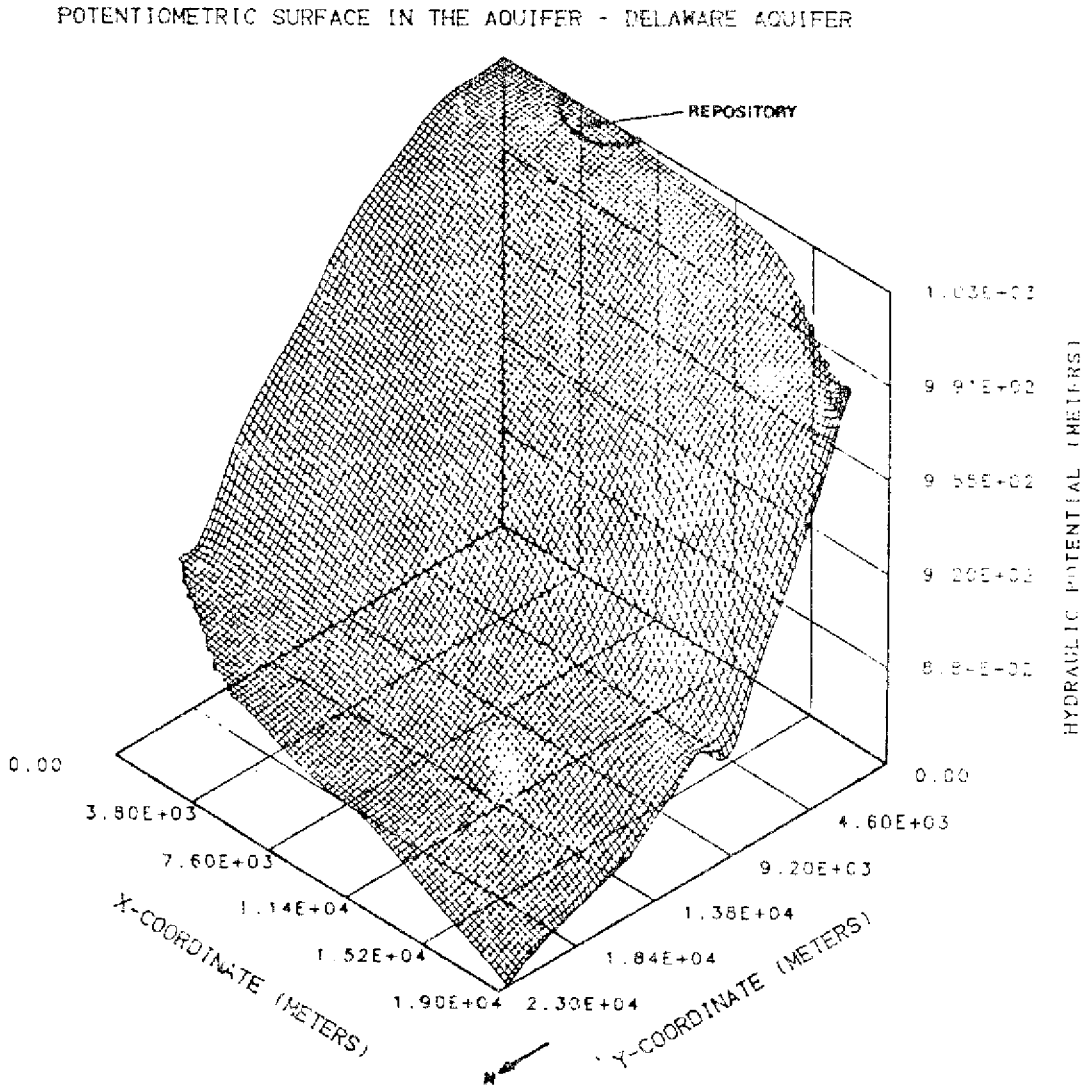


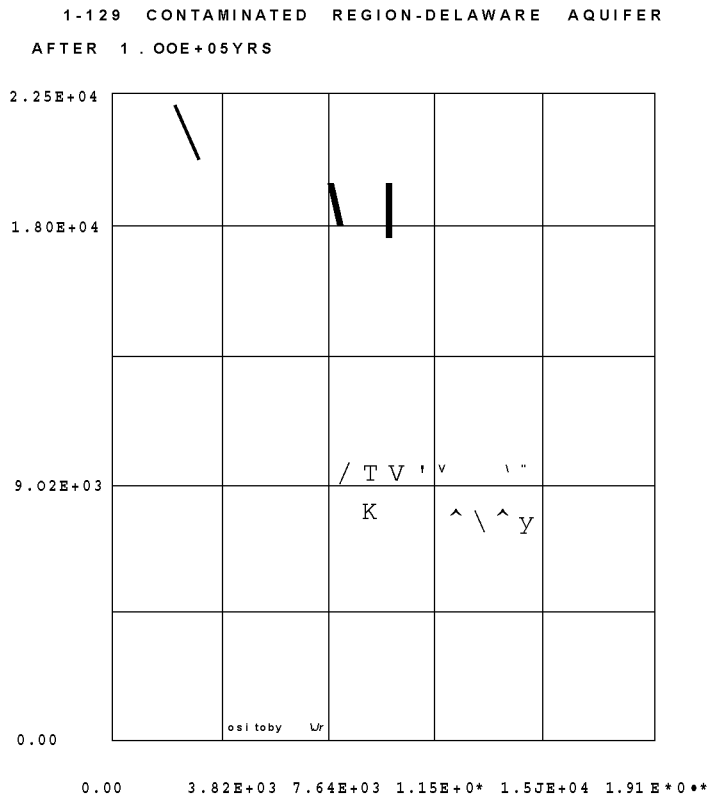
Figure 4.23 The Potentiometrie surface in the Delaware Mountain Group Aquifer.

Delaware aquifer. The absence of irregularities like "valleys" and "hills" indicate that the streamlines will have no confluence or divergent tendencies but exhibit a rather regular pattern. Contrary to the Rustler aquifer, the Delaware aquifer flows northward discharging into Capitan aquifer. As it is shown in Figure 4.24 it would take more than 10^6 years for 1-129 to reach Capitan aquifer.

Besides the discharge into the Pecos River, there is another pathway to the biosphere that can be potentially hazardous to the public health. If a fresh-water-producing well is dug in the shadow region of the repository, deep enough to reach the Rustler aquifer, the water pumped might contain radioactive elements released from the repository.

A typical water producing well flow rate of about 350 m^3/yr was assumed (M2). The calculated potentiometrie surface in the Rustler aquifer was considered and the well location lies inside the shadow region. The well is located at the coordinates: x=15,400 meters and y=12,200 meters (see coordinate system in Figure 4.12 where the well location is defined by a "W").

After superimposing the existing natural hydraulic potential of Rustler aquifer to the potential due to the well (point sink in Eq.(4.3.9)) with above flow rate the resulting potential calculated by HYDRO shows no significant differences from the original Rustler aquifer potential. This is because the



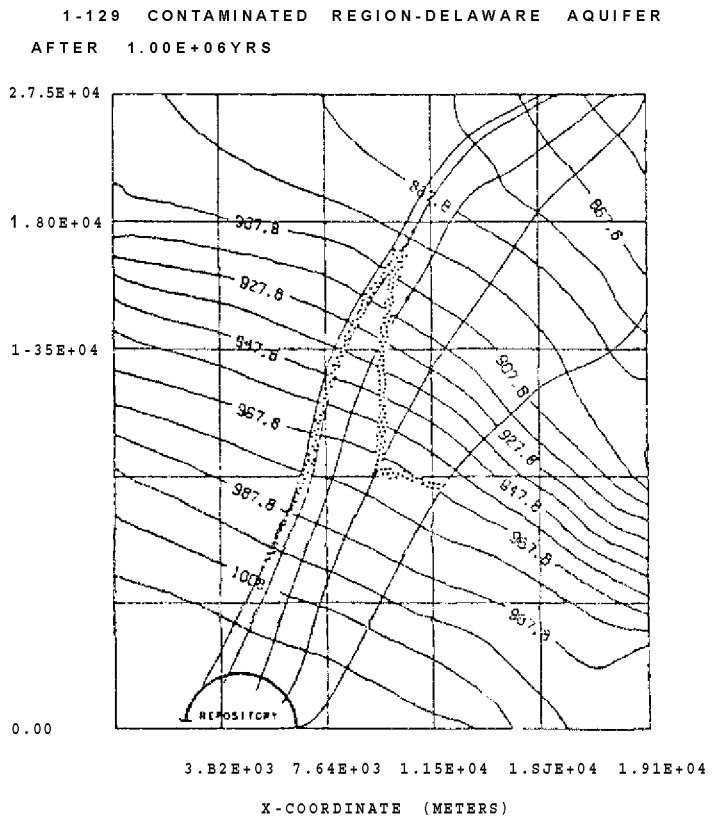
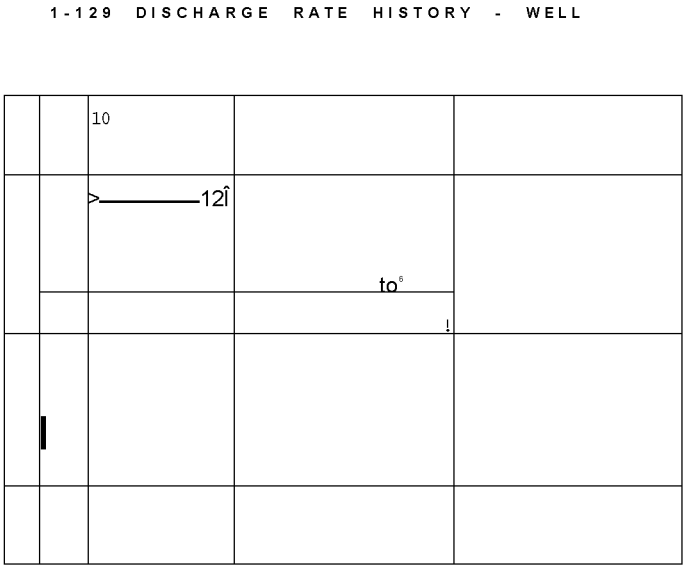


Figure 4 . 24 1-129 contaminated region in Dola'wr? *Vr in tain '"•roup anui'Ter (calculated data) after 10-^ and 10* yrs. Potentials are in meters above MSL.

well flow rate is small compared to the aquifer yield (by a factor of 1000). Therefore, one can use the hydrological calculation already done for the Rustler aquifer with the calculated set of potentiometrie data. Figure 4.11 and Figure 4.12 thru Figure 4.15 are still valid, however, the well location is now part of the biosphere and the discharge rates, nuclide arrival times at the well are different from those quoted earlier.

The water travel time to reach the well is 13,500 years, as compared with the 31,500 years to reach Pecos River. For this water travel time 1-129 and Ra-226 are still the most hazardous nuclides. Figure 4.24a and Figure 4.24b show their discharge rates and cumulative discharge in the well. The maximum water dilution rate for 1-129 is again almost three order of magnitude larger than that of Ra-226. For leach times of 10^{A} years and 10^{5} years 1-129 discharges earlier than Ra-226 and they discharge at different times because they have different retardation coefficient. Since the water arrival time to the well is of the order of 10^{4} years and the unit retardation coefficient, the times of discharge for leach times larger than 10^{A} will1 be equal to the leach times. If, however the retardation coefficient were not unity, then the time of discharge would be controlled either by the leach time or by the product of the water travel time to the well times the retardation coefficient, whichever is larger (see Eq. (4.3.5f)). The maximum 1-129 water dilution rate is about 10 m /yr which 35 times smaller than the well flow rate of 350 m^3/yr.



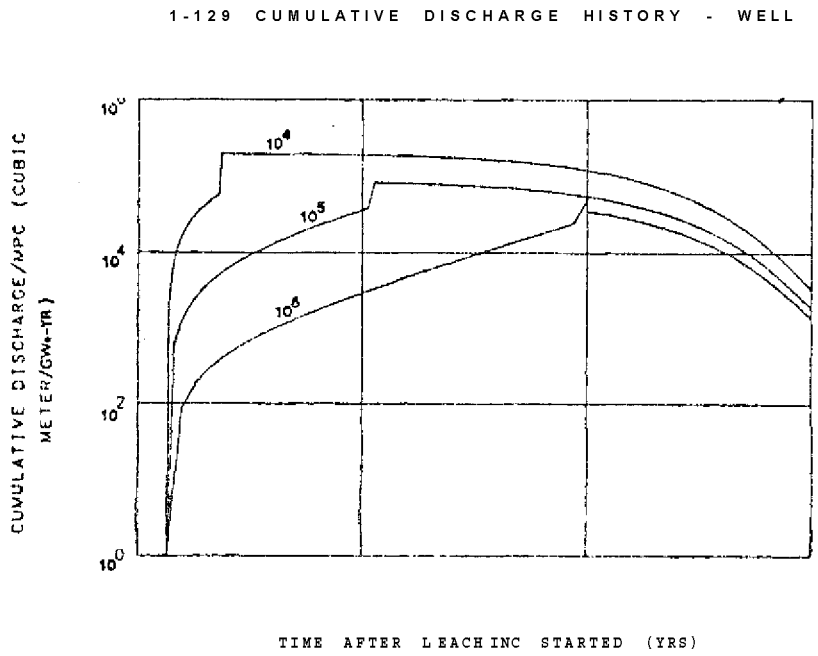
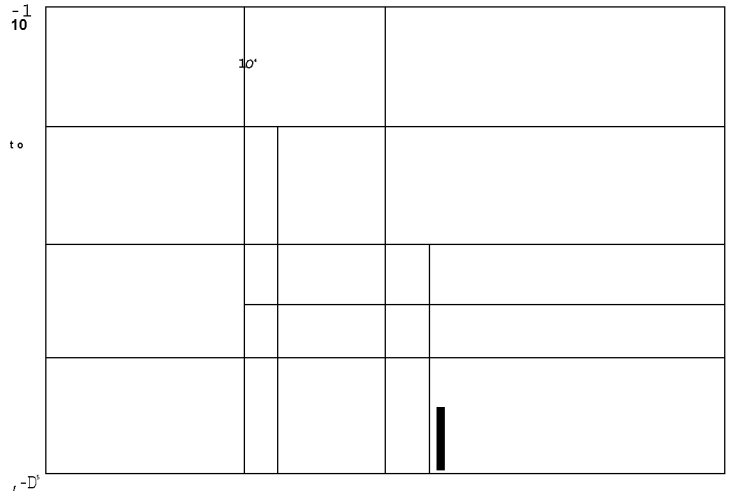


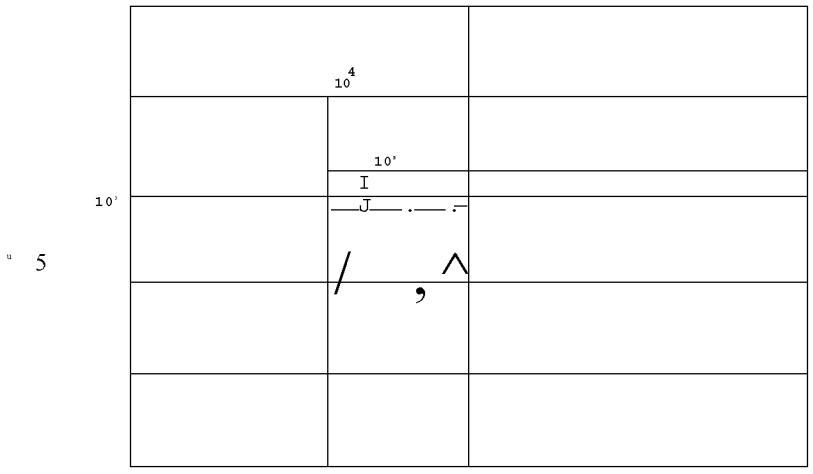
Figure 4.24a 1-129 discharge rate/MPC (water dilution rate) and cumulative discharge/MPC (water dilution volume) at a well in Rustler aquifer shadow region (calculated data). Leach times values are: 10^4, 10^5 and 10^6 years

RA-226 DISCHARGE RATE HISTORY - WELL



TIME AFTER LEACHING STARTED (YRS)

RA-226 CUMULATIVE DISCHARGE HISTORY - WELL



TIME AFTER LEACHING STARTED (YRS)

Figure 4.24b Ra-226 discharge rate/MPC (water dilution rate) and cumulative discharge/MPC (water dilution volume) at a well in Rustler aquifer shadow region (calculated data). Leach time values are: 10^4, 10^5 and 10^6 years

Addendum to Section 4.6

Cole and Bond (C3), also studied the far field migration of radionuclides for the WIPP site. Their work is reviewed in this addendum.

The hydrological calculations in (C3) were performed by the computer program VTT (Variable Thickness Transient Flow, Si). This code solves numerically the governing equation for the groundwater conservation with inhomogeneous aquifer parameters values for the Darcy's flow. For the steady state problem, the model utilizes a finite difference formulation involving Newton's method and a direct Gaussian elimination procedure (see SI for a more detailed description). VTT uses the measured Rustler aquifer piezometric data (Figure 4.7) for the "model calibration" as described in Section 4.4.1. By assuming initial guesses for the aquifer hydraulic conductivity and the boundary conditions, the computer program VTT solves numerically Eq.(4.4.1). The resulting hydraulic head distribution is then compared to Figure 4.7 and by using some arbitrary weighting function to check the consistency between the solution obtained with the measured data new aquifer parameters and boundary conditions are deduced. These new values are used and a corrected solution for the hydraulic head is then derived. This procedure is repeated until an "acceptable" agreement is obtained between the calculated and measured hydraulic head.

One should note that this method does not guarantee uniqueness for the solution since there are infinitely many combinations of aquifer parameters and hydraulic head functions that satisfy Eq,(4.4.1), Therefore, the choice of a particular set of parameter values and the associated hydraulic head distribution by using model calibration is arbitrary,dictated only by the choice of the weighting functions. The resulting Rustler aquifer hydraulic conductivity and hydraulic head obtained by Cole and Bond in (C3) are shown in Figure Al and Figure A2 respectively.

Figure Al shows that the hydraulic conductivity distribution used in (C3) to characterize Rustler aquifer in the region between the repository site and the Malaga Bend is given by only three discrete values of 1,4 and 32 ft/day. The method presented in Section 4.4 (and implemented in UCBNE21) was used for the Rustler aquifer with the calculated data, and a continuously varying hydraulic conductivity from 1 ft/day at the repository site up to about 65 ft/day close to the discharge location at the Malaga Bend was obtained.

The calculated hydraulic head for Rustler aquifer given in (C3) is shown in Figure A2. The shape of the potential lines as well as their corresponding values in feet above the MSL agree well with the calculated potentiometrie data used in this work (Figure 4.8). The shape of the streamlines are also comparable to those obtained in the present work (Figure 4.12) with the

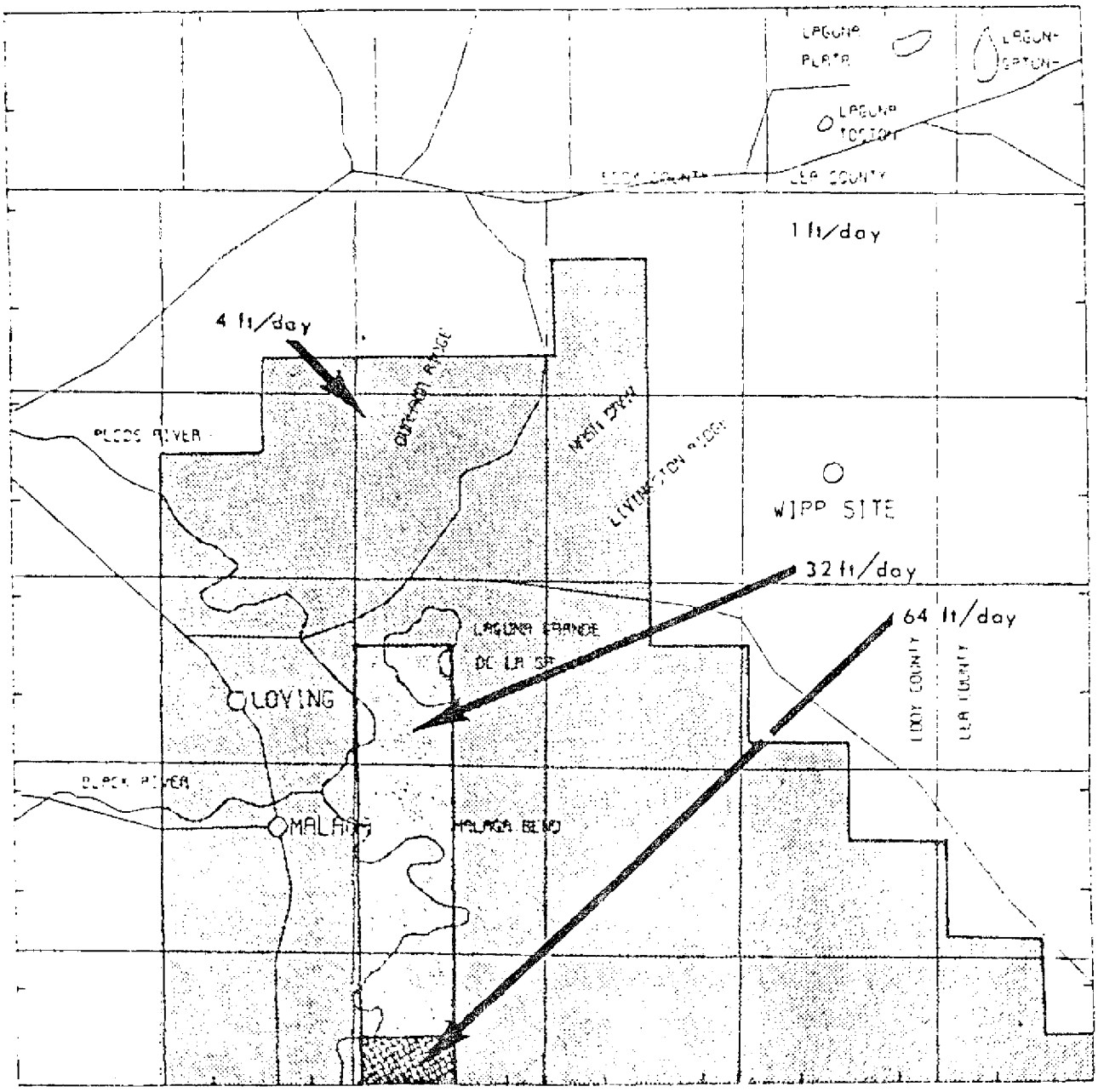


Figure A1 Hydraulic conductivity values used in C3.

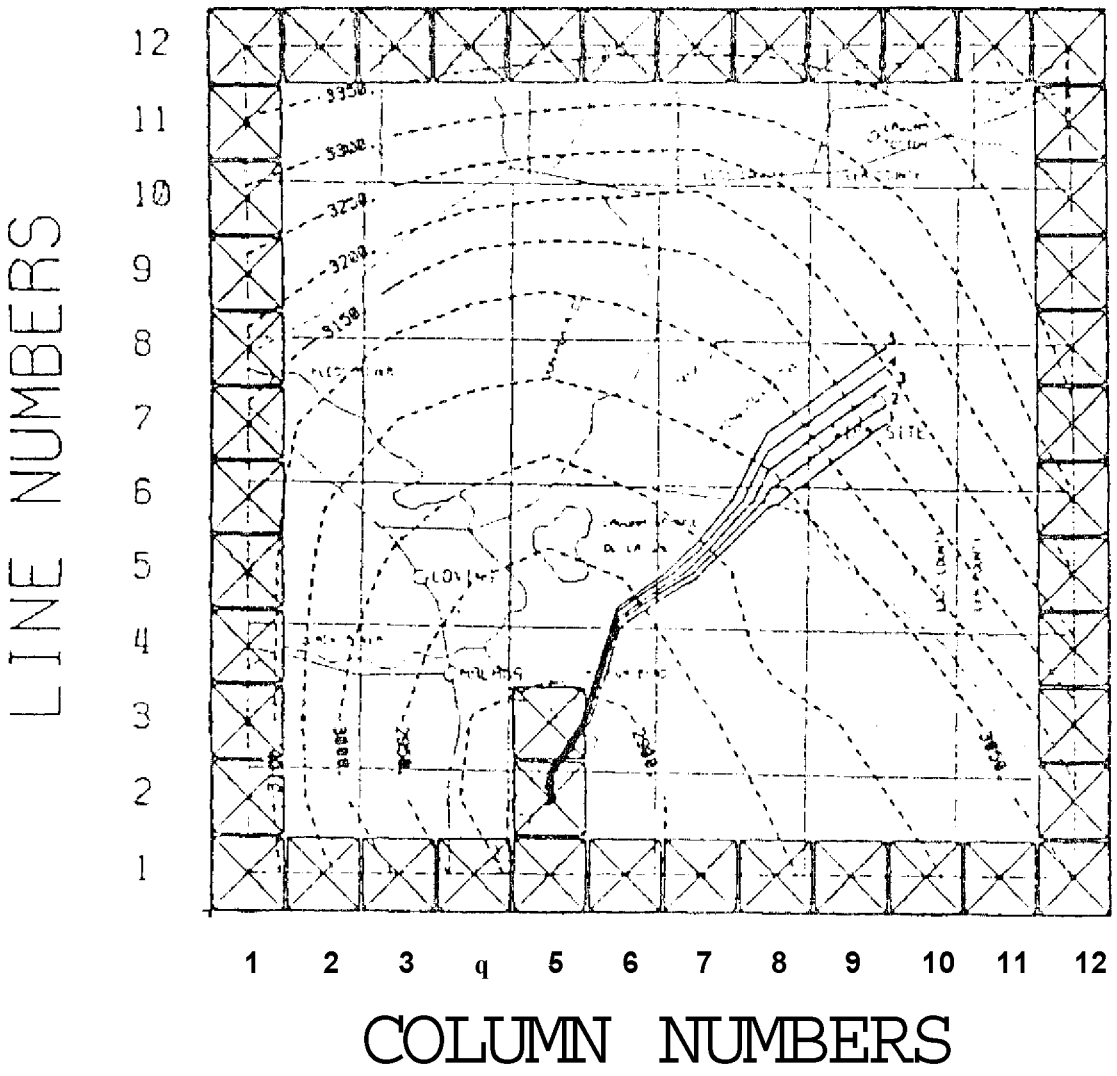


Figure A2 The nodal system usee! in C3 with the calculated hydraulic head distribution and the streamlines of the contaminated region.

A2 which are caused by discrete jumps in the hydraulic conductivity values used.

However, the most serious contention in our review concerns with the fact that the dimensional sealling used in (C3) is about two times smaller than the actual geographical scales used elsewhere for that region. It is stated in (C3) that the distance between two nodal points in Figure A2 is equivalent to 1.5 miles. Using this scaling factor, the distance between the repository site and Malaga Bend is 8 miles, according to Figure A2. On the other hand, data from (D1) indicates that the distance between those same points is 17 miles while data from (M1) and (R1) indicate 18 miles. Furthermore, from (B5) we have the confirmation that the distance is about 17 miles. Therefore, the scaling factor used in (C3) is smaler by a factor of approximately two. Although the values of hydraulic head are not affected by this error, the groundwater velocity (i.e. the gradient of the potential) as well as the distance to the biosphere are affected. Consequently, the water travel time to the biosphere is also affected. The resulting water travel times to reach the Malaga Bend calculated in (C3) by VTT and those obtained in this work calculated by HYDRO are shown in the Table A1 below for comparison.

Table A1 Comparison between water travel times to the Malaga Bend in Rustler aquifer obtained in (C3) and in this work.

Streamline no.	Water travel times (years)	
	Coles and Bond	This work
1	3.43E+3	2.23E+4
2	3.57E+3	3.15E+4
3	3.67E+3	4.65E+4
4	3.72E+3	4.24E+4
5	3.82E+3	4.11E+4

One can notice that the reduction by a factor of two in the dimensional scaling, with a corresponding increase by a factor of two in the local values of the groundwater velocity and in the total distance to the biosphere, caused the water travel time to be decreased by more than an order of magnitude.This difference in water travel time to the biosphere seriouly affects the far-field migration of radionuclides since the arrival time of the first nuclide is greatly diminished and the concentration of a particular nuclide is increased.

Coles and Bond calculated the far-field migration of radionuclides in the WIPP site by using a simplified one-dimensional model. The average length of the five streamlines shown in Figure A2 was used as the equivalent one-dimensional path length and the corresponding average water travel time was

used. The results shown in (C3) also present 1-129 and Ra-226 as being the most hazardous nuclides migrating in the Rustler aquifer.

A quantitative comparison between the one-dimensional calculation carried out in (C3) with the error in the scaling factor and the two-dimensional calculation performed in this work has no important meaning. Nevertheless, the time when the maximum water dilution rate and the corresponding maximum water dilution rate for 1-129 and Ra-226 in Pecos River after discharging from Rustler aquifer obtained in (C3) and in this work are presented in Table A2 for comparisons. The time for beginning of leaching is 1000 years and the leach time is 150,000 years. The initial amount of each nuclide are those present in a LNR reprocessed waste.

Table A2 Comparison between 1-129 and Ra-226 maximum water dilution rates obtained by Coles and Bond and by this work.

	Time of maximum (yr)		Maximum water dilution rate (m Vyr)	
	Coles and Bond	This work	Coles and Bond	This work
1-129	8.70E+3	6.00E+4	1.00E+2	7.00E+1
Ra-226	1.00E+6	1.50E+6	6.10E+0	1.00E-1

In addition, one should also note that in (C3) it is assumed that none of the U-238 present in the spent fuel is lost to the reprocessed high level waste.However, about 0.5% of the U-238 is present in the HLW and is, as our calculation showed, the main source of Ra-226 10^6 years after the leaching started.

4.7 Modelling of the Far-Field Radionuclide Migration at the Site of the Basalt Waste Isolation Project (BWIP) in Hanford, Washington

4.7.1 Review and interpretation of existent hydrological data

Hydrological data used in this work were obtained primarily from the Rockwell International report: "Hydrologie Studies within the Columbia Plateau, Washington" (R2). That report presents an integration of the current knowledge of the Hanford site region hydrology. In this section we present a brief summary of the available information and the reader should refer to above reference for more detailed descriptions.

Among the hydrologie systems present in the Columbia River basalt formation the main studies are centered within the Pasco Basin located in south-central Washington State, particularly that portion of the basin within the Hanford Site (see Figure 4.25). A geological cross section of the Pasco Basin from southwest to northeast is shown in Figure 4,25a. This figure illustrates the structure and stratigraphy of the Hanford Site. Four major groups of flows can be distinguished: the Grande Ronde, the Wanapum, the Saddle Mountains Basalt and the Ringold formation.

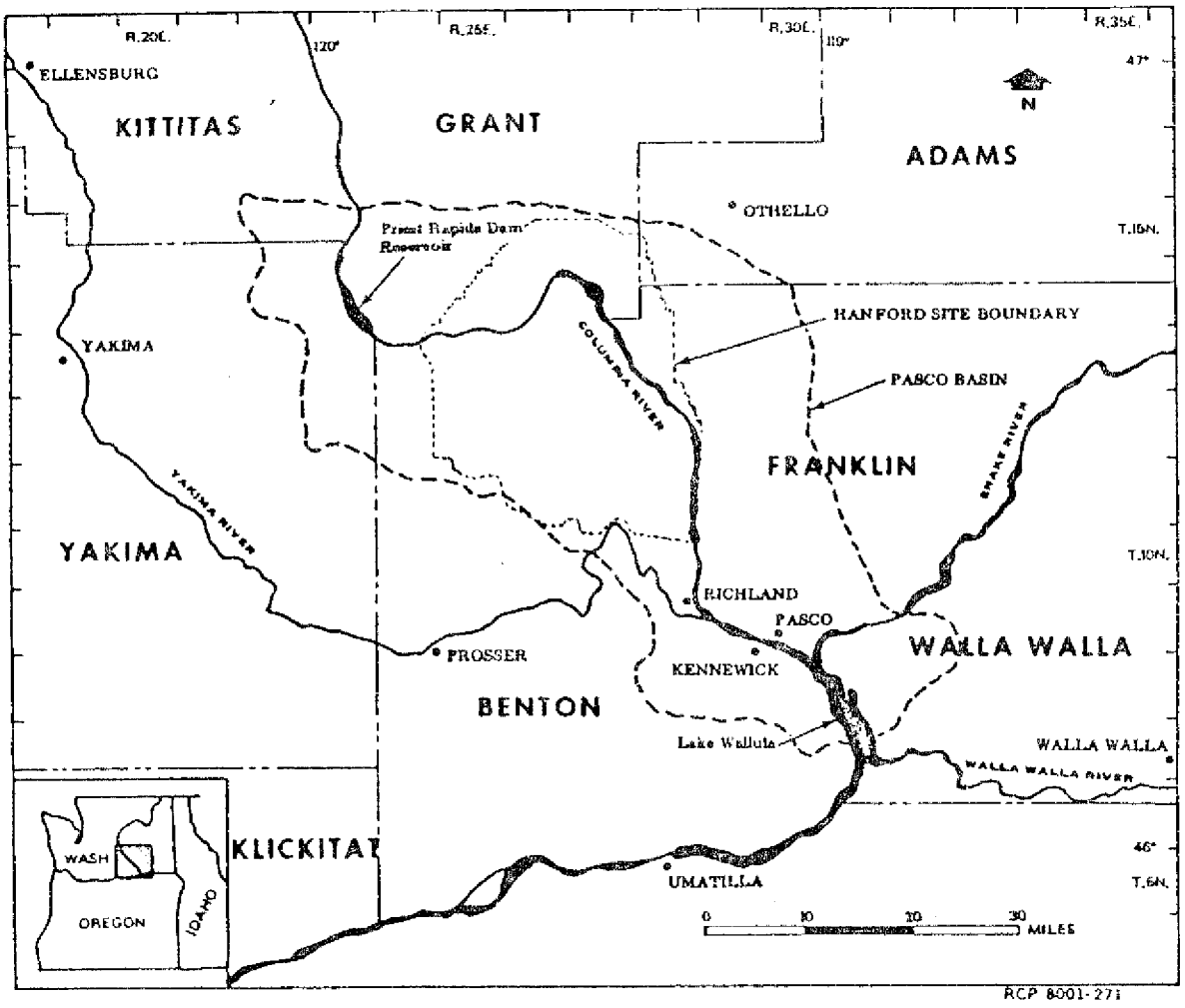


Figure 4.25 Hydrologie modelling region for the Î3T7IP site showing the Pasco Basin boundaries.(from R2)

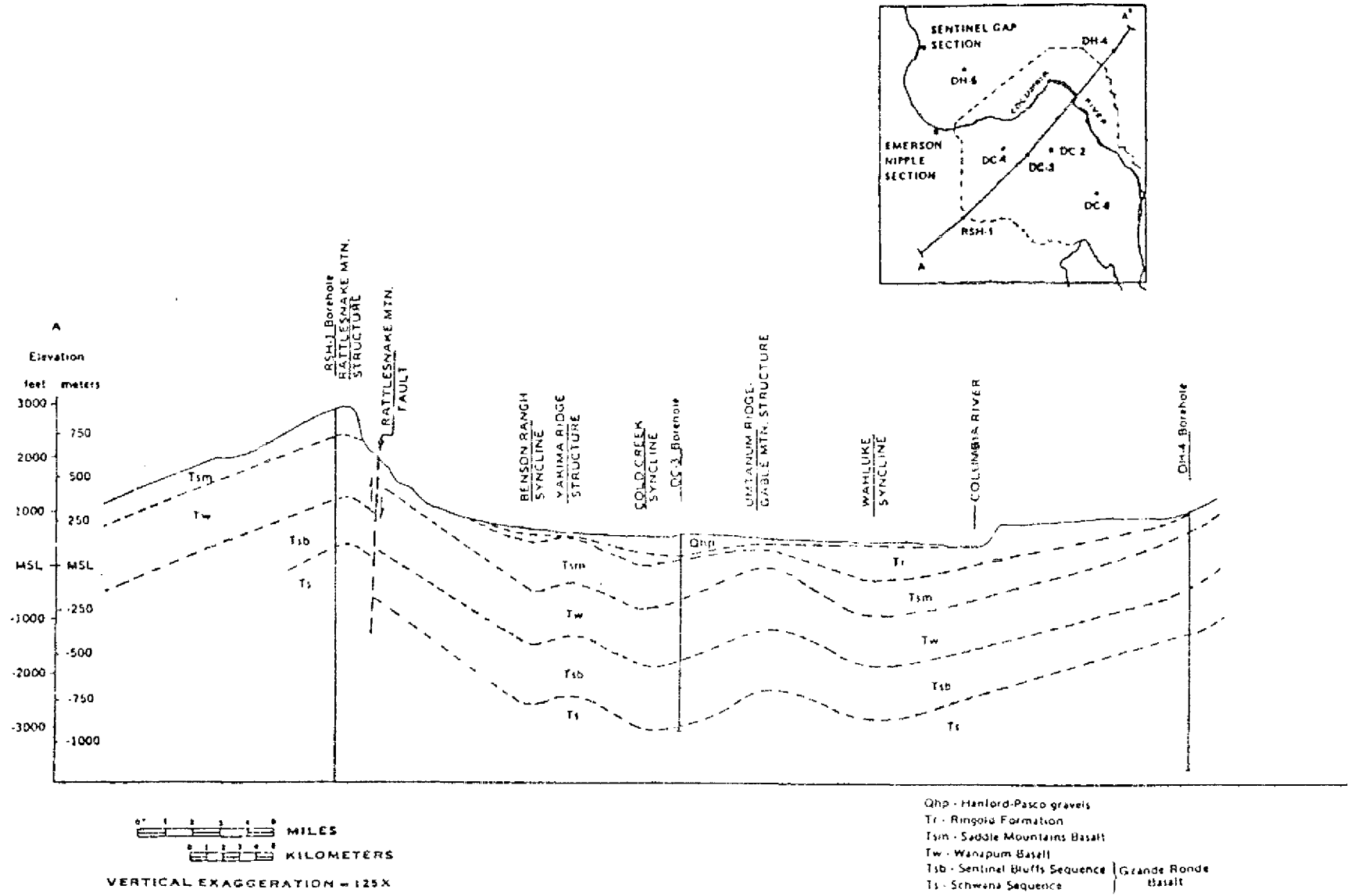


Figure 4.25a Geologic cross section of the Pasco Basin (R3).

