# APPENDIX A - SYSTEM CODE REVIEW

## A.1 System Program Summaries

### AREST

The AREST code was developed by Pacific Northwest Laboratory for DOE. The program takes a modular approach to the problem of making preliminary, quantitative performance assessments of the engineered barrier and near-field systems. Input variables to the code include values assigned to the spent fuel waste package, as well as to variables describing the physical and chemical environments of the repository/near-field system and the waste package.

AREST models the performance of individual waste packages from repository closure to the failure of the cannister, the release of radionuclides from the failed packages, and the subsequent movement of the radionuclides away from the waste packages. Average release rates and cumulative releases over time can be calculated from successive waste package simulations.

The code cannot be considered as a total system code as it treats only various failure mechanisms for the waste packages and not the possible scenario classes creating the conditions for failure.

### SPARTAN

SPARTAN is a simple model developed by Sandia National Laboratories to support DOE's Environmental Assessment of a potential repository at Yucca Mountain, Nevada. Input, consisting of repository, hydrogeologic, waste package, and spent fuel characteristics, is used to simulate the one-dimensional, dispersionless transport of radionuclides in both a porous matrix and a fractured media.

Radionuclide release rates and cumulative curies released are calculated. From this, the performance of the repository can be measured relative to NRC performance objectives and to the EPA standard. The code does not take into account various scenarios.

### TOSPAC

Sandia National Laboratories developed TOSPAC for the Department of Energy specifically for the Yucca Mountain, Nevada site. It considers the one-dimensional transient unsaturated flow and transport of soluble waste materials with coupling between the matrix and fractures.

The code is a FORTRAN 77 program which uses various modules to manage the input and output tasks and to model the differential equations governing water flow, radionuclide transport, and liquid-phase mass transport. A management driver

oversees the interactions between these modules. Input to the code covers the material properties of the geologic strata, the radionuclide properties, and different boundary conditions. Output consists of release over time, nuclide concentrations in the matrix and fractures versus time, and three-dimensional plots of concentration vs. time vs. distance.

## REPRISK

REPRISK is an EPA program which models the long-term radionuclide release and population health effects associated with the disposal of high-level radioactive wastes in mined geologic repositories. It was originally developed for a repository located in a saturated, porous salt media and can address variations in geologic setting, radionuclide inventories, radionuclide release mechanisms and pathways, time frames, and dose uptake pathways.

The code handles four designated "release mechanisms": 1) direct impact of a waste package with release to air and land, 2) direct impact of a waste package with release to an aquifer, 3) disruption of the repository with release to land, and 4) disruption of the repository with release to an aquifer. REPRISK does not treat radionuclide decay chains and does not incorporate a random sampling program (like Latin Hypercube sampling) or any sensitivity and uncertainty analyses.

Consequences of a release to the accessible environment can be expressed as somatic or genetic health effects, a ratio of release amount to limits set in 40 CFR Part 191, and_or total curies released per radionuclide.

## SUNS

SUNS (Sensitivity and Uncertainty Analysis Shell) is a Sandia National Laboratories generic software shell created to perform Monte Carlo and LHS analyses. It is a modular menu driven code with a flexible input editor which can incorporate a variety of application models suitable for such analyses. The user provides replacement statements to equate model variable names to locations in the various SUNS arrays. The program is designed for parametric analyses and correlation studies.

SUNS performs all file management operations. Output is available in both statistical and graphical formats.

## Code Coupler

Sandia National Laboratories developed the Code Coupler programs to provide linkage between a suite of Sandia codes for a total system performance assessment. This linkage is given on two scales: 1) regional to local flow models, and 2) the local flow model and the radionuclide transport model.

Latin Hypercube sampling is used to create a common database for input in order to maintain a consistent description of the system for each of the models. Programs are available to plot estimated flow paths, discharge rates (Ci/day) vs. time (years), and complementary cumulative distribution functions (CCDFs).

## A.2 References


Bonano, E.J., et. al., 1989. Demonstration of a Performance Assessment Methodology for High-Level Radioactive Waste Disposal in Basalt Formations, U.S. Nuclear Regulatory Commission, NUREG/CR-4759, Washington, D.C.

Campbell, J.E. and D. Longsine, 1989. Application of Generic Risk Assessment Software to Radioactive Waste Disposal (Draft), Sandia National Laboratories, SAND89-1419C, Albuquerque, New Mexico.

Dudley, A.L., et.al., 1988. Total System Performance Assessment Code (TOSPAC) Volume 1: Physical and Mathematical Bases, Sandia National Laboratories, SAND85-0002, Albuquerque, New Mexico.

Engel, D.W., et.al., 1989. The AREST Code: User's Guide for the Analytical Repository Source-Term Model, Pacific Northwest Laboratory, PNL-6645, Richland, Washington.

Lin, Y.T., 1985. SPARTAN - A Simple Performance Assessment Code for the Nevada Nuclear Waste Storage Investigations Project, Sandia National Laboratories, SAND85-0602, Albuquerque, New Mexico.

U.S. Environmental Protection Agency, 1983. REPRISK Code Documentation, Arthur D. Little, Inc., Cambridge, Massachusetts.

Document Name:
MOU AB JAN9

Requestor's ID:
MCCARTIN

Author's Name:
codell

Document Comments:
jan 9 revisions of mou appendix b on source term model revie

App B

# APPENDIX B - SOURCE TERM CODE REVIEW

## B.1 Introduction

This appendix reviews models used in previous DOE analyses of the Yucca Mountain repository, and other models related to source term considerations in general. It is not a complete list, but probably covers most of the issues important to the source term for the Yucca Mountain repository.

## B.1 Review of Available Source Term Models Used for assessing the Yucca Mountain Project site

### B.1.1 Early DOE Assessment Models for Yucca Mountain

There are several preliminary, simplified assessments that were performed by DOE for the purposes of scoping the performance of YMP:

a. Environmental Assessment Model

The Environmental Assessment (DOE, 1986) model considered that there were three components of the repository; waste package, engineered barrier and geological barrier. The waste package would last 3000 to 30,000 years, during which time there would be no liquid releases of radionuclides. Their analysis adopted a 3000 year lifetime to achieve "some degree of conservatism". The source term model assumes that there would be congruent dissolution of the matrix, and the release rate is proportional to the water flow past the fuel and the solubility of the matrix. They estimate that for an infiltration rate of 0.5 mm per year, a fuel matrix solubility of 0.05 kilograms per cubic meter, and an infiltration area per canister of 0.33 square meters, there would be a fractional release rate by congruent solution of 2.5E-9 per year. The model does not take into account solubility limits for released radionuclides but assumes that with the exception of carbon, cesium, technetium and iodine, all solubility values would be less than or comparable to the value of the uranium dioxide matrix. The authors recognize that there are other sources of radionuclides in the pellet-cladding gap, hardware and clad, but except for C-14, they argue that the radionuclide inventories would not significantly affect their results for cumulative release. All C-14 releases are assumed to be from the matrix also, neglecting contributions from the cladding and gap compartments. Interestingly, a screening analysis they perform later indicates that most of the radionuclides would never reach the accessible environment except for carbon, technetium and iodine. Since these are the very elements that tend to collect outside of the matrix, neglecting the other compartments may be a weakness in this approach. This model appears to be virtually identical to that presented in Sinnock (  ).

b. The TOSPAC Model

TOSPAC--Total System Performance Assessment Code--is a more sophisticated one-dimensional model by Sandia (SAND 85-002), and considers transient

unsaturated flow in one dimension with coupling between the matrix and fractures. The source term model considers either complete dissolution of the matrix with release of all radionuclides (extremely conservative) or a more-realistic congruent release model. The congruent release model assumes 1) the fractional release rate of radionuclides from the spent fuel inventory is equal to the fractional leach rate of the uranium dioxide matrix; 2) the rate of waste matrix dissolution is a function of the solubility limit of uranium dioxide and the availability of water and 3) transport of dissolved species to the source boundary is instantaneous and the transport behavior in the near field region of the waste package where the rock is thermally and mechanically disturbed is similar in the adjacent undisturbed rock. They neglect any releases from other compartments than the uranium matrix, but acknowledge their potential importance. They limit the amount of release of radionuclide to less than or equal to its solubility in the water contacting the waste. This model would not appear to treat daughter products for chain decay unless all daughters had the same solubility. They claim in most cases that the solubility limit would be greater than the concentration, so the release is truly congruent.

The authors recognize that the assumptions about how liquid water contacts the waste to begin the release process is not well understood. They assume that all of the water intercepted by a container (the product of the infiltration rate and the cross-sectional area of the canister) becomes saturated with waste. They also recognize that additional mechanisms may limit the dissolution of the matrix such as diffusion out of the waste container, and that the advection-only model may be pessimistic.

Waste canisters are assumed to fail at a uniform rate, for lack of any data on actual failures.

### B.1.2 More Recent Modeling of YMP Performance

a. Yucca Mountain candidate site preliminary postclosure risk assessment, Doctor et.al., 1988.

This report describes what is probably the most sophisticated attempt at performance assessment for YMP to date, although it has never been officially published. Releases from the engineered barrier are evaluated using the AREST code (Liebetrau et al. 1987). The AREST model consists of three major components: The engineered system release (ESR) model, the Waste Package Containment (WPC) model and the Waste Package Release (WPR) model. The code treats waste packages individually with no interactions between adjacent waste packages. The WPC model simulates corrosion and degradation leading to package failure. The WPR model simulates release of radionuclides and their migration outward through the waste package barriers. The ESR model integrates the simulated releases from individual waste packages with respect to their failure time distribution. There is also a geochemical model to provide inputs to the three major component models. The authors used the concept of support models

external to the AREST code to perform site-specific calculations that are too time consuming or difficult to include in the overall simulation.

The AREST code uses detailed site specific information about the physical and chemical environment of the waste package and the repository. The code describes the thermal, geochemical and hydrological environments of the simulated waste package. The geochemical model determines the chemical environment of the waste package. The hydrologic model for the unsaturated case determines the time that the waste packages might be rewetted after they cool, although it appears that they only consider porous media and not the possibility of fracture flow near the waste package. For saturated conditions, the hydrologic model calculates the time to achieve resaturation following repository closure. For unsaturated media, the thermal model calculates the time for the waste package to cool to a point where liquid water can come into contact with it.

The containment model assumes several mechanistic models of uniform and pitting corrosion, as well as empirical models derived from site-specific testing. The model does not differentiate between canister and cladding containment. For the present calculation of the Yucca Mountain case however, they did not use a mechanistic code for waste package containment. Instead, they chose arbitrarily a normal distribution of failure times with mean of 1000 years and standard deviation 200 years, with the lower tail truncated at 300 years.

The WPR model takes two approaches, one for saturated and one for unsaturated cases. The saturated model assumes low oxygen levels (leading to low dissolution rate for the uranium dioxide matrix), low radionuclide solubilities and low groundwater flow rates, so that releases are based on diffusive mass transfer. For unsaturated media, the model assumes that the environment is oxidizing and that transport is likely to be convective rather than diffusive. Radionuclides are released from the waste matrix congruently at a rate given by the forward matrix dissolution and the fractional inventory of the nuclide in the matrix. The model chooses the larger of the diffusive/solubility release rate or the convective release rate. The release rate may be solubility limited if the rate of congruent release is high and the solubility of the released species is low. The model also looks at the non-matrix components of the source term, and treats those radionuclides accumulated in the interstices and cladding gap as solubility/transport limited until the inventory is depleted. The modelers recognize that the uranium dioxide matrix dissolution may not be truly controlled by solubility but rather instability in an oxidizing environment, so that the rate could remain non-zero even when the solution becomes saturated with respect to the matrix. The modelers limited the release of the matrix radionuclides on the basis of an oxidized and more-soluble uranium silicate mineral.

Even if release rate is not controlled by the solubility of the matrix and the radionuclide in question is not solubility controlled, the rate of release might still be controlled by diffusion away from the waste form rather than convection if the latter is very small. The models allows for certain of the

radionuclides to form colloidal species. Diffusion of colloids might also limit their release for very low flow rates. Since colloids have much smaller diffusion coefficients than molecular species, this rate must be very small when diffusion limited. It is not likely that both diffusion and convection need to be considered simultaneously for the Yucca Mountain case for any single species.

The WPR model makes no special provision for release of gaseous radionulides such as C-14 dioxide. It assumes that all of this inventory is released upon failure of the canister. The non-volatile radionuclides that are not contained in the matrix generally have high solubilities and do not form colloids in oxidizing environments.

The geochemical model is used to determine the chemical environment of the waste packages. The model calculates the steady state equilibrium concentration of J-13 water in equilibrium with the tuff at different temperatures and in a saturated condition. It does not treat radiolysis reaction between the water and the corroding canister material, sorption of radionuclides, and water vaporization or rewetting. These may be serious omissions that should be tested with support models. In particular, the consequences of corrosion products of the canister and other materials on the rate of corrosion and dissolution of radionuclides, and the effects of concentration of minerals in the near field resulting from the effects of heat and drying should be tested.

### B.1.3 Other Models not developed Specifically for YMP

#### 1. NEFTRAN Model

NEFTRAN is a Network Flow and Transport Model developed by Sandia National Laboratories, primarily for modeling of repository performance at saturated sites. NEFTRAN contains models for solubility limited or leach limited cases. If so desired, the program will determine whether a particular release is limited by leaching or solubility. A third model, mixing cell, assumes that the radionuclides are released into a well-mixed cell. The concentrations of the radionuclides in the cell is governed by flowrate through the cell, volume of the cell and solubility of the radionuclide species.

The source term model follows three radionuclide inventories. The first tracks the total mass of radionuclides remaining in the waste and is called the "unleached inventory". The second inventory is "undissolved"; that which has been released from the matrix by leaching, but whose release to the geosphere is limited by solubility. The third inventory represents dissolved radionuclides. Releases of radionuclides from the matrix depend on the leach rate of the matrix, i.e., congruent dissolution. Releases become part of the soluble compartment if their solubility is greater than the concentration, or part of the undissolved compartment if vice versa. Concentrations of different

isotopes of the same element are taken into consideration for solubility limits by specifying the fraction of the inventories for each isotope.

2. Analytic Models from University of California

The University of California, Berkeley, Earth Sciences Division has published a number of computer codes dealing mainly with the closed-form solution of flow and diffusive transport from waste packages and through the geosphere. Some of these solutions have been incorporated into the AREST code and the PNL assessment of Doctor et al. (1988). Some of the codes that may prove to be useful for defining the source term releases are (as reported by Lee, 1989):

UCBNE-101 - This code calculates the concentration of solubility-limited species as a function of space and time and its mass flux rate from a waste sphere buried in a nuclear waste repository in water saturated rock.

UCBNE-107 - This code calculates the fractional release rate of soluble radionuclides that are released from nuclear waste emplaced in water saturated porous media.

UCBNE-106 - This is a time-dependent version of UCBNE-107.

UCBNE-106D calculates the time history of the diffusion coefficient.

UCBNE-106N calculates the species concentration in the void water as a function of time.

UCBNE-106F calculates the fractional release rate of the species at the void/rock interface as a function of time.

UCBNE-108 calculates the mass flux rate and the fractional release rate at the interface between the first layer of porous material and the next layer of porous material of soluble species released in water-saturated porous media.

UCBNE-102 calculates the mass flux of the non-decaying contaminant outward from a spherical waste form when there is a stationary precipitation at a prescribed distance from the waste separating an inner region of higher solubility and an outer region of lower solubility.

In addition to these codes that are specifically for near field phenomena, there are a set of UCB codes that integrate the source term and the transport models. In order to get analytical solutions, the source term part of these models must be simple, either an impulse (i.e., instantaneous release), a step function in concentration or flux (band release), or a concentration boundary. None of these models can handle solubility limits, because these are inherently non-linear and cannot usually be solved in closed-form. The models can treat the releases of chain-decaying radionuclides in the source, providing their

concentrations can be expressed by the Bateman equations and are not distorted by preferential removal of daughters.

3. CONVO

CONVO is a code developed for NRC to model the performance of the waste canisters and engineered barrier (Ref ). The code was primarily developed for demonstrating compliance with the NRC annual release criteria in 10CFR60.113, rather than the cumulative release criteria of EPA as embodied in 10CFR60.112. CONVO has three models for release of radionuclides, but they all have the same weaknesses in common; they assume that the radionuclides are released at the surface of the waste package through a porous packing material, and that release is limited by diffusion alone. There is no consideration given to the rate at which the radionuclides are released from the $UO_2$ matrix, or other compartments in the fuel. The code was targeted mostly to a saturated, low-velocity, low solubility groundwater system in which diffusion rather than advection was assumed to be the dominant transport mechanism for the release of radionuclides from the waste packages. It appears that in its present form that CONVO would be of little use as a source term model at YMP.

## B.2 References


DOE, 1986 "Environmental Assessment, Yucca Mountain Site, Nevada"

Sandia, SAND 85 - 002

Doctor, 1988

Liebetrau, 1987

NEFTRAN

UCB

CONVO

Document Name:
MOUA1.3

Requestor's ID:
NICHOLSO

Author's Name:
tjm

Document Comments:
appendix 1.3

App C

# APPENDIX C - FLOW AND TRANSPORT CODE SUMMARIES

## C.1 Regional Flow Program Summaries

### SUTRA

SUTRA (Voss, 1984) solves the equations for fluid density-dependent saturated or unsaturated ground-water flow and either transport of a solute in the ground water or transport of thermal energy in the ground water and solid matrix. Solute transport in ground water includes equilibrium adsorption on the solid matrix, production, and decay. Additionally, SUTRA may be used to examine variable density leachate movement and salt water intrusion. While energy transport simulations can be performed with SUTRA, the program only simulates the liquid phase without any consideration for phase changes.

The program uses an integrated-finite-difference method to approximate the governing equations. The finite element mesh can accommodate arbitrary geometries employing quadrilateral finite elements in Cartesian (one or two dimensions) or radial-cylindrical (quasi three dimensions) coordinate dimensions.

Explicit treatment of fractures is not accounted for in the model. However, a dual porosity type of treatment for simulating fracture matrix interactions would be possible through the use of a composite characteristic curves.

### VAM2D

VAM2D (Huyakorn, 1989) is a two-dimensional, finite element program developed to simulate moisture movement and solute transport in variably saturated porous media. In solving the governing equations for ground-water flow the program can take into account hysteretic moisture characteristics and variable (due to moisture content) anisotropy in the hydraulic conductivity of the unsaturated media. The program is capable of simulating the transport of chains of radionuclides that accounts for retardation phenomena via a linear equilibrium isotherm.

VAM2D uses a finite element method to solve the flow and transport equations. Time integration is performed using implicit finite difference approximations with non-linearities being handled with either Picard or Newton-Raphson iteration schemes. Additionally, the iterative methos employs the Preconditioned Conjugate Gradient, PCG, for solving the matrix equations (the PCG method has recently emerged as very promising technique for handling the numerical difficulties of ground-water modeling).

The current version of VAM2D has no capability to handle fracture-matrix problems. Future (1990) development of the program will include a capability to account for fractures via a composite characteristic curve.

TRACER3D

The TRACER3D program (Travis, 1984) simulates two phase mass flow and transport in a three-dimensional, deformable, heterogeneous, reactive porous medium. The program solves the equations for mass conservation of the liquid and gas and a reduced form of the momentum equation. The preogram has the flexibility to solve a one-dimensional, single phase flow problems or include feature such as additional dimensions (up to three-dimensions), the gas phase, and solute transport.

The partial differential equations are approximated using an integrated-finite difference scheme. The iteration procedure is implemented using a Gauss-Seidel or SOR method.

TRACER3D does not explicitely account for fractures, although, the geometric flexibility integrated finite-difference approach would allow for discretizing very small elements which would tend to simulate fractures. However, the program represents the relative conductivity with the Brooks and Corey expression which is reasonable for porous media but may be unacceptable for fractures.

## C.2 Two-Phase Flow and Heat Transport Program Summaries

TOUGH

TOUGH (Pruess, 1987) solves the equations for two-phase flow of air and water in the vapor and liquid phases, and heat transport in a fully coupled way. The formulation used in TOUGH is analogues to that used in multiphase, multicomponent geothermal or steam-flooded hydorcarbon reservoir problems. The governing fluid flow equations account for gaseous diffusion, Darcy flow, capillary pressure, vaporization and condensation with latent heat effects, and conduction and convention of heat are included in the energy equation. Water, air, and rock are assumed to be in thermodynamic equilibrium at all times. The flow domain can include liquid, gas, and two-phase regions, indicating that the code handles both saturated and unsaturated flow problems either individually or simultaneously. The thermophysical properties of liquid and vaporized water are represented by the International Formulation Committee's (1967) steam tables. Air is approximated as an ideal gas and additivity of partial pressures is assumed for air-vapor mixtures.

TOUGH solves three nonlinear partial differential equations simultaneously. These are the conservation equations for air, water, and heat. Air and water can be transported in either the liquid, gas phase, or both. The dissolution of air in water is represented by Henry's law and flow (gas and liquid) by Darcy's law.

The code can simulate flow in one, two, or three dimensions because the method of solution is based on a general integrated finite-difference method. Time stepping is accomplished by a fully implicit procedure. The resulting non-linear difference equations are linearized by the Newton-Raphson technique.

The linearized equations are solved by the Harwell matrix solver that stores only the nonzero elements of a matrix thus reducing core storage requirements for the code.

## NORIA

NORIA (Bixler, 1985) is designed to simulate liquid, vapor, air, and energy transport in partially saturated and saturated porous media. The following mechanisms are included in NORIA: (1) transport of water, vapor, and air due to pressure gradients; (2) transport of water, vapor, and air due to density gradients; (3) binary diffusion of vapor and air; (4) Knudsen diffusion of vaport and air; (5) thermo-diffusion of vapor and air; (6) conduction of sensible heat; (7) convection of sensible heat; (8) evaporation and condensation; (9) nonequilibrium and equilibrium vapor pressure model; and (10) capillary pressure. Nearly all the thermodynamic and constitutive properties in the code can be defined nonlinearly in terms of the remaining dependent or independent variables by the user.

NORIA solves four nonlinear partial differential equations governing the flow of water, vapor, air, and energy. These equations consist of a water-pressure equation, a vapor partial-pressure equation, an air partial-pressure equation, and a heat equation. The equations are solved by the Galerkin finite-element method. Time stepping is accomplished by a two-step time integrator with automatic time step selection. The nonlinear difference equations formed by application of the finite-element method are solved simultaneously by Newton-Raphson iteration. Normally, a one-step iteration is used; however, a multistep iteration is used if the correction on the first iteration is larger than a specified amount.

## PETROS

PETROS (Hadley, 1985) is designed to simulate problems similar to those simulated by NORIA. PETROS solves the same number and types of nonlinear equations and handles the same physical processes as NORIA, but in a slightly different manner. The main difference between the two codes is that PETROS solves only one-dimensional problems, either in linear, radial, or spherical coordinates, and solves the equations with the finite difference method. There are also some difference between the codes in the way the time integrations are performed. PETROS uses a modified version of the time integrator in NORIA.

PETROS solves three mass conservation equations and a heat conservation equation just as NORIA. However, the liquid conservation equation is PETROS is formulated with respect to saturation rather than pressure as in NORIA. The characteristic curves and the thermal conductivity as a function of saturation and temperature are supplied to PETROS through user-written function subprograms. Other parameters such as diffusion coefficients, water viscosity, saturation vapor pressure of water, and default values of the characteristic curves and thermal conductivity are supplied internally in the code as function subprograms. Constants such as gas viscosity, specific heats, and water density can either be set at default values or supplied by the user. The user can also choose between equilibrium and nonequilibrium vapor-pressure models.

The above equations are solved numerically by a finite-difference method. The equations are differentiated in both space and time. Differentiating in time results in fully implicit equations. The saturation and temperature equations are solved with a tridiagonal algorithm. Because the vapor and air pressure equations are stongly coupled, they are solved with a block tridiagonal algorithm.

## C.3 Geochemical Program Summaries

### PHREEQE

PHREEQE (Parkhurst, 1980) was developed to model geochemical reactions between water and rock material. Based on an ion-pairing aqueous model, the program calculates pH, redox potential and mass transfer as a function of reaction progress. The program performs a mass balance of elements in terms of their concentrations in the aqueous phase and uses electrical neutrality and electron balance relations to complete the set of equations needed to solve a given problem.

The program solves a set of nonlinear algebraic equations using a combination of a continued-fraction approach for mass balance and a Newton-Raphson iteration technique.

### EQ3/6

EQ3/6 (Wolery, 1979) was developed to compute equilibrium models of aqueous geochemical systems. EQ3 performs distribution-of-species calculations for natural water compositions. EQ6 uses the results of EQ3 to predict the consequences of heating and cooling aqueous solutions and of irreversible reaction in rock water systems. Reaction path modeling is useful in analysing complex systems wherein analytical data do not permit the definition of reactions by mass balance alone.

The program uses a Newton-Raphson method to solve the algebraic governing equations of chemical equilibrium.

### WATEQF

WATEQF (Plummer, 1976) simulates the thermodynamic speciation of inorganic ions and complex species in solution for a given water analysis. The program provides a general capability to calculate chemical equilibria in natural waters at low temperatures.

WATEQF uses a successive approximation method to solve the mass action and mass balance equations.

CHEMTRAN

CHEMTRAN (Miller, 1983) was developed to simulate one-dimensional transport of chemical species in ground-water. Equilibrium is assumed in all chemical reactions and thermodynamic activities of all reacting species are related by mass-action expressions. The program includes the effects of dispersion and diffusion, advection, sorption via ion exchange or surface complexation, aqueous complexation, precipitation and dissolution of solids, and the dissociation of water.

The governing equations are approximated using a finite difference approach. A Newton-Raphsom iteration technique is used to to solve the system of equations.

## C.4 Transport Program Summaries

SPARTAN

The SPARTAN code is a simple performance assessment code for YMP by Y.T. Lin at Sandia National Laboratories. The model employs a simplistic hydraulic model for flow of water infiltrating the surface and reaching the water table. This model has little in the way of a mechanistic explanation for the way water would flow at YMP. The rate of infiltration in the matrix is assumed to follow Darcy's law, with a gradient of unity, a fixed permeability and fixed effective porosity. For infiltration rates less than 1 mm/year, the speed of groundwater movement is proportional strictly to the infiltration rate and does not take into account the change of hydraulic conductivity with moisture content. For infiltration rates greater than 1 mm/yr the model assumes that a fraction of the water infiltrating will move through the fracture zone faster than through the matrix and with transport properties typical of fractures. The transport model takes radioactive decay and a linear sorption ($K_d$) into account. It allows different retardation factors for daughters and parents.