Here we quote selected segments from (R2) on the description of the Pasco Basin with its flowing groups: "The Pasco Basin, an area of about 2,000 square miles contains one of the largest river systems in the continent, the Columbia River and its tributaries, the Snake and Yakima Rivers.

The water table is found principally in the Ringold Formation. The Ringold Formation is divided into three units: the upper, consisting of bedded fluvial silt and sand with some gravel; the middle, well sorted sand and gravel which are invariably cemented;and, the lower, primarily silt and clay with some interbedded sand and gravel. The reported hydraulic conductivity ranges from 20 to 600 feet per day for the middle unit, and 0.1 to 10 feet per day for the lower unit (R2). The unconfined aquifer attains a thickness of over 200 feet in portions of the basin with the base considered to be the top of the basalt or the thick, low permeable silt and clay of the lower unit of the Ringold formation. Discharge from the unconfined aquifer is primarily to the Columbia River, with lesser amounts to the Snake and Yakima rivers.

Within the Pasco Basin, the Columbia River Basalt Group (confined aquifers) consists of the Saddle Mountains, Wanapum, and Grande Ronde Basalts. The average total thickness of these basalts is about 5,000 feet. The confined aquifers present therein are associated with the more permeable interflow and interbedded zones and are generally located between confining

units composed of the dense, columnar portions of the basalt flows.

The Saddle Mountain Basalt and upper Wanapum Basalt receive recharge from precipitation and from stream runoff in the Rattlesnake Hills, Yakima ridge and the Saddle Mountains. The principal discharge area for aquifers within the Saddle Mountains and upper Wanapum Basalts is most probably to the Columbia River in the southeastern segment of the basin between the city of Richland, Washington and Wallula Gap. Groundwater flow beneath the Hanford Site is generally to the east and south.

Aquifers in the lower Wanapum and Grande Ronde Basalts receive minor or local recharge in the same areas as mentioned for the shallower basalts. Groundwater discharge is probably to the Columbia River, possibly in Lake Wallula, or further south in the Columbia George.

A generalized summary of the groundwater flow system in the Pasco Basin is presented. The unconfined aquifer is essentially a local system, with recharge and discharge contained within the basin. Aquifers in the Saddle Mountains Basalt and upper Wanapum Basalt principally receive recharge and discharge within the basin;although some inter-basin transfer takes place, the system is considered to be local. The lower Wanapum and the upper Grande Ronde Basalt aquifers are tentatively classified as intermediate. The lower Grande Ronde Basalt may be part of a

regional system. Recharge is from within the basin and from the surrounding plateau. Discharges areas have not been identified.

Columbia River flow rates at the aquifers discharge region depends on the electric production at the Priest Rapids Dam Reservoir located upstream. For the 60 year period of record maintained by the U.S.Geological Survey, the average discharge has been 3,250 m^/sec (120,400 cfs).The minimum recorded discharge of 111 m^3/sec (4,120 cfs) ocurred in 1932. In recent years peak flows during spring runoff have ranged from 4 320 m^3/sec (160,000 cfs) to 14,850 m^3/sec (550,000 cfs).

Figure 4.26 (obtained from R2) shows the estimated hydraulic potential map for the Ringold formation aquifers at the Hanford site. Beneath this unconfined aquifer lies the Saddle Mountains Group aquifers and an estimate of the potentiometrie surface in this systems of aquifers is presented in Figure 4.27 (R2). The two groups of aquifers underlying Saddle Mountains Group, the Wanapum and Grande Ronde have insufficient piezometric data to construct a potentiometrie surface for the region of the Hanford site.

At the Hanford site the exact location for the repository has not been defined yet. The proposed scenario to be assumed in assessing the performance of the repository considers an horizontal flow driven by the hydraulic potential gradient through the aquifer in which the repository is located. A crack

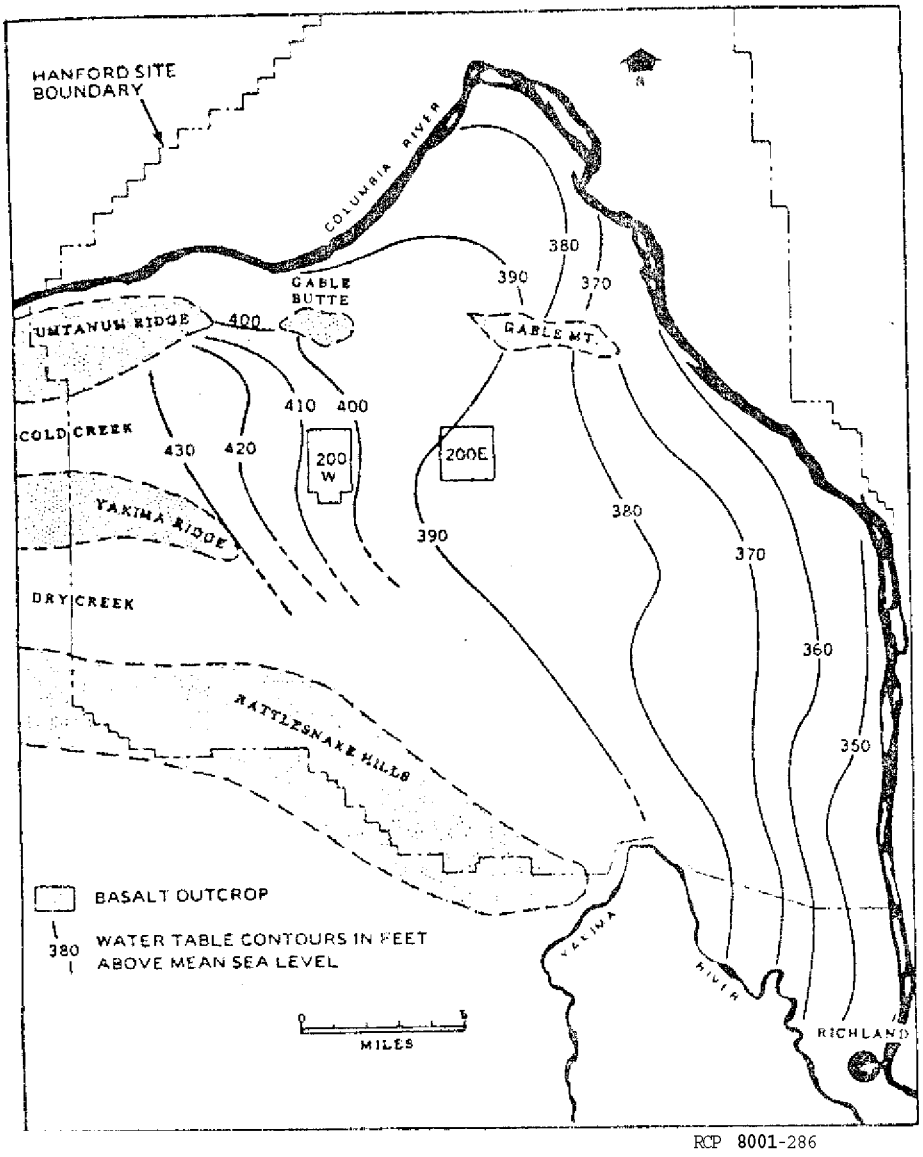


Figure 4.26 Estimated 1944 water table map for the Eanford site (used as Ringold aquifer potentionetrie data,from R2).

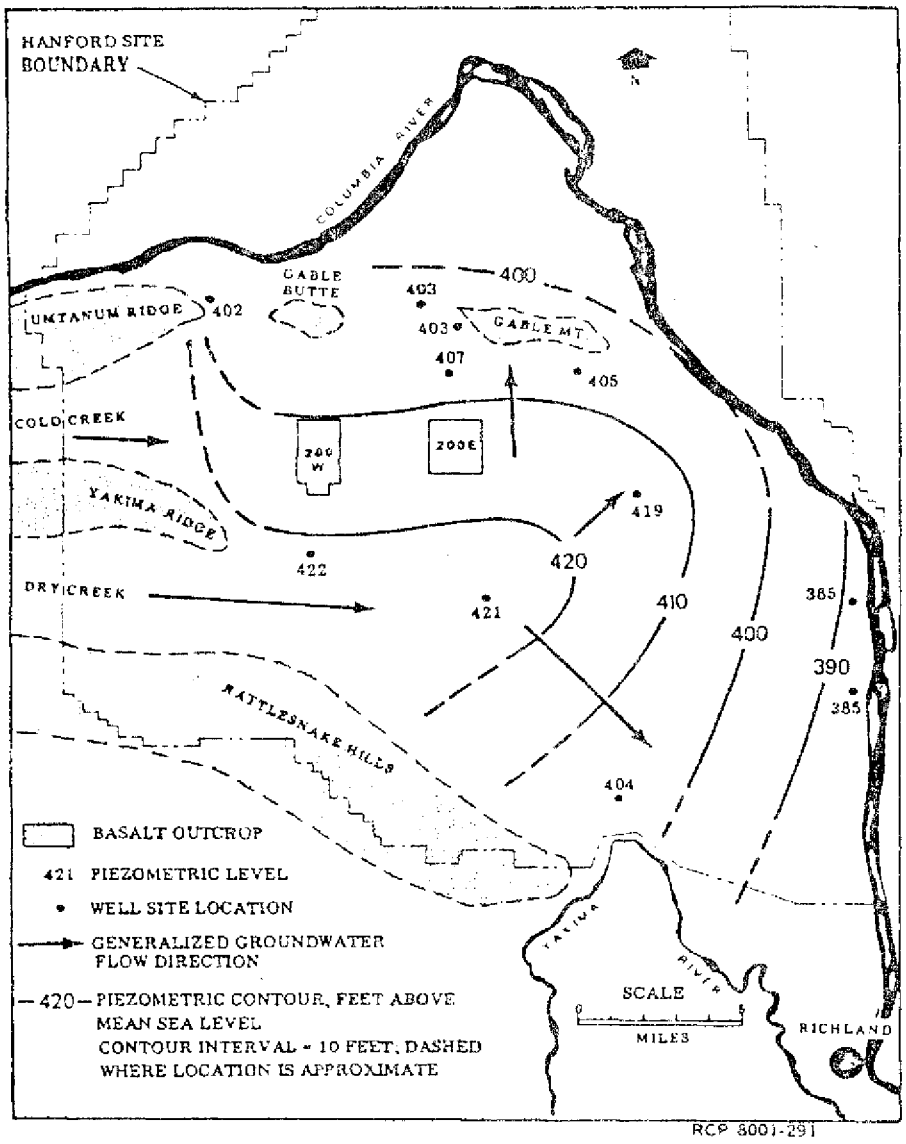


Figure 4.27 Potentiometrie surface used for the Saddle Mountain Group aquifers, from R2.

is assumed to be formed at the repository site. Due to the temperature gradient caused by decay heat in addition to the natural vertical hydraulic potential gradient, groundwater from the horizontal flow is driven vertically upwards after passing through the repository. This contaminated upward flowing groundwater reaches eventually an over]ying aquifer which carries the radionuclides until they discharge into the biosphere.

In this study however, a conservative assumption has been made. In any instance when radionuclides are leached out of the waste package into the groundwater they are instantly placed in the aquifer being studied. It is equivalent to say that the repository is located in the particular aquifer being analyzed. In other words, the time any radionuclide would spend in travelling vertically through the fracture is assumed negligible when compared to the time it spends in the aquifer until the discharge into the biosphere.

Therefore, the repository is placed either in the Ringold aquifer or in the Saddle Mountain Group aquifer. Due to lack of enough piezometric data, Wanapum and Grande Ronde aquifers will not be analyzed although they are possible pathways to the biosphere. Aquifer parameters values obtained from field data show that the hydraulic conductivity and porosity vary over a large range of values (R2,C6), making the choice of a representative value difficult. A summary of the hydrological data used in this work is presented in Table 4.5a (R2).

Table 4.5a Summary of hydrological data at the repository site (R2)

	Ringold aquifer	die Mountain aquifer
Thickness (m)	60	270
Hydraulic conductivity (m/yr)	A range from 10 to 105,used=5O0	3
Porosity	0.1	0.1

4.7.2 Determination of the contaminated regions and radionuclide discharge rates in the BWIP case

Similar calculations as were done for the WIPP site (Section 4.6.2) are repeated here for the BWIP site. Table 4.6 and Table 4.7 summarizes the nuclides parameters used in this case. These tables differ from the corresponding Table 4.2 and 4.3 for the WIPP site because the retardation coefficient of some nuclides are different for basalt formations. Table 4.6 presents the parameters used for the long lived fission products present in high level waste. Again as in the previous case 1-129 with its unit retardation coefficient and long half life requires the largest water travel time to be contained. Table 4.7 summarizes the parameters for the actinide chains present in reprocessed high level waste. Once more Ra-226 which activity is controlled by its precursor U-234 and U-238 is the most potentially hazardous actinide. Table 4.8 is a listing of the most hazardous nuclide in the BWIP site ranked according to the product 1^ (see

Table 4.6 Long Lived Fission Products Parameters for BWIP site

Nuclide		a/ λ_i	(MPC)$_i$ x	c/ M.	$10^{K}V_i$	.001M_i /MPC
	(yr)		(Ci/m^3)	(Ci/GwYr)	(yr)	(m^3/GwYr)
H-3	1.2E+1	1.0E+0	3.0E-3	1.9E+4	1.2E+2	6.3E+3
C-14	5.6E+3	1.0E+1	8.0E-4	1.3E+1	5.6E+3	1.6E+1
Se-79	6.5E+4	1.0E+0	3.0E-4	1.1E+1	6.5E+5	3.6E+1
Sr-90	2.8E+1	5.7E+3	3.0E-7	2.1E+6	4.9E-2	7.0E+8
Zr-93	9.5E+5	5.7E+2	8.0E-4	5.2E+1	1.6E+4	6.4E+1
Nb-93m	1.4E+1	1.0E+4	4.0E-4	5,0E+0	1.4E-2	1.2E+1
Tc-99	2.1E+5	1.0E+0	2.0E-4	3.9E+2	2.1E+6	1.9E+3
Ru-106	1.0E+0	1.0E+1	1.0E-5	1.1E+7	1.0E+0	1.1E+9
Cd-113ra	1.4E+1	1.0E+4	3.0E-5	1.3E+3	1.4E-2	4.5E+4
Sn-126	1.0E+5	5.7E+2	2.0E-5	1.5E+1	1.8E+3	7.4E+2
Sb-125	2.7E+1	1.0E+2	1.0E-4	2.1E+5	2.7E+0	2.1E+6
1-129	1.7E+7	1.0E+0	6.0E-8	1.0E+0	1.7E+8	1.7E+4
Cs-137	3.0E+1	5.7E+3	2.0E-5	2.9E+6	5.3E-2	1.5E+8
Cs-135	3.0E+6	5.7E+3	1.0E-4	7.8E+0	5.3E+3	7.8E+1
Ce-144	7.8E-1	1.2E+4	1.0E-5	2.1E+7	6.5E-4	2.1E+9
Pm-147	4.4E+0	2.5E+3	2.0E-4	2.6E+6	1.8E—2	1.3E+7
Sm-151	8.7E+1	2.5E+3	4, OE-4	3.4E+4	3.5E-1	8.5E+4
Eu-152	1.3E+1	2.5E+3	6,.OE-5	3 « 3H!"^"2	5 « i E X	5.5E+3
Eu-154	1.6E+1	2.5E+3	2 .OE-5	1.9E+5	6.4E-2	9.4E+6
Eu-155	1.8E+0	2.5E+3	2.OE-4	1.7E+5	7.2E-3	8.7E+5

a/:From reference (R2),(B3).

b/:From 10CFR20,Appendix B and (P2).

_c/:For reprocessed high level waste,LWR,10 years decay,0.5% U and Pu loss into the waste,(B2).

Table 4.7 Actiníde Chains Parameters for The BWIP site

Nuclide	K_i a/	$(MPC)_i$ J?/	M_i^0	10T,/K.	,00lM_i°/W
	(yr)	(Ci/m³)	(Ci/GwYr)	(yr)	(m³/GwYr)
Ra-325 4.1F-2	2.8E+3	5.0E-7		7.5E+4	8.7E+5
Ra-226*** 1.6E+3	2.8E+3	3.0E-8		4.4E+3	1.5E+3
Ra-226****1.6E+3	2.8E+3	3.0E-8		7.9E+7	5.5E+1
Th-228 1.9E+0	5.7E+3	7.OE-6		1.2E+0	8.9E+4
Th-229 7.3E+3	5.7E+3	5.0E-7		7.5E+4	1.2E+4
Th-230*** 8.OE+4	5.7E+3	2.0E-6		4.4E+3	3.2E-1
Th-230****8.OE+4	5.7E+3	2.0F-6		7.9E+7	8.4E-3
U-233 1.6E+5	5.2E+2	3.0E-5		7.5E+4	2.0E+2
U-234 2.5E+5	5.2E+2	3.0E-5	1.2E+0*	^.4E+3	3.RE+1
U-235 7.1E+8	5.2E+2	3.0E-5	2.3E-3	1.2E+7	7.7E-2
U-238 4.5E+9	5.2F.+2	4.OF-5	4.3E-2	7.9E+7	1.0E+0
Np-237 2.1E+6	2.8E+2	3.0E-6	1.5E+1**	7.5E+4	5.2E+3
Pn-238 3.6E+1	5.7E+3	5.01X5	5.1F+2	1.5E-1	1.0E+5
Pn-239 2.4E+4	5.7E+3	5.0E-6	4.4E+1	4.2E+1	8.3E+3
Pu-240 6.6E+3	5.7E+3	5.0E-6	2.7E+2	1.2E+0	5.3E+4
Pu-241 1.3E+1	5.7E+3	2.0E-4	1.^E+4	3.1E+1	7.OE+4
Pu-242 3.RE+5	5.7E+3	5.OE-6	1.9E-1	6.6E+2	3.3F+1
Am-241 4.6E+2	1.OE+4	4.0E-6	4.9E+3	4.6E-1	1.2E+6
Am-242m 1.5E+2	1.oE+A	4.OE-6	1.2E+2	1.5E-1	2.9E+4
Am-243 7.9E+3	1.0E+<*	4.0F-6	4.8E+2	7.9E+0	1.2E+5
Cm-242 4.5E-1	3.0E+3	2.0E-5	4.4E+5	1.5E-1	2.2E+7
Cm-243 3.2E+1	3.OE+3	5.0E-6	9.0E+1	1.OE-1	1.3E+4
Cm-244 1.8E+1	3.OE+3	7.OE-6	7.4E+4	5.9E-2	1.0E+7
Cm.-245 9.3F+3	3.0E+3	4.OE-6	9.RE+0	3.1E+1	2.4E+3
Cm-246 5.5E+3	3.0E+3	4.OE-6	1.9E+0	1.8E+1	4.8E+2

•Includes the decay of Pu-218, Am-242n and Cm-242.
**Includes the decay of Pu-241 and Am-241.
***Based on the decay of U-234
****Rased on the decay of U-238
_a/:From reference (R2), (B3).
*hj*From 10CFR20,Apnendix B and (P2).
c/:For reprocessed hicrh level waste,LWR, 10 years decay, 0.5% U and Pu loss into the waste,(B2).
Am-242m is the metastable form of Am-242

Eq.(4.6.2)). As in the WIPP case, 1-129 and Ra-226 are the two first ranked nuclides.

Table 4.8 Potential Hazardous Nuclide Ranking for the BWIP site

Ranking	Nuclide	10T /K(yrs)	I.(m^3 yr)
1	1-129	1.7E+8	7E+9
2	Ra-226	7.9E+7*	2E+8
3	Tc-99	2.1E+6	6E+7
4	Se-79	6.5E+5	3E+6
5	Th-230	3.4E+6*	1E+6
6	Np-237	7.5E+4	5E+5

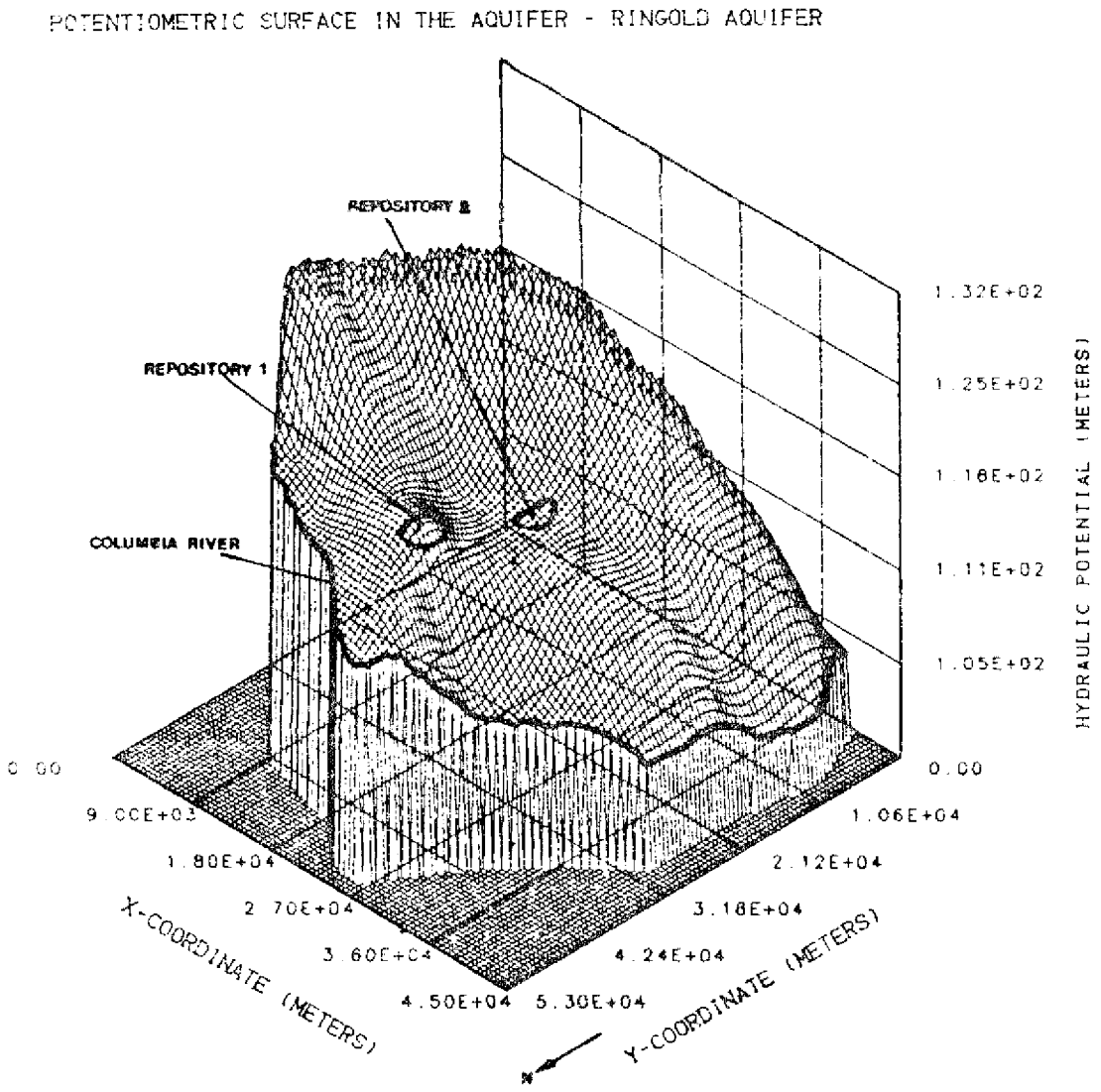
*Ra-226 is assumed to be in secular equilibrium with U-238. Thus values of half-life and retardation coefficient for U-238 were used

Since piezometric data is at present available in sufficient quantity only for the Ringold aquifer and the Saddle Mountain Group aquifer, the hydrological calculations were restricted to these two groups of aquifers, although the Wanapum and Grande Ronde formations are also potential pathways to the biosphere.

Figure 4.28 is the three dimensional representation of the Potentiometrie surface in the Ringold aquifer. Two distinct valleys in the surface indicate that the Ringold aquifer discharges into the Columbia River in two different locations. The projection of the river flow pattern on the Potentiometrie

surface is also showm. Two arbitrary locations have been choosen for a sensitivity study. The first location denoted by "Repository 1" coincides with the present reprocessing plant where low level radioactive **waste has** been placed on the surface. The projection of this first location lies on one of the potentiometric valleys (see Figure 4.20) . The contaminated streamlines converge and then flow eastward until they discharge into the Columbia River. The second location is 2 km away to the south from the "Repository 1". This second location was chosen between the two valleys as shown in Figure 4.28 so that one would not expect any confluence of the contaminated streamlines.

Figure 4.29 is the three-dimensional representation of the potentiometric surface in the Saddle Mountains aquifers. Contrary to the Ringold aquifer this aquifer presents a hill-shaped profile. This type of profile will tend to divide the streamlines. The divergence effect caused by this hill shaped surface is opposite to the confluence effect caused by the potentiometric valleys shown in Figure 4.28. Two different locations for the repository site are again considered: Repository 1 is located on the south, face of the hill and all the contaminated streamlines will flow southward; Repository 2 by its turn is located right on the ridge of the potentiometric hill. In this second case part of the streamlines will flow to the north and part will flow to the south. One should note that these repository locations do not coincide geographically with the two locations assumed for the Ringold formation calculations.



Fig\ire 4.28 Potentiometrie surface in Ringolrl anuifer with nrejection of Columbia River onto the surface.

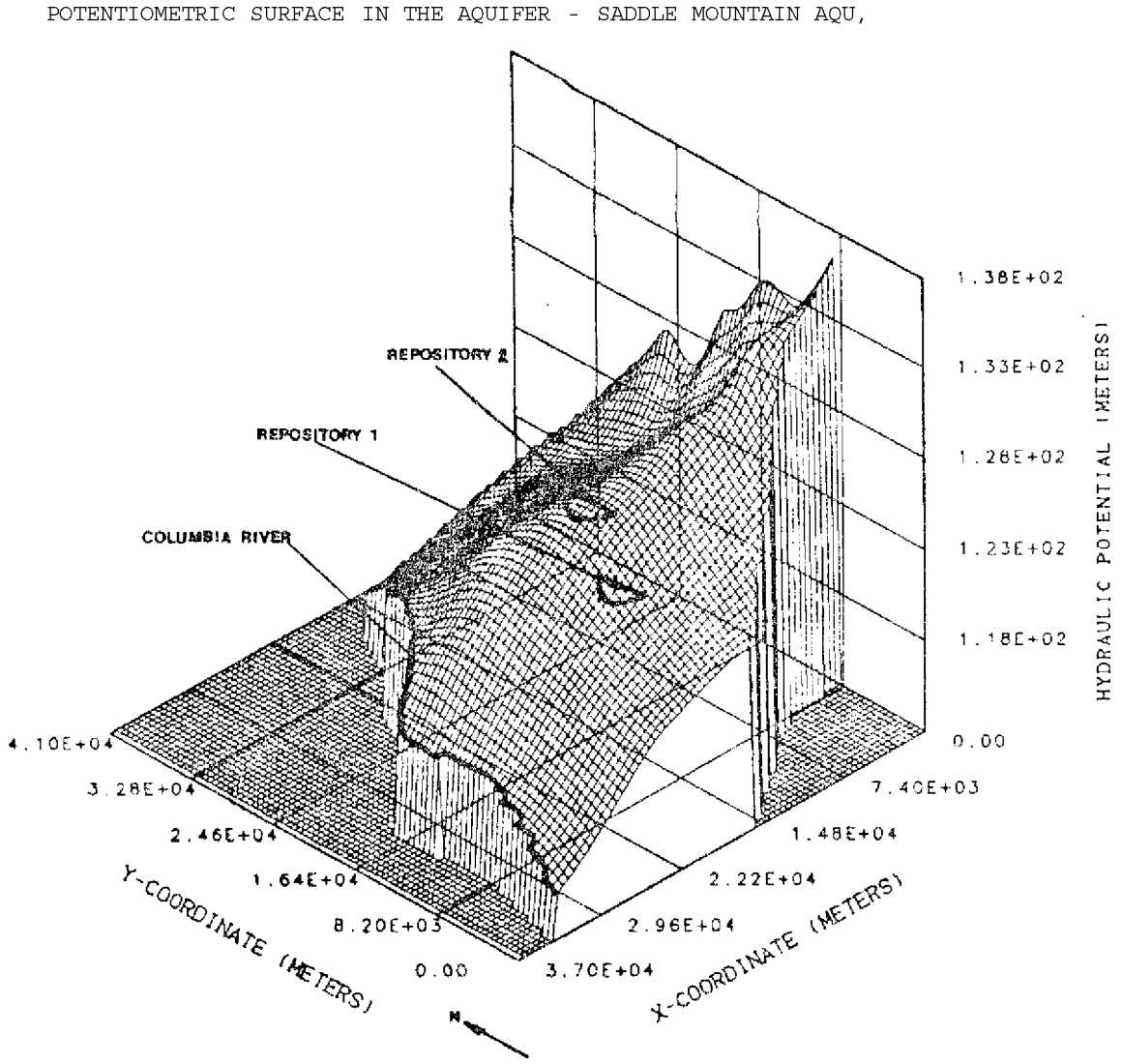


Figure 4.29 Potentiometric surface in Saddle Mountain Group aquifer with the projection of Columbia River onto the surface.

The shadow region in each of the calculations was characterized by five streamlines covering the entire shadow region. Table 4.9 contains a summary of the hydrological calculations results for the two aquifers considered in the BWTP site and it shows the water travel time for each streamline at the biosphere.

Table 4.9 Water Arrival Time (years) at the Biosphere for the BWIP site

	Water travel time (years)			
Streamline no. a/	Ringold repository-1	Ringold repository-2	Saddle repository-1	Saddle repository-2
1	2.67E+2	3.12E+4	1.24E+6	7.84E+6
2	2.93E+2	2.45E+4	1.41E+6	4.63E+6
3	1.95E+2	1.52E+5	9.15E+5	6.46E+6
4	3.41E+2	2.89E+4	1.36E+6	3.6 3E+6
5	5.31E+2	1.22E+4	5.62E+6	1.25E+6

_a/See Figures 4.30, 4.34, 4.38 and 4.41

For the Repository 1 the Ringold aquifer has very small water travel times to the biosphere. Early confluence of the streamlines near the repository causes the water velocity to be greatly increased, reducing the water travel time by orders of magnitude. If the repository were to be located at this position, in an accidental release of radionuclide from the waste into the aquifer,all radionuclides with 10T /K larger than 500

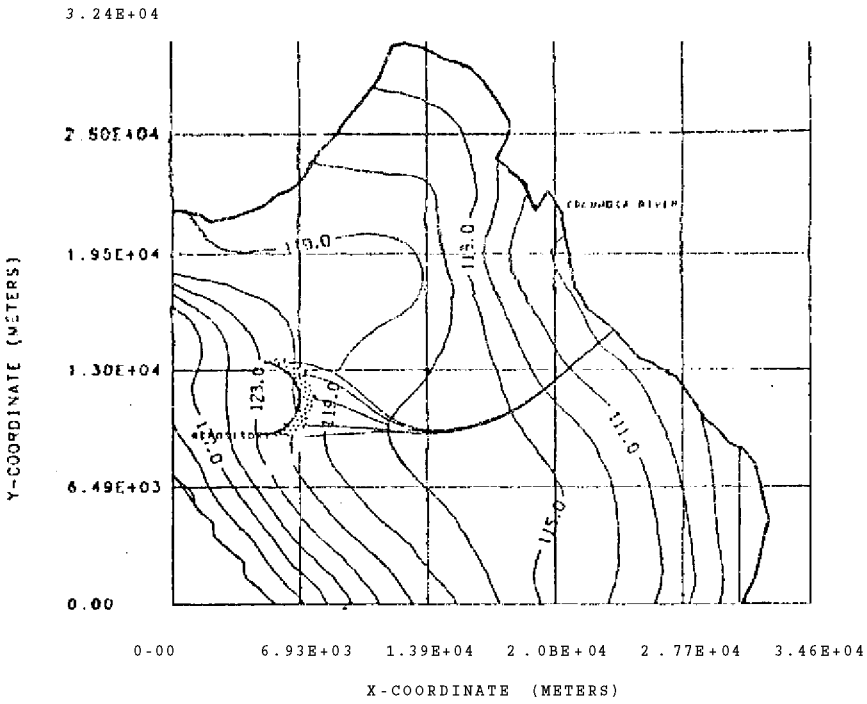
years would discharge into Columbia River. One can see from Table 4.6 and 4.7 that many nuclides should be important. On the other hand, by moving the repository to the second location (Repository 2) only 2 km to the south, the water travel time is increased by two orders of magnitude, reducing greatly the number of radionuclides that might be able to reach. Columbia River.

Table 4.9 shows that the water travel times in the Saddle Mountains Group aquifers to reach the biosphere are larger than 10^6 years for any of the cases studied. 1-129 is the only nuclide that can have a significant discharge rate into the biosphere with such large water travel times.

The 1-129 and Ra-226 contaminated regions in the Ringold aquifer, Repository 1 are shown in Figure 4.30 and Figure 4.31 respectively. The confluence of streamlines takes place close to the repository, which increases the groundwater velocity and reduces the water travel time to the biosphere. It would take about 300 years for 1-129 and about 10 years for Ra-226 to start discharging into the river.

Figure 4.32 and Figure **A.33** shows the discharge rate history of 1-129 and Ra-226 in the Columbia River through Ringold aquifer. Repository 1. Three leach times are considered: 10^4, 10^5 and 10^6, years. For a leach time of 10^4 years, 1-129 dominates the water dilution rate until 10^ years and after 10^ years Ra-226 is the largest contributor although its water

1-129 CONTAMINATED REG10N-R1NGOID AQUIFER AFTER
5.00E+01YRS



1-129 CONTAMINATED REGION-RINGOLD AQUIFER AFTER
2.00E+02YRS

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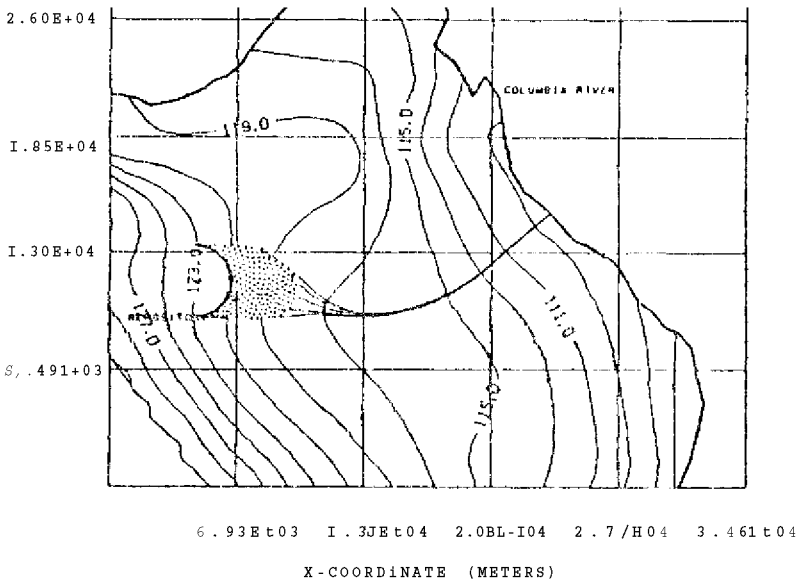

nnre 4.30 1 — 129 c o n t a"! i n a z o r err 5. on \n ii" <~cl" n>
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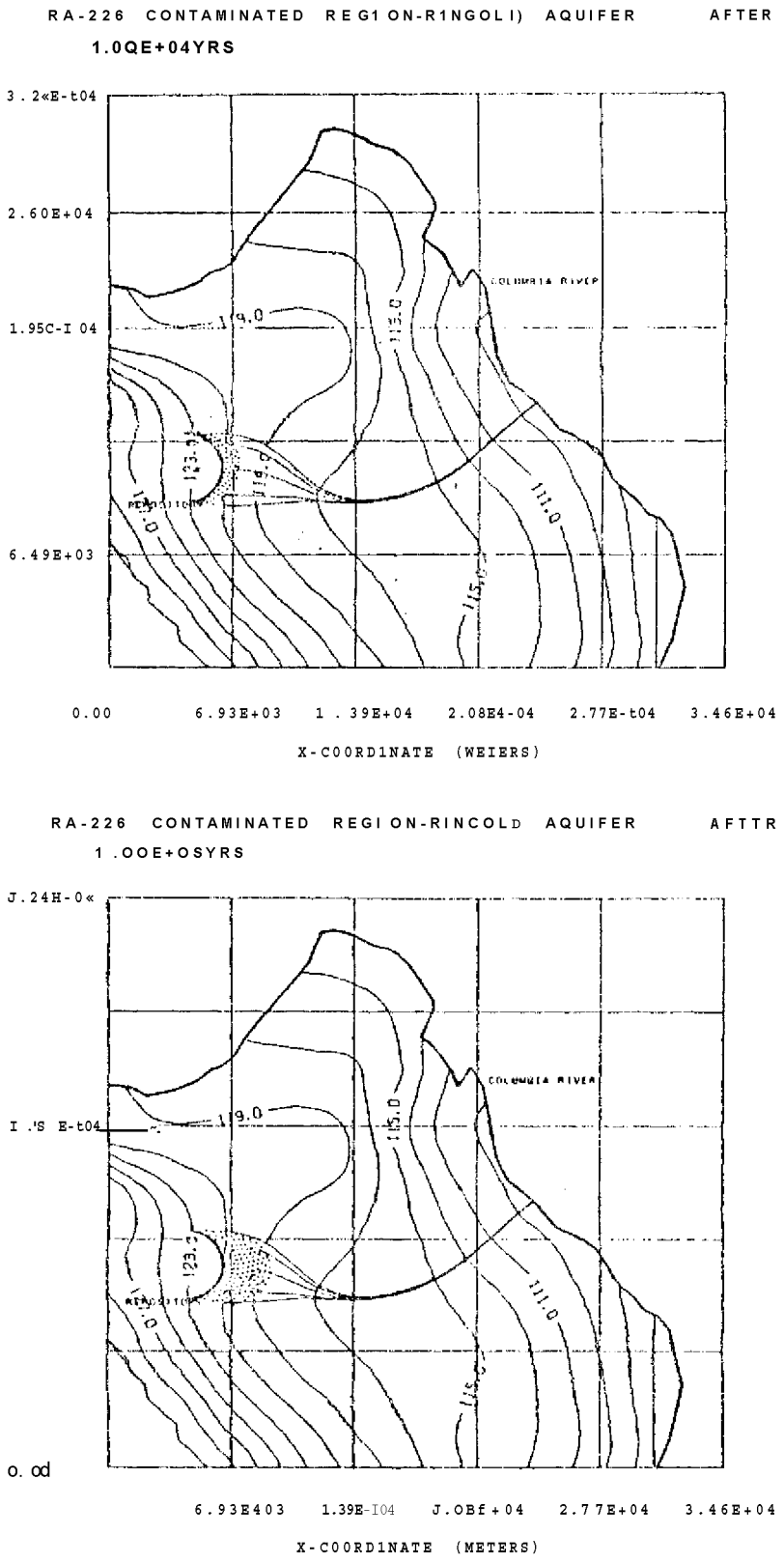


Figure 4.31 Ra-226 contaminated, region in Ringold aquifer (Repository 1) after 10* and 105 years. Potentials are in meters above M.5L.

dilution rate is four orders of magnitude smaller than for 1-129. However, the maximum cumulative discharge of Ra-226 is one order of magnitude larger than the cumulative discharge of 1-129. This is because the total water dilution volume due to the decay of all U-238 present initially at the repository, producing Ra-226 nuclides is larger than the total water dilution rate due to the decay of all 1-129.

In the case of "Repository 2" for Ringold aquifer. Figure 4.34 and Figure 4.35 shows the contaminated region for 1-129 and Ra-226 at different times. Figure 4.36 and Figure 4.37 shows their discharge rate histories. For this second location the water travel times to the biosphere are larger by more than one order of magnitude and the nuclide arrival times are correspondingly larger. 1-129 takes longer than 10^4 years to reach the river while Ra-226 takes more than 10^7 years. The magnitude of the water dilution rates and water dilution volume-for 1-129 and Ra-226 are not significantly changed when compared to the Repository 1 case. However, one must keep in mind that in the Repository 1 case, other nuclides besides 1-129 and Ra-226 (those with $10T^{\wedge}/K_m$ larger than 500) can also discharge into the Columbia River because of the short water travel time to the biosphere. This can increase the total water dilution rate.

1-129 and Ra-226 contaminated regions in Saddle Mountains Group aquifers, "Repository 1" are shown in Figure 4.38 and Figure 4.39 respectively. As expected, the contaminated

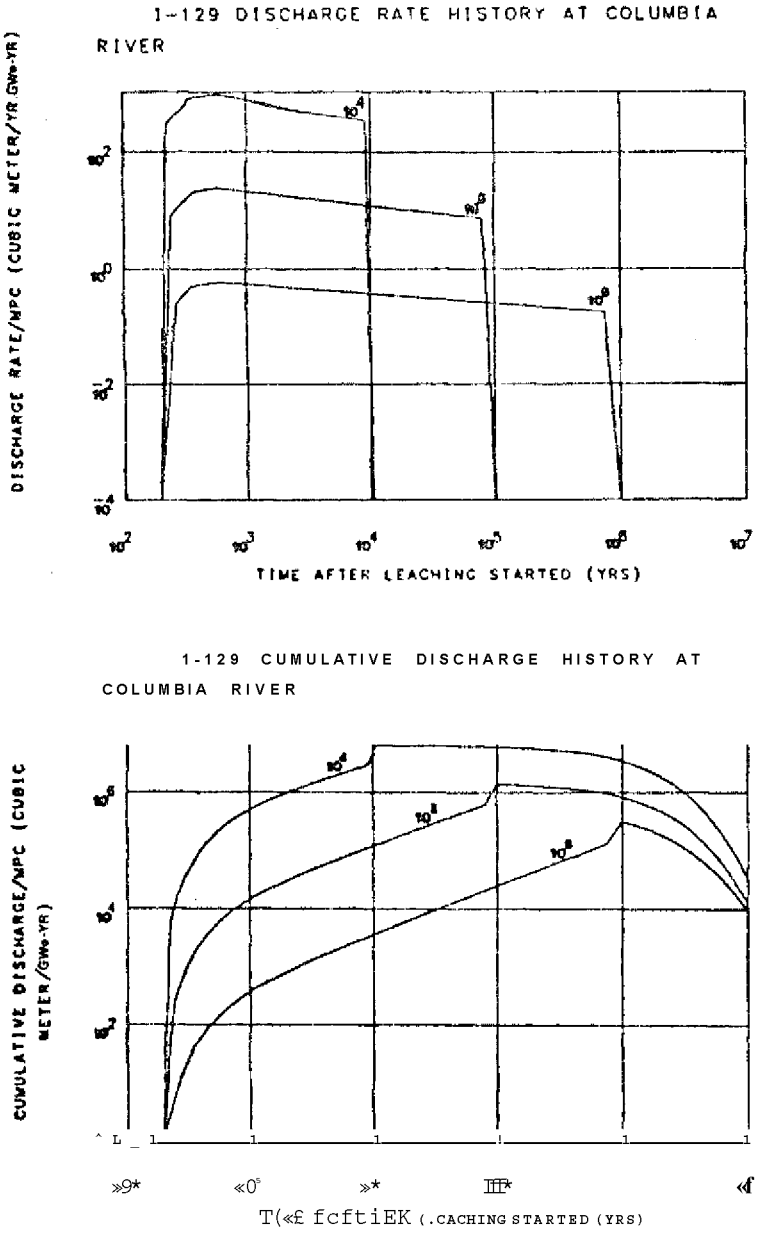


Figure 4.32 1-129 discharge rate/MPC (water dilution rate) and cumulative discharge/MPC (water dilution volume) at Columbia River discharging from Ringold aquifer (Repository 1) for leach times of 10⁴,1()5 and 106 years.

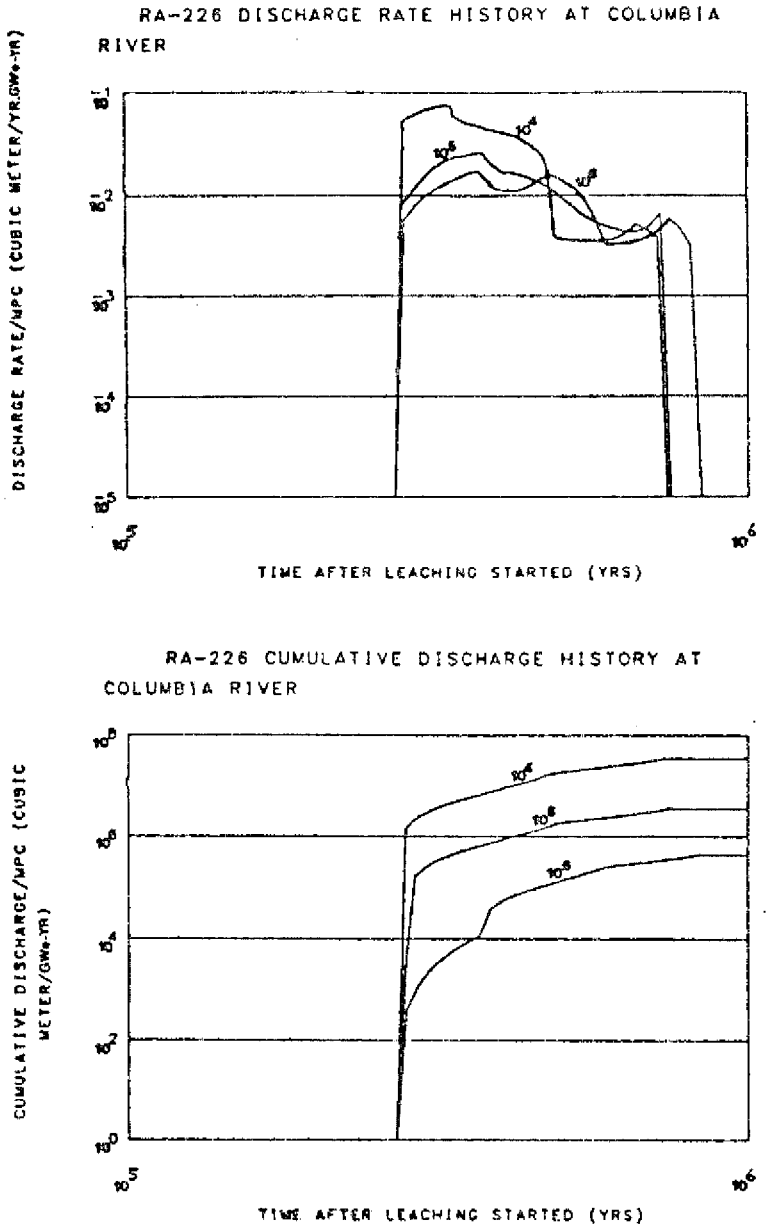
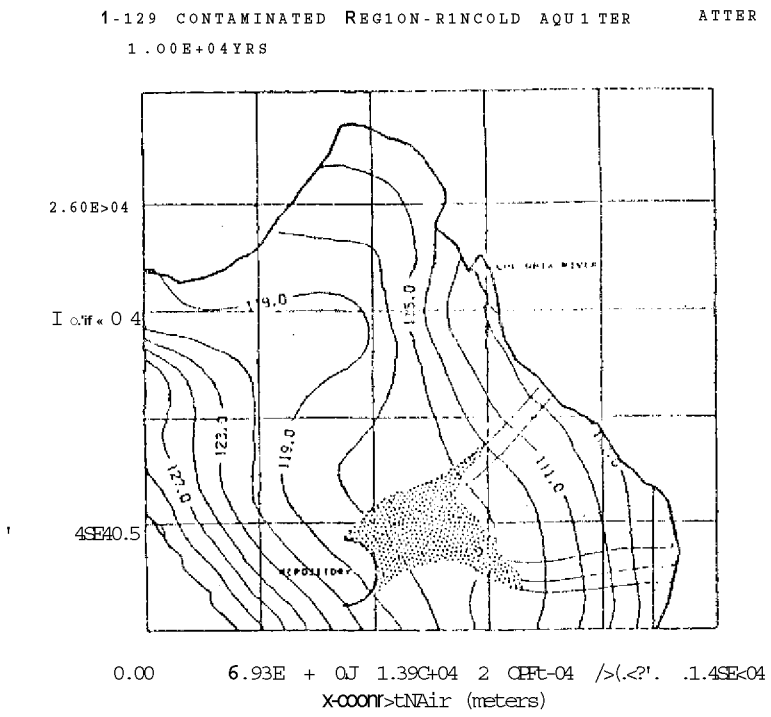
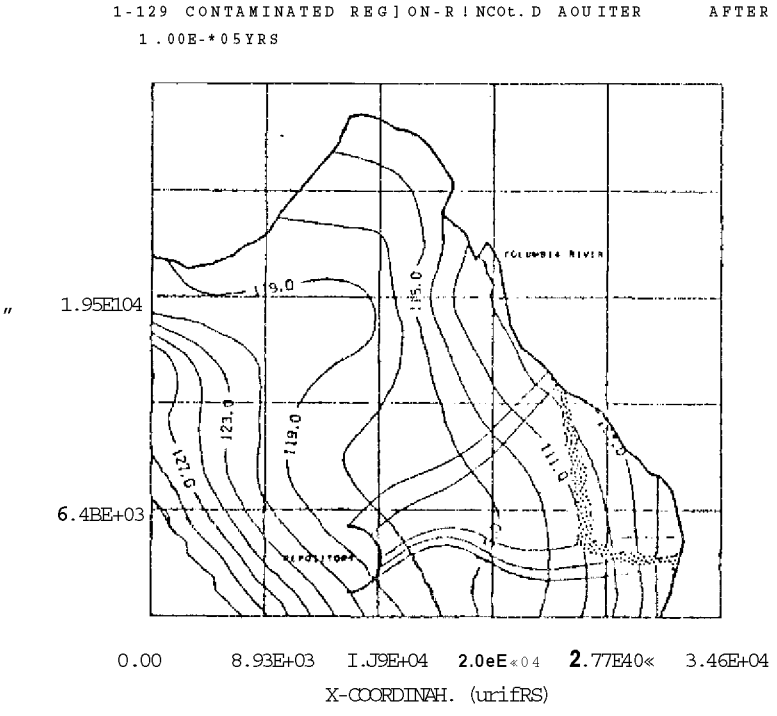
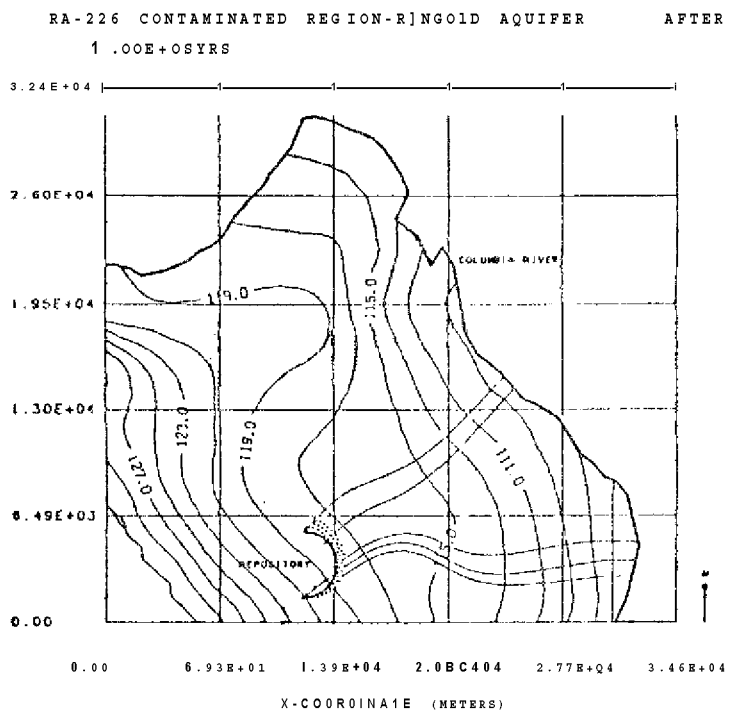


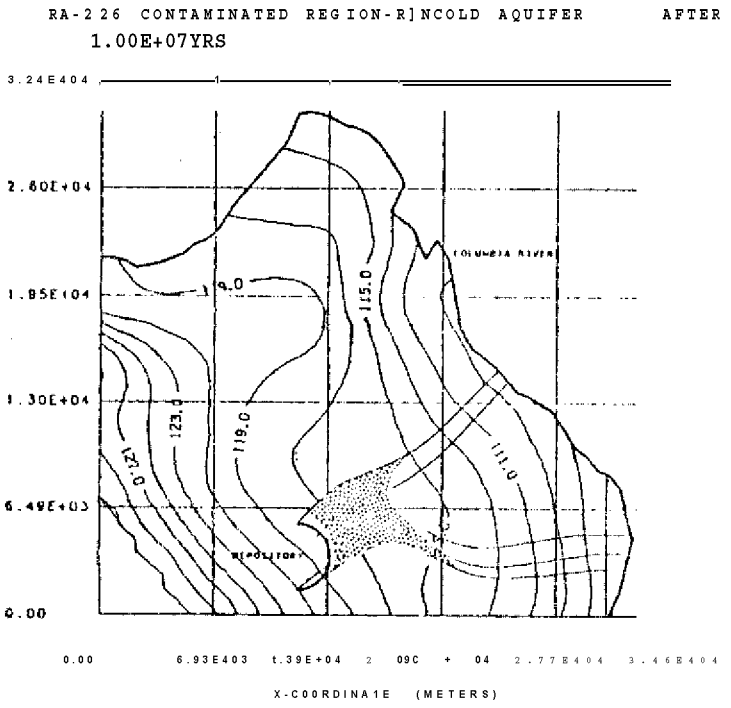
Figure 4.33 Ra-226 discharge rate/MPC (water dilution rate) and cumulative discharge/MPC (water dilution volume) at Columbia River discharging from Ringold aquifer (Repository 1) for leach times of 10^4, 10^5 and 10^6 years





Fiaure ¿.34 1-129 contaminated renion in Rinqold aquifer (Repository 2) after lO'⁴ and 105 vears. Potentials are in meters above MPL.





rrure **A**. 35 Ra-22* contaminated region in Ringold (Repository 2) afterinC and 107 years Potentials are in meters above ᵀT>L.

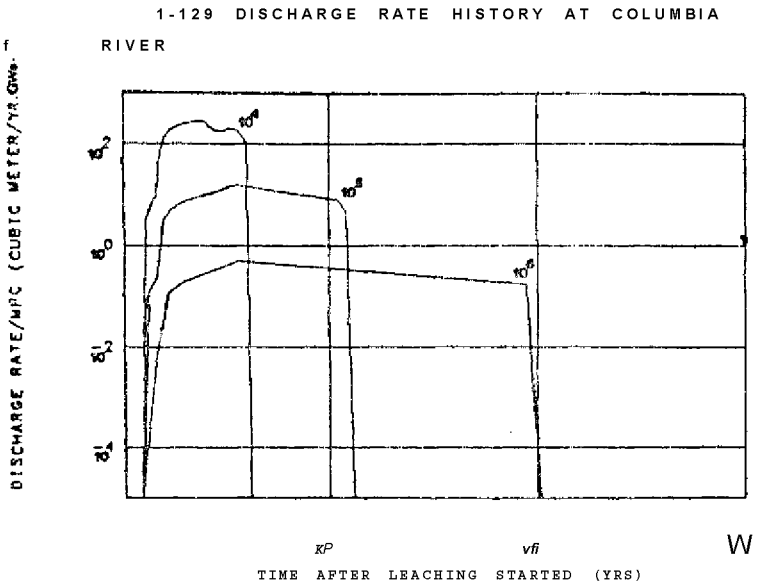


Figure 4.36 1-129 discharge rate/MPC (water dilution rate) and cumulative discharge/MPC) (water dilution volume)at Columbia River discharging from Ringold aquifer (Repositorv *2)* for leach times of 104,IQ5 and 10' years

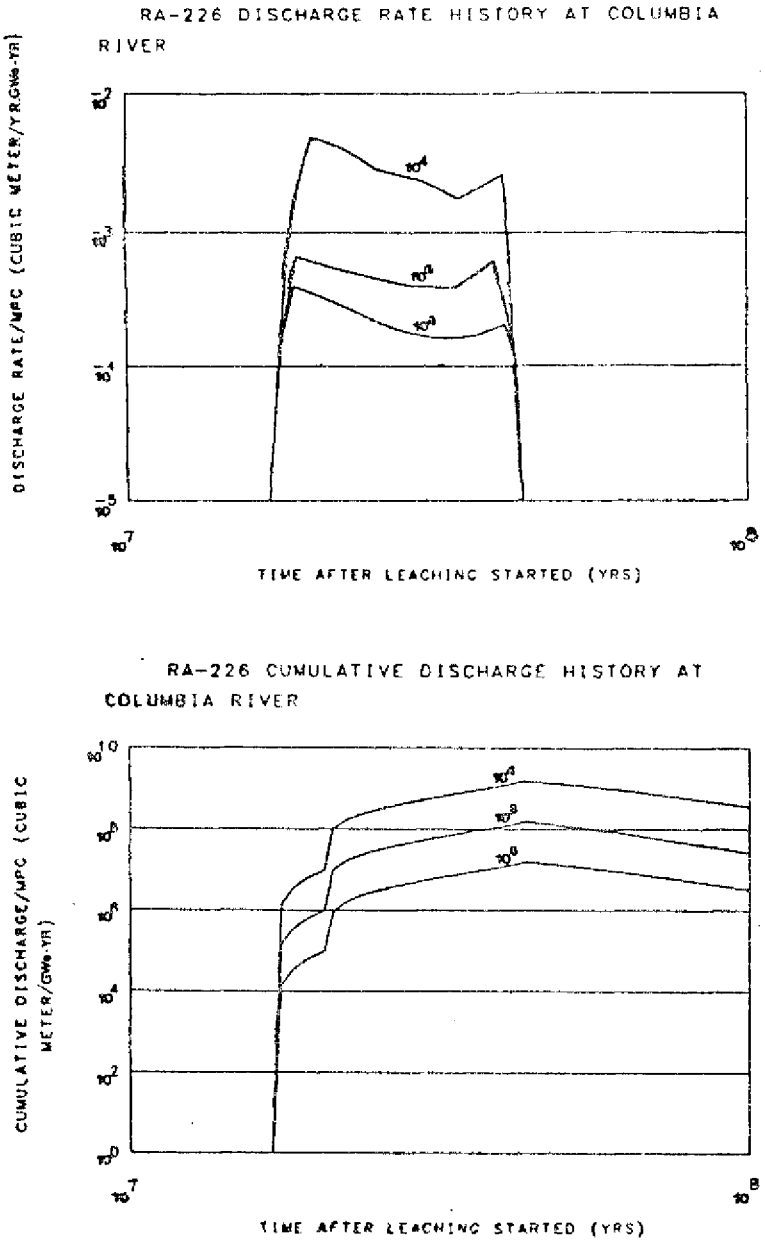


Figure 4.37 Ra-226 discharge rate/MPC (water dilution rate) and cumulative discharge/MPC (water dilution volume) at Columbia River discharging from Ringold aquifer (Repository 2) for leach times of 10^4, 105 and 106 years

streamlines neither confluence nor diverge strongly because the repository is located on the south face of the potentiometric surface. The streamlines develop rather uniformly towards the southeast reaching the Columbia River after about 10^6 years, (see Table 4.9). Ra-226 reaches the Columbia River along with its precursor ^{238}U after 10^9 years. I-129 water dilution rate from the Saddle Mountain aquifer is shown in Figure 4.40.

The last case studied is the Saddle Mountain aquifer with the "Repository 2" location. This second location is on the ridge of the hill of the potentiometric surface. A peculiar behaviour is seen here. Part of the streamlines flow northward discharging into Columbia River and part of them flows southeastward also discharging into the same river, see Figure 4.41.

Although the water travel times at the biosphere for this second case are somewhat larger than those of the first repository (see Table 4.9), the important difference lies in the location of the discharge. In the Repository 1 case the location of discharge is a segment of about 10 km along Columbia River while for the Repository 2 the location of discharge spreads over a distance of about 35 km along the river. The contaminated regions for the Repository 2 are also larger than for Repository 1. Figure 4.41 and Figure 4.42 show the I-129 and Ra-226 contaminated regions for this second repository location in Saddle Mountain aquifer. Figure 4.43 shows the I-129 water

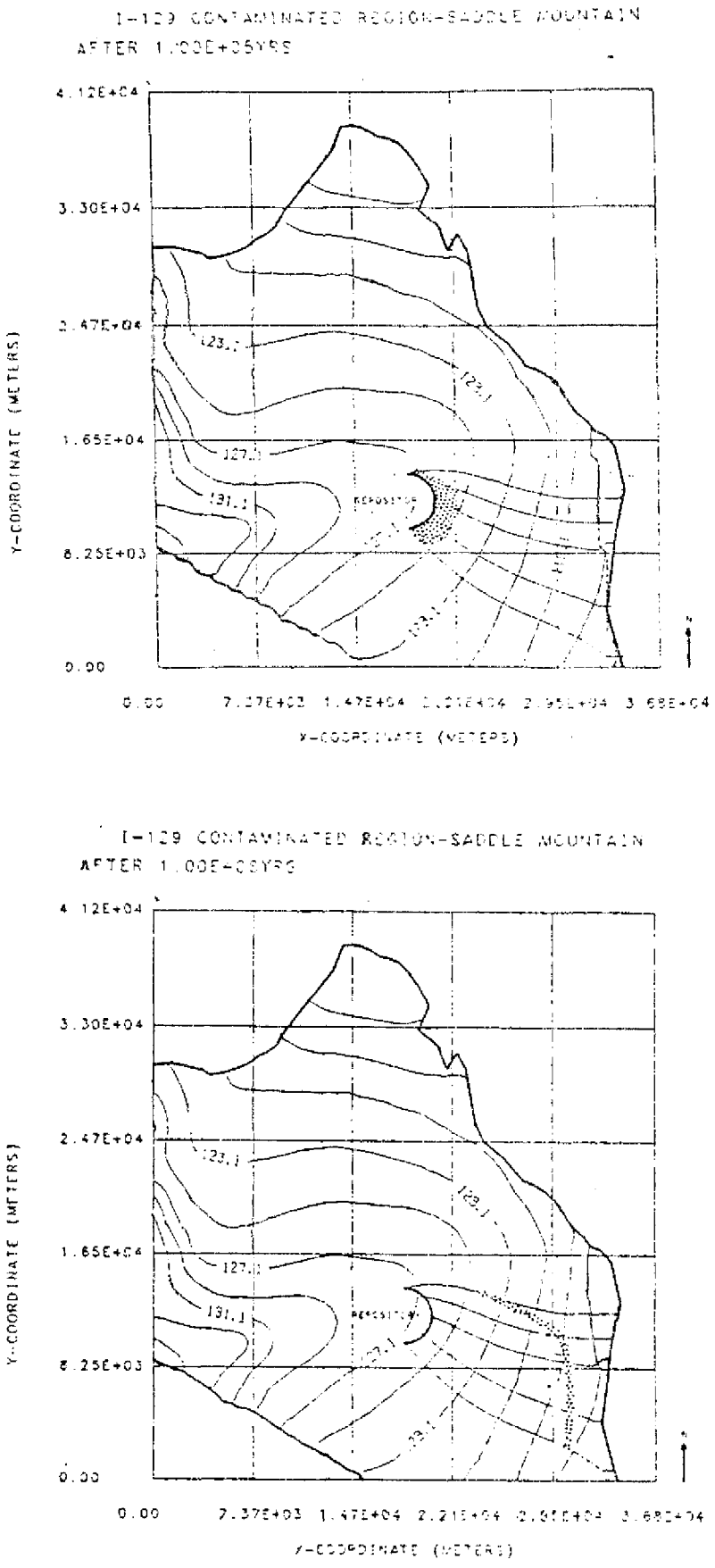


Figure 4.38 1-129 contaminated region in Saddle .Mountain aquifer (Repository 1) after in^ and 10^ years. Potentials are in meters above MSL.

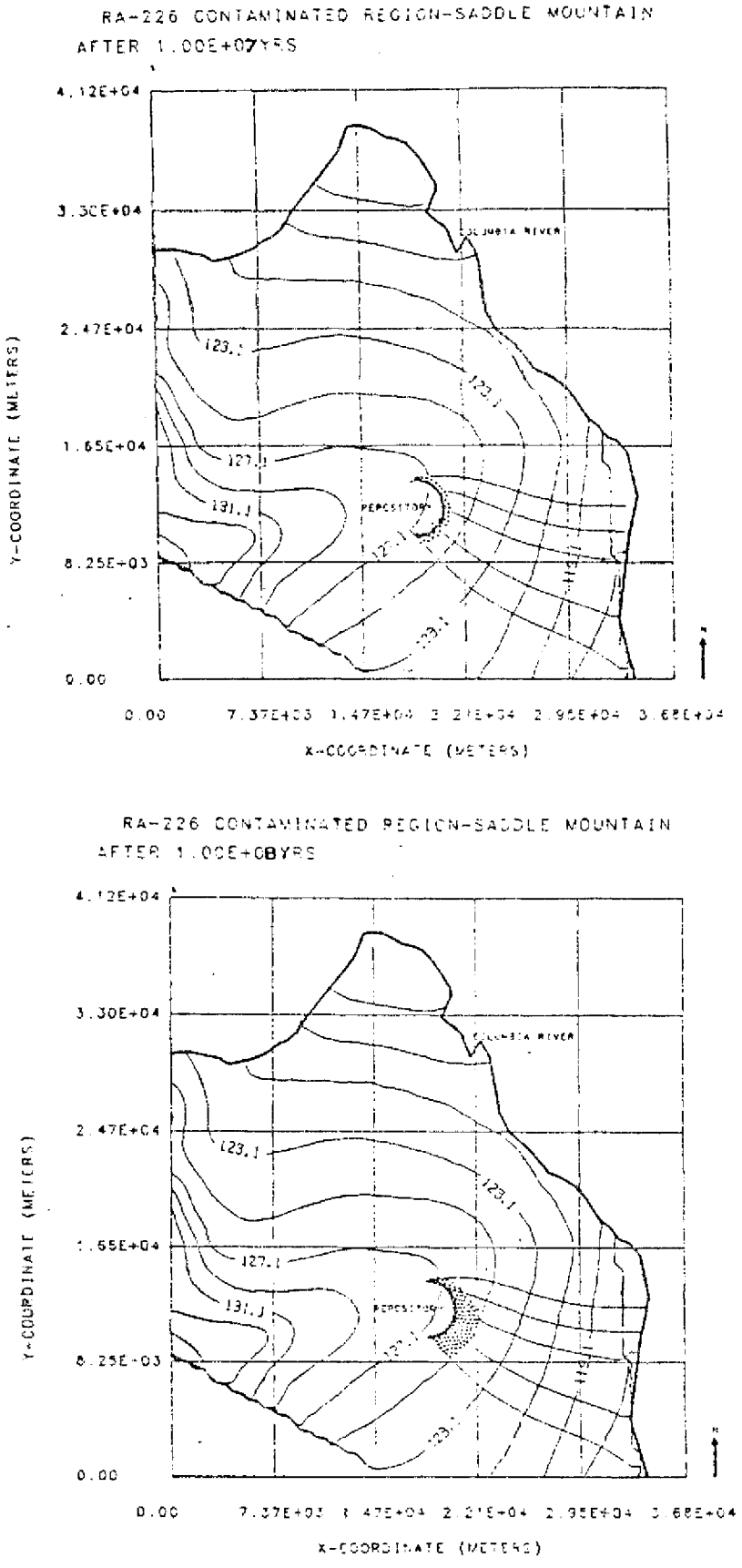


Figure 4.39 Ra-226 contaminated region in Saddle Mountain aquifer (Repository 1) after 10^7 and 10^8 years. Potentials are in meters above MSL.