The SPARTAN code was apparently used for some very preliminary assessments of YMP. The test cases the authors demonstrated considered that there were 2 or 3 pathways for transport which was supposed to represent the different lengths from the repository to the water table. There were two pathways for matrix flow for the case of 0.5 mm/yr infiltration. For 5 mm/yr infiltration, they assumed that the water in excess of what the matrix could carry would travel through a third pathway as fracture flow. For the former case, only I-129, C-14 and Tc-99 would reach the accessible environment within 100,000 years. For the latter case, many more of the radionuclides would be released to the accessible environment.

TOSPAC Model

TOSPAC (Dudley, 1987), the Total System Performance Assessment Code, is a computer program designed to simulate water flow and transport of soluble waste in fractured porous unsaturated rock. The groundwater flow module solves either the transient or steady state partial differential equations for an equivalent porous-fractured medium in which the properties of the matrix and

fractures are combined into one constitutive relationship for saturation versus hydraulic conductivity (or matrix potential versus hydraulic conductivity). The site is represented as a series of one-dimensional flow tubes with no lateral interchange. Within any one flow tube they solve either the steady state or transient flow equation for the equivalent matrix-fracture relationship. For steady state, the solution is iterative to allow the self-adjustment of the hydraulic conductivity and saturation values to correspond to the constitutive relationships for each layer. Once the solution reaches steady state, the hydraulic conductivity is known, and consequently so is the net downward flux and groundwater velocity that can then be used in the transport calculations. The transient solution solve for pressure head with a numerical solution of Richard's equation using Pickard iteration.

The module for radionuclide transport uses the velocities calculated from the flow module. First, the code estimates the fraction of flow in the matrix and fracture flow paths. Concentrations of each radionuclide are calculated for the matrix and fracture compartments with a dynamic coupling between them.

NEFTRAN

NEFTRAN (Longsine, 1987) is a network flow and transport code developed primarily for the NRC program in salt and other saturated rock repositories. The flow model in NEFTRAN consists of an arbitrary network of one-dimensional pipes, connected at nodes. Boundary conditions of pressure are set on some of these nodes, and the hydraulic properties of transmissivity and porosity are set within the pipes. The network model then solves for the steady state velocity and flux within the network. Radionuclides are transported in the network by the calculated flux. The model uses retardation factors to express the speed at which a particular species is transported. It also allows for transport between the actively flowing legs and immobile water adjacent to the leg in order to simulate matrix diffusion. Chain radionuclides can be transported also. There are two models for chain transport; the first model assumes equal retardation coefficients and up to a three component chain. The other model allows arbitrary retardation coefficients for chains up to 6 daughters. The former model is however much less time-consuming. NEFTRAN simulates dispersion along the legs using the Distributed Velocity Method (DVM) which assumes that dispersion is caused by the distribution of velocities in the flow field.

In its present form, NEFTRAN is not ideally suited for performance assessment modeling at YMP for the following reasons:

1. The model is set up for boundary conditions which are appropriate for a saturated site.

2. The flow model is for steady state coditions. (Transient recharge may be an important consideration at YMP)

3. The model assumes that the source term is concentrated in one leg only, and cannot represent source terms highly distributed in time and space. This limitation did not seem to be as important for saturated sites where the flow was more horizontal than vertical, but would be a potentially serious limitation at YMP.

NEFTRAN is being modified now under Research contract A-1266 specifically for the Yucca Mountain case, and some of these limitations should be overcome. Sandia is developing a multidimensional finite difference model to calculate steady state and transient unsaturated flow in porous media. The output of this code will be fed directly into a modified NEFTRAN that can accept flux boundaries and transient flow conditions. If the flow model shows unusual flow patterns, the network in NEFTRAN can be modified to accommodate this, but cannot be modified within a single run for transient conditions. The source term still will not be represented by more than one leg, and therefore cannot truly simulate the highly distributed YMP case. The limitation of a distributed source might be partially overcome by clever sampling of the path length, flow and release times in their systems analysis. (This would hold true for any of the one- dimensional approaches.)

The modified version of NEFTRAN will not be available in time for the present NRC effort on Performance Assessment demonstration.

Analytic codes

There are a large number of analytical codes (i.e., closed form solutions) available that could serve to calculate flow and transport, particularly for one-dimensional steady flow in which there are really few considerations as to whether the flow is saturated or unsaturated. The University of California Berkeley (UCB) codes combine simple source term models with analytical solutions for one-dimensional, steady state flow, and radionuclide transport. The UCB codes have been used in a number of important US studies (e.g., WISP report and AREST code development). These codes are unique analytic solutions due to the fact that they have explicit solutions for chain decay with differing retardation coefficients for each daughter. However, the incorporation of more than one hydrologic layer may not be possible with the solution technique. This would make application to the Yucca Mountain site, where there are several distinct layers with different material properties, difficult.

Another class of analytical codes is Laplace Transform domain solutions (Robinson, Hodgkinson, et al.). The source term, transport model and even stochastic solution can be set up using this method, solving the linear differential equations in the Laplace domain and getting the time domain solution by numerical evaluation of the contour integral in the complex plane. This solution technique should be relatively easy to apply to the problem of transport through multiple layers. The recent development and progress of this solution technique in the United Kingdom needs to be followed for latter use in performance assessment.

## C.5 References

Bixler, N.E., NORIA - A Finite Element Computer Program for Analyzing Water, Vapor, and Energy Transport in Porous Media, SAND84-2057, Sandia National Laboratories, Albuquerque, New Mexico.

Dudley, A.L., et. al., 1987, Total Systems Performance Assessment Code (TOSPAC) Volume 1: Physical and Mathematical Bases, Sandia National Laboratories, SAND85-0002, Albuquerque, NM.

Hadley, G.R., PETROS - A Program for Calculating Transport of Heat, Water, Water Vapor, and Air Through Porous Material, SAND84-0878, Sandia National Laboratories, Albuquerque, New Mexico.

Huyakorn, P. S., 1989, VAM2D - Variably Saturated Analysis Model in Two Dimensions, U.S. Nuclear Regulatory Commission, NUREG/CR-5352, Washington, D.C.

Longsine, D. E., Bonano, E. J., and Harlan, C. P., 1987, User's Manual for the NEFTRAN Computer Code, U.S. Nuclear Regulatory Commission, NUREG/CR-4766, Washington, D.C.

Pruess, K., 1987, Tough User's Guide, U.S. Nuclear Regulatory Commission, NUREG/CR-4645, Washington, D.C.

Parkhurst, D.L., Thorstenson, D.C., and Plummer, L.N., 1980, PHREEQE - A Computer Program for Geochemical Calculations, U.S. Geological Survey, Water Resources Investigations 80-96, Reston, VA.

Plummer, L.N., Jones, B.F., and Truesdell, A.H., 1976, WATEQF - A Fortran IV Version of WATEQ, A Computer Program for Calculating Chemical Equilibrium of Natural Waters, U.S. Geological Survey, Water Resources Investigations 76-13.

Rasmussen, T.C. and Evans, D.D., 1987, Unsaturated Flow and Transport Through Fractured Rock Related to High-Level Waste Repositories, Final Report-Phase II, U.S. Nuclear Regulatory Commission, NUREG/CR-4655, Washington, D.C.

Thomas, S.D., Ross, B., and Mercer, J.W., 1982, A Summary of Repository Siting Models, U.S. Nuclear Regulatory Commission, NUREG/CR-2782, Washington, D.C.

Travis, B.J., 1984, TRACR3D: A Model of Flow and Transport in Porous/Fractured Media, Los Alamos National Laboratory, LA-9667-MS, Los Alamos, New Mexico.

Updegraff, C.D., 1989, Comparison of Strongly Heat-Driven Flow Codes for Unsaturated Media, U.S. Nuclear Regulatory Commission, NUREG/CR-5367, Washington, D.C.

Voss, C.I., 1984, SUTRA (Saturated-Unsaturated Transport) - A Finite Element Simulation Model for Saturated-Unsaturated, Fluid-Density-Dependent Ground-Water Flow with Energy Transport or Chemically-Reactive Single-Species Solute Transport, U.S. Geological Survey, Water-Resources Investigations Report 84-4369, Reston, VA.

Wolery, T.J., 1979, Calculation of Chemical Equilibrium Between Aqueous Solution and Minerals: The EQ3/6 Software Package, Lawrence Livermore Laboratory, Lawrence Livermore Laboratory Report UCRL-52658, Livermore, CA.

Document Name:
AUXPATH JAN 9

Requestor's ID:
MCCARTIN

Author's Name:
codell

Document Comments:
jan 9 revision to c14 pathway

App. D

Appendix D
Auxiliary Analysis - Gaseous Releases of C-14

## D1. Introduction

C-14 is produced in nuclear reactors by the activation of nitrogen impurities in the fuel cladding, and by the activation of O-17, particularly in the uranium oxide fuel and in the circulating water of light water reactors. The release of Carbon-14 from the waste packages is a potentially serious problem at the Yucca Mountain repository because there is at least the possibility of a fast pathway to the accessible environment through the unsaturated fractured rock, excavations and tunnels. Except for the possible relationship between canister lifetime and water influx, the release and transport of C-14 to the atmosphere appear to be largely decoupled from the liquid pathway analyses presented in the body of this report. We conservatively treat C-14 in the liquid pathway analysis by including the total release rate going into solution. In this Appendix we present models for the release of C-14 from the engineered barrier and its transport through the gas pathway to the accessible environment.

## D2. Source Term

Carbon-14 is found in quantities at least ten times greater than would be allowed under 40CFR191 if all were released. It has a half life of 5720 years. The majority of environmental C-14 comes from interaction of cosmic ray neutrons and nitrogen, although it is also created by activation of the rare O-17 isotope in the atmosphere (van Konynenburg, 1987). It is produced in great quantities in atmospheric nuclear explosions through neutron activation. Once in the atmosphere, C-14 is removed from the environment mainly by absorption in the bicarbonate ions in seawater with an apparent relaxation time (i.e., time for half to disappear from the biosphere) of approximately 9 to 15 years (Till, 1983). A portion of the C-14 recycles through the food chain and is very biologically active. The combination of biological activity and long half life lead to relatively large population doses per curie released.

In reactor fuel, C-14 is produced by the same mechanisms as in the atmosphere. The main routes to production are 1) activation of nitrogen impurities in the metallic structure of the reactor and the cladding of the fuel and 2) activation of O-17 in the uranium dioxide fuel and in the circulating water of the reactor, with subsequent deposition onto the cladding and other structural material.

Measurements indicate that about 1/3 of the total C-14 inventory resides on the cladding of PWR fuel, but similar measurements for BWR fuel are not available (van Konynenburg, 1987). The staff expects that BWR fuel will be different because of the different oxidation potential present in the reactors. There is little or no information on inventories for other non-fuel parts of the reactor.

The two mechanisms for producing C-14 in the reactor are important to understanding its availability. Presumably, C-14 created by activation of nitrogen would be dispersed in the cladding because the nitrogen would also be dispersed. Much of the C-14 appears to be from the oxygen activation mechanism, and is adsorbed onto the cladding, fairly close to the surface. This fact may be important because it allows the C-14 to be more readily accessible to the environment than if it were uniformly dispersed in the cladding.

D2.1 Possible release modes at Yucca Mountain

Most of the C-14 is apparently in the form of elemental carbon, metal carbides or oxycarbides (van Konynenberg, 1987). In inert nitrogen and helium atmospheres, spent fuel does not readily release its C-14. Upon exposure to air, however, some of the C-14 oxidizes and is usually released to the immediate atmosphere as C-14 dioxide. About 1 to 2 percent of the available C-14 inventory could be released quickly by this mechanism, but it is mainly the C-14 that is deposited on the surface as crud, or collected on the intergrain boundaries of the fuel (van Konynenburg, 1987). For elemental carbon, release could depend upon oxidation to carbon dioxide and carbon monoxide, the rate of which is extremely slow at low temperatures. Elemental carbon is known to be extremely stable under normal conditions, as is evidenced by the presence of graphite in schists exposed for thousands of years at the earth's surface. There is some experimental evidence to suggest however that carbon will oxidize to carbon dioxide at a temperature of 275°C within a radiation field of 10,000 rads per hour (van Konynenberg, 1987). Temperatures of the fuel may be in this range for the first few decades after storage, but are likely to be considerably cooler near the time required for minimum canister life. Radiation levels of 10,000 rad/hr are likely to be present for up to about 100 years. While the radiation field diminishes with time, we do not have any experimental evidence to indicate that there is a threshold below which no oxidation would occur. For the sake of conservatism, we assume that there is a mechanism available to oxidize available carbon to gaseous carbon dioxide for the lifetime of the repository.

The more likely C-14 release mechanisms at Yucca Mountain are:

- Dissolution of the cladding and oxidation of the C-14 attached to the cladding, e.g., crud.

- Quick release of a small percentage of carbon dioxide gas from the cladding-pellet gap upon failure of the cladding.

- Diffusion of oxygen into the waste form, particularly the matrix, reaction of the carbon with the oxygen and the subsequent diffusion of carbon dioxide out of the matrix.

Other possible mechanisms might also release C-14 but we have little or no direct evidence that they apply:

- Galvanic reaction between elemental carbon in the cladding or metal carbides and the surrounding metal in the waste form.

- Reaction of metal carbides on the zirconium or uranium with water to form acetylene gas (Katz and Rabinowitz, 1951).

- Biological action of carbon or some carbon compound in the waste.