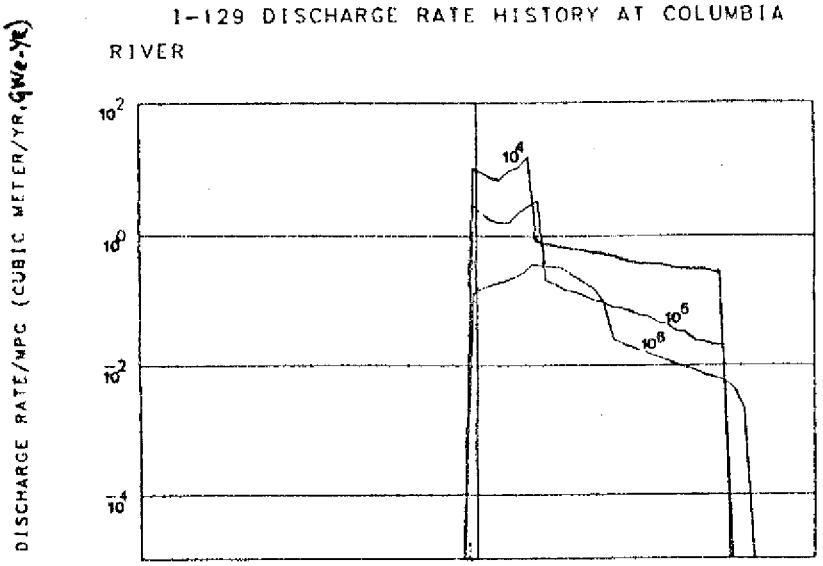
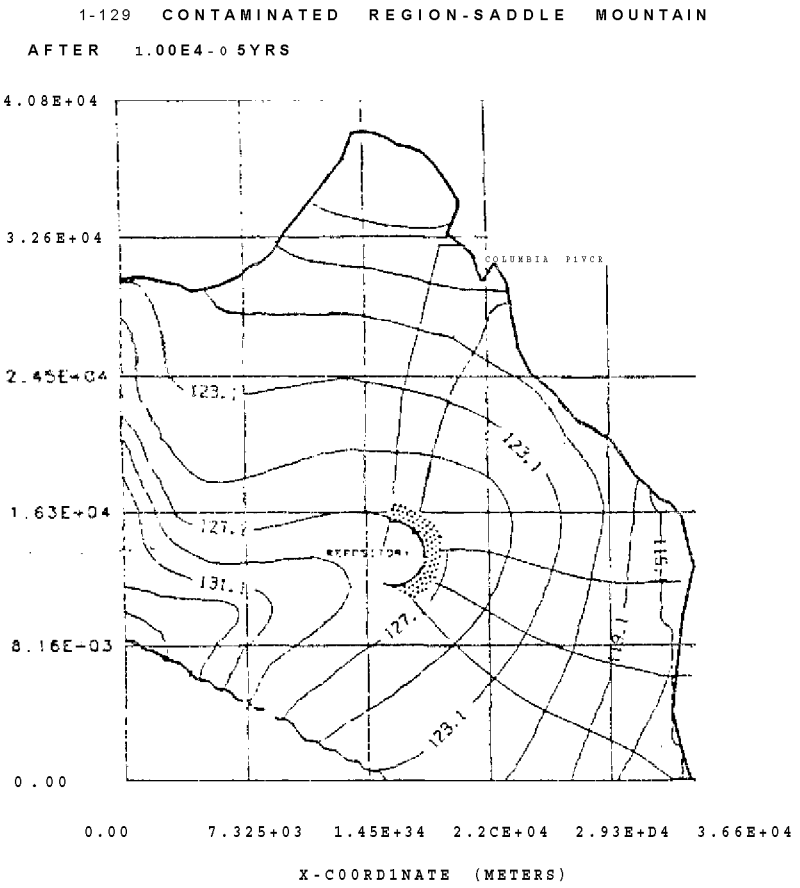


Figure 4.40 1-129 discharge rate/MPC (water dilution rate) and cumulative discharge/MPC (water dilution volume) at Columbia River discharging from Saddle Mountain aquifer (Repository 1) for leach times of 10 , 10^5 and 10^ years.



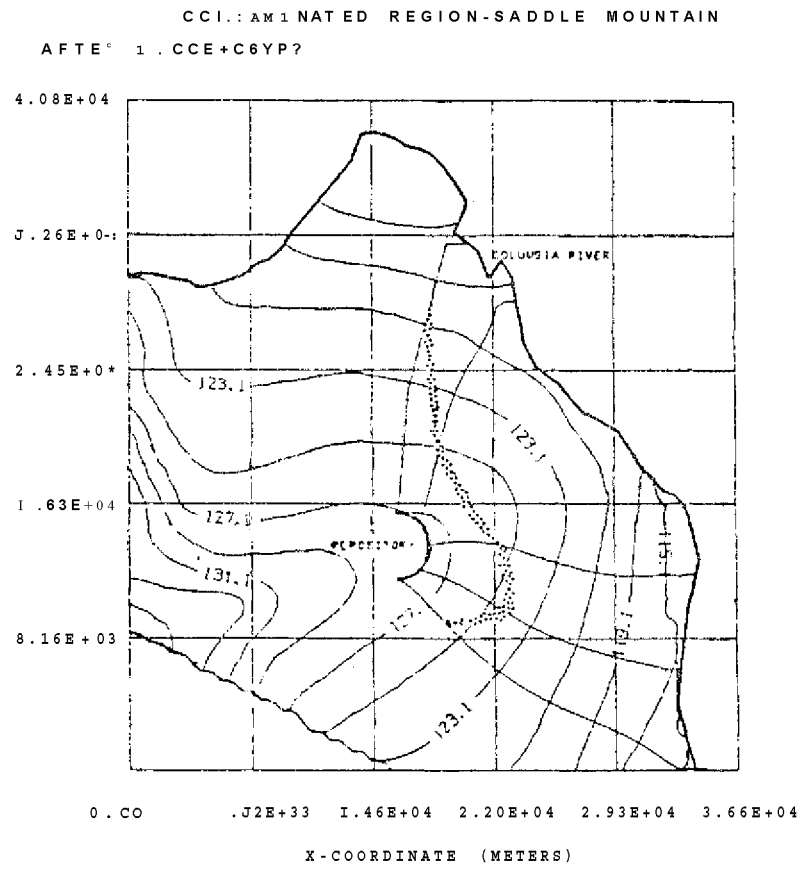
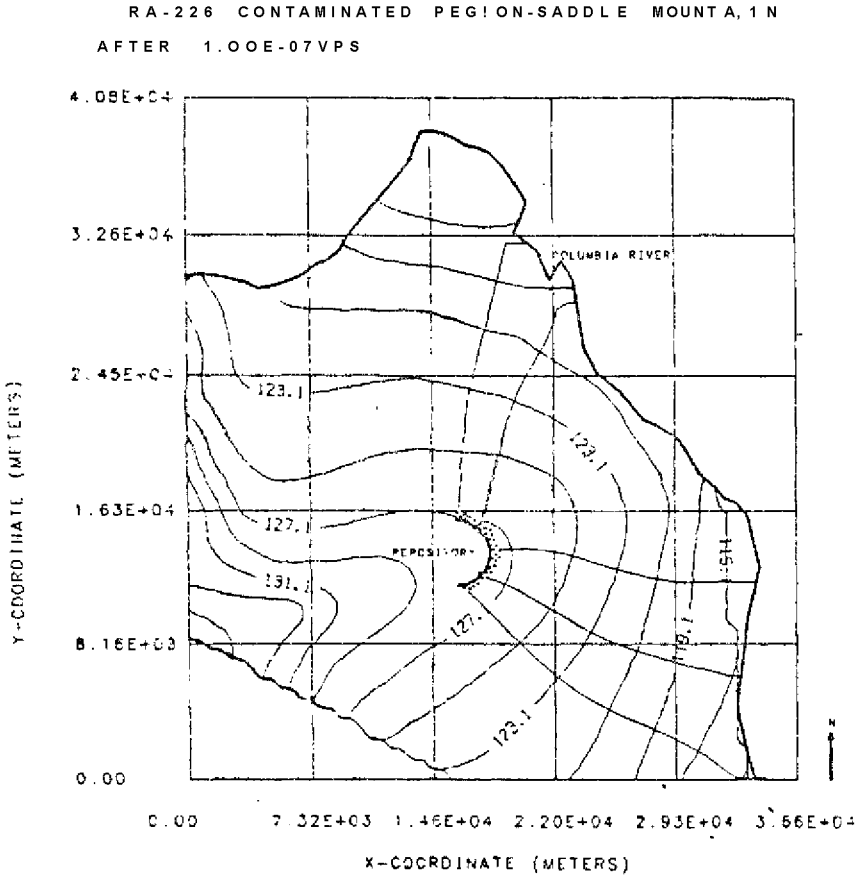


Figure 4.41 1-129 contaminated region in Saddle Mountain aauifer (Repository 2) after in^ and 10^ years. Potentials are in meters above MSL.



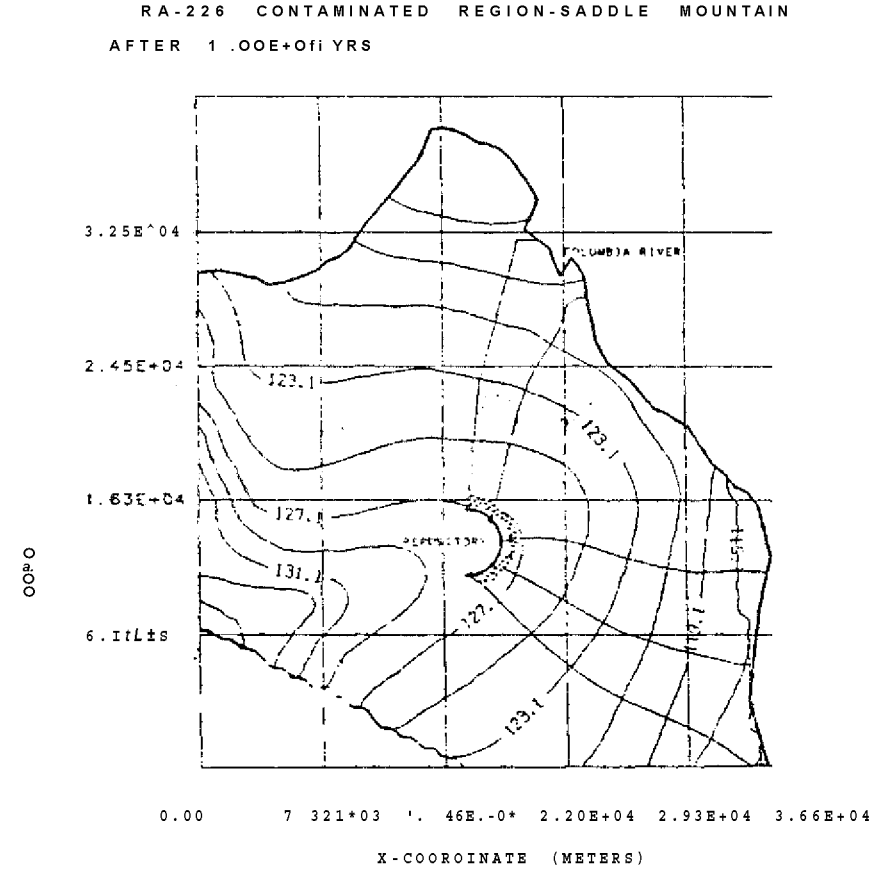


Figure 4.42 Ra-226 contaminated region in Paddle Mountain aquifer (Repository 2) after 10^ and 10' years. Potentials are in mters above ™.SL.

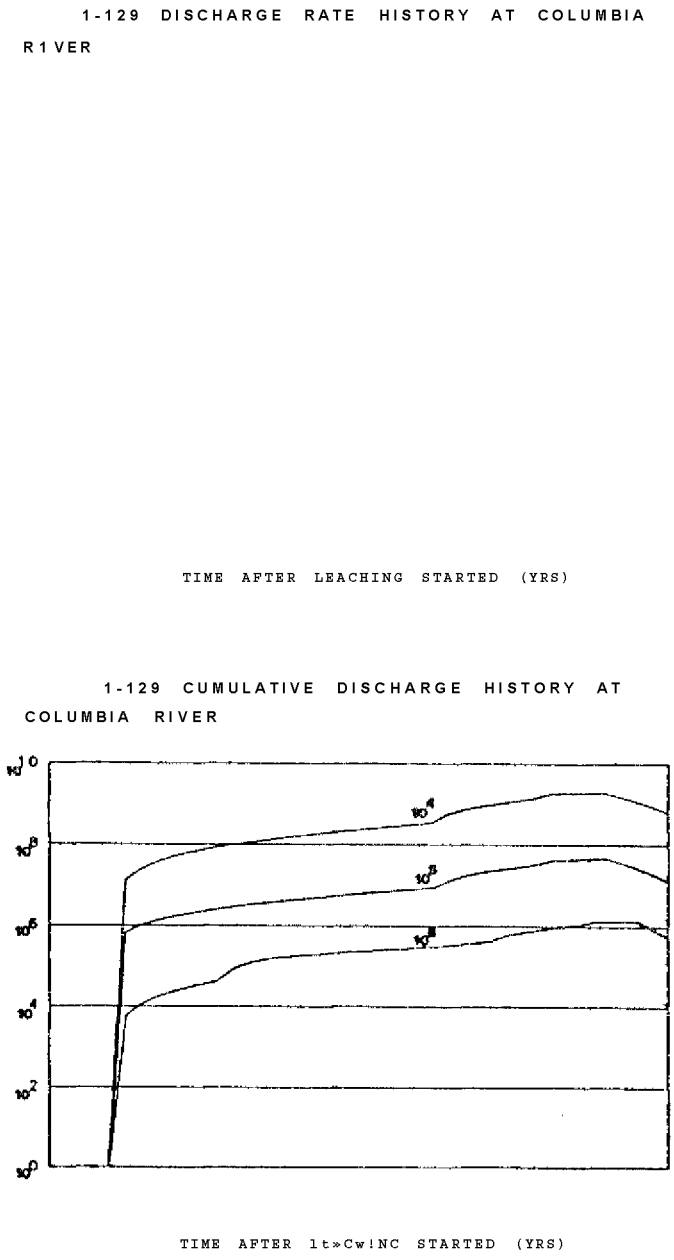


Figure 4.43 1-129 discharge rate/MPC (water dilution rate) and cumulative discharge/MPC (water dilution volume) at Columbia River discharging from Saddle Mountain aquifer (Repository 2) for leach times of 10^4, 10^5 and 10^6 years.

dilution rate at Columbia River.

The following Table 4.10 shows the maximum total water dilution rate as defined in Eq. (4.4.22) for each of the four cases studied in the BWIP site .These values are contrasted against the recorded flow rates in the Columbia River.

Table 4.10 Maximum total water dilution rates and Columbia River flow rates

Columbia River flow rates:	Maximum:4.9E+11	(m /yr)
(60 years record)	Average :1.1E+11	
	Minimum:3.7E+09	
Ringold aquifer,"Repository 1"	.....1.0E+03	
Ringold aquifer,"Repository 2"	•«••a««•2•0E*t*02	
Saddle Mountain aquifer,"Repository 1". . . .1.5E+01		
Saddle Mountain aquifer,"Repository 2". . . . 1.5E+00		

4.7.3 Effects of variations in the initial nuclide activities, in the time for beginning of leaching and in the nuclide MPC values

In this section we discuss how to extend the calculations to the disposal of unreprocessed fuel instead of high level reprocessed waste. In addition, the effect of variation of the

delay time for beginning of leaching on the results obtained previously as well as the effects of changes in MPC values are discussed.

The extension of the calculation for spent fuel disposal.

The initial activities of each nuclide present at the time of burial were the result of reprocessing the spent fuel of a LWR after generating 1 Gw(e)yr of electricity with a load factor of 80%, thermal efficiency of 34% and a burnup of 30.4 Mwd/kg. These spent fuels are reprocessed after 150 days cooling period and 0.5% of the Pu and U are lost to the waste. The time lapsed between discharge and emplacement in the repository is assumed to be 10 years. To study the case of spent fuel disposal rather than reprocessed high level waste, the present analysis would still apply. Since only the initial activities of U and Pu are affected during the reprocessing one must multiply the Ra-226 discharge rates and cumulative discharge by 200 to account for the fact that 100% of the discharged U-233 will be initially in the waste instead of only 0.5%. This is possible because the nuclide arrival times to the biosphere are large enough so that only the decay of U-238 is important, if the nuclide arrival time

at the biosphere were shorter than 10^5 years one must also consider the contribution of the Pu-238 decay. The hydrological calculations are of course not affected. The contaminated region as well as nuclide arrival times are also not affected.

The effects of the variation in the delay time for beginning of leaching on the calculations.

The value used throughout the calculations for the delay time in starting the leaching, to represent the durability of the waste package and, the engineered barriers was 1000 years.The first nuclide arrival times (Eg. (4.4.19)) of all nuclides present were such that only 1-129 and Ra-226 (U-238), whose effective half lives are larger than 10 years, reach the biosphere. In view of this fact, increasing the delay time for beginning of leaching to up to 10 years will not change significantly the initial concentrations of these nuclides at the beginning of leaching. Therefore the. results obtained for the concentrations and water dilution rates are not affected although the actual time for the nuclide to reach the biosphere is increased accordingly. If the set of retardation coefficients was such that other nuclides might also arrive at the biosphere (e.g.Pu-242,Pu-239,etc.) an increase in the delay time for beginning of leaching could affect the water dilution rates at the biosphere.

The effects of the variation of the nuclides MPC.

ICRP-30 (II) has recommended new biological uptake factors for some of the nuclides considered here. They can be translated into adjusted estimates of maximum permissible concentration (MPC^) for the purpose of calculating water dilution rates and water dilution volumes. The most significant changes affect Np-237 with a 200 times reduction in the MPC value and Ra-226 with a

60 times increase in MPC, (C4). These changes in MPC values does not invalidate the present results. Since the MPC are linear (inverse) multiplication factors, to convert the old water dilution rates and water dilution volumes into the new corrected values one would simply multiply the water dilution rates obtained in this work by the ratio of the new MPC divided by the old MPC. One can therefore extend the present calculation to include new values of MPC.

4.7.4 Summary and conclusion

Utilization of the present two-dimensional analytical solution to the radionuclide transport equation provided some qualitative informations about the migration of radionuclides through geologic media which the one-dimensional calculations lacked. These are the description of the two-dimensional contaminated region in the aquifer from the repository site to the discharge location at the biosphere at any time after the leaching started, and the determination of the location of discharge at the biosphere. Furthermore, by considering the aguifer as being two-dimensional should produce more realistic quantitative numerical results than one-dimesional calculations.

The calculations performed in Section 4.7 to assess the potential hazard to the public due the failure of the repository at the BWIP site have shown that the most potentially hazardous nuclides present in the waste are the I-129 and the Ra-226 (produced by the decay of U-238). In the event of an accident the contamination of the Columbia River does not exceed the allowed maximum permissible concentration for every nuclide present in the waste even when the river flow rate is assumed to be at its minimum recorded flow rate.

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Appendix A. Description of the computer code UCBNE25

UCBNE25 evaluates the analytical non-recursive solution to the one-dimensional transport equation without dispersion for the i-th member of a radioactive chain of arbitrary length.

A.1 Data input description. (See the program structure in Figure A.1).

Card 1: FORMAT(212)

Variable	Description
NCIIAIN (12)	Number of chains to be studied.
NGRAPH (12)	<0 produces a plot with the concentration history of every member of the chain for each set of parameter.
	>0 no plots are produced,only a printout.
	=0 produces a plot with the water dilution rate history of every member of the chain for each set of parameter.

Card 2: FORMAT(3(2F9.3,I2),F9.3,I2)

Variable	Description
Z0 (F9.3)	First value of path lenth (m) to be evaluated.
DELZ (F9.3)	Multiplying factor for the next MZ cases of path length to be evaluated.
MZ (12)	Number of different cases of path length to be

evaluated $Z=ZOx(DELZ)^{n}$; n=1,2,....MZ.

VWO (F9.3) First value of water velocity to be used (m/yr).

DELVW (F9.3) Multiplying factor for the next MVW cases of water velocities to be evaluated.

MVW (12) Number of different cases of water velocities to be evaluated $VW=VW0x(DELVW)^{m}$; m=1,2,_____MVW.

TBLO (F9.3) First value of the time for beginning of leaching to be evaluated (years).

DELTBL (F9.3) Multiplying factor to obtain the next MTBL cases of time for beginning of leaching to be evaluated $TBL=TBL0x(DELTBL)^{k}$; k=1,2,.... MTBL.

DELLT (F9.3) Multiplying factor to get the next MLT cases of leach time.Each nuclide can have a different first case value for the leach time and these values are specified in the individual nuclide specification cards (see next cards).

MLT (12) Number of different cases of leach time LT to be evaluated $LT=LT0x(DELLT)^{j}$; j=1,2,_____MLT.

The next set of cards (Card 3 through Card 4+1) must be repeated for every chain being studied. In other words one need NCHAIN set of these cards.

Card 3: FORMAT(110,12)

Variable Description

NTIME (110) Number of time intervals that the contaminated time of each nuclide is to subdivided. The calculations will be performed for each time interval.

I (12) Number of members the chain has,

Card 4 to Card 4+1: FORMAT(12,A7,5F10.4), a total of I cards

one for each member of this chain.

Variable	Description
NUMBER (12)	Hierarchy in the chain, NUMBER=1, 2, ... I
NNUCL (A7)	Nuclide name (e.g. TH-230).
THALF (F10.4)	Nuclide half life (years).
K (F10.4)	Nuclide retardation coefficient.
LT (F10.4)	Nuclide leach time (years).
C (F10.3)	Nuclide total activity at the time of burial (Ci).
TOX (F10.4)	Nuclide Maximum Permissible Concentration (Ci/m^3)

Figure A.1 Structure of the program UCBNE25.

Initialize

Read data input

Do every chain,NT=1,NCHAIN

Do every case of time for
beginning of leachinrr,
TBL=TBL0*(DELTBL)**N;N=1,..MTBL

Do every case of water velocity
VW=VW0*(DELVW)**J;J=l,...MVW

Do every case of leach time
LT=LT0 *(DELLT)**K;K=l,...MLT

Do every case of path length
Z=Z0*(DELZ)**M;M=1,....MZ'

Do every nuc ide in the chain
NU=1,I

Determine the contaminated time
for every nuclide

Do every time interval
NT=a,NTTME I

Evaluate the concentration and
the water dilution rate

Plot water dilution rate curves NGRAP¡1=0
Plot concentration curves NGRAPH<0
No graphs,just printouts NGRAPH>0

```
  P I A. 3 6 8 3 0 1 , T I N G , D
'INPUT  62D0C  22.22.50   ¿0  SEP  81   VIA  CR04                                  265
.IDs
•USERPR
:OPY,  INPUT/RR »OUTPUT/PR.
)I  SPOSE,OUTPUT=PR,PA=IF.

PROGRAM  UC3NE25
DANIEL  K.S.  TING
DECEMBER  1980
DEPARTMENT  OF  NUCLEAR  ENGINEERING
JNIVERSITY  OF  C ALIF CRNIß »BERKELEY
B E R K E L E Y , C A . , 9 4 7 2 0



**  CONTROL  CARDS  LISTING  **

t JOBCARD]
f PASSWORD]
*J SERPR
MNF4.
F E T C H P S , I D 0 S , U L I 8 , U L I B X „
F E T C H P S , G P A C 8 N 7 , G P A C , V A 8 ^
L I N K , F = L G O , F = G P A C , P = U L  I B , X .
G R A P H I C , F N = F I L M , F T = V A .
E X  I T .
D U M P , 0 .
GR'JMP.



**  PR33RAM  LISTING  **

        PROGRAM    MAC1(INPLT,CUTPUT,TAPE5=INPUT,TAPE6=0UTPUT,FILMJ
C
C           INITIALIZE  THE  PRCGPAM
C
        ZOMMON/IGSZZZ/ZMCCE12C0)
        DIMENSION   XNAMEf 5C),YNAMEI50),TNAMEII50 >
        DOUBLE  T10
        DIMENSION   NIdOI ,t»2(10 J,W3(10»
        DIMENSION  OCtS.^SI.VIIOI.EIIOI.CdOI.TCXdOI, TH ALF (10 I , B( 10, 10 ),
       5.3ETA(10,IO),DI(S,<;,S),A(10,10>,S(10),ST(III ,NNUCL( 101, TMAX( 10 ) , NUM
       S3ER(10I,rfD(20 0»,TIMEC2 00»
        DOUBLE  PRECISION  K(10> ,N(200),LT(10),NMAX(10)
        DIMENSION   TINLOGC2C0I,WCL0G1200)
        DOUBLE  PRECIS ICN  A,ADS,APRO,AT,B, BATEMAN,BETA,C, CMAX,C1,C2,C3,C4,C
       $5»DELLT,DELTA,DELTEL,DELVW,DELZ»Dt,DIFF,DM,DM  AX,OS,01»02,03,04,05,
       SD8,E,ERROR              P,S,ST,S1,S2  »S3,T,TBL,TBL0,TDNAX,TEMP4,THALF,
       $TIME,TIMLQG,TMAS,TMAX,TMAZ,  TMIN,  TCX,  T  T,TTMAX,TI,  T2,V.VIN,VM,VWO,WA
       SLOG , WAPRt WO'tWCLCG, WMAX ,W1,W2,W3,W6,X1  , X2,X3,X4,Y,Z,ZO
        DOUBLE  PR1,PR2
        DOUBLE  EE,EEE,BB
        DOUBLE   EO,EE, EBCeCE.BOEC, S1M,S2M,S3M
C
C           READ  DATA  INPLT
C
        READ  (5,201»  NCHAIN,NGRAPH
   201  FORMAT(2I2)
        IE AD  I 5,105 J  Z0,0ELZtHZtVWO,OELVW,MVW,T8L0 ,DELTBL,MTBL,DELLT,MLT
   105  FORMAT (2F7.3,I2,2F9.3,I2,2F9.?,I2,F0.3,I2i
```

```
    IF (NGRAPH.LE.C) CALL MCDESG(I MODE,6,0. I
    30  89  NC-1.NChAIN                                                    266
    RE AD(5, 20 0) NT IKE,I
200 FORMATI 110,12)
    DO 99 N'J=1 , I
    RE AD I 5» 106 J  NUMBER (NL ) ,NNlJCL ( NU J ,THALF{NU) , K{NU),LT(NU),C(NU>,TOXt

    E ( NU ) =ALOG(2. I/TFALF(NUl
106 FORMAT! 12,A7,5FI 0.A )
 99 CONTINUE

       EVALUATE B A T E KAN S FUNCTIONS
    :ALL  8ATEMAN(I,E,C,B)

       EVALUATE  EVERY  CASE  OF  TIME  FOR  BEGINNING  OF  LEACHING

    T BL=TBLO/CELTBL
    DO  61  ITBL = 1,MTBL
    T BL = TBL *D EL TB L

       EVALUATE  ACTIVITIES  AT  THE  BEGINNING  CF  LEACHING

    DO 60 I 1*1, I
    Y = 0.
    DO 62 I I 1 = 1,I I
    A6--EII  11   )*TBL
 62 Y = Y*B{11,111)*DE XFIW6)
 60 C I I I l = Y*E ( I I M C I 1 l/E ( 1 J

       REEVALUATE E A T E N AN S FUNCTION
    :ALL  BATEMAN( I,E,C,B »


       EVALUATE  FOR  EVERY  CASE  CF  WATER  VELOCITY

    VW=V^O/DELVW
    DO 63 IVW = 1 ,MVH
    VW=VW*DELVk
    DO 6 4 I J = 1,I
 64 VI I JKVw/KIUS

       EVALUATE  THE  BETA  FUNCTIONS

    DO 21 M 1 = 1, I
    DO  22  ¥J=l, I
    IF!MI.F2.MJ)  GO  TC  22
    IF{V(MJ).EG.V(MI I l GO TO 59
    BETA(MI,MJ!MEIM)*VIMJ>-E(M)*VIMI))/(V(MJ)-V(MII)
    3 E T A(M J,M I )= B E T A{p I,HJ )
    50  TO  22
 59 B E T A ( MJ , M I 1 = 0.
 22 CONTINUE
 21 CONTINUE
       EVALUATE  EVERY  CASE  OF  LEACH  T I M E

    DO 65 ILT = 1 , I
 65 LH ILT »=LT ( IL T J/DELL T
    DO 66 I 3 = 1,ML T
    DO  67  14=1,1
 67 L H I 4 ) = L T ( 14 I * D E L L T
```

```
:          EVALUATE FOR EVERY PATH LENGHT
C                                                                    267
      Z^ZO/DELZ
      30 68 15=1,MZ
      Z=Z*DELZ
C
C            INITIALIZE GRAPHING SYSTEM
C
      IF(NGRAPH.GT.C) GCTO 41
      VM=0.
      DO 7 7 K S= 1 » I
   77 IF(V(KSI.GT.VM) VM=V(KS)
      VIN=1.0D10Q
      DO 78 KL=1,I
   78 I F(V(KLI.LT.VIN) UN = VIKL)
      L3=IDINT(DL0G10(Z/VM)}
      L4= IDINT(DLGG10( Z/V IN•LT(1 )) +1
      T3 = FL0AT(L 3)
      T4 = FLOAT(L4I
      Z Vr Z /VW
      CALL SUBJEG(ZMCDE,T3,-3.,T4,5. I
      IF(NGRAPH.LT.O)CALL SUPJEGIZM0DE,T3,- 4.,T4 ,5.I
      CALL OBJCTCCZMCDE»20.,20,,9C.,30.)
      CALL SETSMG(ZM0DE,45,1.5)
      DIVX = 1 .
      DIVY=2.
      CALL GRIDG(ZM0DE,0IVX,DIVY,0,0)
      CALL LABELGCZMODErO, DIVX, 0, 3•
      CALL LABELGIZMODE,1,DIVY,0,3 !
      ENCODE ( 50, 1C0CXN&VE I
 1000 FORMAT(*           TIME AFTER LEACHING STARTED {Y R S ) * )
      ENCODE(50,1C01 ,YNAME)
 1001 FORMAT( *   WATER CILUTION RATE (CU3IC ME TER/YP,*GWYR8 * I
      IF(NGRA PH.LT.O> ENCCDE(50, 1002 , YNAME)
 1002 FORMAT(*             DI MENSIONLESS CONCENTRATION*)
      ENCODE(150,10C3,TKAME»ZV,LT(1»,TBL
 1 003 FORMAT(<W A T ER TRAVEL TIME    1PE8.2,* (YRS),LEACH TIME = *,1PE 8.2,*
     $ (YRS) ,TIME FOR BEGINNING OF LEACHING =* .1PE3.2,* (YRSI*)
      CALL TITLZS(ZMCDE,1,1,1.0»
      CALL TITLEG(ZMCDE,50,XNAME,50,YNAVE,1 50,TNAME)
C         EVALUATE THE CCNCENTRAT ICN FOR EVERY N'JCL I DE
C
   41 DO 50 11=1,1
C         DETERMINE TFE T I f* E DOMAIN FOR EVERY NUCLIDE
C
      VMAX=0.
      DO 36 Kl= 1,II
      IF(V(K1».GT„VWAX» V^AX^V(Kl»
   36 CONTINUE
      VMIN=1.0E100
      DO 3 7 K2«l,II
      IF(V(K2).LT.VMIN) VMIN=V(K2)
   37 CONT INUE
      TMIN'Z/VMAX
      T = L T(I 1)
      TMAZ=Z/VMIN*T
      DEL T A=(DLCG10IT fA Z)-DLOG10(TMINi) /NTIME
C
C         EVALUATE TFE CCNCENTRATICN AT EVERY TIME STEP
C
      CMAX=0.
      TTMAX=0.
```

```
    DO 38 K2 = 1.»NT!ME
    T10=DLOG10(TMIN}*CELTA*K3                                          268
    TT=10.**T10

       EVALUATE THE STEP FUNCTIONS

    DO 39 K 4 = 1, I
    S(K4I=0.
    S T ( K4 5 = C«
 39 CONTINUE
    DO 40 K5=l,I
    IFIV(K5»*TT.GE.ZI S t K 5)=1.0D00
    I FÍVU5JMTT-TI.GE.Z) ST ( K5J=1.OD00
 40 CONTINUE
    C1 = 0.
    DO 51 12=1,II
    ED=(-El 12»*(TT-Z/V(Il I»)*OABS I S I I 1»-S T ( II» >
    CALL EXPO(ED.EE)
 51 C 1 = C1 + B (11,12)*E E*Í S (I15-STÍÍ1)J
    EB=(-E(UI*Z/VII1M*DABS(S(I1»-STU1!)
    CALL EXPOIEB.EEEI
    Cl=Cl*EEE*lS(I1S-ST(Il)I
    C5 = 0.
    IF( 11.EC.1 » GO TO 71
    WMAX=0.
    00 521 L=l, 11 -1
    DO 531 M=L,I1
    DS = S(M Í-STIN I
    ADS^DAB St 0 S)
    DO 541 NR=L,I I
    IFINR.EC.»* > GC TO 541
    DO 551 J=I » L
    W l (J) = ( -BETA(NR,M)*UT-Z/V(Kn-E(M)«Z/V(M) l*S(M)
    -<2lJ» = (-T*(E(Jl-3ETA(NP,M»i-BETA(NR,Mi*{TT-Z/V(M»l-E(Mi*Z/V(MM*ST
   tl M )
    W3(J)=(-E{J)*(TT-Z/V(M))-E(M)*Z/V(M)I*A0S
    1 F(BETA(NR,Ml.EC.C.I Wl(J 1=0.
    IF(BETA(NR,M).EC.C.) V»2(J I=0.
    IF(BETA(NR,M).EQ.C.) W3(J)=0.
    I F Í Wl(J).GT.WMAX) aNAX-Wl(J I
    IF(W2(J).GT.WMAX) V>PAX=W2(J)
551 I F(W3(J ) .GT.WMAX I WMAX=W3(J »
541 CONTINUE
531 CONTINUE
521 CONTINUE
    I F ( WMAX.GT.60C. I C I FF = V.MAX-600.
    I F(WMAX.LT.60C. >DIFF=0.
    DO 52 NJ=1,II-1
    C4=0.
    DO 5 3 NM = NJ,I I
    C3 = 0.
    DO 54 NP = NJ,I 1
    I F(NR.EC.NN » GO TC 54
    <i2"0&
    DO 55 NK*1 ,NJ
    PR1=1.0DOO
    DO 58 NC=NJ, I 1-1
 58 PR1=PR1*E(NCI*K(NCI
    PR2=1.0DOO
    DO 57 NC«NJ,I1
    IF(NQ.ECNR) GO TC 57
    I Fl NQ. ECNP » GC TC 57
```

```
    PR2 = PR2ME(N3)*K(NC)*(K{NPJ-K(NMH*E(NM)*K(NM)*(MNC)-KINRN«-E(NR)
   S*K(NRI*IK{KM1-K(NC)!)
 57 CONTINUE                                                          269
    X1=3(NJ,NKI*(K(NP)-K(NM))**(IJ-NJ-1I
    Xl=Xl/(E(NK)*K(NR»-E(NKI*K(NM)-EINP)*KlNR)tE(NM|*K(NMJ|
    Xl=(X1+PR1»/PR2
    S1 = (-BETA(NR,N«I*UT-Z/V(NM)I-E(NV)*Z/V(NM))
    S2=(-T*lE(NKI-3ET«(NPtNMII)fS1
    S1=S1*S(N*»
    S2=S2*ST(NP)
    S3 = (-E(KKi*TT-(E(K^}-E(NKII*(Z/\/(NM)1!
    S3 = S3*DABS(SI KM>-STihH))
    51 = S1-D IFF
    52 = S2-0 IFF
    S3=S3-0IFF
    CALL EXPO(51,X3)
    IF(BETAINR,NM).EC.C.) X3 = 0.
    X3=X3*S(NM>
    CALL EXPO(S2»X2J
    IF(BETA(NR.NM1.EQ.C.» X2 = 0.
    X2=X2*ST(NMJ
    CALL EXP0(S3,X4)
    X4=X4*(S(Nf I-STCNsv)>
    C2=C2+X1*(X3-X2-X4)
 55 CONTINUE
    C3=C3+C2
 54 CONTINUE
    C4rC4 + C3
 53 CONTINUE
    C5=C5*C4
 52 CONTINUE
 71 IF(II.EC.I>DIFF=C.
    TEQ= (E(ii•mn/(Eiu!*K{iin
    IFEC5.GT.TEQ) GO TC «5 7
    IFSDIFF.GT.6.0DC2» GO TO 97
    M(K3)=C1+C5*DEXP(CIFF)
    IF(NIK3I.LT.O.» GC TO 97
    TIME(K3}*TT
    WD{K3)=MK3I*C(1I*EII1)/(E(1I*T0X(I1I*TI
146 IF(N(K3l.GT.CPAX>TTMAX=TT
    IF(N(K?).GT.CMA>) CMAX=N(K3)
 38 CONTINUE
    30 TO 222
 97 30 98 IX=K3,NTIME
    Hi 1X1=0.
    T10=DL0G1C(TMIN1+DELTA*IX
    TT=10.**T10
    TIME(IX)*TT
    *D(  IX)=1.0C-200
 98 IF(IX.EG.1» GO TC 146
222 NMAX(m=CMAX*C(l)*E(Il.MEm*TOXlIi)*TI
    TMAX(III=TTMAx
    WRITE(6,101*
101 FORMAT(IH1,5X,*NL"BEP*,2X,*NUCLIDE*,2X,*HALFLIFE(YR)?t,2X,*S0RPTI
   SON CONSTANT*, 2X, *LEACH TIME (YRJ*, 2X, ^INITIAL ACTIVITY (CI) *, 2X,
   SPC  (CI /M**3)*)
    WRITE(6,10C) II,NNLCLI11», THALF(IU,K(I1»,LT(I1»,C(I1t,TOX(II>
100 =r)RMAT(7X,I2,4X,A7,5X,lP0 3.2,9X,lPD8.2,10X,lPDfl.2.10X,lPL)8.2,12X,I
   $PD3.2)
    WRITE(6,102» Z,V«,NMAX(II», TMAxl I1»
102 FORMAT(//,2X,*PATFLENGHT=#,1PD8.2,*(*)*,2X,*WATERVEL.=*,IPD8.2,
   $MM/YR)«,2X,*MAX.hATERDIL.RATE=*,1PD8.2,*(M**3/GW*YR*»2i*,2X,*TIM
```

```
      SE OF MAX,(YRJ**,1PD8-2 I                                                    270
       WRITEU,102)
  103 FORMAT(//,8X,«TIME (YR)*,3X,*DIMENSIONLESS CONC.*,3X,*WATER OILUTI
      SDN RÄTE { «**3/Gk*iR**2M)
       00 80 NLCG=1,NT IKE
       WCLQGlNLOGI=WD(M.CGJ
       IF(NGRAPH.LT.OI hCLOG(NL CG)=N(NLG G)
       IF(WCLOGINLOGI.LE.l.OD-3 » WCLOG i N LOG!-• 1.00-3
       HCLOGINLOG»=ALOGIO(WCLOGlNLOGIJ
   80  TINLQG(NLOGi=CLCGlC!TSME(NLOGn
       DO 56 K3=l,NT I ME
       WRITE(6,104 I T I F E ?K3) »NCK3I • VdD C K3 !
  104 F0RMAT(8X,1P0B.2» 6X,1P08.2,13X,1PD8.2)
   56  CONTINUE

       IF(NGRAPH.GT.C> GC TO 50
C           DRAW CURVES FDR EACH NUCLIDE
C
       IFIWCLOGI l).GTo-3.) WCLOGl1J=-3.
       CALL LINESG(Z«GDE,NTIME,TINLOG»WCLOGJ
   50  CONTINUE
       IF(NGRAPH.LE.OJ CALL FRAME
   68  CONTINUE
   66  CONTINUE
   63  CONTINUE
   61  CONTINUE
   89  CONTINUE
       IF(NGRAPH.GT.O) GC TO 43
       CALL EX ITG(ZMQDE)
   43  STOP
       END
       SUBROUTINE BATEMAM I»E,C»B)
       DIMENSION EUOI, C(10», B(10,10>
       DOUBLE PRECISION E,C,E
       DOUBLE TEMPI
       DO 27 L1=1, I
       DO 28 L J=1, I
       TEMP1=0.
       DO 31 LM=1,LJ
       TEMP2=1.
       30 29 LR=LM,LI
       TEMP2=TEMP2*E(LP I
   29  CONTINUE
       TEMP3=1.
       DO 30 LL=Lt"» L I
       IF(LL.EC.LU GC 1C 30
       TEMP3=TEMP3*(E(LL1-EILJI)
   30  CONTINUE
       rEMPl=TEMPlMC(LM)*El1J/(C(1>*E(LM)))*TEMP?/(E(LI)*TEMP3>
   31  CONTINUE
       B(LI,LJ)=TEMP1
   28  CONTINUE
   27  CONTINUE
       RETURN
       END
       SUBROUTINE EXPO I X, Y)
       DOUBLE X,Y
       I F (X.LT.-6.002 I GC TO 501
       Y=DEXP(X I
       30 TO 502
  501  Y=0.ODCC
  502  RETURN
```

Appendix B Description of the computer code UCBNE20.

B.1 Data input description.

1) 1st card: Initial system description:

VARIABLE	FORMAT	DESCRIPTION
NNUCL	12	total number of nuclides being considered
	E12.4	first value of path length to be used (meters); (zé + 0)
	E12.4	first value of leach time to be used (yrs); (T<t> ± 0)
	E12.4	first value of water velocity to be used (m/yr); (v# 4 0)
TBU	E12.4	first value of time for beginning of leach (yr); (TBLtf ^ 0)

2) 2nd card: System parameters variation description

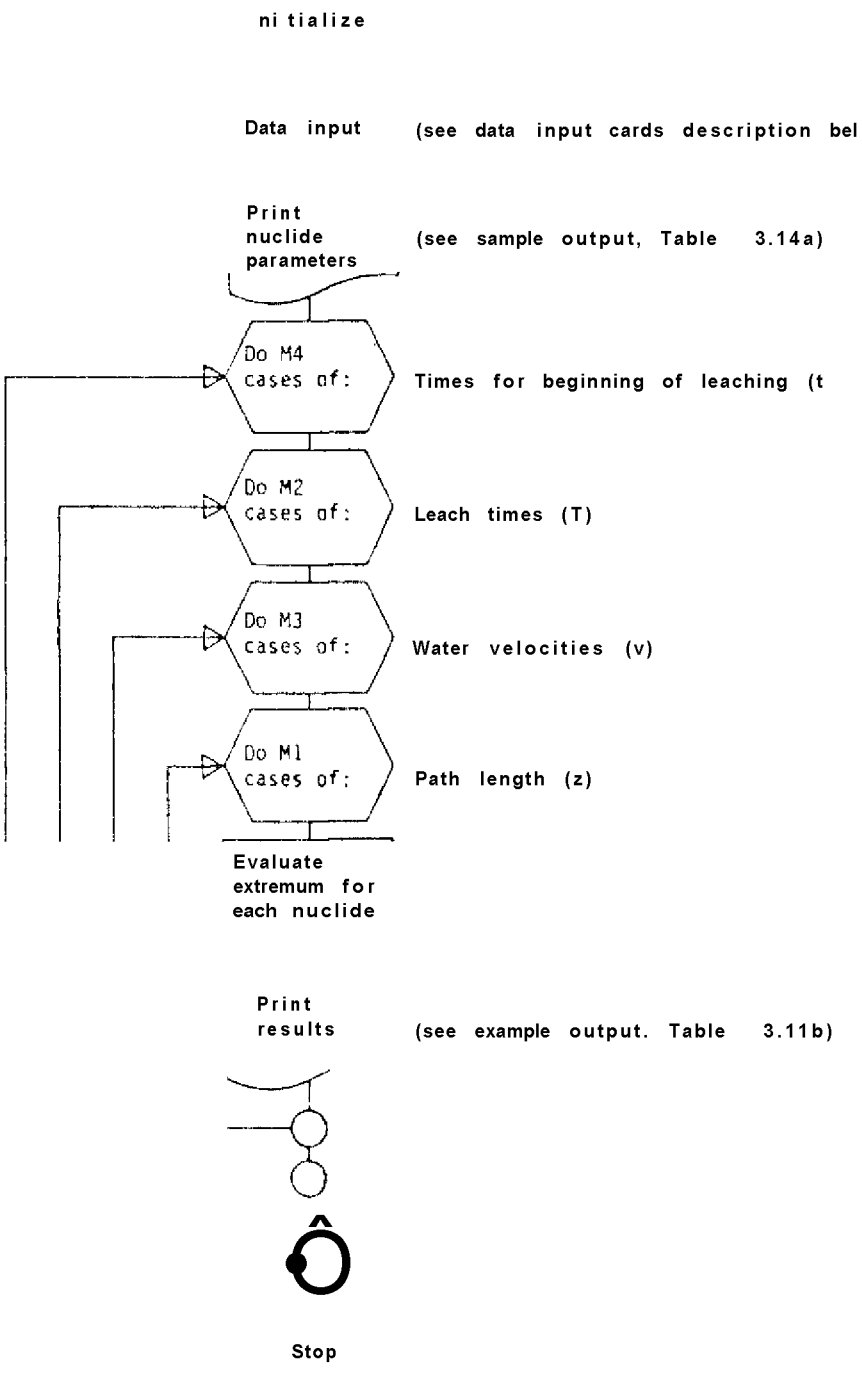
VARIABLE	FORMAT	DESCRIPTION
Ml	12	total number of different path length cases to be evaluated Ml = 1,2 ...
DEL1	E10.4	multiplying factor for different path length cases: z = x x (DEL1)^{n}; n = 1,2 ... Ml
M2	12	total number of different leach time cases to be evaluated M2 = 1,2 ...
DEL2	E10.4	multiplying factor for different leach time cases: T = T0 x (DEL2)^{n}; n = 1,2 ... M2
M3	12	total number of different water velocity cases to be evaluated, M3 = 1,2 ...
DEL3	E10.4	multiplying factor for different water velocity cases vw = v0 x (DEL3)^{n}; n = 1,2 ... M3
M4	12	total number of different time for beginning of leaching cases to be evaluated, M4 = 1,2,3 ...
DEL4	E10.4	multiplying factor for different time for beginning of leaching cases TBL = TBl# x (DEL4)^{n}; n = 1,2 ... M4

3) 3rd through (NNUCL _+ 2)th card: Nuclides description

It is required one card for each nuclide being considered, for a total of NNUCL cards. Each card has the following inputs:

VARIABLE	FORMAT	DESCRIPTION
NN	12	Nuclide identification number
NUCL	A6	Nuclide name (e.g., TH-229)
NH	12	Nuclide hierarchy: NH = 1 : if it is a first member of a chain NH = 2 : if it is a second member of a chain NH = 3 : if it is a third member of a chain NH = 4 : if it is in secular equilibrium with the nearest long lived precursor
NP1	12	NP1 = identification number of the 1st precursor if NH = 2 or 3. NP1 = identification number of the nearest long lived precursor if NH = 4. NP1 = 0 if NH = 1
NP2	12	If NH = 3, NP2 is the identification number of the 2nd precursor. NP2 = 0 otherwise
HFLV	E12.4	Nuclide half-life (yr)
KD	E12.4	Nuclide sorption coefficient, KD = 1 + LLZ_JL!D J, e S U
TOX	E12.4	Nuclide maximum permissible concentration (MPC); (Ci/m³)
C	E12.4	Initial activity at the time of emplacement, i.e., t<- = 0, (Ci)

Figure B.1 Structure of the program UCBNE20.



```
FIA • 968301,TING.0
NPUT  620 CC  12.2°,04   12  SEF  51   VIA  CP04
D =
FY, INFI'T/RR ,0LTFUT/RR .
SFOSE ,0UTFUT= FP .F<J=1*.

CGRAM  UC BNE 20
M E L  K.S.  TING
F1L,196C
F ART HF NT CF N L C Lti. AR ENGINE. EF ING
IVfFSITY  CF  C*LIFCRNI£tEt*K£LE Y
RKFLcY.CA. ,S4720


 CCNTFCL  CARDS  LISTIfG  **

CBCAR CI
ASSWORC1
SERPR
N4.
C.
IT.
KP,Q,
UHP.


 FRCGFAH  LISTING  **

     PFCGRAH HAX1 < I KF L T, CUT FL T , T A PE 5 = IN ? UT , T AP EE =C IT PL T )
     DIMENSION f'CT FCC ( 1 0 0 )
     0 IHL NSICN NLC L ( 1c C ) , NN (1c C ) , fsPl ( i CO ,'J°2 ( 1C? ) , Nh (l'JD) , HFLV(lCC),
    SVK(iOO) , C(10CMCX10Q) , TMX(100) , D"AX(100) JIFt. (100)
     INTEGER S2 (3, 3) , S3 (3,3 )
     OIKN3ICNV (3 ) , V2 (3) , AL (3 ,3 ) ,EE ( 3 ,3) , 7 ( ICG) , FRL CSF (ICC 5 , h (ICC)
     REAL LACBCA(1Q0) , KD (1S0KNNAX(100)

            RFA C  CATA  INRJT

     RLAD  (5,200)  NM'CL »Z0»T0»V0,TSLQ
200  F CF rAT (12,4112.4)
     READ ( 5 , 4 2 C ) H1 , DELl»K2»OELt, ^3»DfiL3, "'*tDTL4
420 F CRM AT (12 , C10 .4 , 1 I , E 10 . 4 , I 2 , E 10 . «.,12, £ 10 • M
     DC 2C 1 = 1 , NM'CL
     READ (5,2 [1 ) NN (2 ) tM'CL C I ) , N F (I) , NF1 ( I >, NP2 ( I ) , hF L V (I 5 , KC (I) , T C X (I
    n  , c (i)
201  F CRM AT (12,Ac, 12 , 2 12- 12 . 4 >
 20  CCM3NLE
     DC  10  I=1,NNUCL
     LAKECA(I)=0.6 93/HFLV(I)
     E (I) =LA HE CA (I >
 10   AT(I) = LAMEDA(I)*XC(I)

         EVALLATF THE ACTIVITIES AT EACH T I Mc F C R BEGINNING LEACHING

     TEL = TBLC/CELU
     DC  4 1 3  J413=1,M4
     T EL=TBL*CEL4

         KFITF. PROGRAM 7 IT Lt. , CASF FEING SOLVED AN C MCLI CE FAF A PF. TEF< S
```

```
    WRITE (6,2 (4 ) TEL
>04 F CR HAT (1H1, /T HE MCL ICES F^RAHETERS AP.E LISTED E E L 0 W t , 5X , iT I H E FCC
   $ EEGINMNG OF LEACHING IS t , 1 X •i=»c a . 2 , IX , * ( YR ) * )
    DC 414 I=1,NNUCL
    IF (NH (I ).EQ .3 ) GC TC kls
    GC TC 414
1(15 J1 = NF2 (1)
    J2=NP1 (I)
    AX=C (J1) *E (J2) »E (I) » ('ZXF (-E (J1) *TBL) / ( (E (J2) -E (J1) M (? (I) -E (JD) ) *
   *E>P (-E<J2 ) *TBL) / ( (£ (Jl ) -E (J2 ) ) * (c (I)-r (J Z) ) ) (-F. (I >*TBl) / I (E (Ji
   I)-E'       (I)) ME (J2) -£ (!) ) ) )
    AY = C (J2) »CC) * (EXF (-F (J2) «TEL) -E:XP (-; (I) 'T5L) ) / (E (J) -r (J2>)
    AZ = C (I) *c>P (- £ ( I ) *T? L)
    C (I) = A X *A 1 + AZ
    1 F (C (I) .LT . 1. CE-2 (o) C (I) = 1.0E-2C0
414 CCM IMF
    DC 4 1 6 1= 1, NNUCL
    IF (NH (I) .EQ.2 ) GC TO 4 1 7
    GC TC 416
417 J4 = NF1 ( 1)
    C (I) =C ( I) *EXP (-E (I ) *T?L) *C (J4) *E (I) * Vi X? <-E ( J 4 ) *TEL (-E ( I ) *T5L
   S) ) / (t (I ) -E (J4 ) )
    IF (C (I ) .LT . 1 , OE-2 CO) C (I) = 1.0E-200
416 CCM3NUE
    DC 18 1= 1, NNUCL
    IF (NH (I) .EQ .l> GC TO M1 ?
    GC TC 418
419 C (I) =C ( I) *E XP <-E (I ) * T 3 L )
    IF (C (I ) .LT . 1 . OE-2 00) C ( I ) = 1 . OE-2 00
418 CCM INLF.
    DC 4 62 I-=1, NNUCL
    I F (N H (I ) . EQ .4 ) GC TO V i i
    GC TC 462
461 J 5 = N F1 ( I)
    C (I) =C (J5 )
    I F (C (I ) .LT . 1 . Gfc. -2 CO) C (I > = 1 . GE-20 0
462 CCM2NUE
    WRITE (6 , 2 05 )
2 05 FCRMAT (// , f MJ*Efc; F * , 2 X , * f L C L ICC* , 2 X, * HE M 9F F * , 2X , * H . A L F-L IPE (YF ) t, 2>
   I, /SORPTION CONSTANTS/ .2>, *  HFC (CI/M* »3)   * » 2/ , / INITIAL ACTIVITY
   S (CI) * , 2>, /ATENL'ATICN FACTCR (1/Y~) / )
    DC 3 0 1=1 .NNUCL
    WRITE (6 , 2 (6 >NN ( I ) , NUCL ( I ) , NH ( I ) , HFLV ( I ) , KO ( I ) , TCX« I ) , C { I ) , A r ( I )
20 6 FCRMAT (3X,I2,4X,Afc,5> , 12, ;X,1FES .2,9<,1' EP .?, 10X , l°cB .2,13X,l>-"Ee .2
   f, 33X , 1FE s .2 )
 30 CONTINUE
    T = T0 / DEL2
    DC 411 J127=1,M2
    T=T*CEL2
    V K = V C/DEL3
    DC 412 J27=l,*3
    VW=VW*CEL3
    Z = Z0 /DELI
    DC 650 Jl23=1,hl
    Z = Z *CE L1
    DC 11 1=1 , NNUCL
 11 VK (I) = VW / KD ( I)

        E VALLATE THE F XTRE HUH C F THE FIRST MC" E L J

    DC 4 C 1=1 , NNUCL
```

```
    GC TC 40
500 THAX (I ) = Z / V < { I)
    MFTHCD( I)=*E#
    NKAX(I}=t>P(-LAHECA(I)»TNAX(I))
    OPAX(I)=NNAX(I)«C(I)/(T*TCX(I))
    TI HE (I)=T
 40 CCHTIKLE

       EVALUATE THE f XTFF HUH CF THE SECOND MEFBER

    DC 50 I=i,NNUCL
    IF (NH (I ) .EC .2 > GC 10 6C0
    GC Tc 50
600 J=NP1(I>
    CALL AFFOX2 (I ,Z ,T thHAX,CHAX.THAX,TI1i ,N'1.LAHECA ,C, \<K.TCX,fETHCC)
 50 C C M INL'E

       E VALLATE 7HE t XTRE HUH CF THE THIRD HE KEEP

    DC 6 C 1 = 1 ,NhUCL
    IF(NH(I).EQ.3) GC TO 11C&
    GC TC 60
100 J1=NF2(I)
    J2 = NP1 { 1)
    J3=I
    V C1)=VK (J 1J
    V (2) =VK U 2 )
    V (3) =VK (J3)
    AlrLAMECA (J 2) -L AH EDA ( J 3)
    A2 = LAHECA IJ3) -LAHECA(Jl)
    A3 = LAHECA ( Ji) -LAHECA ( J2)
    0 = 1. / (V (1 )*Ai»V<2)*A£*V<3MA3)
    AL(1,3)=A2/ (V (3 ) -V (1 ) )
    A L (2 ,3 )=A 1/ (V (2 i-V (3 ))
    AL (1.2>=A3/ (V (1 )-V (2 ) )
    A L(3,i)=AL(1,3)
    AL (3,2)=AL ( 2, 3)
    AL (2 ,1 ) =AL (It 2)
    EE(1.3) = (LAHECA(Jl)*V(3)-LAr'ECA(J3)*V(l))/(V(3)-V(l))
    BE(2,3) = (LAH6CA(J2)*V(3)-LAHeCA(J3)»V(2))/(V(3)-V(2))
    8E(1,2)=(LAHB0A(J1)*V(2)-LA^ECA(J2)*V(1))/(V(2)-V(1))
    BE (3,1)=EE(1,3)
    BE (2,1)=BE(1,2)
    BE (3,2>=8fc <2* 3)

       EVALUATE THE FLNCTICNS S2 (I, J ) AND VZ (I)

    IF (V (1 ) ,LT . V( 25 ) GC TC ICE
    IF (V (2) .GT.V(3) ) GC TC 104
    S2(1.3)=0
    S2(2,3)=-l
    Sc (1 ,2) =1
    IF (V (1 ) .GT , V( ?) ) GC TO 1C 3
    VZ (1 )=V (2 )
    VZ (2 ) = V (1 )
    VZ (3 ) = V (3 )
    NF=3
    N !>=!
    NS = 2
    S3 (1 .3) =-1
    S3 (2 , 3 ) = - 1
```

```
GC  TC  IOS
VZ (1 ) = V (2 )
VZ (2 ) = V (3 )
VZ (3 ) = V (1 )
N Fr 1
N h = 2
KS = 2
S3  (1 , 3 ) = 1
S3 (2 . 3 ) = G
S2 ( l i2 ) = l
GC  TC  109
S2  (1» 3 ) = 1
S2 Í2 , 3 ) -1
S2  (1 , 2 >= 0
VZ (1> = V (3 )
VZ (2 ) = V (2 1
VZ (3 ) = V (1 )
NF = 1
Nt" = 2
NS = 3
S 3 (1 » 3 ) = 1
S3 ( 2 , 3 ) = 0
S3 ( l , 2 ) = í
GC  TC  103
IF (V (1 ) .LT .V( 3) )  GC TC  10 6
52  (1 , 3 ) = 1
32  52 . 3 ) = 1
S2 ( i  .25 = 0
V Z (i ) = V (3 )
VZ (2 ) = V (1 )
VZ (3 ) = V (2 )
NF = 2
N f- = l
NS = 3
53  (1 , 3 ) = 0
S3  (2 , 3 ) = 1
S3  (1 , 2 ) = - l
GC  TC  108
52  (1 » 3 ) = - l
S2 ( 2 , 3 ) = 0
S2 ( 1t 2 ) = - 1
I F (V (2 ) , GT • V ( 3) )  CC TC  1C 7
VZ (1 ) = V (1 )
VZ (2 ) = V (2 )
VZ (3 ) = V (3 )
NF = 3
NF = 2
NS = 1
S  3 ( 1 , 3 ) = - 1
53  (2 , 3 ) = - J
S3  (1 , 2 ) s 0
GC  TC  108
VZ (1 ) = V (1 )
V Z (2 ) = V (3 )
VZ (3 ) = V (2 )
NF = 2
N h = 3
NS = 1
S3 ( 1 , 3 ) s 0
S3  (2 , 3 ) = 1
S3  (1 . 2 ) = - l
CALL  A P R O 3  (I « Z . T . C . N ^ AV .  rfAX . T '- IAX . TIVF» VZ . S3 , S2 . NF , Nr - , NS . AL . LAHE 0
```

```
   $A,C.V,VK,TC>,SE,Ji.J2,J3,fc.Tr-CD1
 60  CCNTINLE

        EVALUATE- THE CCSE FCF- THE KUCLICIS IN S £ C U L A F EOUILIEFL I'

     DC 7C I = 1,NNUCL
     IF (NF<I>,EG.41GCTC1600
     GC TC 70
300 J=NP1(I)
     RATIC=VK(J)/VK(I)
     IF (NH(J).E0.2 ) GC TC 1601
     IF INHJ1.EC3 ) GO TO 16C2
     NrAX(I)=NNAX(J)«C(J>*VK(I)/(C<I)*VK(J>)
     GC TC 1603
501  J2=NF1(J?
     NNAX (I)=NHAX(J) *LAMEDA (J)*C<J2)/(0(I)*LAMGDA (J2)*KATIC)
     GC TC 1603
602  J3=NF2(J)
     NHAX(I)=NNAX(J)*LAMECA(J)«C(J3)/(C(I>»LAMEQA(J3)*FA7IC)
603  THAX(I)=THAY(J)
     0HAX(I)=NNAX. (I)*C(I)/(7*TcX(I))
     T1HE(I)=TIME(J)
     METHOD (I) =METHOC (J )
 70  CCNTINLE
     TCTAL=0.
     DC 90 I=1,NNUCL
 90  TCTAUTCTf LONAX (I)
     DC 91 1 = 1 ,NNUCL
 91  FRDCSE(I)=(CMAX(I)/TOTAL)M0C.
     WRITE(6 ,2 (2)
202 FCRMAT (1H1»6X,tLEACHTIHE(Y-.. ) t,3X,*PAIHLENGHT(M) i,3X,tWATE«?V
    SELCCITY  1f/YR)*)
     WRITE (6,2(3)T,Z,Vfc
203 FCRHAT(8X,1PE12.«t,9X,1PE12.4 ,EX,!Ptl2.4)
     WRITE (6 ,2 17 )
20 7   FCRMAT(lHQ»*NC«*t2X,*NUCL3CE*»3X,<HEM3ER*t3X»<lST*»3X,*2NC#,3X«*7I
    3HEOFPEAK(YF)*,3X,*HAXIHUNN/NCt,3X,*KAT.0IL.(M**3/CW*Yc**25*,3X
    S* *CONTAN.TIHE (YR ) * )
     DC 8 0 1=1 .NNUCL
 80  WRITE(6,2(9)NN(I),NUCL(:),NH(I),N"1(H,NP2(I),THA>(I),HVAX(I),CMA>
    <(I),TIHE(2)
209  FCRHAT(IX,I2,3X,A6,6>,I2,7X,I2,«X,I2,7X,lPE3.2,9X,LPR*.2,13y,lFEe.
    J2,14X,IFFc.2,7X,CFF6.3,EX,¿1)
650  CCNT INUt
412  CCNT INL'E
411  CONTINUE
413  CCNT IMF
     STOP
     ENC
     SUBROUTINE  APrtGXZn.Z.T.NHAX.CMAX.TMAX.TIHF.NPiiLAMenA.CIVK.TOX.N-
    STFCD)
     DINENSICN Hf.THCC (100 )
     DIHENSICN TMAX ( 1GG),TIME (100),O^AX(13G),NPl(10C) ,C(10C),V<(100) ,TC
    $X (100)
     REAL NH.AX (100 ), LAHECA (ICC )
     METHCO ( 11 - tA*
     A=LAHECA(I>/VK(I)
     J=NP1(I )
     C1=C (I)/LAMEDA(I)
     C2=C(JI/LAKBOA1J)
     3=LAHECA(J)/VK(J)
     TC i\v fT\ rr w*/ t\\ rn TO T O
```

```
     If(A.GT.B)  GO  TC  7QC                                                -
     THAX (I ) = Z/VK(I)
     NNAX (I) = (C1/C2+LAHECA(J)M*VK(I)/A3S(V<(J)-VK<I) ) ) *EXr(-A*Z)
     GC  TC  7 01
7C0  B 12= A 85 (LAMED A( J5*VK (I) / < VK (I)-VK (J) ) )
     Q1 = ALCG (( C1+C2*T*E12) t(C2*T*E12n
     Q2=B-A
     QQ=Q1/Q2
     IF (Z .GE.QC)  GC  TC  711
     THAX  (IU2/VKCI)
     NhAX(I)=(Ci/C2*LAr'ECMJ)*T*VK(I)/A9S(V<(J)-VK(I)))*EXt'(-A*Z)
     GC  TC  701
711  THAX (I) = Z/VK(J)
     H2 = 0 .
     H2T=0.
     IF (VK (I )* 2/VK (J ) . C-E. Z>  F2 = l.
     IF (VK(I )* (Z/VK(J)-T) .GE.Z )  H2T=1 .
     NhAX(I)=(Cl/C2)*EXF(-LANECA(I)*Z/V<(I))'(H2-H2T)*T»E12*EX-(-LAfECA
    $(J)*2/VK(J))
     GC  TC  701
712  TT=2*Z/VK «1 )
     hNAX (I ) = < C1/C2) *EXP( -LAHECA (I )*TT> * (LAM3CA (J ) / (LAMBCA (I ) -LAh ECA (J)
    S) )* (EXF (-LAMBDA (J ) )*TT-EXF (-LAM3DA (I )*TT ) )
     THAX  (I)=TT
701  DHAX  (I)=NHAX(I)*LAHEDA(I)*C(J)/(T*TOX(I)*LAMECA(J))
     IF (C (D/TCX (I ).LT.0.1)  GC  TC  62 5
     IF (VK (I KLT . VMJ ) )  GO  TC  627
     IF (Z/VK (J J-Z/VK C ).GT.T)  GC  TC  626
     TI HE (I)=T
     GC  T C  625
625  TIHt(I) = Z/VK(J)-Z/VKC)
     GC  TC  625
627  T1 HE (I) = Z/VK( I )-Z /VK(J)*T
     GC  TC  625
628  TIHE (I)sAES (Z/VK (I) - Z / VK (J))
625  RETURN
     E NC
     SLEROUTINE  APFCX3 (I,Z,T.C . NHAX.O MAX,T HAX,TIHE,VZ ,S3 »S2,NF,NH ,NS,AL
    J,LAMEDA,C,V,VK,TC>,E£,J1,J2,J3,ME-TH0D)
     D I HE NSICN  METHCC(IOG)
     DINENSICN  AL(3,3),C(lC0),V(3),VK(lGG),TOX(lG0),tf;{3,3>
     D IHF HSICN  T IMl (1CC),C"AX(1CG),TMAX(1CQ),V7(3>
     REAL  NHAX (100),LAHBCA (100 )
     IMEGfc R  S3 (3, 3) ,S2 (3,3)
     A23(Z,T)=-AL(2,3)*Z-BF(2,3)»T
     A13(Z,T)=-AL(1,3)*Z-3E(1,3)*T
     A12(Z,T) = -AL(l,2)*Z~er<l,2)*T
     Bl = C (J2 )* L AH8 CA (J1) / (C (Jl )* LA HBO A (J2) )
     3=LAH8CA(J2)»T*3i*V(3)/(V(2)-V(3))
     A=IAHBCA(J2)*T*V(3)*D*LAMEDA(J1>
     ME T H CD(I)=*A<
     W1 = 8*BE (2 ,3 ) / (A* (EE (NH,NF) -BE (NF,NS) ) )
     W2 = B'BL (2 ,3 )/ (A* ( Ft ( NM , NS ) -EF (NF , NS) M

        EXTRE HU N  IN  REGION  1

     T L=Z/VZ (3 )
     TR = Z/VZ (2 )
     X2=Z*(AL(HH,NF)-AL(NF,NS))
     X3 = EE (NH,NF J-BE (NF ,NS)
     IF (VK(J1) .EQ.VZ (3 ))  GC  TC  33C
     r £ M / L/ / i 4 \  tr r  11"7 # «- » *  l- r~  f f  -t -i *
```

```
XH=i.o-e/ß
X4= XK*EFUM»NF>/EfC (NF.NS)
    (X4.LT.C») GC TC 312
X1=ALGG (X4)
TT= (X1-X2 1/X3
IF(Wl.GE.1.3) GO TC 332
IF (TT.LE.TP) GO TC 333
T1rZ/V2(2)
GC TC 334
IF (TT.GE.TL) GO TC 335
T1=Z/VZ (2)
GC TC 334
T1=TT
GC TC 334
T1=Z/VZ(3)
GC TC 334
XH=A/(A-e)
X4=Xh*EE(NH,NF)/EE(NF,NS)
IF (X4.LT.0.) GC TC 312
Xl=ALOG (X4)
TT= (X1-X2 )/X3
IF (W1.LE.-1.0) GC TC 336
IF(TT.LE.TP) GO TC 337
T1=Z/VZ (2)
GC TC 334
IF (TT.GE.TL) GO TC 33«.
T1=Z/VZ(2S
GC TC 334
T1=TT
GC TC 33U
T1=2/y2 (53
GC TC 331.
Xh=1.0
X4=Xf*eL(Nf,NF)/E6 (NF.NS)
IF (Xi..LT.C.) GO TC 312
X1=ALCG(Xi)
TT= (»EX2 1/X3
IF (TT.LE.TR) GC TC 311
T1=Z/VZ(2)
GC TC 334
IF (TT.GL.TL) GC TC 333
T1=Z/VZ Í2)
GC TC 334
T1=TT
X2 3=A23(Z,T1)*AGS(S3(2,3))
X13=A13(Z.T1)*IA9£(S3<1,3))
X12=A12(Z,71)*IAES(S3(1,2))

CCNC1=(E-A)*EXP(X23)*S3(2i3) 4A»f.XP(XI3)*S3(1,3)-A*EXP(XI25*S3(1,2)

 EXTREMLM IN FEGICN 2

TL=Z/VZ(2)
TR=Z/VZ(1)
Y2=Z•(AL(KM,NS)-AL(NF,NS))
Y3=BE(Nh,NS)-9E(KF•NS)
IF (VK(Jl) .EC.VZ (3)) GC TC 3~C
IF (VK(J1) »EG.VZ (2)) GC TC 341
Yf=1.C
Y4=Yf*EL(NM»NS)/Er(NF,NS)
IF {Y4 • LT «C.) GO TC 411
Y1=ALOG(Yfc)
T T = (vi vx
```

```
      IF (T7.IF.TF.)  GC  TC  342
411   T2= Z/VZ (2 )
      GC  TC  3*3
342   IF(TT.GE.TL)  GC  TC  34^
      T2=Z/VZ (2 )
      GC  TC  343
344   T2=TT
      GC  TC  343
341   YN" = A/(A -9 )
      Y4 = YN**6E ( NM ,N S) / EE (N'FiNS )
      IF (YU.LT .0.5  GC  TC  411
      Y1 = A LCG<Y4)
      TT= ı Y1-Y2 )/Y3
      IF(W2 . L E . -1 .0 )  GC  TO  345
      I F (TT.LE.TR)  GO  TC  346
      T2= Z/VZ (2 )
      GC  TC  343
346   IF (TT.GE.TL)  GO  TC  3 47
      T2=Z/VZ (2 )
      GC  TC  343
347   T2=TT
      GC  TC  343
345   T2=Z/VZ (1 1
      GC  TC  343
340   Y H = 1 ,0 - E / A
      Y4=YN*B6 (KM,N S) / E E (N F , NS )
      IF (Y 4.L T.C.)  GC  TC  411
      Y 1=A LOG (Y4)
      T T = (Y1-V2 J/Y3
      IF (W2.GF . 1. 0)  GC  TC  35 Q
      IF (TT.LE.TK)  GC  TC  351
      T2 = Z/VZ (2 !
      GC  TC  343
351   IF (TT.GE.TL)  GO       352
      T 2= Z/VZ (2 )
      GC  TC  3 43
352   T2 = TT
      GC  TC  3 43
350   T2=Z/VZ (1 )
343   Y 23=A23 (Z ,125 *I AES (S 2(2 ,3 Ï )
      Y 13= A13 (7 ,T2) *IAE5 (S 2 (1 ,3 ) )
      Y 1 2 = A 1 2 ( Z , T 2 > M A E S ( S 2 ( : , 2 ) >
      C C N C 2 = ( E - A ) * E > P ( Y 2 3 > * S 2 ( 2 , 3 ) * A * E X P ( Y 1 3 ) » 3 2 ( 1 , 3 ) - A » E X P ( Y 1 2 ) * £ 2 ( 1 , 2 )
      IF(CCNC1.GT.COKC-2>  GO  TC  4 73
      CCNC=CONC 2
      TN=T 2
      GC  TC  483
«73   CCNC=CC NC1
      TN=T1
, e 3  T3=Z/VK (I )
      IF ÍVK (I ).£Q.V2(3 ) )GO  TC  491
      U2 3=A23(Z,T3í*IAES(S2(2,3))
      U13=A13(Z»T3)  *IAES(S2(1  .3))
      U12=A12(7,T3)*IAES(S2(1,2))
      XN=(E-A)»EyP(J2  3)*S2(2,3)+A*EXP(U13)*S2(1,3) - A*LXP(ü12)''S2 ( í ,2)
      GC  TC  492
»91   U2 3=A23(Z,T3)*IAES(S3(2,3))
      U 13= Al 3 (Z ,T 3) -IAES (S3 (1 ,3 ) )
      U12=AI2 (Z,T3) *IAES (S3 (1,2))
      X M= (E-A )* E X F(L2 3 ) * S3 (2,3) •A*EX"(Ui3)*?3 ( 1 ,3) - A    XP ( L 12 ) * S 3 (1,2)
»9 2    CCSC3=(C(J3)»LAfECA(JÍ)/(C(Jl)*LAK5DA(J3)))»EXF(-LAr'ECA(I)*T2^X»'
      IF(CCNC.GT.CO NC 3)  GC  TC  4 90
```

```
     NrAX (I ) =C CNC3
     T h AX (I ) =T 3
     GC TC 1500
490  N hAX (I ) =CCKC
     THAX (I)=T •
500  DHAX(I>=Nr-AX(I)*LAHeDA(I)«C(Jl>/(T*LA"9DA(Ji)'TCXII))
     IF (C (IJ/TCX (I ).LT . C C I) GC TC 523
     IF (VK(I ).EG.VZ(1) ) GC TC 525
     IF (VK (I ).£C .V Z (2 > ) GO TC 527
     IF(Z/VK (I UT.GT.Z/VZ (1 ) ) GC TC 526
     T I HE <I)=2/VZ(i) -7/VK (I )
     GC TC 4 05
526  Tiff (I)=T
     GC TC 40e
527  IF (Z/VK (I H T . C-T .2 /VZ (1 ) ) GC TC 525
     T1 HE (I) = 2/VZ(1)-Z/VZ(3)
     GC T C 406
525  T I HE II> = 2/VK(I)-Z/VZ(3)»T
     GC TC 406
528  TIHE (I) = Z/VZ(1)-Z/VZ(3)
4Q8  RETURN
     F KD
```