- Release of methyl iodide created from the reaction of carbon and iodine present in the fuel This could be a potential release mechanism for I-129. Methyl iodide would be volatile at temperatures of about 200°C expected in the repository during the first few decades after site closure.

The staff has little direct evidence to support a model for C-14, but have chosen what we consider to be the most likely mechanisms, and cover them below in their order of expected importance. We apply these mechanisms to our C-14 release model and have in all cases chosen conservative ranges of parameter values to apply to these models. We must stop short of stating that the overall models are conservative, however.

### D2.1.1 Releases due to Oxidation of Uranium Dioxide

We assume that the C-14 trapped within the uranium dioxide fuel will be released at a rate coupled to the rate of oxidation of the fuel. Uranium dioxide is unstable in an oxidizing environment, and oxidizes to other forms, with corresponding increases in volume, porosity and fracturing in many cases. If the reaction proceeds fast enough, the $UO_2$ will spall, becoming more porous and less dense. The increase in volume could promote continued cracking of the cladding, allowing more pellets to be exposed.

Spallation is an indication that significant oxidation has occurred and may also provide for increased exposure of the C-14 to oxidants. Both $UO_2$ and C will be competing for the oxidants. From thermodynamic considerations alone, carbon would be oxidized first at low oxygen activities, followed by oxidation of $UO_2$ at higher oxygen activities. However, the relative rates of the competing reactions probably govern how the components of the spent fuel will be oxidized. Einsiger and Woodley (1985a) state that for irradiated fuel the uranium dioxide crystalline structure is damaged and pellets are fragmented, thereby opening more surface area to oxidation. In addition, gas bubbles and fission products may migrate to the grain boundaries where the interconnected paths can form, making grain boundaries preferential sites for oxidation. The radiation field can ionize or excite atmospheric oxygen or water, possibly enhancing the oxidation rate.

Einsiger and Strain (1984) present two curves bounding the time to spallation $t_s$ as a function of temperature T:

$$\log t_s = (0.78 \times 10^{-4}/T) - 13.01 \qquad \text{(D1)}$$

$$\log t_s = (1.03 \times 10^{-4}/T) - 15.9 \qquad \text{(D2)}$$

where $t_s$ is in given in hours, T in degrees Kelvin, and log denotes the base 10 logarithm. Equations D1 and D2 are not directly useable to determine the rate of release of C-14 because they are formulated with steady temperatures in mind. Since the fuel temperature changes with time, it is more convenient to convert spallation time to an oxidation rate. If we assume that the rate of oxidation $\lambda_s$ is the reciprocal of the spallation time $t_s$, we can then define a time-dependent rate of C-14 release:

$$\lambda_s = 1/t_s \qquad \text{(D3)}$$

This model may be conservative from the standpoint that the time for the onset of spallation does not signal the total oxidation of the fuel pellets. On the other hand, the rate of release of C-14 may not be as low as indicated for long spallation times that occur at lower temperatures.

D2.1.2 Oxidation of Zirconium

A large fraction of the C-14 inventory may be in the cladding, caused by neutron activation of O-17 picked up from the circulating water particularly in BWR's, or nitrogen impurities in the metal itself. Corrosion of the zirconium may be the first step in releasing the C-14 to the atmosphere, although it is possible that this corrosion may not be necessary to initiate release. In addition, cladding corrosion leading to perforation could expose the $UO_2$ to oxidation.

Oxidation of the cladding has been studied for the case of dry cask storage of spent fuel. Einziger and Kohli (1984) present a rate equation for zirconium cladding in terms of temperature:

$$L = 3.68E8 \times t \times \exp(-15810/T) \qquad \text{(D4)}$$

where L is the oxide thickness in millimeters, t is the time in years, and T is the absolute temperature, degrees K. To find the growth of zirconium oxide layer with time, we first convert Eq.D4 to a rate, and integrate from the time of failure $t_f$, using the expected temperature of the waste:

$$L = \int_{t_f}^{t} 3.68E8 \quad \exp(-15810/T(t))\, dt \qquad \text{(D5)}$$

The calculated oxide thicknesses are presented in Table D1 for a typical fuel temperature ranging from a high of 320 to 110 degrees C over 10,000 years.

Table D1 - Calculated zirconium oxide thickness

| Temperature | t-yrs | L-mm |
|---|---|---|

| | | |
|---|---|---|
| 320 | 5 | 4.9E-3 |
| 300 | 25 | 1.25E-2 |
| 275 | 50 | 1.52E-2 |
| 250 | 75 | 1.59E-2 |
| 230 | 100 | 1.61E-2 |
| 200-110 | 10000 | 1.62E-2 |

A typical cladding thickness is 0.61 mm, so the maximum oxide growth is only about 3% of the total thickness. Most of the oxidation takes place when temperatures are highest, with virtually none after about 100 years.

Einsiger and Woodley (1985a) also describe a possible condition that might affect the rate of cladding failure in the absence of oxygen. Canisters might contain a few tens of milliliters of water from rods stored in cooling pools. The radiolysis of the water could provide oxidants that could oxidize the cladding (Reed, 1987).

The ramifications of zirconium oxidation are not entirely clear. It appears that there would be relatively little oxidation of the zirconium in the repository. If the fuel is kept cool; e.g., in wet storage casks prior to being placed in the canisters, the reaction would not proceed very far. It would be more oxidized in dry storage, but might be inhibited by the presence of inert atmosphere in the canisters. Although the percent oxidation may be small, most of the C-14 might be close to the surface as crud, or attached to an existing oxide coating since it might have been picked up externally from the circulating water. The fact that little if any oxidation of the zirconium alloy occurs at temperatures lower than about 230 C leads to a tentative conclusion for the purposes of this study that there will be little additional zirconium oxidation after canister failure. We will assume therefore that only the readily available portion of the C-14, about one percent, will be driven off during the pre-canister-failure period, and that there will be no additional releases from the zirconium compartment. Corrosion of the cladding might be relatively more important if it causes perforation, allowing oxygen to reach and oxidize the spent fuel matrix.

## D2.2 Proposed Source Term Model

We have chosen for the Phase 1 study to employ the following model for the release of gaseous carbon from the engineered barrier incorporating the mechanisms discussed above:

- Canisters fail at a rate predicted by a normal probability distribution. We chose two different distributions to demonstrate the sensitivity of the C-14 release to the waste package lifetime.

- At the time of canister failure, oxygen will enter the canister and become available immediately to react with the uranium dioxide in the fuel rods. Although most fuel rods will have additional protection from oxidation based on resistance to corrosion of the zirconium alloy cladding, we will

assume for the purpose of conservatism that all fuel rods are available for release of their C-14 inventories.

- On failure of the canisters, a small fraction of the C-14 inventory is released rapidly. This fraction represents the C-14 inventory of the cladding-pellet gap and the C-14 close to the outside surface of the cladding or crud that would be readily oxidized.

The cumulative fractional release rate of C-14, f(t), is calculated based on the random failures and oxidations of a large number of canisters to which is added the fractional prompt release $f_p$ from the canisters at the time of failure $t_f$:

$$f(t) = \frac{1}{N} \sum_{i=1}^{N} \int_{t_{fi}}^{t} [\lambda_{si}(t) + f_p \, \delta(t-t_f)] \, dt \qquad \text{(D6)}$$

where N is the number of canisters, and $\delta$ is the Dirac delta function at time $t = t_{fi}$.

D2.4 Results of Source Term predictions

Figure D1 illustrates the fraction of the total C-14 inventory released up to 10,000 years for two different assumed canister failure models. The higher release curve (solid) corresponds to canister failure with a mean failure time of 550 years, a standard deviation of 150 years and an upper and lower limit of 100 and 1000 years respectively. The lower (broken) curve corresponds to a mean failure time of 1000 years, a standard deviation of 300 years and an upper and lower limit of 200 and 1800 years respectively. The maximum cumulative releases were about 13.2% and 2.5% respectively, illustrating the strong dependence of C-14 release on waste package lifetime.

D2.5 Limitation of the C-14 Source Term Model

The C-14 release model has been based on the following limiting assumptions:

- A non-mechanistic failure of all canisters in a time short relative to the half life of C-14 and the 10,000 year period of interest.

- An influx that upon canister failure of sufficient oxygen to cause unimpeded fuel oxidation. Oxygen will not be consumed by other reducing agents such as the canister walls and metal components of the fuel assemblies.

- The highly corrosion-resistant cladding on the fuel is assumed to offer no protection from oxidation.

- A prompt release from the cladding and pellet-gap inventories for 100% of the fuel rods. Actually the prompt release might occur only from failed fuel rods.

- Rate of oxidation equal to the reciprocal of the spallation time. Actually spallation time may be more representative of the oxidation of only a fraction of the fuel. This might be conservative at high temperatures, and may not be a conservative assumption at low temperatures.

D3. Gaseous Transport Model

Once released from the fuel, the C-14 would probably be carbon dioxide or another gas such as methane or acetylene. Van Konynenburg (1987) estimates that there would be no more than 22 kilograms of C-14 in the repository, as contrasted to greater than 300,000 kilograms of dead carbon in the immediate vicinity of the repository as carbon dioxide and even more as carbonate and bicarbonate ions. Part of the dead carbon will be available to exchange with the C-14 along the transport pathway. The effect of this exchange will be to retard the speed at which the C-14 could be transported to the accessible environment. A potentially important reaction is the precipitation of calcite (calcium carbonate) by the reaction of calcium ions and carbon dioxide to form a low solubility precipitate (Ross, 1988). The significance of retardation of C-14 or its removal by precipitation will depend on the relative rates of exchange between $CO_2$ gas, bicarbonate and calcite, and the velocity of air flow through the rock.

Several reports propose C-14 transport models. Knapp (1987) describes a one-dimensional model for C-14 transport by advection with exchange between the gas phase and the bicarbonate in the groundwater. The results of this study show that for Yucca Mountain, C-14 released as a pulse from the repository horizon at 2000 years after repository closure would reach the surface within 6000 years.

Amter et al (1988) expand on the concept of a C-14 transport model with more computational detail. Their model accounts for two dimensional gas and liquid advection, diffusion and exchange between liquid and gas compartments. They assume that gas and water are in equilibrium for carbonate species because of the rapid diffusion of carbon dioxide. Dissolved bicarbonate ions in the rock are considered to be essentially immobile because of the relatively high velocity of gas flow to liquid flow. Liquid phase diffusion is also ignored because liquid phase diffusion constants are much smaller than gas phase diffusion constants. The presence of the C-14 components in the liquid will have the effect of reducing the speed of transport by a retardation factor.

D3.1 Chemical Modeling

The chemical retardation of C-14 depends on equilibrium between carbon dioxide, bicarbonate ion and solid carbonate. The equilibrium between C-14 as $CO_2$ and

bicarbonate is tied to several possible chemical factors including the presence of calcite, $CO_2$ partial pressure and pH. Ross (1988) assumes that $CO_2$ dissolved in water is immobile, a conservative assumption for atmospheric releases since there is likely to be a net movement of groundwater to the water table from the ground surface. $CO_2$ is produced naturally in plant roots. The the decline in the concentration of $CO_2$ with depth seems to indicate that it is being removed by some mechanism, most likely calcite precipitation. Ross speculates that this would require a source of calcium ions infiltrating the site. Although the groundwater is not saturated with calcium carbonate and it does not appear to be precipitating naturally, an increase in repository temperature might cause precipitation by evaporation, thereby concentrating the calcite. Calcite solubility is retrograde, decreasing with increasing temperature. This trend leads to some interesting possibilities how the bicarbonate ions in the heated area would react and whether there would be an irreversible deposition of C-14 in precipitating calcite.

Amter et al (1988) present the results of geochemical modeling to determine the complicated equilibrium among the C-14 gas, liquid and solid phases. The conceptual model of the geochemical system had three principal features:

"1. Sufficient calcium carbonate is present in the unsaturated zone to dominate the aqueous chemistry and buffer the pH of the water.

2. A relatively minor amount of calcium is derived from silicate weathering reactions. As a first approximation, it can be assumed that calcium concentrations are the result of equilibration with calcium carbonate.

3. Fractionation plays a negligible role in removing carbon-14 from the gas phase, and concentrations of carbon-14 are proportional to those of carbon-12."

The effect of isotopic equilibrium between phases is to reduce the speed of transport by a factor B, defined:

$$B = 1 + \frac{\theta_T - \theta_D}{\theta_D} \frac{C_T^*}{C_T} \qquad (D7)$$

where $\theta_T$ = total porosity

$\theta_D$ = drained porosity

$C_T^*$ = concentration of carbon ion in the liquid phase at equilibrium

$C_T$ = concentration of carbon ion in the gas phase at equilibrium

Ampter et al (1988) determine the equilibrium concentrations needed for Equation D7 using the PHREEQE reaction path model. There are few data available on the chemistry of water in the unsaturated rocks of the repository, and therefore the data used in the analyses are somewhat subjective.

The results of the PHREEQE calculations were functions expressing the dependence of retardation on temperature for the hydrogeologic units. The expected retardation coefficients ranged from about 20 to 90 over the expected temperatures and concentrations of carbonate in the rock.

D3.2 Gas Phase Transport Modeling

Several mechanisms potentially drive the gas flow, but Amter et al (1988) consider two mechanisms to be dominant:

- Temperature-driven circulation caused by repository heat and the geothermal gradient;
- The difference in density between the moist, warm air in the rock and the cool dry air in the atmosphere.

The authors considered and eliminated the following potential mechanisms for transport of C-14:

- Liquid phase advection - The downward flux of liquid water is likely to be about one tenth the gas flux during the period of repository heating that is most important to HLW performance assessment.
- Diffusion - Using a travel distance of 350 meters and a retardation factor for C-14 of 70 gives a travel time for diffusion of 43,000 yrs, which is much larger than either the ambient of heat-driven travel times for the repository.
- Binary diffusion - A mass flow of air from higher to lower temperatures in the rock will be driven by diffusion, but this flow was shown to be much smaller than the temperature-driven flow.
- Mixing by seasonally alternating flow - Under ambient conditions, gas within Yucca Mountain will move upward in winter and to a lesser extent downward in summer, but would move C-14 molecules only a few centimeters per season, much smaller than even the molecular diffusion effect.

The C-14 transport model relied on a temperature field developed by Tsang and Preuss (1987) that showed a gas phase velocity of meters to thousands of meters per year resulting from the repository heat, as shown in Figure D.2. The model of Amter et al (1988) predicted travel times for C-14 of several hundred years to several tens of thousands of years, depending on the location in the repository and the depth of the overburden, as shown in Figure D.3.

D3.3 Staff's C-14 Transport Model

The staff used the estimated travel times calculated by Amter (1988), as shown in Figure D.3 to develop a scoping model which accounts for transport of carbon dioxide from the repository to the surface of the earth. The model considers radioactive decay using the average travel time for C-14 from the repository to the surface. Amter calculated the travel times along a transect of the repository at zero, 2000 years, 10,000 years and 50,000 years. The fractional release $f_i$ at the earth's surface for a parcel of C-14 released at time $t_0$ was determined by integrating along the path from the repository to the surface assuming that the velocity of the parcel would be everywhere equal, but varying with time (This is not necessarily a good assumption, because the velocity is known to vary in space within the complicated convection currents predicted by Tsang and Preuss, 1987):

$$L(t) = \int_{t_0}^{t} v(t)\, dt \qquad \text{(D8)}$$

Where L(t) is the normalized distance that the parcel has traveled relative to the distance to the surface, v(t) is the normalized velocity, defined here as the reciprocal of the travel time at time t, and $t_0$ is the time of release. The integral was evaluated graphically to find the time t when L(t) = 1. The object of the integration was to find the travel time of the parcel and determine if it could reach the surface within the stated time limit, i.e., 10,000 years. Once the travel time $t_i$ was determined for each parcel with release time $t_{0i}$, the fraction $f_i$ released at the earth's surface was determined by radioactive decay:

$$f_i = \exp(-\lambda t_i) \qquad \text{(D9)}$$

Where $\lambda = \ln 2/t_{1/2}$. The results of these calculations are summarized in Table D2 for releases at 500 to 6500 years. The fractional release ranges from a maximum of 0.91 to a minimum of 0.65. Releases after about 6500 years do not arrive at the surface of the earth before 10,000 years.

Table D2 - Release Fraction as function of release time

| Time of release, years | Fraction Reaching Surface |
|---|---|
| 500 | 0.86 |
| 1500 | 0.91 |
| 2500 | 0.86 |
| 3500 | 0.82 |
| 4500 | 0.74 |

| | |
|---|---|
| 5500 | 0.71 |
| 6500 | 0.65 |
| beyond 6500 | none in 10,000 yrs |

D.3.3.1 Limitations of C-14 Gas Transport Model

Some of the limitations of the Staff's transport model are given below:

- There is the possibility that gaseous releases from the repository level may follow the shortest path and that there may be ample ground transport between one part of the repository and another because of the network of drifts, shafts and fractures. The effective travel time for C-14 released anywhere in the repository may therefore be more characteristic of the shortest travel time calculated.

- There is evidence that in natural waters, $CO_2$ is not in equilibrium with the atmosphere, partially because of unfavorable mixing conditions and the slowness of the gas transfer reaction (Stumm and Morgan, 1970). The chemical model for C-14 behavior is based on the assumption of equilibrium. Failure to attain equilibrium would have the effect of reducing the retardation of C-14.

- In their transport and chemical models, Ampter et al (1988) assume intimate contact between the gas and water phases. Such contact is unlikely at Yucca Mountain because under unsaturated conditions water would be present primarily in the smallest rock pores, and the flow of air would be most prevalent in the largest rock pores and fractures. Therefore, the potential for close air-water contact would be diminished, having the effect of reducing the retardation of C-14.

D4. Conclusions and Recommendations

The results of Amter et al (1988) and Knapp (1987) for transport of C-14 from the Yucca Mountain repository to the surface of the earth predict travel times ranging from a few hundred to a few thousand years, and are shortest during the period where there is significant heating from the radioactive decay. This period of short travel times coincides roughly with the period when the present model predicts most of the C-14 releases to occur, but any release depends on the failure of the waste canisters. The release of C-14 is very sensitive to the lifetime of the waste package in the present modeling approach, particularly because early failure times lead to faster and more complete oxidation of the uranium dioxide. Considering the 5720 year halflife of C-14, there would be relatively little attenuation of the cumulative release of C-14 at the earth's surface because of holdup in the geologic barrier.

The present release and transport models have been formulated for mechanisms which the staff considers to be conservative, but there is little direct evidence that the model is correct. We have identified the following areas where the collection of additional data would be most fruitful:

- We should strive to investigate the mechanisms for C-14 release, including the available information on dry cask storage, and the investigations to be performed by DOE. There is considerable scatter in the data on spallation of the uranium dioxide fuel, and this could be a potential source of uncertainty. We should not rely however on a secondary measure such as spallation to determine the rate of release for C-14 from the fuel. We should urge DOE to collect data leading to more direct measurements of C-14 releases from the various compartments of the fuel.

- We should investigate geochemistry of calcite precipitation at the Yucca Mountain site under repository conditions to determine whether the released C-14 is removed effectively before reaching the accessible environment. There are several counteracting factors involved in the effectiveness of this mechanism for removing C-14. Knapp (1987) states that "Water-rock interaction is probably insignificant due to the low abundance of calcite at the Nevada site and due to the prediction that calcite will not precipitate". However calcite solubility diminishes with increasing temperature, leading to the possibility that repository-induced heating would cause calcite precipitation. At the present time, the staff believes that this mechanism will be ineffective in removing C-14.

## D5. References


Beahm, E.C., W.E. Shockley and O.L.Culberson, 1985, "Organic iodide formation following nuclear reactor accidents", NUREG/CR-4327

Einsiger, R.E. and R.E. Woodley, 1985a, "Evaluation of the potential for spent fuel oxidation under tuff repository conditions", HEDL-7452

Einsiger, R.E. and R.E. Woodley, 1985, "Low temperature spent fuel oxidation under tuff repository conditions", HEDL SA-3271, Hanford Engineering Development Laboratory, Richland Washington

Einsiger, R.E., and R.E. Woodley, 1987, "Predicting spent fuel oxidation states in a tuff repository", Westinghouse Hanford Company, HEDL-SA-3267

R.Einziger, R.Kohli, "Low temperature rupture behavior of zircalloy-clad pressurized water reactor spent fuel rods under dry storage conditions", Nuclear Technology, Vol 67, Oct 1984, pp 107-123

HEDL "Evaluation of the potential for spent fuel oxidation under tuff repository conditions", HEDL-7452

B.Grambow, "Spent fuel dissolution and oxidation - an evaluation of literature data", SKB 89-13, Swedish Nuclear Fuel and Waste Management Company, March 1989

Amter, Steven, E.Behl, B.Ross, "Carbon-14 travel time at yucca Mountain", Appendix to Yucca Mountain Candidate Site Preliminary Postclosure Risk Assessment, P. Doctor, et.al, June 1988 (Draft)

Tsang, Y.W. and K.Preuss, "A study of thermally induced convection near a high-level nuclear waste repository in partially saturated fractured tuff", Water Resources Research, vol 23, pp 1958-1955, 1987

B. Ross, "Gas-Phase transport of carbon-14 released from nuclear waste into the unsaturated zone", Material Research Society, Symposium Proceedings, Vol 112, 1988

R. van Konynenburg, C.F.Smith, H.W. Culham, and H.P. South, in Scientific Basis for Nuclear Waste Management, Material Research Society Proceedings, Vol 84, pp 185-196, 1987

D.T.Reed, R.A. Van Konynenburg, "Effects of ionizing radiation on moist air systems", Material Research Society Symposium on the Scientific Basis for Nuclear Waste Management XI, Boston MA 1987.

Knapp, R., 1987, "An approximate calculation of advective gas transport of C-14 at Yucca Mountain, Nevada", Lawrence Livermore National Laboratory, UCRL-97805 (preprint)

Stumm. W., and J. Morgan, 1970, Aquatic Chemistry, Wiley-Interscience, New York

Katz, J.J., and E. Rabinowitz, 1951, The Chemistry of Uranium-The Element, Its Binary and Related Compounds, National Nuclear Energy Series, Division VIII, Vol.5, Dover Publications Inc, New York

Till, J., 1983

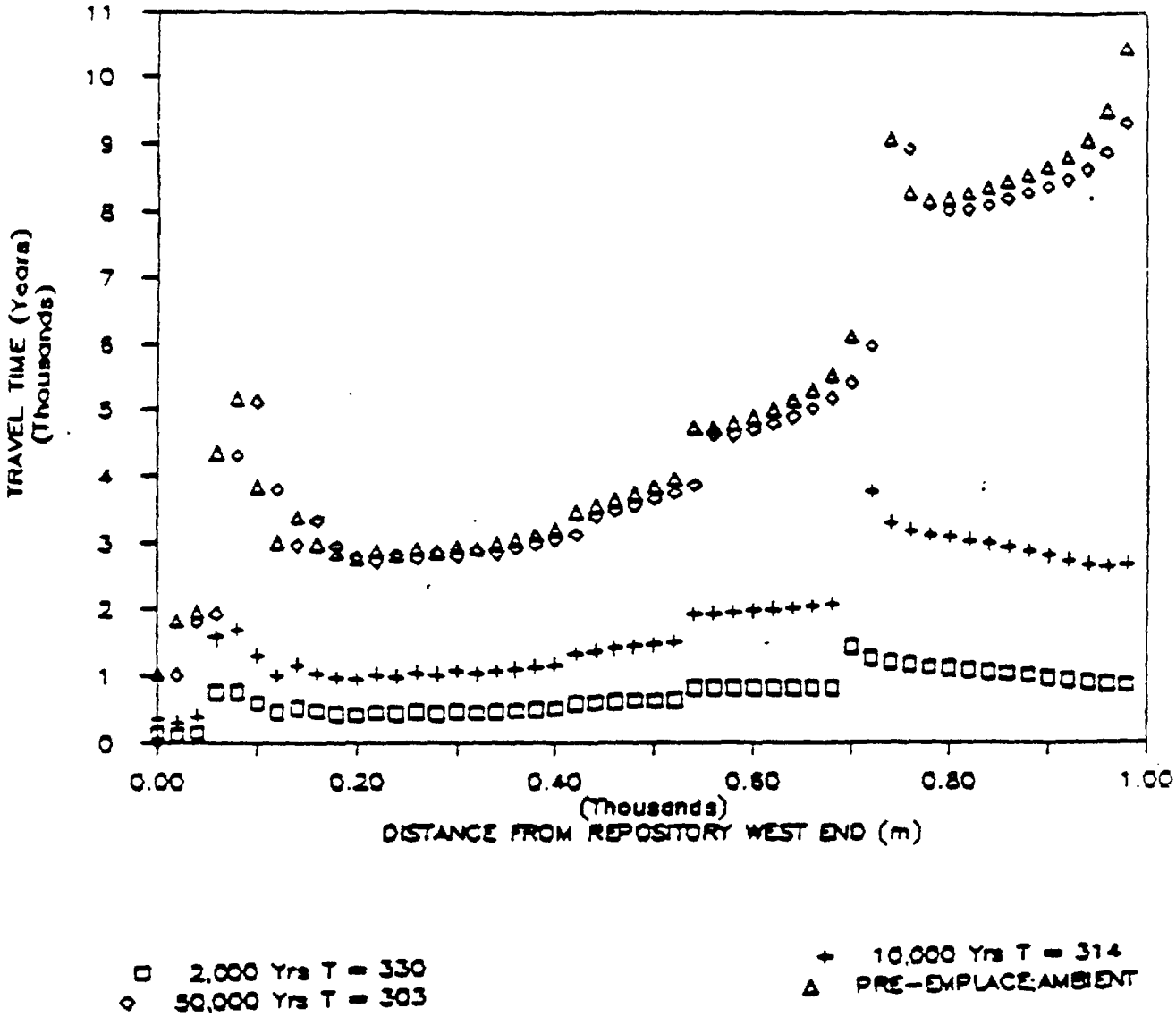



Figure D3 Carbon-14 travel time from the repository to the surface for ambient conditions, 2,000, 10,0000, and 50,000 years. (After Ampter, 1988)