Appendix C. Description of the computer program UCRNE21

C.1 Subprogram HYDRO data input description

Subprogram HYDRO determines the streamlines of the contaminated region and evaluates the hydraulic conductivity and the water travel time along these streamlines for a two-dimensional groundwater flow. Hydraulic head distribution can be input either by analytical expressions or by measured field data.

Card 1: FORMAT(5F10.3).

Variable	Description
XMIN (Fl0.3)	Minimum abcissa of the region of interest (m).
XMAX (F10.3)	Maximum abcissa of the region of interest (m).
YMIN (F10.3)	Minimum ordinate of the region of interest (m).
YMAX (F10.3)	Maximum ordinate of the region of interest (m) .
DEL (F10.3)	Grid size in the x-direction and y-direction (m)

Card 2: FORMAT(5F10.3,110).

Variable	Description
XREP (F10.3)	Abcissa of the center of the repository arc (m).
YREP (F10.3)	Ordinate of the center of the repository arc (m)
RAD (F10.3)	Radius of the repository arc (m).
TETAI (F10.3)	Initial angle of the repository arc (radians) zero is the positive x axis, it is positive counterclockwise.

TETAF (F10.3) Final angle **of** the repository arc (radians). Same orientation as for TETAI.

NTETA (110) Number of streamlines to be considered on the **repository arc.**

Card 3: FORMAT(110,5F10.3). This card is required even if no point sinks or sources are being considered.

Variable Description

NW (110) Number of point sinks or point sources. NW=0 if no point sinks or sources are being considered.

VINFI (F10.3) Horizontal uniform flow velocity (m/yr). VINFI=0 if no uniform horizontal flow exist.

EPSILON (F10.3) Constant aquifer porosity.

THICK (F10.3) Thickness of the aquifer near the point sinks and sources.

COND (F10.3) Hydraulic conductivity (m/yr) for the point sinks and point sources system.

CONREP (F10.3) Hydraulic conductivity at the repository site.

Card 4 : FORMAT (3F10. 3) , one. card for each point sink/source. If NW=0, no cards 4 are required.

Variable Description

XP (F10.3) Abcissa of the point sink/source (m).

YP (F10.3) Ordinate of the point sink/source (m).

QS (F10.3) Flow rate of the point sink or source (m/yr).

Card 5: FORMAT(5F10.3), this card input the field

piezometric data, it is required at least 8 of these cards. It is not necessary to specify the number of these cards being input.

Variable	Description
XWORK (F10.35	Abcissa of the data location (m).
YWORK (F10.3)	Ordinate of the data location (m).
CONDX (F10.3)	Reserved for future use.
CONDY (F10.3)	Reserved for future use.
POT (F10.3)	Aquifer potential at the data point (meters above the mean sea level).

Comment: If no field data is being used, no cards 5 are required,

```
MA.368301,TING,0
MPUT  6200C  23.01.13   20  SEP  81   VIA  CR04                                  286
5=
SERPR
?Y, INPUT/RR.OUTPUT/RR.
5P0SE,CJTPUT=PR,PA=1F.
DGRAM UC8NE21  SUBPROGRAM  HYDRO
M I EL K.S. TING
GUST 1981
PAPTMENT OF NUCLEAR ENGINEERING
I VERS ITY OF CALIFCPNIA,BERKELEY
RKELEY,CA.,54720


 CONTROL CARDS LISTING **

OBCARD]
ASSW3RD ]
SERPR
F4.
THLIB.
TCHPS,SDL,ULIXjULIB.
NK»F=LGQ,P=ULI X,X•
• TAPE,TAPE11 = /TING/MAC2/EX PER IE , 3 748 2.
IT.
MP,0.
UMP.


 PF-D3RAM LISTING **

     PROGRAMMAC2 ( INPUT,OUTPUT,TAPE5^INPUT,TAPE 6 = OUTPUT , TAP Ell,FILM I
     LEVEL  2,XSTR,YSTR,TSTP,P0TEN,PSTR
     : QMMON/DUMMY/XSTR{50, 100 t,YSTR(50,100 »,TSTR!50,1 CO I,POTEN(1 00,100»
    S,PSTR150,ICO)
     LEVEL  2,C,XP,YT,NV,VINFI
     3DMM3N/SIG/Ol100),XP(100l,YTI100) ,NW,VINFI
     LEVEL  ?,CCNDX,CCNCY,EPS,POT
     CCMMIN/HYDRO/CONDX(200 ) ,CONDY(200I , EPS(200),PCT(200)
     LEVEL 2,DPX,DPY,XGR ID,YGRID,NX,NY» D P H I
     2OMM3N/0P/DPX{ICC ,10CJ ,DPY(100,100),XGRID(100I ,YGRID(100),NX,NY,DP
    SHI ( 100, 100 I
     LEVEL2,OX,CY
     3OMMIN/DE/DXC 10 0,100 8 rDYl100,100)
     0 1 MENS IGN Y{3),WCPKI21 ), IW0PK{10!
     3IMENSICN ARRWCRK(ICO, 100 J
     3 I MENS ICN XBDARR(IOC) , YBDARR{100)
     3DMM0N/DOT /XWORK ( 2 00 ) , YWORK ( 200) , DATWOP.K { 2 0 0) , I WKARP (1 0 0 0 »
     DIMENSION  YP{3 »,PY(3 )
     EXTERNAL F,DP C T
* * * *}EAD  DATA  INPUT        ********** t ****'****** ************
     RELERR-1.CE-6
     A8SERR = 1. OE-5
     NTAPE = I 1
     READ(5,IOC)  XMIN,>MAX,YMIN,YMAX,DEL
100 'CRM4T(5F10.3 )
     MX = INT ( (XMAX- XM IN I/DEL M )
     1 F I A MOD ( I XMAX-XMIN) .DELUGT.O. > NX = NX O
     XMAX = XM IN*CEL >MNX- 1 I
```

```
    \JY=INTUY*AX-YMIIU/DEL+T)
    IF (AMODI (YM4X-YMIN) ,DEL ) .GT. C• ) NY=NY *• I                    287
    YMAX=YMINtDEL+(NY- 1 »
    READ! 5, ICI) XREP,YREP,RAO,TETAI,T°TAF,NTETA
 01 FORMAT(5FIO.3,I1Cî
    READ(5,132) N>», V I NF I, EPSILON, THICK, CCND, CONREP
 02 FORMAT(I10.5F10.2 )
    I F(NW.LE.O I GO TC 10
    30 11 J-1 , NW
    READ(5,103S XP(J),YT(J ) ,CS
.03 FORMAT (3F10.3 •
 11 3 ( J ) - QS/( EPSI L CM THICK*6.2R32 )
 10 WRITE(NTAPE,112 I Xf I N, XMAx , YM îH , Ax , DLL , Nx , NY» NTETA
.12 FORMAT(IX,5E9.2,3 15 »
    NDATA=C
 14 I F(EOF{5)a N E» 0» ) GO TC 13
    NDATA=NCATA+1
    READ(5,107 I XWORK{NCATAJ, YWORK(N'OATA) , CONDX(NDATA) , CONDY(NDATAI, POT
   $(NDATA(
i 07 FORMAT !5F10.3 »
    GO TO 14
 13 0 EL X = DE LY = DEL
    NDATA=NDATA-l
    : ALL BGNGPD
    J JX=NX
    XM= XMIN
    XX=XMAX
    J JY-NY
    YM=YM I N
    YX=YMAX
    ;ALL SETGRCi J JX, X P«, XX, JJY, YM, YX)
 EVALUATES POTENTIAL FINCTION FOR A DISTRIBUTION OF SOURCES AND SINKS
    DO 50 JX=i , JJX
    XGRIDlJX) XM*OELX*(JX-1)
    PX=XGRIC(JX)
    DO 51 JY=1 , JJY
    YGR I D( J YÎ YP+DELY'UJY-1)
    PY( 1 I=YGPIC(JY )
    SUM=0.
    I F(NW.LE.C ) GG TC 25
    DO 52 JS=1,NW
    PAR=SQRT( (XGRIC(JXJ-XP(JS>)**2» (YGRI0(JY»-YT(JS))**2)
    IF(PAR.LEoC) GO TC 52
    SUM = SUM<• C ( JS »*ALCG(PAR »
 52 CONTINUE
 25 ³UTEN( JX, JY) = -VlNFl*XGRID( JX)-SU'4
    POTEN(JX, JY»^ PCTEMJX, JYl * EPS I LON / CON D
    I F ( Nw. LE. C ) GC TC 54
    CALL F(PX,FY,YP)
    DX(JX, JY»=-1./YPÎ 2)
    DY(JX,JY)=-YP(1)/Y P(2 I
    3X(JX,JYl=DX(JX,JY)*EPSILON/COND
    DY ( JX,JY)=CY(JX,J\)*EPSIL0N/C0ND
    GO TO 51
 54 D X(JX t JY i = C.
    DY(JX,JY)=C.
 51 CONTINUE
 50 CONTINUE
    IF(NDATi.LE.O ! GC TO 26
    30 24 ICATA=1 , NCATA
 24 DATWORKÎ I CATAl-PCTtICATA)
    lALLCLCGPDt XWORK,VWORK ,DATWORK,ND AT A, ARRWORK,100 ,100, IWKAPP,1 0000)
```

```
   :ALL  CLCBNC(XrfORK ,YWORK,CAT WORK,NDATA,i,100,XBDARR,YBDARR,INMBND»
   CALLCLCPLMXBDAPP,YBDARR,INMBND,1,-999999.,APPWQRK,100,100>
   IALL  DERI V(APRWORK)                                                  288
   I ALL  DERI2(ARRWCPK,DPH I,XGRID,YGRID, NX , NY)
   GO  TO  53
26 DC  27  JX=i,JJX
   DO  28  JY=1,JJY
   ARRWORK(JX,JY>=0.
   DPHI(JX,JY)=0.
   DPX(JX,JY »-0.
   DPY(JX,JY)=0.
28 CONTINUE
27 CONTINUE
53 DC  69  MX=1,NX
   DO  61  MY-1,NY
   POTEN(MX,MYI=APRVCRK(MX,MY)+PnTEN(Mx,VY)
   DPX(MX,MY J=DPX(MX,HY)+DXIKX,MY>
   DPY(MX,MY»^DPY(VX,VY)•DY(MX,MY)
61 CONTINUE
69 CONTINUE
   3ELTA= (TETAF-TETAI)/(NTETA-1)
   DD  55  LX=1,NX
   DO  56  LY=1, NY
   WRITE(NTAPE,111)  FCTEN(LX,LY)
11 F0RMAT(1X,E13.5)
56 CONTINUE
55 CONTINUE
   WRITE(6,12?l
.22 FORMAT(IH1,*  *** PCTENTI AL FUNCTION MATRIX (METERS ABOVE MEAN SEA
  SLEVEL I ****I
   CALL  WRITER(PCTEN,NX,NY,XGRID,YGR!D»
   WRITE(6,123)
.22 FORMAT(lHi,*  *  *  < POTENTIAL GRADIENT IN THE X DIRECTION *****
   CALL  WRITER(DPX,NX,NY,XGR ID,YGRID )
   wRITE(6,124 )
.24 FORMAT(1H1,*  *** POTENTIAL GRADIENT IN THE Y DIRECTION ****>
   CALL  WRITER(OPY,NX,NY,XGRID,YGRID !
   DETERMINATION OF TFE SHADOW REGION
   DO 33 NT=l,NT ETA
   IETA=TETAI+<NT-1MDELTA
   XR=XREP»RAD*CCS(TETA>
   yR=YREP*-RAD*S IN IT ETA j
   NINI=0
   DO 34 NS=1,NX
   IF(XGRICINSJ.LT.XP)  GO TO 34
   NINI =NS
   GO TO 70
34 CONTINUE
70 IF(N INI.EC.l ) GC TC 71
   IF(NINI,FC.O» N I N 1= NX
   X=XR
   Y(I )=YR
   Y(2)=ALCG(CCNREP)
   Y(3>=0.
   DO 72 I N=1,N I N I- 1
   XOP=XGR IDIMNl-l >-DEL* ( 1N-1 )
   IFL AG=1
   NEQ- 3
   C ALL RKF(DFOT,NEC,Y,X,XOP,RELERR, ABSE PR, IF LAG,WORK,IWORK}
   XS TR (NT ,N IN I- IM =*CP
   YSTR(NT,NIM-IN)=V (1 )                ,'t'- -
   PSTR(NT,NIM-IN1 = EXP(Y(2M             I
```

```
      TSTRINT,NIM-IM y(3i
     X=XOP
      IF(Y(3».LT.0. > TSTP(NT,NINI- INi=0.
      IF(Y(1).GT«,YMAX) GC TO 73
      IF(Yd).LT.YMIN) GC TO 74
      GO TO 72
75    YSTRINT,NIM-IN > OMAX
      rSTP(NT,NIM-IN)=C.
      30 TO 72
74    YSTR(NT,NIM-IN)=tVIN
      TSTR(NT,NïM-  ÎN»=C
72    CONTINUE
      DD 44 IX=1,NIM-1
      KX-NINI-LX
      IF(KX.FC. I) GC TO 44
      DS=TSTR(NT,KX»-T$TR(NT,KX-1 I
      IF(DS.GE.0.I GC TC 45
      3D TO 44
45    DO 43 MX=1,KX
      XSTRINT,MX)=XSTRlM,KX)
      YSTP(NT,MX)=Y STR(NT,KX >
      PSTR(NT,MXl = PSTR(NT» KX !
      TSTR(NT,MX»=TSTR(NT,KX>
43    CONTINUE
      GO TO 71
44    CONTINUE
71    X=XR
      Y(1)=YR
      Y Í 2)=ALCG(CCNREP)
      Y(3 > =0.
      DO75ÎN=NINI,NX
      XCP=XGP ID(N IN I)«-CEL*(IN-NINI J
      I FLAG=1
      MEQ=3
      CALL    RKFIDPCT,NEC,Y,X,XOP,RELERR,ABSERR,IF LAG,WORK,I WORK »
      XSTRINT,INí-XCP
      YSTR(NT,INi=Y(ll
      PSTR(NT,IN)=EXPlY(2) )
      TSTR(NT,IN)-Y(3 I
      I F(Y(3).LT.O. ) TSTR(NT,IN) = 0.
      IF (Y(1»•GT.YMAXl CC TO 76
      IF(Y(1)•IT•YMIN) GC TO 77
      GO TO 75
75    YSTRINT, IM-YM.AX
      TSTR(NT,IN)=0.
      GO TO 75
77    YSTRÎNT,ÏM=Y*IK
      TSTR(NT, IN 5=0.
      X=XOP
75    CONTINUE
      DO 41 LX=NINI,IX
      IF(LX.EC.MNI GO TO 41
      DS=TSTR(NT,LXI-T!1P(NT,LX-1)
      IFIDS.LE.O. » GC TC 42
      30 TO 41
42    3D 46 MX=LX,NX
      XSTRINT,MXi=XSTR(NT,LX I
      YSTR(NT,MX)=YSTR(NT,LX)
      PSTR(NT,MX ! = PSTR(NT,LX )
      TSTP(NT,MX)-TSTR(NT,LX)
46    CONTINUE
      GO TO 33
```

```
41  CONTINUE
33  CONTINUE                                                                290
    OC 62 Nl=ltNTETA
    TE TA= TE TA I +CELTA* (M-l )
    ANGLE=(TETA*180. 1/3.14 16
    kRITE(6,108)   M, ANGLE
.08 =DRMAT(1H1,11X,*STREAMLINE NO.*,I4,3X,*ûNGLE IN REPOSITORY IS*,F10
   S.3,*  DEGREES* I
    rfRITE(6,125)
.25  CRMAT(IX,*NX*,5X,*X-(VETFRS>*,5X,*Y-{METFPSI *,5X,*TRAVEL  TIME  (YR
   il*,3X,<CQKDUCTi\/1TY (M/YRl*I
    DO 65 N2=l»NX
    WRI TE (NTA»E,1 16 > XSTP (N 1,N2 » .VSTRI NI ,N2l , Î'S TR( NI , N2 >
.16 FORMAT(IX» 3E13.5 í
    WRITE(6,110)  N2,XSTR(N1.N2) «YSTR(M,N?»,ISTR(NI,N21,PSTR(NI,N2 >
.10 FORMAT(IX,14,3X,4(1PE13.6,3X>>
65  CONTINUE
62  CONTINUE
    CALL  ENCGRC
    STOP
    END
    SUBROUTINE DERIV(M

    THIS VERSICN OF CERÏV EVALUATES THE PARTIAL DERIVATIVES USING A
   CENTRAL DIFFERENCE APPROXIMATION Ahi AY FROM THF BOUNDARY


    LEVEL 2,DP>,0PY,XGRID,YGPID,NX,NY,DPHI
    CÛMMON/OP/DPX{10C,1CC»,DPY(100,100»,XGRID?100J,YGR10(100t,NX,NY,DP
   $3I(100,100!
    DIMENSION  M ICO, ICO)
    DELX=(XGRIC(NXi-XCFID(1»!/{NX-D
    DELY=(>GRIC(NY)-YGFIC(1))/(NY-1)
    DO 10 LX=1,NX
    30  20  LY= 1,NY
    M2=LX+1
    M1=LX-1
    M2^LY+l
    N1=LY~1
    3=2.*DELX
    IFILX.EC.1) M1=LX
    IF(LX.EC.Î) D=DELX
    IFILX.EC.NXI  M?" LX
    IF (LX.EC.NXI  C=DELX
    IF(LY.EC.1» Nl=LY
    ÎF(LY.EC.NY)  N2=LY
    IF(LY.EC.1) D=DELX
    IF{LY.EC.NY) C=DFLY
    DPX(LX,LY)=(A(M2,LY)-A(M1,LY))/D
    DPY(LX,LY)=(A(LX,N2)-A(LX,N1))/D
20  CONTINUE
10  CONTINUE
    RETURN
    END
    SUBROUTINE DER12(«,DPH!,XGRID,YGR!D»NX,NYI
    LEVEL  2,DPHI,XGRIC,YGRID,NX,NY
    DIMENSION A(1C0,1C0),XGRID(100),YGRID(100),DPHI(100,1001
    DELX=(XGRIC(NX)-XGFIC(Il i/(NX-1>
    OELY--(YGRID(NY)-YGFID(1))/ÎNY-I)
    DO 10 LX=1,NX
    DC20LY=l,NY
    M2-LX+1
```

```
      H1»LX-1
      N2=LY«-1

      IFUX.EQ.lJ  M1=LX
      IF(LX.EC.NX»  M2=LX
      IF(LY.EC.1)N1=Ly
      IFUY.EC.NYI  N2=LY
      PXMMM2,LY>-2.*MLX,LY)4&(M1,LY))/(3ELX**2.I
      PY=(A(LX,N2)-?.*A(LX,LY)+A(LX,N1>  )/(DELY** 2.)
      3PH1(LX,LYi=PX*PY
   20 CONTINUE
   10 CONTINUE
      RETURN
      END
      SUBROUTINE  DPCTt X,Y,YP )
      LEVEL  2,DPX,DPY,XGRIC,YGRI 0.NX,NY , O^HI
      COMMJN/OP/CPX(100 ,100 ) ,DPY(100,100),XGRID( 100) ,YGR ID(100) ,NX,NY,DP
     SHI(100,100)
      DIMENSION  Y(3 >,YP(3 )
      NS=NX
      DO  10  I X=1,NX
      IF(XGRIDl IX).GE.X )  N S= IX
      IF(XGRIC( IX).GE.X)  GO  TO  40
   10 CONTINUE
   40 NG=NY
      DO  20  IY=1,NY
      I F(YGR I C(IY».GE.Y(1>iNG'IY
      IF(YGRIC(IY).GE.Y(l)I  GO  TO  30
   20 CONTINUE
   30 IF(NG.EC.1I GC TC 50
      A=DPY(NS,NG)-CFY(\S,NG-?.)
      3=(Y(1l-YGR ID(NC-1) )/(YGRID(NGI-YGRID(NG-1 )I
      DPDY=A*8+CPYf NS,NG-1 !
      C=DPX(NS,NG)-CPX(NS,NG-1)
      DPDX=C*E*DPX(NS,NG-1>
      GO  TQ  6C
   50 D PDY=DPY(NS,NG I
      DPDX=DPX(NS,NG>
   60 IF(DPDX.EC.O. )  D PDX=1.OF-290
      rPl1)=DPDY/DPDX
      YP(2»=-CPHI(NS,NCl/DPDX
      I F(Y(2).GT.730.)  GC TO 77
      VX=DPDX*FXF(Y(2)}
   77 I Ft Y(2».GT.73C.)  vX=I.OE-290
      IF (VX.EC.C.)  VX=1.0E-290
      YP (3 )=- l./VX
      RETURN
      END
      SUBROUTINE  WRITER(A,NX ,NY,B,C>
      LEVEL 2,A,B,C ,NX , hY
      DIMENSION  M100.100I,B(100),C(100)
      ARG=NX/11.
      SIPAGE=I M ( ARG )
      IF(AMOC(FLCAT(NX»,ll.).GT.O.)NPAGE=NPAGE+1
      DO  10  NP=i,NPAGE
      I F(NP.EC.1)WR I TE16,100)(B(I),I=1,MI NO(11,NX))
  100  F0RMAT(2X,//,IX,*>(METERJ*,2X,11(IPEIO.3,1Xa(
      LF I N  I NP-1)*1 1+10
      I F(N').GT.1)WR I TE(6,102)(B(I),1=(NP-1)*11,MINO(LF I N,NXU
  102  -ORMAT(lHl,*X(ME7ERi*,3X,ll(lPE10.3,lXM
      WPITE(6,1C3 )
  103 FORMAT(IX,*Y(METER I t )
```

```
    DO  20  LINE=1,NY
    IF(HP,GTo 1 )  GC  TC  2C                                          292
    rfRITE(6,101) C(L I N E ) ,( M J,LINE ) ,J = 1,M!NO(' 1,NXI )
    GO  TO  20
 30 1F i NP. EC. NPAGEUP HE (6 ,101 )C(LINE \ , (A ! J, LI NE) , J = ( NP-1 ) *11 ,NXI
    IF(N?.LT.NPAGEIWRITE(fc,101>C(LlNEI,(A(J,LINEf,J=(NP-li*ll,(NP-ii*i
   $1+10)
101 FORMAT ( IX , 12( 1PE10.3 , 1X) )
 20  CONTINUE
 10  CONTINUE
    RETURN
    END
    SUBROUTINE  F{ X,Y ,YP)
    LEVEL   2,C,XP,YT,Nh,VINFI
    CUMM3N/SIG/C(10C»,XP(1COl,YTt100i,NW,VINFI
    DIMENSION Y(3 ) ,YP 13 )
    SUM1=0.
    SUM2=0.
    DO  10  J«1,NV»
    A=(X-XP(J»I**2.KY(1)-YT(J))**2.
    IF{A.EQ.O.)  GC  TC  10
    SUM1 = SUM1HQ(J)*(X-XP(J)))/A
    SUM2=SUV2+(Q{JI*(Y(II-YT(JiII/A
 10  CONTINUE
    DX=-VINFI-SUM1
    DY=- SUM2
    YP{1 )=DY/CX
    YPC2j=-l./CX
    RETURN
    END
```

C.2 Subprogram PLOTMAC data input description

Subprogram PLOTMAC evaluates the concentration of the i-th member of a radioactive chain of arbitrary length along the streamlines of the contaminated region of the two-dimensional groundwater flow.

Card 1: FORMAT(2A10,F10.3)

Variable	Description
H0LL1 (A10)	Hollerith to be displayed in the graph.
HOLL2 (A10)	continuation of H0LL1.
POTPLOT (F10.3)	If less or equal to zero no graphs are generated only a printout. Otherwise a plot is produced.

Card 2: FORMAT(5F10.3,I10,F10.3)

Variable	Description
XREP (F10.3)	Abcissa of the center of the repository arc (m).
YREP (F10.3)	Ordinate of the center of the repositoty arc (m).
RAD (F10.3)	Radius of the repository arc (m).
TETAI (F10.3)	Initial angle of the repository arc. Zero is the positive x axis (radians), positive counterclock.
TETAF (F10.3)	Final angle of the repository arc (radians).
NTETA (I10)	Number of streamlines to be considered on the repository line.The streamlines are equaly spaced.
ANGNO (F10.3)	Angle between the north direction and the positive x axis.

Card 3: FORMAT(415,2F10.3). PLOTMAC allows the user to zoom in a region inside the original region of interest defined in HYDRO*i* producing an amplified view of a given part of the region of interest.

Variable	Description
NXPLMX (15)	Maximum grid number in x-direction to be shown in the plot.
NXPLMN (15)	Minimum grid number in x-direction to be shown in the plot.
NYPLMX (15)	Maximum grid number in y-direction to be shown in the plot.
NYPLMN (15)	Minimum grid number in y-direction to be shown in the plot.
SUMAX (F10.3)	Maximum value of the potential function (m).
SUMIN (F10.3)	Minimum value of the potential function (m).

Card 4: FORMAT(110,4F10.3). This card is equal to card 3 in HYDRO, see section C.1.

Card 5:FORMAT(3F10.3). These cards are equal to cards 4 in HYDRO, see section C.1.

Card 6: FORMAT(2(I10,2F10.3))

Variable	Description
NMEMBER (I10)	Number of members in the chain.
TLEACH (F10.3)	Leach time (years).

TBEGIN (F10.3) Delay time for beginning of leaching (years).

NTIME (110) Number of different time values after the leaching for which calculations are to be done.

TIMEO (F10.3) The first value of time to be used (years).

DTIME (F10.3) Multiplying factor for the NTIME cases of times to be evaluated:TIME=TIMEO*(DTIME)**K;K=1,..NTIME

Card 7 to Card (7+NMEMBER): FORMAT(A7,5F10.3),one of these cards are required for each member of the chain, the cards must be ordered as the chain is.

Variable	Description
NNUCL (A7)	Nuclide name (e.g. Ra-226).
THALF (F10.3)	Nuclide half life (years).
K (F10.3)	Nuclide retardation coefficient.
C (F10.3)	Nuclide total activity at the time of burial (yr).
RCG (F10.3)	Maximum Permissible Concentration (Ci/m^3).
GRAP (F10.3)	If GRAP is larger than zero a plot for this nuclide is produced, otherwise only the print-out of this nuclide concentration is generated.

Card 8+NMEMBER: FORMAT(2F10.3), these cards describe the biosphere by given a number of coordinates, any number of cards is accepttable. If biosphere is not to be shown in the plots no card is included in this section.

Variable	Description
XBIO (F10.3)	Abcissa of the biosphere coordinate (m).
YBIO (F10.3)	Ordinate of the biosphere coordinate (m).