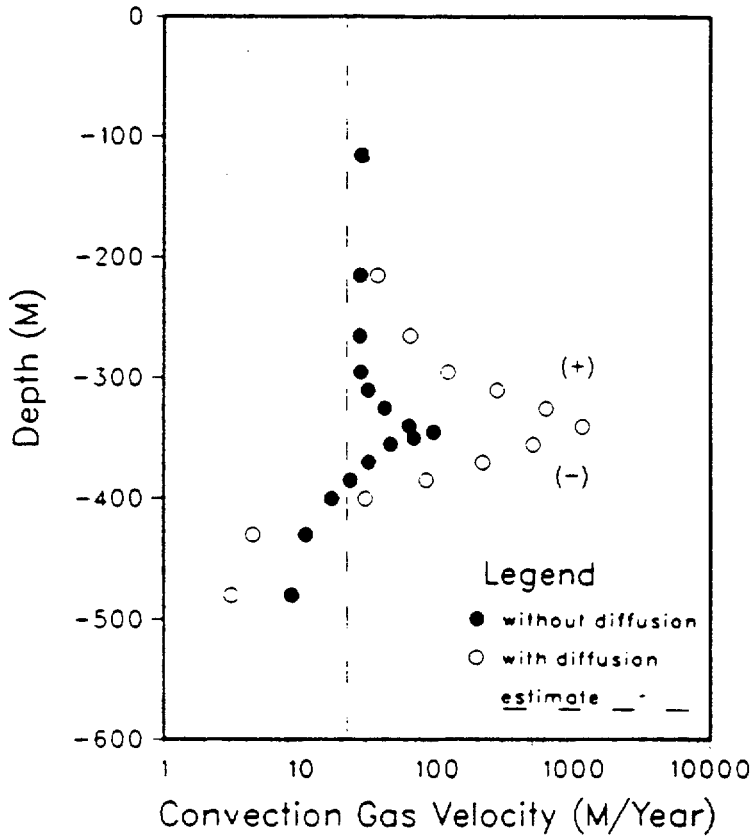



Fig. D2 Gas convection velocities along the repository center line at 100 years after waste emplacement. Plus and Minus signs refer to upward and downward fluxes at the repository depth for the case with binary diffusion. (after Preuss, 1987)

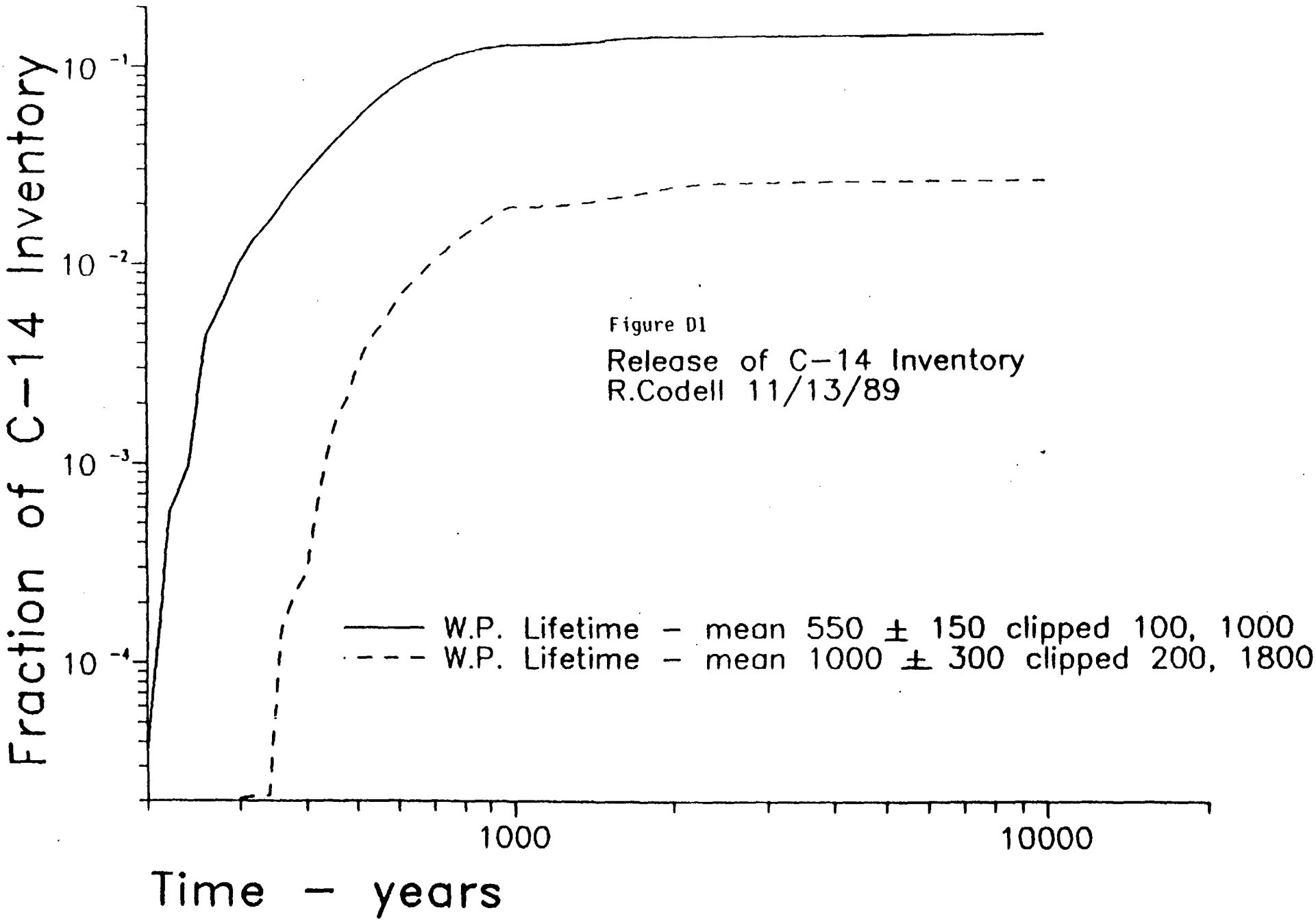



Figure D1

Release of C-14 Inventory
R.Codell 11/13/89

Document Name:
CONVERGE/

Requestor's ID:
RINN

Author's Name:
codell

Document Comments:
aux analysis on statistical convergence

typ E

## APPENDIX E - TESTING STATISTICAL CONVERGENCE

The Latin Hypercube Sampling method is an efficient method for performing Monte Carlo analyses (Helton, 1961). As with all Monte Carlo analyses, increasing the number of samples increases the convergence of the statistical results. We are usually interested in minimizing the number of repetitions, particularly for complicated, time-consuming calculations. A rough "rule of thumb" for LHS analysis is that the minimum number of samples should be 4/3 the number of independent variables for good statistical convergence. It is not clear however whether the rule of thumb is meant to apply both to the generation of the CCDF curve and the sensitivity analysis or just the latter. The following example was designed to test whether or not this "rule of thumb" applies to highly nonlinear problems like the present calculation.

There are 47 independent variables sampled in the present analysis. The rule would therefore predict that about 63 samples would be sufficient to generate an acceptable output distribution; i.e., the CCDF of EPA release Fraction. To test this hypothesis, we generated the 10,000 year CCDF for the base-case scenario from 500 LHS samples in order to have a smooth benchmark curve representing a statistically converged distribution. We then generated 5 CCDF curves for the same distribution, but using only 100 LHS samples each, with each case employing a new random seed. The results are shown in Figure ~~XX~~ E.1. Only one of the five CCDF curves generated with the 100 point samples was close to the 500 point CCDF curve. Convergence was best in the low-release region, and generally poor in the high-release region. The 100-point case leads to a spread in the release in the high-consequence portion of the curve of about two orders of magnitude. This result indicates that the "rule of thumb" in this case is inadequate, and many more samples would be required.

The probable explanation for the inadequacy of the "rule of thumb" in this case is that there were relatively few samples giving high release, and many cases where there was no release at all within 10,000 years. The low-release samples were far more prevalent, as demonstrate by the generally good agreement in that portion of the curve. The result of this exercise points to the need for care in using the LHS method to assure that enough samples are generated for statistical convergence. We should also pursue some of the more sophisticated sampling methods such as Fast Probabilistic methods and Importance Sampling (e.g. CNWRA, 1988).

### References

Helton, J.H.,1961, SIAM Review, Vol 12, no 1

CNWRA, 1988, "Fast Probabilistic Performance Assessment (FPPA) Methodology Evaluation", Center for Nuclear Waste Regulatory Analysis

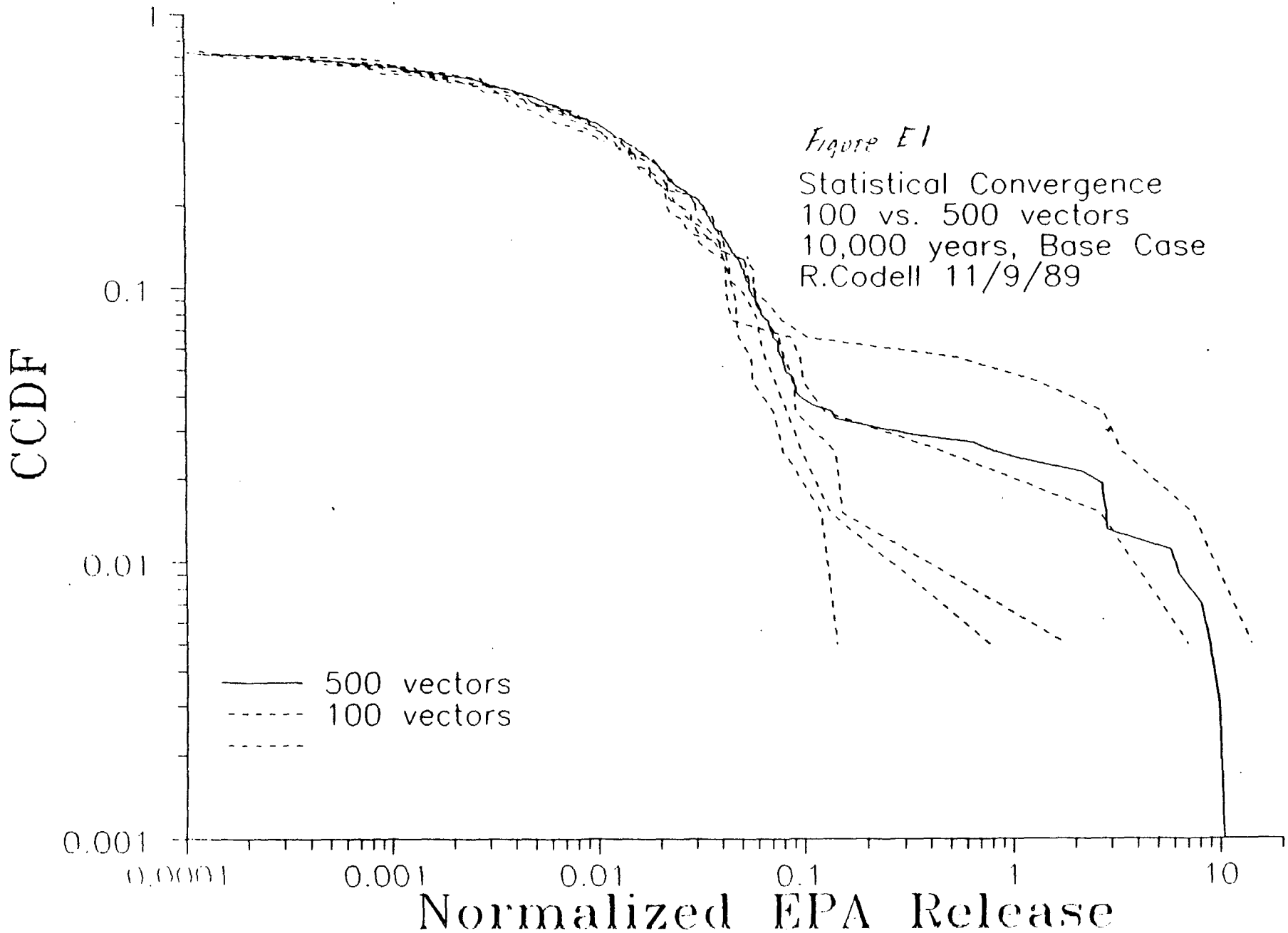


Figure E1
Statistical Convergence
100 vs. 500 vectors
10,000 years, Base Case
R.Codell 11/9/89
500 vectors
100 vectors
CCDF
1
0.1
0.01
0.001
0.0001
0.001
0.01
0.1
1
10
Normalized EPA Release

Document Name:
MOUA2.3

Requestor's ID:
RINN

Author's Name:
tjm

Document Comments:
appendix 2.3

App. F

## APPENDIX F - AUXILIARY ANALYSIS OF HYDROLOGIC DATA

An auxiliary analysis of hydrologic data was conducted to determine if spatial correlations could be identified for porosity and hydraulic conductivity parameters. This analysis did not identify any spatial correlation with depth for saturated hydraulic conductivity data or for Calico Hills unit porosity data. A large scale trend of decreasing porosity with increasing depth was identified for the Topopah Springs unit and a small scale correlation length of less than 40 meters was identified in data from two holes in the Topopah Springs unit.

The identification of spatial correlation is important to performance assessment modeling, because longer correlation lengths increase the probability that contaminated ground water pathways will be encountered which might provide quicker transport of radionuclides to the water table. To look for correlation lengths the program GEO-EAS (Geostatistical Environmental Assessment Software)(Englund, 1988) was used to generate scatter plots, histogram plots, cumulative distribution plots (probability plots) and variograms of depth, porosity, and saturated hydraulic conductivity data for the Calico Hills and Topopah Springs units. A variogram is a means of quantifying the commonly observed relationship that samples close together will tend to have more similar values than samples far apart. In this analysis the scatter plots were used to look for trends with depth, while the variograms were used to look for spatial correlation in the vertical distance between pairs of measurements.

Since, unsaturated zone hydrology parameters were of interest, this study only used core data. The data input files were created from a Lotus spread sheet of Yucca Mountain hydrologic parameters from DOE data. An example page from this spread sheet is attached. In all runs depth is in meters, porosity is unitless, and saturated hydraulic conductivity is in meters/second.

Histogram plots of Topopah Springs and Calico Hills porosity data were prepared using all the porosity data from these units in the data base. The histogram plot of the Topopah Springs porosity values was made from 6 wells and 200 samples. The histogram plot of the Calico Hills porosity values was made from 6 wells and 174 samples. From the histograms it was concluded that (1) the Topopah Springs unit tends to have lower porosity values than the Calico Hills unit, (2) the distribution of Topopah Spring porosity data is skewed to the lower porosity values, (3) the Calico Hills porosity data is skewed to higher porosity values and is bimodal (Figures F-1 and F-2). These results probably reflect the difference in matrix porosity values between the nonwelded Calico Hills unit and the welded Topopah Springs unit.

Scatter and variogram plots where made only for holes which had enough data to conduct this type of analysis. Data from 5 holes (holes: USW GU-3, USW G-1, USW G-4, USW H-1, UE25a-1) were used in the analysis. Separate plots of saturated hydraulic conductivity, porosity, and distance were made for each hole by formation.

No correlations with depth could be identified in scatter plots and variogram plots of saturated hydraulic conductivity from either the Topopah Springs or Calico Hills units. In addition no correlations with depth could be identified in plots of porosity data from the Calico Hills unit.

However, a trend of decreasing porosity with depth was identified in scatter plots of some of the holes in the Topopah Springs unit (UE25a-1, USW GU-3, and USW G-4) (Figures F-3, F-4, F-5). This trend is probably the result of increasing welding with depth, resulting in decreased porosity with depth. Porosity variogram plots of the Topopah Springs unit for two holes (USW GU-3 and USW G-1) contained a pattern. However, this pattern could be due to the trend noticed in the scatter plots. Therefore, the trend was removed from the data, by using GEO-EAS to calculate least squares fits and the corresponding slope for all the scatter plots. A Lotus program was then used to remove the slope from the input data for each hole by calculating the slope intercepts for each "X" value (depth) and then subtracting the "Y" value (porosity) from the "Y" value at the intercept. With the trend removed, there appears to be spatial correlation displayed in variograms for holes USW G-4 and UE25a-1 (Figures F-6 and F-7). In both cases the variogram has a sill of 40 meters or less, indicating that beyond a 40 meter separation distance there is no spatial correlation for porosity.

In summary, this analysis did not identify any spatial correlation with depth for saturated hydraulic conductivity or for Calico Hills unit porosity data. A large scale trend of decreasing porosity with increasing depth was identified for the Topopah Springs unit and a small scale correlation length of less than 40 meters was identified in data from two holes in the Topopah Springs unit.

## REFERENCES CITED

Englund, E. and Sparks, A., 1988, GEO-EAS (Geostatistical Environmental Assessment Software) User's Guide, U.S. Environmental Protection Agency, EPA/600/4-88/-33a

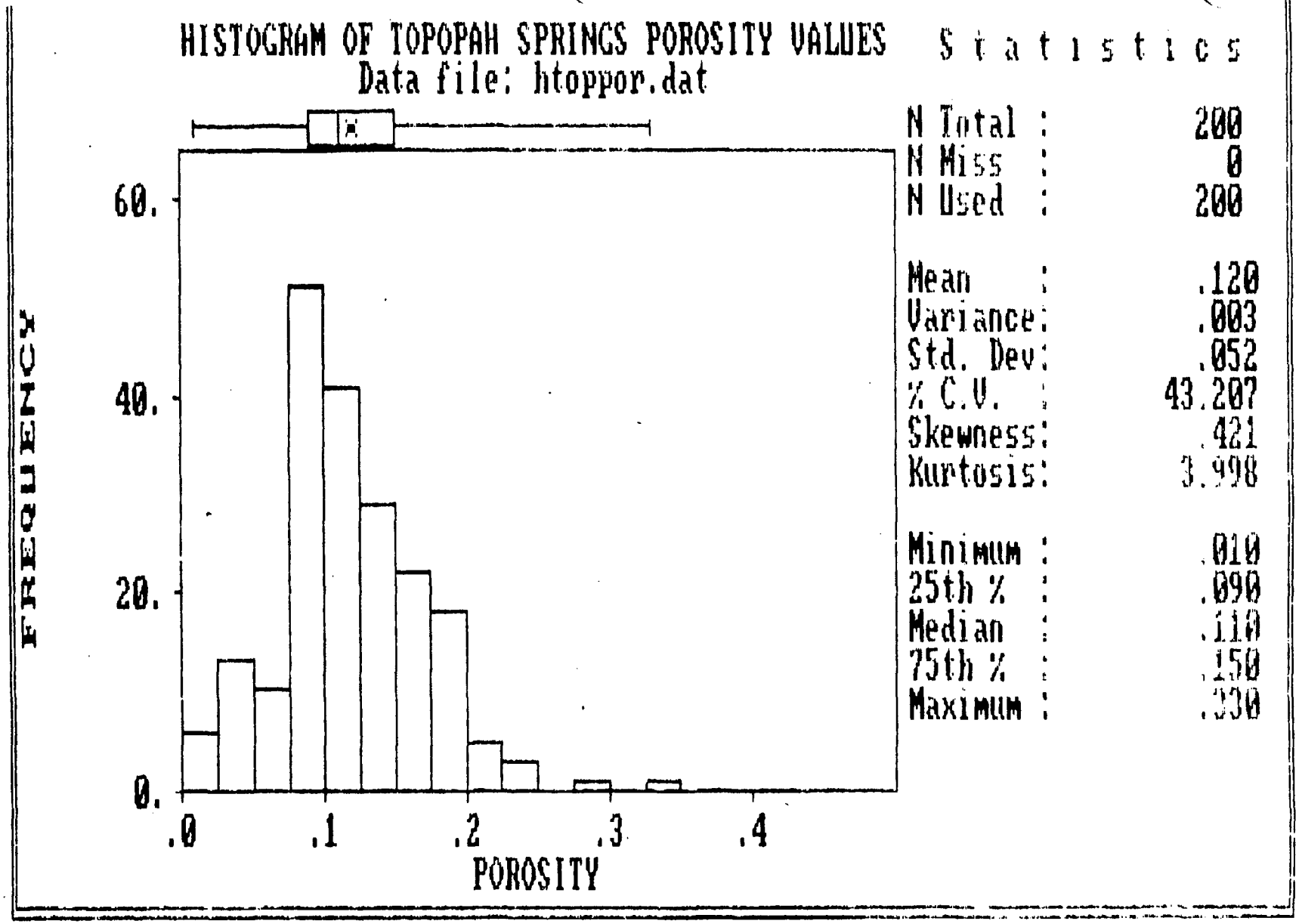



Figure ~~2-1~~ F-1 Histogram of Topopah Springs Porosity Values

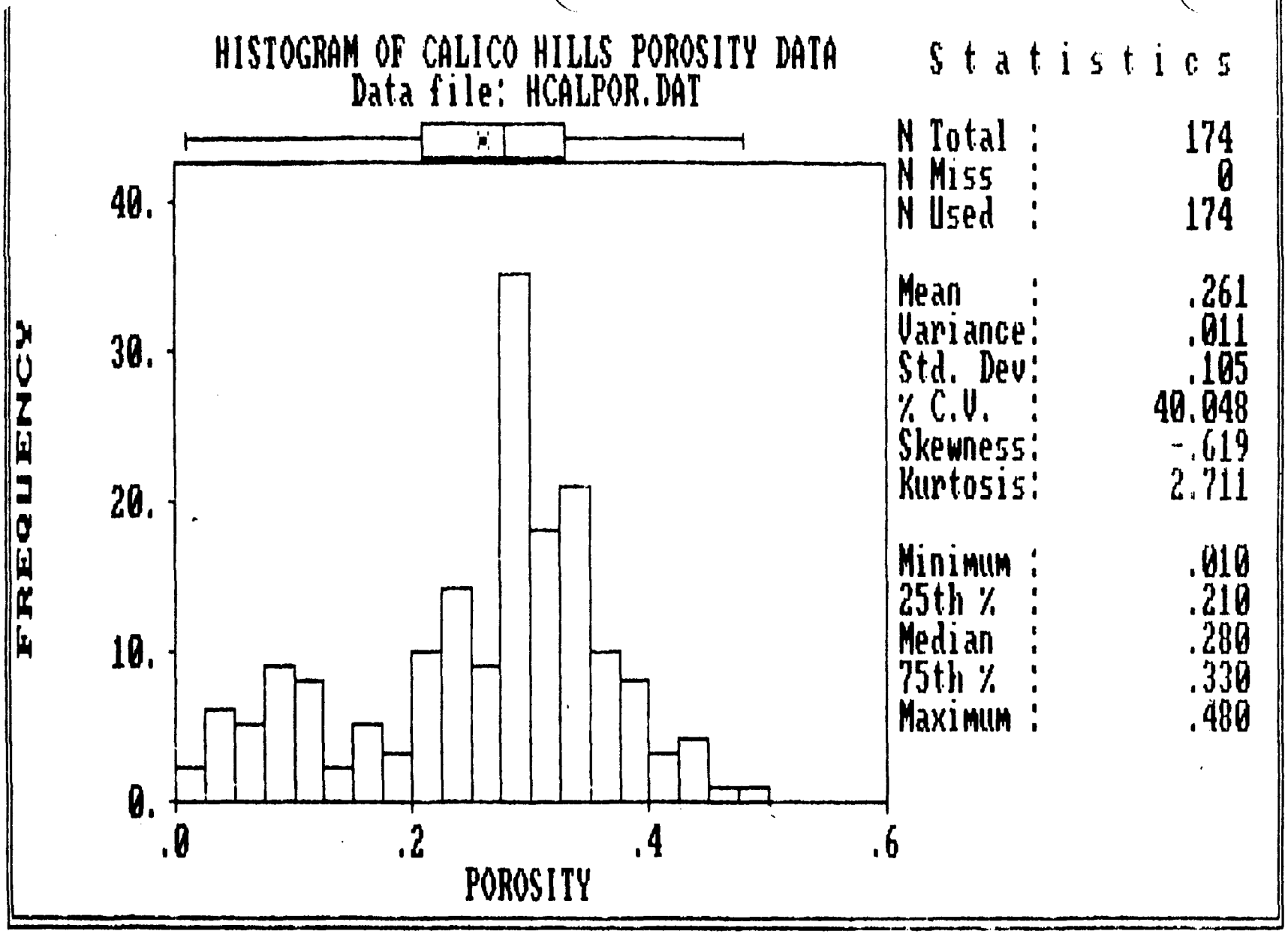
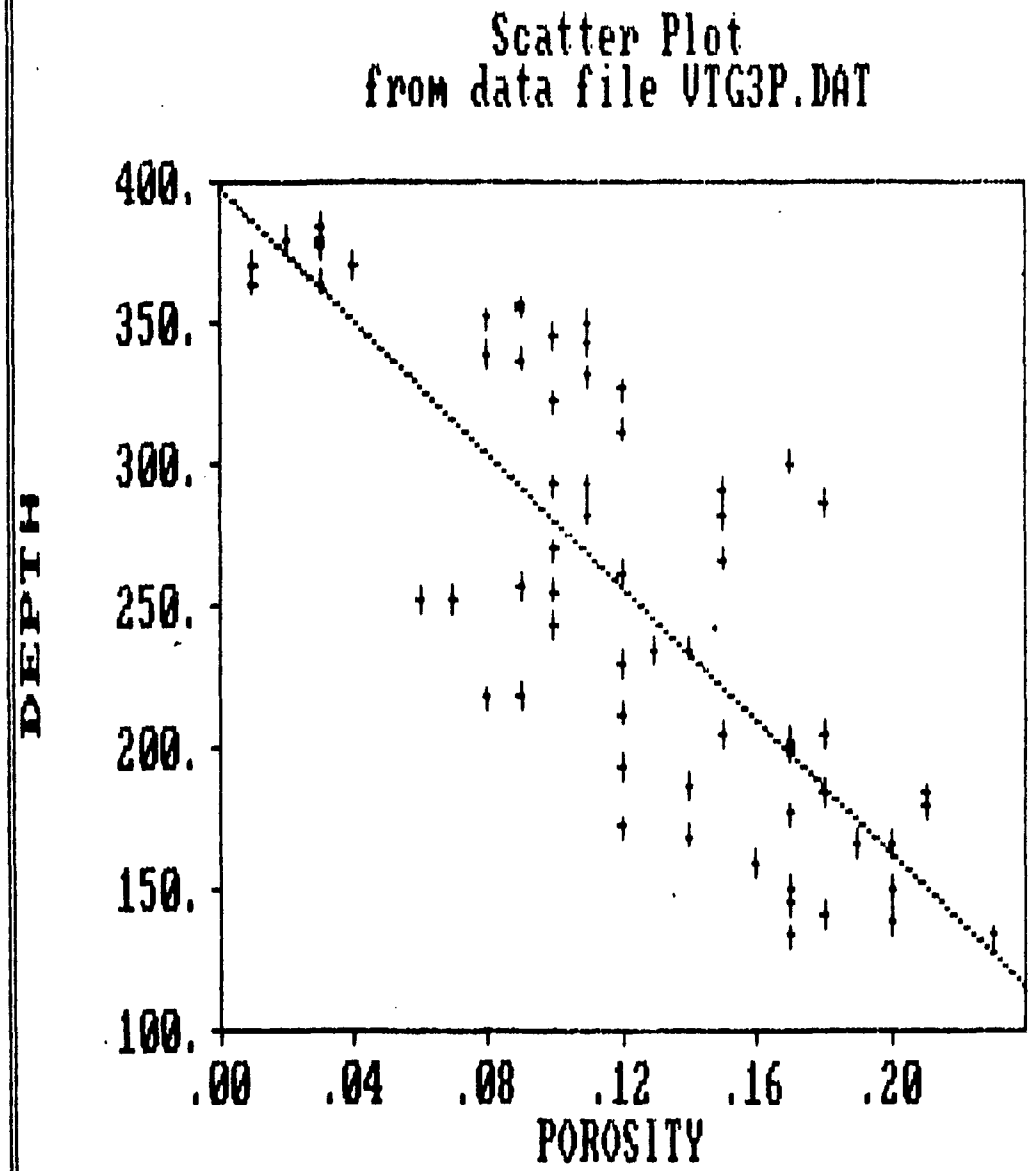