Comment: The coordinates must be sequentially input.

```
 IA.368301,TING,0
 PUT  62J0C  23.27.27   2C  SEP  81   VIA CR04

IERPR
'Y,ISIPUT/RR,0UTPUT/RR.
-POSE,OUTPUT=PR,PA=.\F.

)GRAM  UCBNE21  SUBPROGRAM  PLOTMAC
JIEL  K. S.  TING
iUST  1981
'APTMENT  OF  NUCLEAR  ENGINEERING
! VERSITY  OF  CALIFCPNIA,BERKELEY
IKELEY.CA.,94720



 CONTROL  CARDS  LISTING  **

DBCARD1
ASS»I3RD ]
SERPR
' 4.
rCHPS,IDDS,ULIB,ULI8X.
rCHPS,GPACBN7,GPAC,VAEN.
TTAPE,TAPE11=/TING/MAC2/PUSTLE3,3   74   0 3 .
NK,F=LGO,F=GPAC,P=UL IB,X.
APHIC,FN=FILM,FT=VA»
IT.
1P.0.
JMP.



 PP 03 RAM  LISTING  **

      PROGRAM PLCTMAC ( INPUT, OUTPUT, TAPE5- INPUT, TAPE6-OUTPUT, TAPEU , FILMI
      COMMON/IG SZZZ/ZMCCE( 200)
      DOUBLE  SRPMX,SPPMN,TIE
      DIMENSION  XBIC(2C0),YBIO(2OO)
      JIMENSICN VEXI1),VEYl1),PLOT(40)
      DIMENSION ABST(20!,BACT(20I,ABSM(20!,3ACM(20i,ABSL(20i,BACH2Ot
      DIMENSION  XWELL(2C),YWELL(20),S(20)
      DIMENSION MAX(40),7fiX(20>
      DIMENSION  ZHAX(20i,ZMIN(20!,DIFFEUOO>
      DIMENSION  NN.UCK 2C) ,GR AP(2 0)
      COMMON/AN AME/XKAMEf 50 ?,YNAMF{5J!,TNAME(100 J,ZNAME(50)
      LEVEL 2,E, K,C,RCG,TvMEMBER, TLE&CH, TBF.G IN
      DOUBLE  THALF,K(20),E(2C),C12C)
      COMM,DN/CONC/N*EMBEF,TLEACH,TBEG IN,E,K,C,RCG(208
      LEVEL 2.XSTR,YSTR,TSTR
      COMMON/STREAM/XSTR(50, 100),YSTR(50,1CO), TSTR( 50, 100)
      LEVEL 2,POTEN
      COMMON/CUMMY/PCTEN(100,100)
      DIMENS IGN  XWORK(2C0 I ,YWORK(200I,DATWORK(?OOI,ARRWORK(1 00,100I
      SJTAPE=11
      READ(5,100)  HCLL1,H0LL2,P0TPL0T
100   FORMAT(2A10,F10.3)
      RE AD(5,120IXREP,YFEP,RAD,TE T A I,TETAF,NTETA,ANGNO
120   FORMAT(5F10.3,I 10,F10.3)
      READ(5,13 0 1 NXPLNX,NXPLMN,NYPLMX,NYPLMN,SUMAX,SUM IN
120   FORMAT(41 5,2F10. 3)
```

```
LIO FORMAT ( 11 0, 4F 1Q . 3 »
     IFINW.LE.C»  GC  TC  56
     DO  57  J = 1 » NW
     READ I 5 , 12 1 » XWELLÎ J ¡ , YwELL(J) , QS
121  FORMAT Î 3F 10» 3 )
 57  J(J I=QS/(EPSIL0N*ThlCK*6 . 2 822 >
 56 3 E A D I 51105 >NUMBER, T L E ACH, T B EG IN » NTI MF, T I MEO , D T I ME
105  FORMATI2( I 10,2F10.3) )
     30  12  1=1,NM£V8EP
     READ I 5,106 J NNUCL(I « » THAL F iK ( I ) , C íI ) ,RCG(I I , G P Ap( I)
106  FORMAT « A7,5F10.3 I
 12  E(i ) = DLCG(2.DOO I /TFALF
     READ(NT APE,112) XV IN,XMAX,YMIN,YMAX,0EL»NX,NY,NTETA
112  FORMAT(IX,5E9* 2,3 If)
     DO  10  LX=1,NX
     DO 11 L Y = I » N Y
     READÎNTAPF.,11 1 )  PCTEN I LX, L Y )
111  FORMAT(IX,E13.5 »
 11  CONTINUE
 10  CONTINUE
     DO  15  Nl=l,NTETA
     DO  16  N2= 1 ,NX
     READ(NTAPE,116t   XSTR(Nl,N2l,Y5TR(Nl,N2i,TSTR(Nl,N2>
116  FORMAT(lX,3E13.5 )
 16  CONTINUE
 15  CONTINUE
     SIDA TA = C
 14  I F(EOF(5 J.NE.O. )  GC  TO  17
     SIDATA-NCATA+1
     READ(5, 10 2 1  XBIOUCATA) ,YBIC(NDATA)
102  FORMAT I2F10.3»
     3 0  TO  14
 17  XV.AX = XMINMNXFLMX - 1J*DEL
     XMIN=XMINf(NXPLMN-1»*DEL
     XMAX^ XV AX-XMIN
     XREP = XP EP-XMIN
     X TRANS = XM IN
     XMIN=0.
     YMAX = YMINKNYPLMX - 1 )*DEL
     YMIN=YMIN+ (NYPLMN- 1 >*D EL
     YMAX=YMAX-YMIN
     YREP = YREP- YMIN
     VTRANS=YMIN
     YMIN=0.
     NDAT A=NC ATA- 1
     3D  20  JX--NXPLMN,NXPLMX
     DD  21  JY=NYPL*N,NYFLMX
     MX-JX-NXPLMN*1
     MY=JY-NVPtMN*1
     POTEN(MX,MYI=POTEN(JX,JY»
 21  CONTINUE
 20  CONTINUE
     DC 22  MET A = 1,NTETA
     DO  23  IX=KXPLMN,NXPLMX
     MX =IX-NXPLMN*1
     XSTR(META,MXl=XSTR(META,IX»-XTRANS
     rSTR(META,MX)=YSlF(META,IXI-YTRANS
     TSTR(META,MX)=TSTP(META,IXJ
 23  CONTINUE
 22  CONTINUE
     NIX = NXPLMX-NXPLMN • 1
     NiY=NYPLVX-NYPLMN*1
```

```
    DTA=(TETAF-TETAI 1/INTE TA-1 )
    I F ( A3S IXREP- XM IN » . CT . ABS ( XREP- XMAXM KD' -1
    1FIA3SIXREP-XMIN1.LE.ABS(XREP-XMAXII  KD=1
    IFUXMAX-XMINJ.GT.(YMAX-YMIN)I  GO  TO  43
    A3=80.
    A2=A4=2C.
    Al=( (XMAX-XMIN)*( «3-A4 ) )/(YMAX-YMIN J•A2
    GO  TO  44
 42 41=80.
    A2=A4=20.
    A3= ( tYMAX-YMN»*(ai-A2))/lX"AX-XMIN)»AA
 44 DIVX=(XVAX-XMIN)/5.
    DIVY=(YMAX-YMIN»/5.
    AN=(3.1416*ANGNC)//80.
    AA=A1*3.
    VEX(1I-AA+5„*CCS(ANJ
    VEYl1)=20..5.*5INfAM)
    DIF=TETAF-TETAI
    ANG1~ITETAI*18C.)/2.1416
    3ANG=(DIF*180.1/3.1416
••••'DRAW  POTENTIAL  LINES  AND  STREAMLINES  OF  THE  SHADOW  REGION
    CALL  M0DESG(ZMCOE,6,CI
    TIME=TIMEC/DT IME
    DO  13  ITT-1,NTIME
    TI ME=TIME*CTI ME
    DO  41  LU=l»NMEMB5R
    SRPMX=-1.OD+300
    SRPM,=1.0C+?00
    DO  31  JU=1,LU
    SRPMX"DMAX1(SRPMXtK{JU)J
    SRP"N=DMINKSRFMN,K(JU))
 21 CONTINUE
    ZMAXt LU)=T IME/SFF^N
    TIE=(TI ME-TLEACH)/SPPM X
    ZMINtLUi=DPAXl(O.CCO,TIFi
    WRITEI 6,103)  NNLCL(LU) ,ZMAx(LU) ,ZMlN( LUI
103  FORMAT(IX,47,2(1PES.2,3X)(
 41 CONTINUE
    DO  29  NU=I ,NMEM8EP
    ^RITE(6,104)  NNUCL(NU)
104  FORMAT!IX,A7)
    IF(GRAP(NL).LE.O.>  GO  TO  29
    C ALL  SU8JEG(ZM0DE,XMIN,YMIN,XMAX,YMAX
    CALL OBJCTClZMCDE,¿2,A4,Al,A3)
    CALL  SETSMG(ZMQDE,4 5, 1.5J
    CALL  GRlDG(ZMDDE,CIVX,DIVY,C,Oi
    C ALL  LA3ELG(ZMOD6,C,DIVX,0,-9.2)
    C ALL  LA3ELG(ZM0DE,I,DIVY,0,-9.2)
    ENCODE{50,1CO0,XNAME I
000 FORMAT(*                  X-COCRDINATE  (METERS}*)
    ENCODE!50,1001,YN4ME I
001 FORMAT t *          Y-CCCRDINATE (METERS)*>
    E NC ODE( 10C.10C3, T\JAME)NNUCL(NMEMBER) ,HCL L\,H0LL2,TIMF
0D3 FORMAT( A7,* CONTAMINATED REGI ON- *,A10,A10, *4FTER*,1PE9,2,*YPS
    CALL  TITLZSIZMCDE,1.1.1.0)
    CALL  TITLZSIZMODE,1,2,1.El
    CALL TITLEG(ZMOOE,50,XNAME,50,YNAME,100,TNAME i
    CALLSETSMG(ZMCDE,45,1.0)
    DO  4 5  NT=1,NTETA
    DC  46  MX-=1,NX
    XWORK(MX)=XSTR(NT ,MX)
 46 YWORK(MX)=YSTR(NT ,MX
```

```
 45  CALL  LINESG(ZMQBE»NX»XV*ORK,Y*ORK)
     DO 47 JJ=1,NX
     DC  48  NN~1,NY
     ARRWORKlJJ,NN>=PC TEN(J J , NN )
 48  CONTINUE
 47  CONTINUE
     XO= A2/1C0.
     Y0=A4/1C0.
     CALL CCNZSIZMCDE,I, 8, XO)
     CALL  CCNZS(ZMQDE,1,9,Y0}
     CALL  CCNZSIZMCDE,1.18.1>
     C ALL CCNZSIZMCDE,1,17,1)
     CALLCCNRECIARRtoCRK,100,NX,NY,SUMAX.SUMIN»-10.,-1,-1,0)
******* DRAW REPOSITORY.BIGSPHERE AND NORTH DIRECTION ********** ****
     CALL SETS*G(ZMCDE,185,1.0J
     C ALL CIRARG(ZMODE,XREP,YREP,RAO,ANG1,DANG»
     IF INDAT A.GT.O )CALL LINESG5 ZHODE,NCATA,X310,YR10)
     CALL  SETS"G(ZM0DE,14,3.0)
     CALL VEC2XYIZMCCE,AA,20.,4.,ANGNO,0., 0., 11
     IVAL'JE=IHN
     CALL  SETSMGtZMODE,189,0.51
     CALL SETSVG(ZMCDE,84, I VALUE I
     CALL  POINTGtZMGDE,1,VEX,VFY)
     CALL  SETS^GIZMODE,14,0.)
     IF(NW.LE.O)  GC  TC  59
     CALL  SETSMGIZMODE,189,0.4)
     DO  55  NWEL L=1,NW
     DC  54  1=1,F
     ANGU=((l-l)*45.*3.1416)/180.
     ANGULO=(I- 11*45.
     1DMX= AMAXI((YMAX-tMN) , JXMAX-XMIN) )
     RAD IUS=RDMX/30.
     SENGHT=C.8*RACILS
     AX=RADIL'S*CCSS ANGL )
     AY=RADILS*SINtANGL)
     XARR=XWELL(NWELLl-XTRANS
     YARR=YWELL(NWELL!-YTRANS
     IF(Q(NWELLI.LT.C.)  XARR=XAPR+AX
     IF(0(NWELL».L T.C. i  YARR-YARP*AY
     I F ( CMNWELL I.LT. C. )  ANGLLC= ( I«-3)*45.
     CALL VEC2XYIZMCDE,XARP,YARR,SENGHT,ANGUI 0,0.,0., 1»
 54  CONTINUE
 55  CONTINUE
 59  CALL  SETSMG(ZMCDE,189,Q.5>
     IF(POTPLOT.LE.O,t  GO  TC  83
     CALL  SFTSMG(ZH00E,45,1.0)
     CALL  SETSMGIZMCDE,50, 0.i
 83  :)D  24  NSTR=1*NTETA
     D IM I N=• 1.0E+300
     DO  30  LX= 1, NX
     DIFFE(LX)=ABS(TSTF(NSTR,IX)-ZMIN(NU)1
     DIMIN=AMIN1(0IMIN,DIFFE(LX)I
 20  CONTINUE
     DO  51  LX= 1 ,NX
 51  IF(DIFF E CLXl . EO. D ININ»  KX= LX
     IF(T STP(NSTR,KX).EC.O. )  GO  TO  18
     ABSTINSTR)=XSTR(NSTR,KX)
     8ACT(NSTR«=YSTR(N$TR»KX»
     GO  TO  15
 18   TETA=TETAI+(NSTR-1)*(TETAF-TETAI)/(NTETA-1)
     A3SUNSTRi«XREP*RAC*CCS(TETAJ
     3ACT(NSTR)=YREP>RSC*SIN(TETA)
```

```
 19  WRITE16 ,131»  NSTR,ABST(NSTR»»BACT(NSTR»
.31  F0RMAT(1X,*TRAILING*,2X,I4,3X,2.PE9»2, 3X,1PE9.2!                    300
 24  CONTINUE
     I VALUE=1H*
     CALL    SETSMG(ZMODE,84,IVALUE»
     CALL    SETSMG(ZMODE,45,1.0!
     IT(GRAPLNUI.GT.O. (CALL  PC I ntg ( ZMODE, n t et A, ABS T,B ACT I
     00  35  J5=l,NTETA
     WRITE(6,106)  J5
L08  FORMATIlHl,lOX, *STpEAMLINE NC.*t I4)
     dRITE(6,147 )
147  FORMAT(2X,*NX*,3X,*X- IMETERI*,3X, *Y- (METERbx,*SIGMA (YR»*, 3x, *N
    $/N0*,3X,*QILUTICN  RATE  (CUBIC  METER/YEAR I*)
     TAX(J5)=-1.0E+300
     00  36  J6=1,NX
     Z-TSIR( J5,J6>
     CALL  MACKNU,Z,TIME,A,BS
     XWORM J6>-E
     WRITE(6,105)J6,XS1RIJ5,J6),YSTR(J5,J6),TSTP(J5,J6),A,B
109   FORMAT(1X,I4,3X,5I1PE9.2,3X))
 36  CONTINUE
     DO 38 LX=1,NX
 28  TAX(J5)=AMAX1{TAX(J5J,XWOPK(LX))
     DO  53  LX^1,NX
 53  IF(TAX(J5),EQ»XW0FK(LX))  KX=LX
     ABSM(J5  J=XSTR(J5,KX1
     8ACM(J5)-YSTR(J5,KX)
     IF(A8SM(J5J.E2«AeST(J5J»  GO  TO  26
     GOTO26
 26  IF(BACM{J5).NE.RACT(J5))  GO  TO  28
     ABSM(J5J = XSTR(J5,KX+KO>
     BACM(J5YSTR(J5,KX*KD!
 28  WRITE(6,133I  J5,ABSM(J5! ,BACM(J5)
125    FORMAT(IX,*MAXIMU»*,2X,I4,3X,lPE9.2,3X,lPE5.2i
 35  CONTINUE
     DO  33  J3=1,NTETA
     3IMIN=*UOE«-300
     DO  34  LX"1,NX
     DIFFE(LX>=ABS(TSTP(J3,LXJ-ZMAX{NUI>
     DIMIN=AMIN1(DIMIN,CIFFE(LXM
 34  CONTINUE
     DO  52  LX=1,NX
 52  IF(DIFFE(LX».ECOW IM  KX" LX
     A3SL(J3 J = X 5TR(J3 ,KXi
     BACL(J3 )=YSTR(J2,KXi
     riRITE(6,1»2 I  J3, AESLIJ3»,BACL(J3 »
132   F0PMAT(1X,*LEADING*,2X,I4.3X,1PE9.2,3X,1PE9.2)
 32  CONTINUE
     1VALUE-- 1H*
     IF(GRAP(NU».GT.O.»CALL PCINTGlZMODE,NTETA,ABSL,BACLI
     CALL  FRAME
 29  CONTINUE
 13  CONTINUE
     CALL  EXITG(ZMCDE»
     STOP
     END
     SUBROUTINE MAC1I11,Z,TT,P,W)
     DIMENSION  TCX(20)
     COMMON/D/B,EETA
     LEVEL  2,1,T,TeL,E,K,C,TOX
     LEVEL  2,B,BETA
     CCMMON/CONC/I,T,TEL,E,K,C,TOX
```

```
 DOUBLE  E(2C)»K(2C),Cl20i»Bl20»20l»BETA(20,20l
 DOUBLE  S1T S 2 » S 3                                                    301
 DOUBLE   Cl»C2»C3»C4,C5,Xl»X2,X3,X4,PRl»PR2
 DOUBLE E3 » EC » EE » EEE
 DIMENSIGN  Wl(20),wZI 20 ),W3(20>
 DIMENSICN  S(20), SU20) ,V(20)
 CALL BATEMAN( I ,E,C,B)
 DO  60  11=1,1
 Y=0.
 DC  62  111=1,ÏI
 rV6*-E( I I I »*T3L
 Y=Y+B( II ,1 U i*EXPIK6l
 C(II l = Y*ElIÎ)*Cll)/£î.î )
 CALL  BATEMAN(I,E,C,B )
 VW=1.
 DO 64 I J = l, I
• \/(lJ} = V»/K(IJS
 DO  21  Mi=i,ï
 DO  22  MJ = I,I
 I F ( MI . ECJ. MJ > GC TC 22
 IFIVÍMJUEC.VÍMI II  GC  TO  59
 3ETA(MI,MJlME(MII*\/(MJ>-E(MJ>+\MMIl»/(V(MJ)-V(MIN
 BETAIMJ,MII=BETÄ(MI,FJ)
 GO  TO  22
) BETAIMJ,MI ) = 0.
Ï CONTINUE
 CONTINUE
 DO  39  K4=l,I
 S(K4)=0.
 ST(K4»=0.
! CONTINUE
 DO  40  K5=1, I
 IFfV(K5i*TT.GE.Z I S ( K5 i~ 1 .
 IF(V(K5)*(TT-T).CE.Z I  ST(K51=1.0
I CONTINUE
 C1=0.
 DO  5 1  12=1,11
 ED= ( - E ( 12 >*(TT- Z/V ( II »    ABS(S(I1»-STfI1»)
 CALL EXPO!EO, EE I
 Cl = Cl + B ( I l , I > » * E E * ( S ( i l ) - S T U i n
 EB= (-Etilí*Z/V( IlII* ABS ( S ( I 1 i- ST ( 11 i »
 CALL  EXPCt EE,EEE )
 C1 = C1*EEE*(S(I1)-ST(I1>J
 C5 = 0.
 I F ( I I . E C U  GO  TC  71
 WMAX=0.
 DO  521  L»l,11-1
 DO 531 f. = L ,11
 D S - S I M I - S K H I
 ADS=ABS(DS   J
 DO  541  NR = L,I 1
 IFINR.ECMI  GC  TC  541
 DO  551  J=1,L
 Wl(J) = (-BETA(NR,w|*(TT~Z/V(M)) - E(MI*Z/V(M)>*S(Mi
 ^2(Jl=(-T*(E(Jl-BETA(NR,Mi)-BETA(NR,", t*(TT-Z/v/(M»>-E(Mi*Z/N/(M»)*ST
$ I M )
 W3(J) = (-E(JI*(TT-Z/V(M)-E(M)*Z/V(M||*ADS
 IF(BETA(NR,Mi.EQ.C.»  wl(J  - 0.
 IF(BETA(NP,MJ.EC.C. I W 2 S J  = 0.
 IF(BETA(NR,M|.ECC.>K3(J  = 0.
 I F IW1ÍJI.GT.WNAXJ  nMAX=Wl  JI
 I F(W2(J ».GT.WMAX )  WMAX = H2  Ji
```

```
51  IF (W3( Jl.GT.WAX »  hMAX=W3(J>
41  CONTINUE                                                                  302
.31 CONTINUE
21  CONTINUE
    IF(WMAX.GT.600.) CIFF=WMAX-600.
    IFIWMAX.LT.60C.)  CIFF=0.
    DO  52  NJ- 11 U-l
    C4=0.
    DO  53  NM=NJ,I 1
    C3=0.
    DO 54 NR = NJ 11 1
    IF(NR.EC.KF)  GO  TC  54
    C2=0.
    DO  55  NK=1,NJ
    PR1=1.DOO
    DO  53  NQ=NJ,I 1-1
58   PR1=PR1*E(NCf*K(NC.
    ?R2=1.DOO
    DO 57 NC = NJ »I 1
    IF(NO.EC•NR>  GO  TC  57
    IFtNQ.EC.NH»  C-C  TC  57
    PR2=PR2*lEtNQ»*K(NC)*(KtNR)-K(NM)>t-E(NH)*K(NM)*(K(NQ)-K(NR))+E(NR)
   $*K(NRJ*(K(NM,-K(NC))»
57  CONTINUE
    X1=B(NJ,NK)*(K(NP)-K(NM,,**(I1-NJ-l)
    Xl=Xl/(E(NKl*K(NRl-E(NK,*K(NMl-E(NRi*K(NP»*E{NMl*K(NMi.
    Xl=(X1*PR1J/PR2
    S1=t-BET4(NR,NMI*tTT-Z/V(NM)S-E(NM)*Z/V(NMI!
    S2=rJ-T*(E(NK>-8ETMNP,NM>>>*S1
    S1=S1*S(NM)
    S2=S2*SY(Nf I
    S3M-EtMa*TT-(E(NM,-ElNKN*{Z/V(NM)))
    S3=S3*ABS(SINKJ-ST(NMI)
    S1=S1-DIFF
    S2=S2-DIFF
    S3=S3-DIFF
    CALL  EXP0(S1,X3)
    IFtBETAlNRtNMI.EC.C.J  X3=0.
    X3=X3*S(NM»
    CALL  EXP0(S2,X2J
    IF(BETA(NR»NMI.EC.C.>  X2=0.
    X2=X2*ST(NHi
    CALL  EXPO(S3,X4)
    X4=X4*(SINK»-ST(N*))
    C2=C2+XI*(X3-XZ-X4>
55  CONTINUE
    C3=C3*C2
54  CONTINUE
    C4=C4+C3
53  CONTINUE
    C5=C5+C4
52  CONTINUE
71  IFUl.EC.ll DIFF-C.
    TEC=(E(1»*K(\JI/(E(II)*K(111)
    IFIC5.GT.TEC1  GO  TC  97
    IF(DIFF.GT.600..  GO  TO  97
    P=C1+C5*EXP(DIFFi
    IF(P.LT.O.I  P=0.
    ,V=P*C(1l*E(II»/(E(1>*TOX(11>*T)
    GO  TO  58
97  P=0.
    W=0.
```

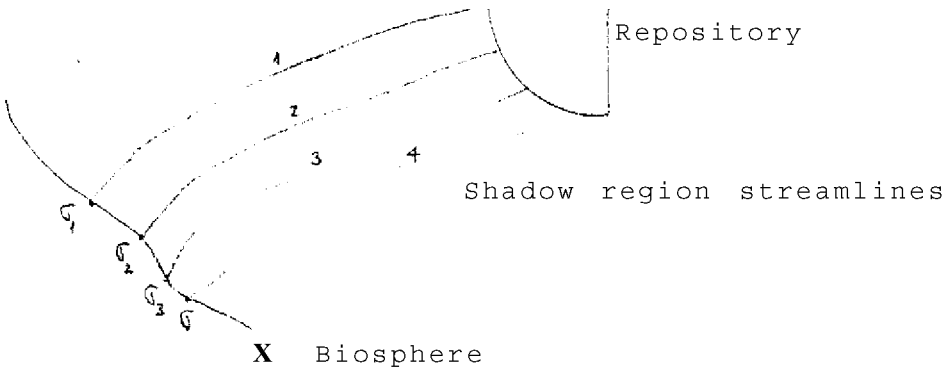
```
 98  RETURN
     END                                                                    303
     SUBROUTINE  B4TEM AM I,E ,C,B)
     LEVEL 2,E,C,B, I
     DIMENSION E(20,,C(2G),B120,20J
     DOUBLE  C,E,TEMPI,E
     DO 27 L 1 = 1 , I
     DO 28 LJ=l , I
     TEMP1=0.
     DO 31  LM'1,LJ
     TEMPZ-1.
     DO 29 LR=LM,L I
     TEMP2=TEMP2»E(LR )
 29  CONTINUE
     TEMP3=1.
     DO 30 LL=LM,L I
     IFILL.EC.LJ»  GC  TC  20
     TEMP3~TEMP3*lEILLJ-E(LJ> )
 3D  CONTINUE
     TEMP1=TEMP1*(C( If* »*E(1»/(C(1I*E(LM)M*TEMP2/(E(LI)»TEMP3)
 31  CONTINUE
     3(LI,LJ1=TEMP1
 28  CONTINUE
 27  CONTINUE
     RETURN
     END
     SUBROUTINE EXPOlX , Y )
     DOUBLE  X, Y
     IF(X.LT.-6.0D2 >  GC  TO  501
     Y=DEXP(X )
     GO  TO  502
501  Y=0.0D00
502  RETURN
     END
```

1111111. 111111111. 111311111.111111111.11II11111.111111111.1111111 11.111111

C.3 Subprogram DCHARGE data input description

Subprogram DCHARGE evaluates the discharge rate, the water dilution rate rate, the cumulative discharge and the water dilution volume at the biosphere for a i-th member of a radioactive chain of arbitrary length migrating in groundwater through a two-dimensional geologic media.

The subprogram DCHARGE is entirely independent of the PLOTMAC program. It is related to HYDRO subprogram only by the water travel time at the biosphere which must be read out of the HYDRO printout. Another set of data that must be obtained from the HYDRO print outs are the volumetric flow rates between the streamlines of the shadow region. Suppose the system studied can be represented by the following sketch



The values of o(1),o(2)o(NTETA) as well as Qd),Q(2),____Q(NTETA) can be obtained from HYDRO. The fractional volumetric flow rate is defined as

$$RQ(J)=Q(J)/\sum_{J} Q(D_{J}),J=1,2,...NTETA \qquad (C.3.1)$$

Once the hydrology is defined by HYDRO, DCHARGE can evaluate the water dilution rate and the water dilution volume Eq. (4.2.26) and Eq. (4.2.27) respectively for any radionuclide chain at any point inside the shadow region. The particular location where the calculations are to be performed is not characterized by a coordinate pair but rather by the correspondent water travel time value at that point.

Card 1: FORMAT(110,2(F10.3,I10))

Variable	Description
NTETA (110)	Number of contaminated streamlines to be considered. It is not necessarily the same as in HYDRO. (NTETA must equal or larger than two).
TBLO (F10.3)	First value of delay time for beginning of leaching to be used (years).
DELI (F10.3)	Multiplying factor for the next NTBL cases of time for beginning of leaching to be evaluated.
NTBL (110)	Number of different cases of time for beginning of leaching (TBL) to be evaluated. TBL=TBL0x(DEL1) ;k=1,2,___NTBL.
TO (F10.3)	First value of leach time to be used (years).
DEL2 (710.3)	Multiplying factor for the next NT cases of leach time to be evaluated.
NT (110)	Number of different cases of leach time (T) to be evaluated :T=T0x (DEL2)^{j};j=1,2,...NT.

Card 2 through Card 2+NTETA: FORMAT(2F10.3). NTETA of these cards are required, one for each streamline describing the shadow region.

Variable	Description
SIGMA (F10.3)	Value of the water travel time at the location where this streamline intercepts the biosphere (years).
RQ (F10.3)	Fractional volumetric flow rate as defined in Eq. (C.3.1) for this streamline.

Card 3+NTETA: FORMAT(315)

Variable	Description
NTIME (15)	Number of time intervals that the contamination time of a radionuclide at the biosphere is to be divided.NTIME does not affect the accuracy but to produce a smooth plot it is recomended that NTIME be equal to 20 or larger.
NMEMBER (15)	Number of members in the radioactive chain.
KS (15)	Number of intervals that the biosphere curve is to be subdivided between two consecutive streamlines. The accuracy of the calculations is very sensitive to this number. If leach time is small compared to the arrival time of the nuclide this number should be increased. A first try is KS=50.

Card 4+NTETA through Card 4+NTETA+NMEMBER:

FORMAT(A7,5F10.3). One of these cards is required for each member of the chain. The cards must be ordered in the same way the chain is.

Variable	Description
NNUCL (A7)	Nuclide name (e.g. RA-226).
THALF (F10.3)	Nuclide half life (years).
K (F10.3)	Nuclide retardation coefficient.
C (F10.3)	Nuclide total activity at the time of burial (Ci)
RCG (F10.3)	Nuclide maximum permissible concentration (Ci/m^3)
CALC (F10.3)	If CALC <0 the program does not calculate for this nuclide although uses its parameters for its daugthers calculations.If CALO 0 the program prints and plots the results for this nuclide.

Figure C.I Structure of the subprogram DCHARGE.

Initialize

Read data input

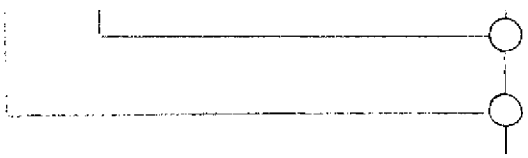
Do every case of time for
for beginning of leaching
TBL=TBL0*(DELI)**K;K=1,..NTBL.

Do every case of leach time
T=T0*(DEL2)**J;J=1,...NT.

Do every member of the chain
1=1,2,...NMEMBER.

If CALC > 0 evaluate the water
dilution rate (Eq.4.4.20) and
water dilution volume (Eq.4.4.21).

If CALC >0 plot and print the
results for this nuclide:the water
dilution rate and the water dilution
volume. I



```
'IA. 8 68301 ,T INGt 0
iPUT  6200C  13.23.39  10 SEP 81  VIA CR02                                  309
) =
'Y, INPUT /R.R, OUTPUT/RR.
5P0SE,0JTPUT=PR,PA*1F.

) CRAM UCBNE21  (SUBPROGRAM OCHARGE)
*4IE L K.S. TING

'ARTMENT OF NUCLEAR ENGINEERING
[\ECSITY OF CALIFORNIA, 8ER«t£L£V
?KELE ^,CA. ,94720



 CONTROL CARDS LISTING **

0BCARC1
ASSWOFD)
SERPR.
F<.,L*0.
THLIB.
TCHFS,IDOS,ULIB,ULIBX.
TCHFS,GPACBN7,GPAC,VA3N.
NK, F=LGO,F=GFAC, P=ULIB,X.
APHIC»FN°FILM,FT=VA.
IT.
MP,0.
JMP.



 PROGRAM LISTING

     PROGRAM OCHARGE (INPUT • OUT PUT , T£P£5=INPUT , TAP£6*0 UT PUT , F ILM1
     COMMON/IGSZZZ/ZMCDE(201)
     COMMON/CONC/NKEhEER,T ,T3L ,E,K,C,RCG( 20 )
     DIMENSION  X(2Q),H(2Q)
     DIMENSION NKUCL (20 ) ,CALC ( 20)
     DOUBLE  TMAX , TMIN
     00U3LE  ZMIN,ZMAX
     D0U3LE  THALF,K(20),E(2C),C(20) ,SRFMX , SRPMN,SMAX, SMIN
     DIMENSIONXNAME(70J , YNAHE ( 70 ) » TNAHE(15G >
     DIM-INSION ZMIN (20>,ZKAX (20 ) , SIGMA ( 2L) ,RQ<20)
     DIMENSION PLCTES <1GQ I ,1 IMEPC1C0)
     DIMENSION RATE (5*100 ) tTOTAL (5* 100) «T IKE ( 5 1100 )
     DIMENSION RN (18 0Q) .TOXRATE (5 ,10t) .TOXTOT A (5. 1QCI
     READ (5,100! NTETA,TBLC, DELI, NTBL, TO, OEL2 , NT
100  FORMAT (I 10• 2(2F10.31110>>
     DO  22  ITETA=1,NTETA
     READ (5 ,1011  SIGfA (ITETAJ , RQ (I TET A)
1 01  FORMAT (2F10.3)
 22  CONTINUE
     READ (5,102)  NT I h£» N ME M8E R,KS
102  FORMAT (3 15)
     DO  10  1=1,NMEMBER
     READ(5,103)  NNUCL(I),THALF»K(I),C(I) ,RCG(I) ,CAL3 CI)
1C3  FORMAT (A7,5FI0.3)
 10  E(I) =DLOG(2.D00)/THALF
     READ (5,107)  HOL1.HCL2
107  FORi AT (2A8)
     TBL = T3L0/DEL 1
```

```
      DO  IODO   IT BL = i» NTBL
      TBL= TB L* CE L1                                                    310
      DO  11  NU C= i f NMEK BER
      IF(CALCíNUC) .LE.O. )  GO  TO  11
      TMAXs-1. 00*300
      TMIN*1.00*300
      TsTO/DEL 2
      DO  1QÜ1   IT=i,NT
      T=r»0EL2
      SRPIXs-1.0*300
      SRPMN= 1. 0*300
      DC 12  JU=1, KUC
      SRPMX=DMAXi(SRPMX,K(JU>i
 12   SRPMN= DMIN1(SRPKN,K(JU) )
      00  13   NS TR= 1,NTETA
      2MAX  (NSTR)x SIGMA (NSTR)*3RPMX*T
 13   ZMIM(NSTR) = SIGMA(NSTR) *3RP MN
      SMAX       D*300
      SMIM = 1.D*300
      00  14   NS TRsl ,NTETA
      SHAXsDMA XI (SMAX,Z*AX (NSTR) )
      SKIN =D M I M (SMINtZKINÍNSTR) )
 14   CONTINUE
      00  17   NSTR = 1,NTETA
 17   X(NS TR) = FLOAT (KS*NSTR)
      00  18   NS TR = 1,NTETA
      00 19  NS=1, KS
      NN=KS*NS TR • (NS-1)
      RN(NN) =RQ (NSTR) /KS
 19   CONTINUE
 16   CONTINUE
      CALL  POLINT (NTETA, X, SIGMA, Hi
      DELT A= (DLOGiOlSMA » -DLOGl C(SMIN))/(NTIM£-1)
      DO  15   IT IMEsl,NTIM£
      AXPA sDLOGlO  (SMIM*(ITIM£-1 >*DELTA
      TlMi  (IT, ITIME)*10. ••AXPA
      TT = TIME(ITtITIME)
      TGTALOT  ,ITIME)=Q.
      RATE(IT,ITIME)=0.
      DO  20   NSTR=KS,NTETA*KS
      XX=FLOAT  (NSTR)
      CALL  POL YVL (0, XX, Z, YP, NTETA, X, H, WORK , 1 ERR)
      CALL   MA CK NUC, Z, TT, SMIN, P, W)
      RATE(IT,IT  IhE)=RATE(IT,ITIME)*P»C(1)*RN(NSTR)/T
      TOTA L(IT,ITIMt) = TOTAL(IT, ITIML > *W»C(1)»RN(NSTR)/T
 20   CONTINUE
      TOXRATE(IT, ITI ME I = RATE(IT,ITIME)/RCG(NUC)
      TOXTOTAÍIT,ITIME)=TOTAL(IT,ITIME)/RCG(NUC)
 15   CONTINUE
      WRITE(6,104)   NNUCL(NUC),T 8L,T
LC4   FORMAI 11H1 ,5X, *NUCLIDE  -  11A7 , 3X ,* DELAY  TIME  (YRS )  =*,1Pt 8.2,3X,*L
     tEAC-(  T IME  (YRS)  =*,1PE8.2)
      WRITEÍ6,1Õ5)                                                  ,
LC5   FCRMAT í//,lX,jcTIME  (Yt) í , 2X, * D ISCH ARGL  RATE  (CI/YRGWYR) *,2X,íCUMUL
     SATIVE  OI SC HAR GE  (CI/GWYR) * ,2X ,/RATE/MPC  (M3/YRGWYR)t,2X,tCUMULATIi
     SE/MPC   (M3/GWYR)t)
      00  16   IT IME = 1, NTIME  '
      WRITE(6, 106)  TIHEÍIT, ITIME), RATE (IT, ITIME) ,TOTAL {IT , III ME í ,TOXRATE
     K I T , ITIME) , TCXTCTA(IT,ITIME)
1C6    FORMAI(IX,1PE8.2,12X,1PE8.2,2 0X,1PE6.2,20X,1PE8. 2,¿0X,1 PE 8.2)
 16   CONTINUE
      TMAX=DMAXi  (SMAX,TMAX)
```

```
   T HI N=D MI M (SMIN,TMN)
 1 CONTINUE                                                              311
   CALL MODESG (ZMOOE,6,0)
   RATE MXs-1. OE+300
   RATE MN'i«.QE*300
   TOTALMX=-1. CE+300
   TOTALMN* i.QE*300
   DO 1003 IT«1,NT
   00 23 IT IME=1» NTIfE
   IF(TOXRAT£(IT, ITIMEKLT.1. GE-<. > TOX* ATE C IT, ITIME I =1.
   IF(TOXTOTA(IT•» ITZME i»LF.1• 0» TOXTOTA(IT,ITIME>«1.0
   TIME(IT, ITIMEJsALOG1O (T IME (IT, IT XWE) >
   RATE MXBAMAXI (RATEMX, TOXRATE (IT, IT IME) I
   RATE MN = A Ml NKRATEMN, TOXRATE (IT .ITIME > )
   TOT A LMX= AMAX1 (TOTALMX, TOXTOTA (IT, ITIME ) )
   TOTA LMN= AMIN1(TCTALMN, TOXTOTA(IT, ITIME))
   T OX* ATE < IT, IT IME UALOG1O (TOXRATE (IT, ITIME) )
   TOXTOTA( IT, IT IME) =ALOGiG (TOXTOTA (IT, ITIME) )
23 CONTINUE
03 CONTINUE
   XMAX =F LOAT (IOINT(DLOG1u (T MAX)))*1 .0
   XHIN=F LO AT (IOI NT (DL061C (TMIN) ) )
   OIVXs1.O
   DIVYs1.O
   AsALOG1O (RATEMN)
   YMINsF LOAT (INT(A))
   IF(A•LE•0.) YMIN=FLOAT(INT(A)) -1.
   BsAL OG10 (RATEMX)
   YMAXsFLOAT(INT(8))*1.
   IF(3.LE. 0.) YMAX=FLOAT(INT(B))
   IF( A BS (Y MAX-YMIN). GE.&.) OIVY=2,0
      PLOT THE CISCHARGE RATE
   CAL. SUBJEG «ZMCDE,XMIN, YMIN, XMAX, YMA X)
   CALL OBJ CIG<2MGQE,30,,20.,90•,60,)
   CALL SETSMG(ZMCCE,45,1.5)
   CALL GRIOG(ZMOOE,CIVX,DIVY,0,0)
   CALL LABELG (ZMOOE,0,0IVX,0,3)
   CALL LABELG(ZMOOE,1,DIVY,0,3)
   ENCODE (50, 20C0 , XNAME )
00 FORMAT (1 OX,/TIME AFTER LEACHING STARTED (YRS )* )
   ENCODE (70,2001, YNAME)
01 FORMAT (2 X, it DISCHARGE RATt/MPC (CUBIC MLTER/YR)/)
   ENCODE (150 , 20C2,TNAME ) NNUCL(NUC ) ,H0L1 ,HOL2
02 FORMAT(A7,* CISCHARGE RATE HISTORY AT/.2A8)
   CALL TITLZS(ZMOOE,1,1,1. )
   CALL TITLZS(ZMODE,1,2,1.81
   CALL TITLEG (ZMODE,50, XNAME, 50, YNAME, 15U, TNAME)
   00 1004 ITs1tMT
   TOXR ATE (IT » 1) = YMN
   TOX*ATE(IT,NTIME)=YMIN
   00 100 5 IT IME = 1 ,NT IME
   TIM£P( IT IME) =TIhE(IT, IT IME )
05 PLOTER(ITIME) = TOXRATE(IT, ITIME)
   CALL LINESG(ZMCDE,NTIMc,TIMEP,PLOTER)
IC CONT INUE
      PLOT THE CUHMULATIVc DISCHARGE
   CALL FRAME
   D1VY=1.0
   WNAXsFLOAT( INT(ALOG10 (TOTALMX) >) +1.0
   WMIN=FLOAT( INT(ALOGlu (TOTALMN) I)
   IF((WMAX-WMIN) .GE.6.) DIVY=2.0
   CALL SU3JE6(ZMOOE,XMIN.WMIN,XMAX,WMAX)
```

```
    CAIL  06JCTG(ZMOCE,30.,20. , 90 . , 60 . Î
    CALL  SETSMG (ZMOCE,45,1.5)
    CALL  GRIDG(ZMOOE,CIVX,ûIVY,û,G)
    CALL  LA6ELG(ZM0DE,û,OIVX,0,3)
    CALL  LABELG(ZMCDE»1»DIV Y» 0,3)
    ENCOOL (7 0, 20 03 , YNAME)
 03 FORMAT it CUMULAT ! VE 01SCHARGE/MPC  CCUBIC  METE R ) *)
    ENCOOE(150,2004,TNAME)  NNUCL(NUC),HOL1,H0L2
 04 FGRMAT (A7, *  CUMULATIVE  0ISCHARGE  US TORY  AT/ ,2A8)
    CALL  TITLZS(ZMOOE,1,1,1. )
    CALL  TITLZS (ZMOOE,1,2,1.8)
    CALL  TII LE G(ZMODE,50,XNAME,50,YNAME,15Û,TNAMEJ
    OO  100 6  IT-i.NF
    00  1007  IT IM£=i,MIM£
    T IME P ( IT IME ) = T U E ( IT , IT ÎME !
107  PLOT ER(ITIME)=TCXTOTA(II,ITIMEî
    CALL  L INESG(ZMOCE, NT îM.., T I ME P , PLOTER)
    OELTAl* ( XMAX-T IME ( IT » NT IME ) ) / ( NT I »/E -1 )
    DO 150 0 IT IME = 1 » NT IME
    T IME P( IT IME) =TIME(ITtNTIM£)*(ITÎME-1)*OELTAi
    AXP= 10 .»*T IMEP ( ITIME)
    PLOTER (ITIME) = TOXTOTA (IT , NT IME )»£XP( -E (NUC) *AXP)
;CC  CONTINUE
    CALL  L INESG(Z MCCE , NT IME , T IME P , FL CTER )
Î06  CONTINUE
    CALL  F R A Me.
 11  CONTINUE
JOC  CONTINUE
    STOP
    END
    SU3ROUTI NE  MAC1 (Il, Z, TT , T A ,P , W )
    DIME NSIGK  TOX (20 I
    CC.-M 0N/L>/B,8ETA
    COMMUN /CONC/I,T,TBL ,E,K,C, TOX
    00U3LE  E(20),K(20),C(2û),6(20,20),BETA(20,20)
    CÛU3LE   Al,A2,A3,Y1,Y2,Y3,D1,Q2,D3,D4,Pi,P2,P3,P4
    OOUBLE   S1,S2,S3
    OOU3LE  E Z, EY , T A, £W, EF
    DOU3LE   A F,AZ
    DOUBLE   C1,Ci,C3,C4,C5,X1,X2,X3,Xt.,PR1, PR2
    DOUBLE   E B,cD,EE,EEE
    CIME NSION  hi (20) ,W2(2Û» ,W3 (20 )
    DIMENSION  S <2C ) ,ST (20 ) , V(20)
    CALL  BATEMAN( Il ,E,C,8*
    OC 60  11=1,11
    Y*0•
    O O  b Z  111=1,11
    X6=-E(III)*T8L
 62  Y=YfB(II.HX)*£XP(H6>
 60 C(II ) = Y'£(II;j*C (i)/EC11
    CALL  BATEMAN(I1,E,C,B)
    VH=1 .
    OO  Q*,  IJ=1,I1
 6-,  V (I J) = VW/K(IJ)
    OC  21  MI=1,11
    OO 22 MJ=1, Il
    IF(MI.EQ.MJ)  GC  TO  22
    IF(V(MJ) .EQ» V (MI))  60  TÛ  5 9
    BETA  (MI,MJ)s(E (MI)'V(MJ)-E(MJ)*V(MI)) /(V(MJ>-V(MI))
    BETA  (MJ,HI) = BETA(MI,MJ)
    GO T 0  22
 59  BETA(MJ,MI)=0 .
```

```
22  CONTINUE
21  CONTINUE
    DO 39 Ki.=l,I 1
    S(K4)= 0.
    ST(K4)=0 •
39  CONTINUE
    00 <tQ K5si,Il
    IF(V K 5 ) *T T»GL .Z) S (K5)=l.
    IF(V (K5J * t TT-TJ .GE.Z) ST ( K5 ) *1 • 0
40  CCNTINUE
    Pl=û .
    Ci=Q .
    ÛC 51 12*1,11
    £0= (-E (121 * 4TT-Z/1? (Ill) I* ÂBSISîîiî-ST ( I D )
    CALL EXPO(ECEE)
    IF(TT.GE.K(I1)»Z) GO TO 30
    EF = £ Z= 0. 000
    GO TO 31
30  IF(TT.GE.(K(ID*Z*T>) GO TO 32
    IF(TA,LE.K(I1)»Z) GO TO 33
    EF=-E(I2 1*(TA-Z/V(11) I
    EZ=-E(I2 )* (TT-Z/V ( I D )
    GO TO 31
33  EF=0•
    EZ=-E(I2 )MTT-Z/V(ID )
    GO TO 31
32  IF( T A. GT .K ( I D *2) GO TO 34
    EF=2 .
    EZ=-E(12)*(TT*T)
    GO TO 31
3i. IF ( T A. GT ,(K ( ID»Z*T) ) GO TO 35
    EF= -E (12 >* ( T A - Z / V d l M
    EZ=-E (12 )• CTT+T)
    GO TO 31
35 EF = £ Z=0 .
31  CALL EXPü(EF,EY)
    CALL EXPO(EZ,EH)
    P1*P1*B( II .12 ) • (EY-EM)/£ (12)
51  C1=C l«-8( Il .I2)*EE»(S(I1)-ST(ID)
    EB= ( -c (II) *Z/V ( I D ) * A 3 5 ( S UD - S T ( I D )
    CALL EXPO(EB,EEE)
    Cl«Cl»EEE* (S ( I D -ST ( I D )
    C5=0 •
    P5 = 0 .
    IFCIl.EQ.ll GO TO 71
    KMAXxC .
    00 5 21 Lsl,11-1
    00 5 31 H=L ,11
    DS=S (M)-sT (M)
    ACS= ABS ( OS)
    OC 541 NR=L ,11
    IF(NR,EC «M) GO TO 541
    CO 551 J=1,L
    Hl( J) = (-BETA (NR,W MTT-Z/V (M) ) -L (M)*Z/V(M) )»S(M)
    H2 (J ) = (-T» (E (J) - 8ETA( )^,K) ) -BETA (NR, M) » (TT-Z/V (M ) )-E(M) »Z/VIM) ) *ST
  S (M)
    K3(J) = (-E(J)*(TT-Z/V(M))-E (M)»Z/V(M))»ADS
    IF(3ET A(NR,M) .EQ.O.) Hl(J)xQ.
    IF ( BETA ( NR ,M ) .ECO . ) H2( J) =0,
    IF(8ET A(NR ,»/).EQ.O.) W3(J)xO.
    IF(W1(J).GT.HMAX) WMAX=W1(J)
    IF (W2 ( J) .GT. WMAX) WMAX=W2 (J)
```

```
51  IF{H3(J) .GT.WMAX) HMAX=H3(JS
1.1 CONTINUE
31  CONTINUE
21  CONTINUE
    IF<WMAX.GT.600.)  DIFF=WMAX-OC0.
    IF(WMAX. LT.600.)  OIFFsÛ.
    OC  52  NJ=1,11-1
    C4=Q •
    Pi» = 0 •
    00  53  NM=NJ,I1
    C3=0 .
    P3=0.
    DO  5 k  NR=NJ,U
    IF(NR.EQ .NM)  GO TO  5%
    02=0 .
    P2=0«
    DO  55  NK=1, NJ
    PRlr 1. DO 0
    00  58  NQ=NJ,I1-1
58  PR1=PR1*E(NQ) *K(NQ)
    PR2=1. DOC
    00  57  NQ=NJ,I1
    IF(NQ.EQ.NR)  GO  TO  57
    IF(NQ.EQ.NM)  GO  TO  57
    PR2=PR2ME (NQ) »K(NQ> • (K(NR)-K (NM) ) •£ (NM) »K (NM) »(K(NQ)-K (NR) > *E(NR >
   $»K(NR)»  (K(NM)-K(NQ)))
57  CONTINUE
    X1=3 (NJ, NK )*(K(NR)-K (NM) )»»(I1-NJ-1i
    X1=X1/ ÍE (NK> *K (NR)-E ( NK) *K (NM) -£ (NR) »K (NR) +E (NM) *K ( NM) )
    Xl= ( X1*PR1 )/PR2
    Sl= ( -BETA( NR ,NM) * (TT-Z/V (NM) ) -E (NM)»Z/V (NM))
    Ai= Í -BEIA(NR,NM)«CTA-Z/V (NM) ) -E (NM) *Z/V (NM) )
    IF(TA. LT.K (NM) »ZI  Al=-£(NM) *Z*K ( NH)
    S2=(-T*(E(NK)-BETA(NR.NM)))*Sl
    A2= (-TME(NK) -BETA (NR,NM) ) ) +A1
    IFdA.LT. (K (NM)*Z*T) )  -Ü2=-T*£ ( NK )-£ ( NM ) » Z*K ( NM )
    51=S1*S(NM)
    52=S2*ST (NM Î
    S3= (-E (NK) *TT-(E(NM)-E(NK) )*(Z/V (NM)))
    A3= (-E (NK) • ÎA- iE (NM) -E(NK) )» (Z/V (NM) ) )
    IF(TT. GL.K (NM)*¿)  GO  TO  8 C
    AF=A Z=0-
    GO  TO  81
80  IF(TT. Gt «(K (NM) *Z*T) |  &0  TO  82
    IF(TA.LE.K (Il)*2)  60  TO  83
    AF=A 3
    AZ=53
    GO  TO  81
83  AF=-E(NM)* Z*K (NM Ï
    A7=53
    GO  TO  81
82  IF( TA. GT «K (NM) *Z)  GO  TO  84
    AF=-E(NM) * Z*K(NM)
    AZ= -E ( NK ) * T -E (Nh >*Z*K (NM)
    GO  TO  81
84  IF(TA.GT.(K(NM)*Z+T))  GO  TO  85
    AF=A 3
    AZ=-E(NK )*T-E (NM)*Z*K (NM)
    GO  TO  81
85  AF=AZ=0.
81  AF=AF-01FF.          .          .          .          .          .
    AZ=A Z-DIFF
```

```
    At = A 1 - D l FF
    S 2 = S 2 - D I F F
    A 2 = A 2 - O I F F
    S 3 = S 3 - D I F F
    C A L L   E X P C ( S 1 , X 3 )
    C A L L   E X P 0 ( A 1 , Y 3 >
    I F ( 3 £ T A ( N R , N M ) . E Q . f l . )     X 3 = 0 .
    I F i B E T A ( N R , N M )  • E Q . O . )   ¥ 3 = 0 « ,
    X 3 = X 3 * S ( K M )
    0 3 =  ( Y 3 - X 3 )  *  ( K ( N R ) - K ( N M I ) » S  ( N M )  / ( t  ( N M ) • < ( N R ) - E  ( N R  I » <  ( N M )  )
    C A L L   E X P 0 ( S 2 , X 2 )
    C A L L   E X P 0 ( A 2 , Y 2 I
    I F  ( 3 E T A { N R » N H )  . E Q . O . )   X 2 = 0 .
    I F ( B E T A (  f \ R » N M )  . E Q . O . )   Y 2 = 0 .
    X 2 = X 2 * S T ( N M )
    D 2 =  ( Y 2 - X 2 )  *  ( K ( N R ) - K ( N M )  ) • S T  ( N M )  / ( E  ( N M >  » K  ( N R )  « E  ( N R  ) * K  ( N M )  )
    C A L L   E X P O ( S 3 , X < . )
    C A L L   E X P O ( A F , Y i )
    C A L L    E X P O ( A Z . D i )
    Qk= ( Y l - 0 1 )  / £  ( N K )
    X < i = X < . *  ( S  ( N M ) - S T  ( N M )  )
    C 2 = C 2 * X 1 * ( X 3 - X 2 - X 4 )
    P 2 = P 2 « -   X l * ( 0 3 - 0 2 - D < » )
55  C O N T I N U E
    C 3 = C 3 * C 2
    P 3 = P 3 * P 2
5k   COM  I N U L
    Ck=0k*-CZ
    Pk=Pk*P3
53  C O N T I N U E
    C 5 = C 5 * C 4
    P 5 = P 5 « - P 4
52  C O N T  I N U E
71  I F ( I l . E Q . l )   D I F F = 0 .
    T E Q = ( t  ( 1 ) » K ( 1 ) ) / ( E ( I 1 ) * K ( I 1 )  )
    1 F ( C 5 .  G T . T E Q )   G O   T O   9 7
    I F ( P S . G T . T E Q )   G O   T O   9 7
    I F  ( O I F F .  G T . 6 C L . )   G O   T O   9 7
    P = C 1 * C 5 * E X P ( D I F F )
    W = P 1 * P 5 * E X F  ( D I F F )
    I F ( P . L T . 0 . )   P = 0 .
    I F ( * < . L . T . 0 . )   H s O .
    G O   T O   9 8
97  P = 0 .
    w=o.
98  R E T U R N
    E N D
    S U B R O U T I N E  B A T E f . A N ( 1 1 £ « C « B )
    D I M E N S I O N  E ( 2 C )  , C ( 2 0 )  , 8 ( 2 0 , 2 0 )
    D O U B L E   C , E , T E M P I , B
    D O   2 7   L I = 1 , I
    D O   2 8   L J  = 1 , I
    T E M P 1 = 0 .
    D O   3 1   L M « 1 , L J
    T E M P 2 = 1 .
    D C   2 9   L R = L M , L I
    T E M P 2 = T E M P 2 » E  ( L R )
29  C O N T I N U E
    T E M P 3 * 1 .
    0 0   3 0   L L * L M , L I
```

```
      IF(LL.EQ.LJ)  GO TO 30
      TEMP3=TtMP3* IE<LL>-E(LJ)>
30    CONTINUE
      TEMP1=TEMP1 + IC(LM) *E(11 /<C(1)»E(LM)>>•TEMP2/IE(LI)»TEMP3)
31    CONTINUE
      B(LI,LJ)sTEMP1
28    CONTINUE
27    CONTINUE
      RETURN
      END
      SUBROUTINE EXPO(X,Y>
      DOUBLE X,Y
      IF(X .LT.-6.002)  GO TO 501
      Y=DEXP(X1
      GO T0 502
01    YsO.ODfiO
02    RETURN
      END
```

C.4 Subprogram POT3D data input description

Subprogram P0T3D produces a three dimensional plot of the hydraulic head distribution used in the subprogram HYDRO.

Card 1: FORMAT(2A10,2F10.3)

Variable	Description
H0LL1 (AlO)	Hollerith to be displayed in the graph legend.
H0LL2 (AlO)	Continuation of H0LL1.
SUMIN (F10.3)	Minimum value of the potential function (in), see HYDRO printout.
SUMAX (F10.3)	Maximum value of the potential function (m), see HYDRO printout.

r, INPUT /RR» CUTPUT/RR.
POSE,0J TPUT=PR,PA«1F.

GRAM UC8NE21 (SUBPROGRAM POT 3D)
IEL K.S, TING

ARTMENT OF NUCLEAR ENGINEERING
VEFSITY OF CALIFORNIA,BERKELEY
KELE t.CA. ,94720

CONTROL CARDS LISTING

```
BCARC1
SSHCRD]
ERPR
4.
CMPS,IDOS,ULIB,ULIEX.
CHPS,GPAC8N7.GPAC,VA8N.
TAPE,TAPE11=/TING/J/AC2/RUSTLE3,37483.
K,F=LG3,F=GFAC,P=ULI8,X.
PHIC,FN=FILM,FTsVA.
T.
P.O.
MP.
```

PROGRAM L ISTING •*

```
    PROGRAM POT 3D(INPUT,OUTPUT,TAPE5=INPUT, T APE6=0UT PUT,TAPE11,FILM)
    COMMON/IGSZ22/ZMCOE(2    0 0)
    DIMENSION VEX (1) , V£Y (1) , PLOT U0)
    COMMON/ANAME/XNAME(50),YNA ME(5 C) » TNA ML(10 0),ZNAME(5 0)
    DIME NS ION XWORK (100) » YMORK(1 0 0)» ARRW ORK (10 0, 10 0)
    READ(5,100)  HOLL1,HOLL2,SUMIN.SUMAX
CO  FORMAT (2 A1 0 , 2F10 » 3)
    MA P E= 11
    READ (NTAPE,112)XMIN,XMAX, YMIN, YMA>,DEL,NX, NY,NTETA
12   FORMAT(IX,5E9.2,315)
    00  10  LX=1,NX
    DO  11  LY=i,NY
    READ (NTAPE,111)  ARRWORK (L X, L Y )
11  FORMAT (1X,E13.5)
11  CONTINUE
10  CONTINUE
    IF ({ XMAX-XM IN) .GT . ( YMAX-YM IN ) >  GO  TO  43
    A3 = 3 0.
    A2 = A 4=20 .
    A1= ( (XMAX-XM IN )* (A3-A4) ) /( YMA X-YMIN) *A2
    GO TO 44
43 A1 = 3 0.
    A2 = Ah= 2C .
    A3=(  (YMA X- YMIN >• (A1-A2I )/( XMAX-XMIN) *A<.
4h   DIVX=(XMAX-XM1N)/5.
    CIVY=(YMAX-YMIN)/5.
    DIVZ=(SUMAX-SUM1N)/5.
    rat!      m nn F^a  t rnnrF .A . n i
```

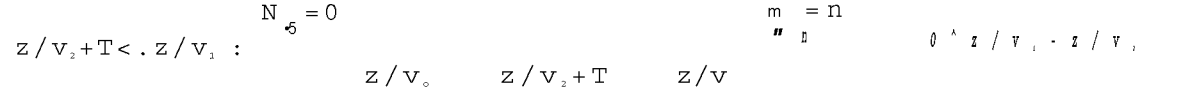
```
      CALL  BEGIN3 (PLOT)
      PLOT (1 UXMIN
      PLOT (2 )= XMAX
      PLOT (3 )= THIN
      PLOT (<» ) = YMAX
      PLOT  (5USUMIN
      PLOT (6 ) = SUHAX
      PLOT <7)=9Q.
      PLOT (3 1*1.
      PLOT (19) «1.
      PLOT(26)=2* 6
      PLOT (27) =io0
      CALL  SU6U3D(ZMODE,PLOT|
      CALL  0BJCTG(ZM0CE,A2, A<.,Ai,A3>
      CALL  GRI 03 0 (ZMGCE,PLOT,QI \,X,DI VY, DIVZ)
      CALL  SETSMG(ZMG0E,45,1.2)
      CALL  LABL3D (ZMODE .PLOT, 1, Ol VX, 2, 9. 2)
      CALL  LA8L3D(ZMODE,PL0T,2,DIVY,2»9.2)
      CALL  LA8L30(ZMC0E,PL0T,3,0IVZ,2,9.2)
      ENCODE(5 0, 100C,XNAME)
JOG   FORMAT (*                  X-COORDINATE  (METERS) t)
      ENCDOE (5 0. 1001 .YNAME)
301   FORMAT It                 Y-COORCINATE  (METERS)?)
      ENCODE (5 0. 1Q04.ZNAME)
304   FCRMAT It             HYDRAULIC  POTENTIAL  (METERS)/ )
      ENCODE ( 100 , 1006.TNAME ) HOLLI, HOLL2
306   FORMAT It       POTENT IOMc TRIC  SURFACE  IN  THE  AQUIFER  -  *,A1G,A1C)
      CALL  TITL3D(ZMODE,PLOT , 50,XNA ME,50,YNA ME,50,ZNAME,100,TNA ME)
      00  54  K1=1,NX
      XWORMK1}=XMIN* (K1-1)*0E L
 54   CONTINUE
      DO  55  K2=1,NY
      YWORK(K2 ) = YMIN-KK2-1) *OEL
 55   CONTINUE
      CALL  SURFCE(ZMOCE,PLOT, XWORK,YKORK,ARRW0RK,10 0,NX,NY,Q)
      CALL  EXITG(ZMODE)
      STOP
      END
```

Appendix D-Derivation of The Contamination Time Interval and the Contaminated Reaion for the Second and Third Member Nuclides when $N_{0} \neq N_{1} \neq 0$.

D.1-Determination of the contamination time interval θ_{2} for the second member when $N_{0} \neq 0$ (Table 3.7).

The solution for the concentration of the second member is expressed by Eq.3.4.8.The contamination time interval is defined as the time interval in which the concentration is non zero at a fixed position.The first term on the right hand side of Eq.3.4.3 is non zero in the time interval $(z/v + T - z/v_{1} \geq T)$ because the function $S(v_{2}t - v_{2}(t-T))$ is non zero in this interval.Likewise,the second term is non zero in the interval $(z/v_{2} - z/v_{1})$ if $v_{2} < v_{1}$ or $(z/v_{2} - z/v_{1})$ if $v_{2} > v_{1}$ .When the two terms are added the resultant concentration is non zero in the superposition of the above tire intervals when each individual term is non zero.The different confimirations resulting from the superposition are shown in the foillowina diagrams

Wien $v_{1} < v_{2}$ two possibilities arise



No = 0

z/v₀+T>z/v.

z/v. z/v^ Z / V₂ + T

Above results are summarized in Table 3.7.

D.2—Determination of the contaminated region R₀ for the second member when N. ^0 (Table 3.7).

The contaminated region is defined as the region in which the concentration is non zero at a fixed time t.The first term in Eg.3.4.8 is non zero at a fixed time t in the region defined by (v₂t-v₂(t-T)=v₂T) because the function S(v₂t;v₂(t-T)) is non zero in this region.The second term is non zero in the region (v₀t-v^t) if v₂>v^ or (v^t-v t) if ᵛi>ᵛ2,because the function S(v-^t;v₂t) is non zero in this intervals.By adding the two terms,the resultant concentration wi11 be non zero in the superimposed region of the two individual non zero regions.The different possibilities are shown in the following diagrams

N =0

V ᵛ 2 9 ᴿ2 = ᵛl t - ᵛ2 (t - T)

v₂ (t-T) V^t V₁t.

When v^< v_^ two different possibilities arise

N₉ = 0

v₂ (t-T)>v₁t ᴺ2 ᵃ° , R^ = v₂t - v₁t

vₓt V₂(t-T) V₀1

v, (t-Tk v t $N_2=0$ $v_2(t-T)$ v, t $v_2 t$ $N_2=0$ $R_2=v_2 T$

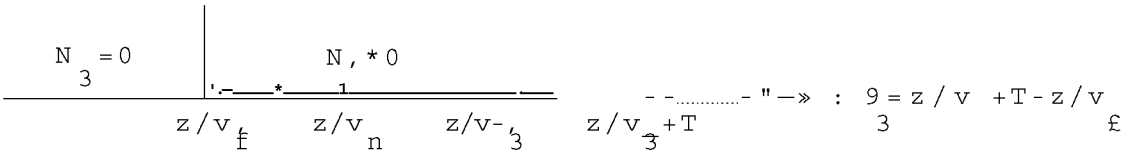
These results are summarized in Table 3„7.

D.3-Determination of the contamination time interval for the third member when $N^{\wedge}_0 \neq 0$ (Table 3.10).

The solution for the concentration o{the third member is expressed by Eq.3.5.15.One can distinguish two terns : the first term which represents the contribution of the third member nuclides initially present at the repository and the second term (brackleted term) which represents the contribution from the decay of the precursors.At a fixed position,the first term is non zero in the time interval (z/v^+T-z/v =T) because the function S(v t ;v^(t-T)) is non zero in this interval.The second term is non zero in the time interval (z,/v -z /v_) where v is the slowest
s f s
nuclide velocity and v^ is the fastest nuclide velocity.This is because at least two of the functions S(v.t?v.t) are non zero in this interval (see Table 3.8).When the two terms are added,the resultant concentration will be non zero in the sunerinnosed interval of the individual non zero time domains.The following diagrams show the different possibilities for the contamination time interval depending on the relative magnitude of the nuclide velocities.

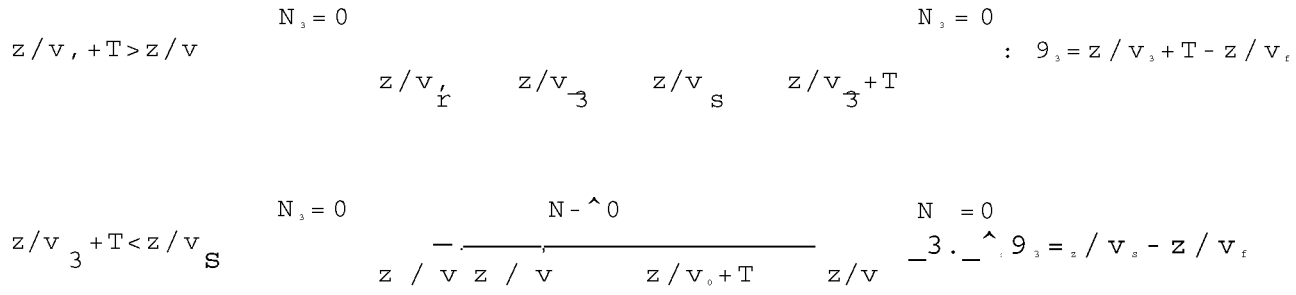
1)-When the third member is the slcwest nuclide,i.e. v =v$_t$

(case 1:v$_1$>v$_2$>v and case 6:v$_2$>v i>V3 in Table 3.3)



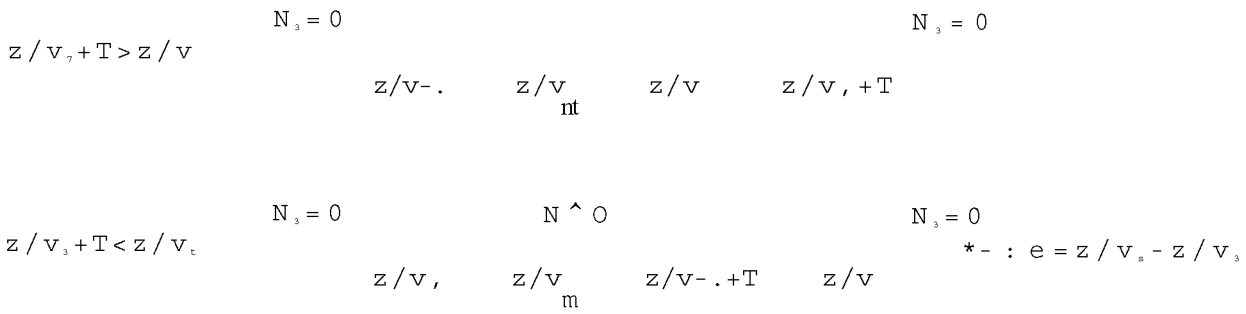
2)-When the third member has the intermediate velocity,i.e

v$_3$=v$_m$ (case 3:v$_1$>v$_3$>v$_2$ and case 4:v$_1$>v$_3$>v$_2$ in Table 3.5)



3)-When the third member is the fastest nuclide,i.e. v^=v

(case 2:v$_3$>v$_2$>v-^ and case 5:v3>v]>v? ^n Table 3.8)

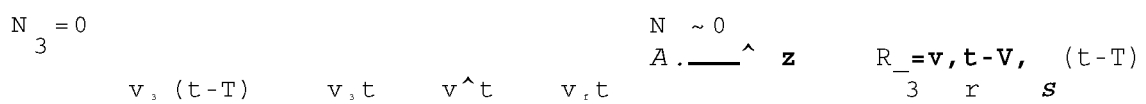


Above results are summarized in Table 3.10.

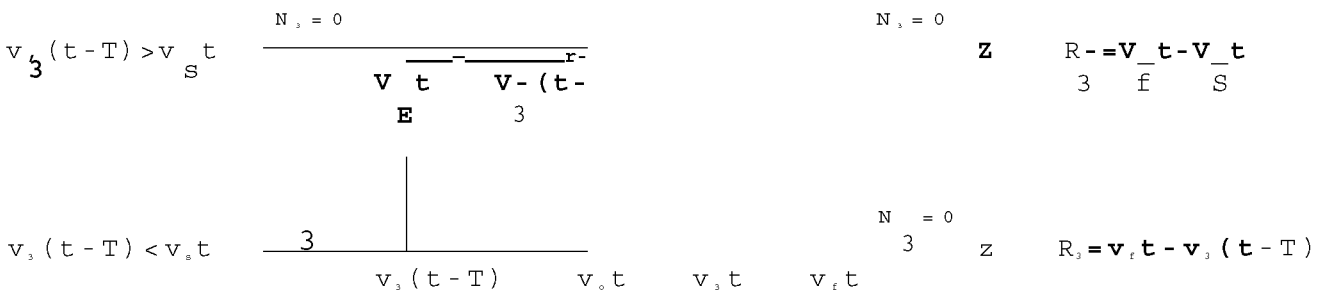
D.4-Determination of the contaminated region R_3 for the third member when N^^Vo (Table 3.10) .

Let us consider aoain the concentration distribution for the third member,as beina the superposition of two terms as discussed in D.3.At a fixed time,the first term is non zero in the reaion defined by ($v_3t-v(t-T)=v^T$) bdcause the function $S(v^t;v_3(t-T))$ is non zero in this region.The second term is non zero at a fixed time in the region (v t-v t) where,again,v stands for the slowest nuclide velocity and v_f stands for the fastest nuclide velocity.This is because at least two of the functions $(v^t;v..t) are non zero in this region (see Table 3.8).When the two terms are added,the resultant concentration wall be non zero in the region of the superposition of the two individual non zero concentration regions of each individual term.The following diagrams show the different possibilities for the contaminated region dependinn on the relative maanitudes of the nuclide velocities.

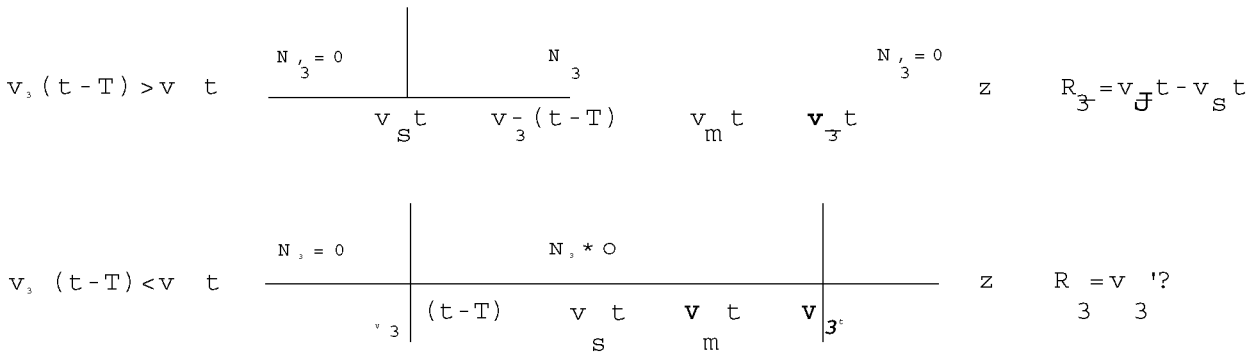
1)-When the third member is the slowest nuclide,i.e. $v_3=v_s$ (case $1: v_1>v_2->v_3$ and case $6: v_2>v_1>v_3$ in Table 3.3)



2)-When the third member has the intermediate velocity,i.e. $v_3=v_m$ (case $3: v^>v_3>v_2$ and case $4: v_3>v_3>v^$ in Table 3.8)



3)-When the third member is the fastest nuclide, i.e. $v_3 > v_f$ (case 2: $v_3 > v_2$ and case 5: $v_3 > v_f$ in Table 3.8)



Above results are summarized in Table 3.10.