Figure F-2 Histogram of Calico Hills Porosity Data




Regression Results:

| | | |
|---|---|---|
| # Pairs | : | 81 |
| Slope | : | -1183.699 |
| Intercept | : | 398.172 |
| Correl. coeff. | : | 1.000 |

Figure F-3 Scatter Plot, Hole USW GU-3, Topopah Springs Unit

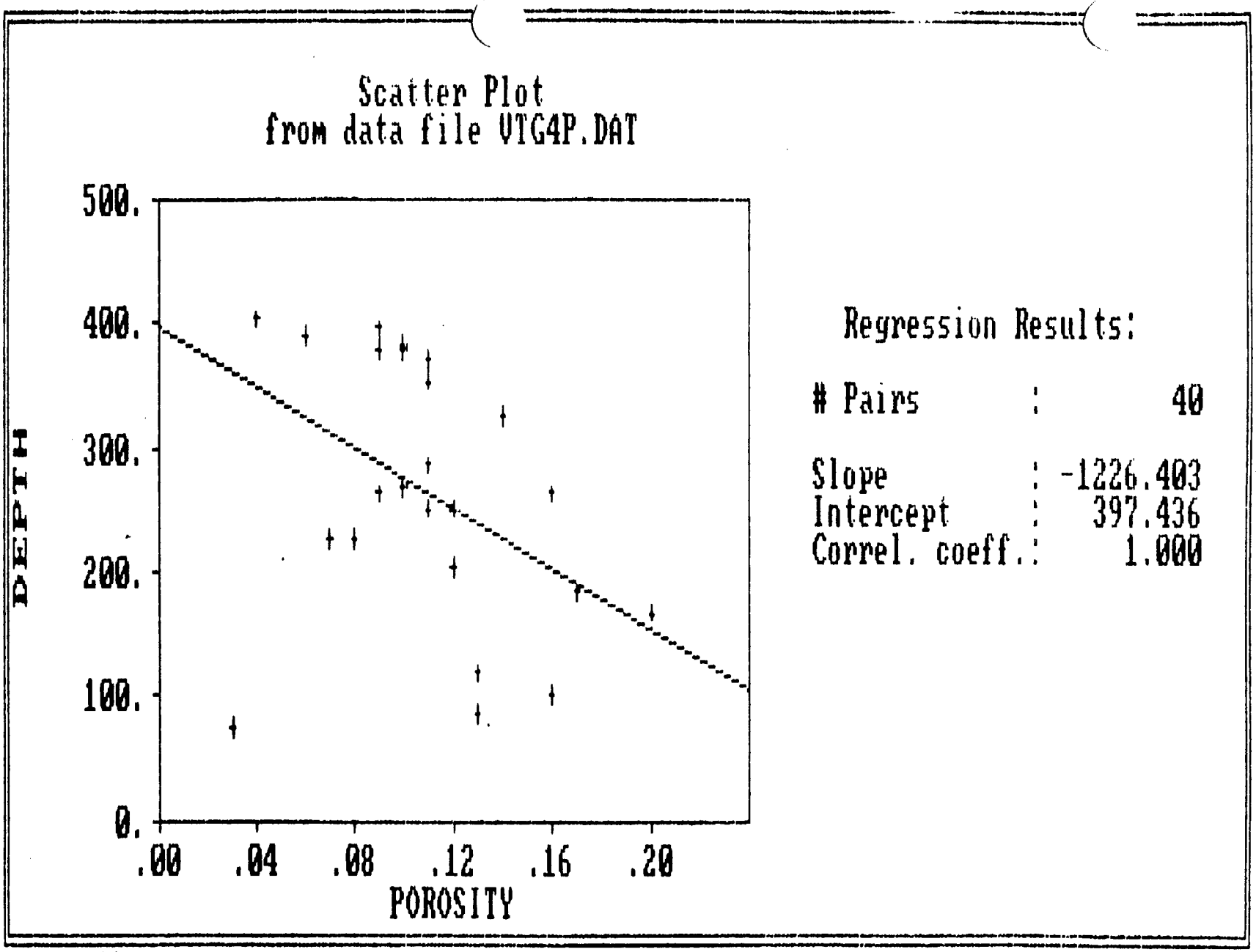
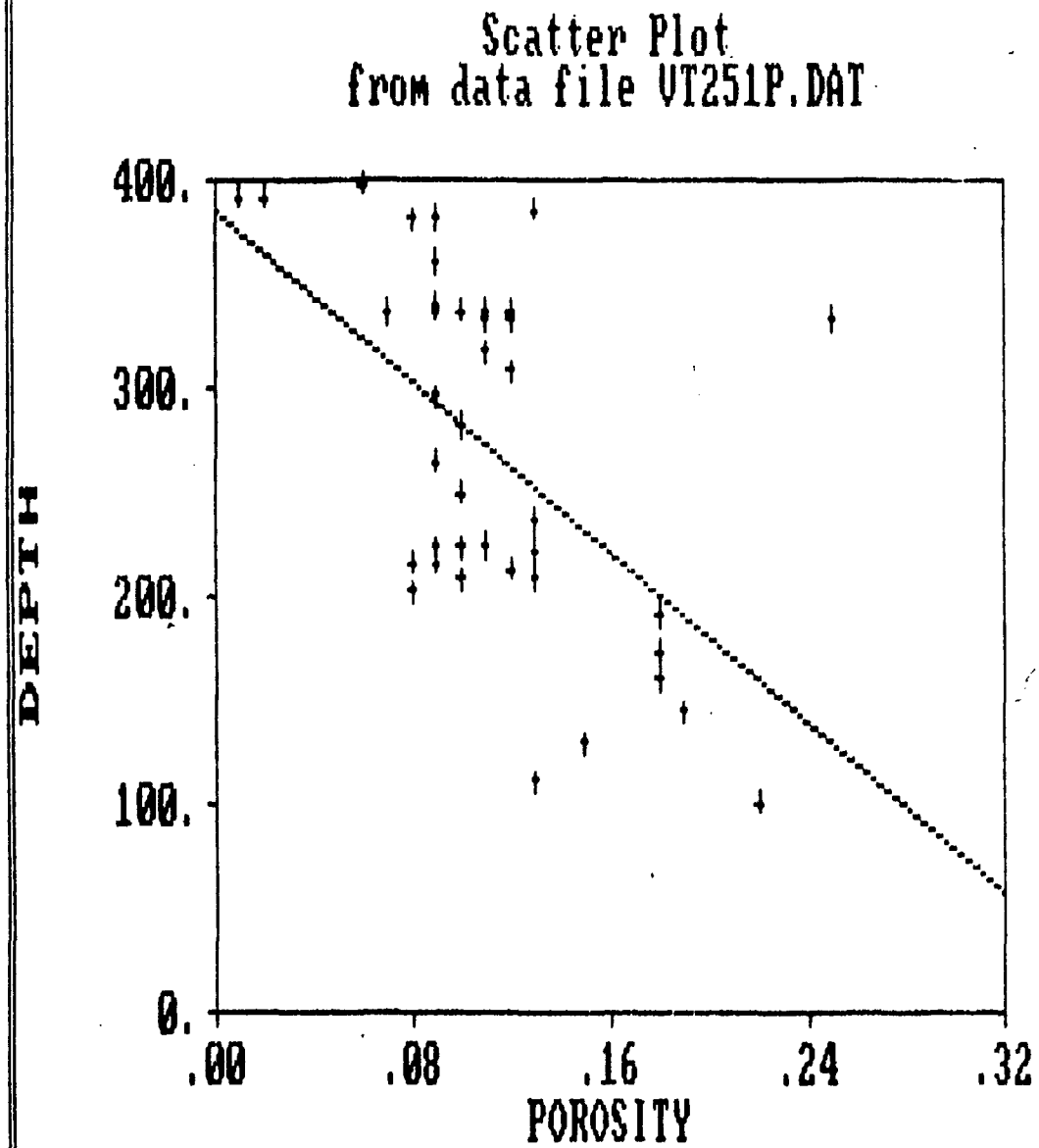



Figure F-4 Scatter Plot, Hole USW G-4, Topopah Springs Unit




Regression Results:

| | | |
|---|---|---|
| # Pairs | : | 45 |
| Slope | : | -1025.763 |
| Intercept | : | 383.412 |
| Correl. coeff. | : | 1.000 |

Figure ~~E-5~~ F-5 Scatter Plot, Hole UE25a-1, Topopah Springs Unit

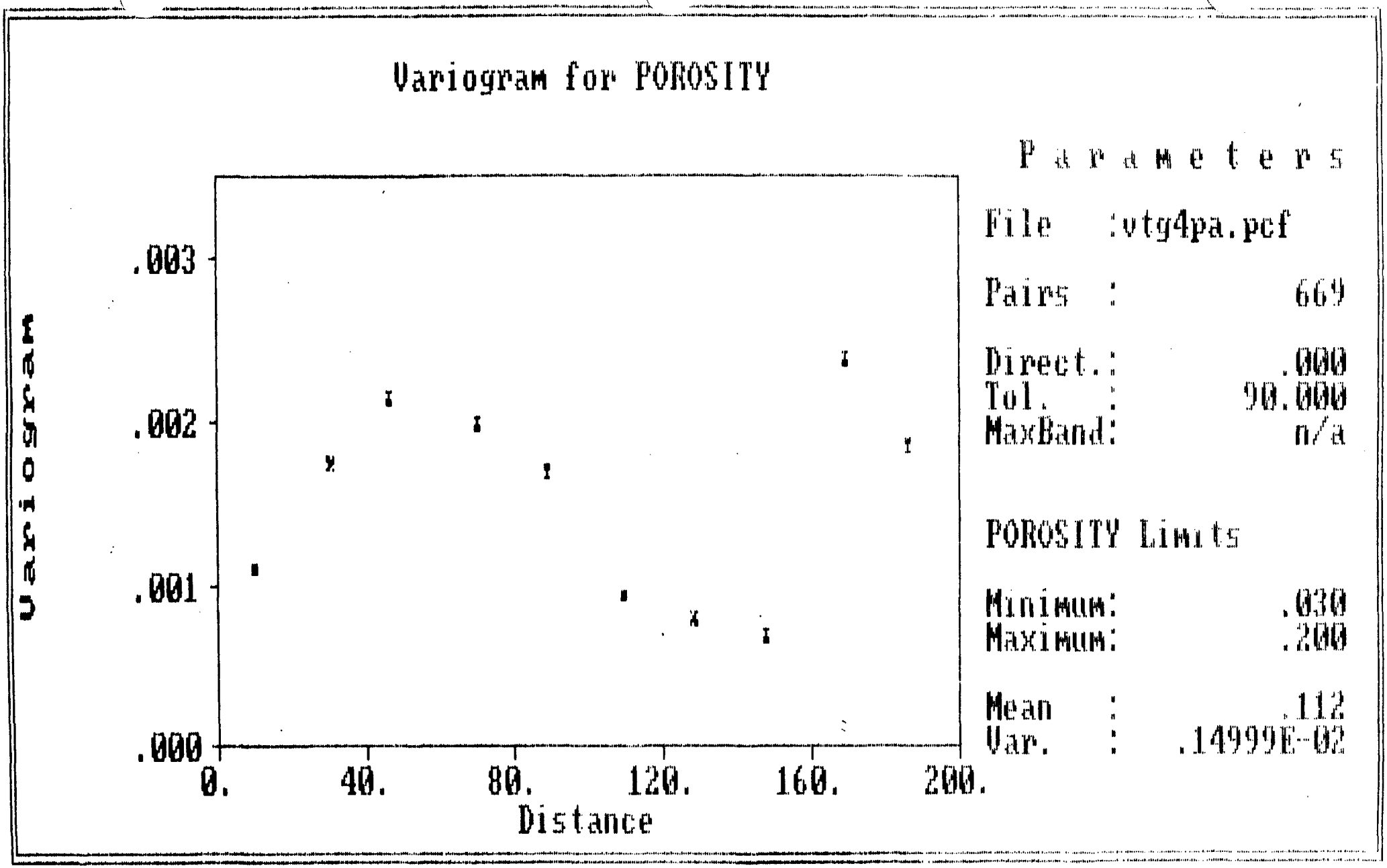



Figure F-6 Porosity Variogram, Hole USW G-4, Topopah Springs Unit

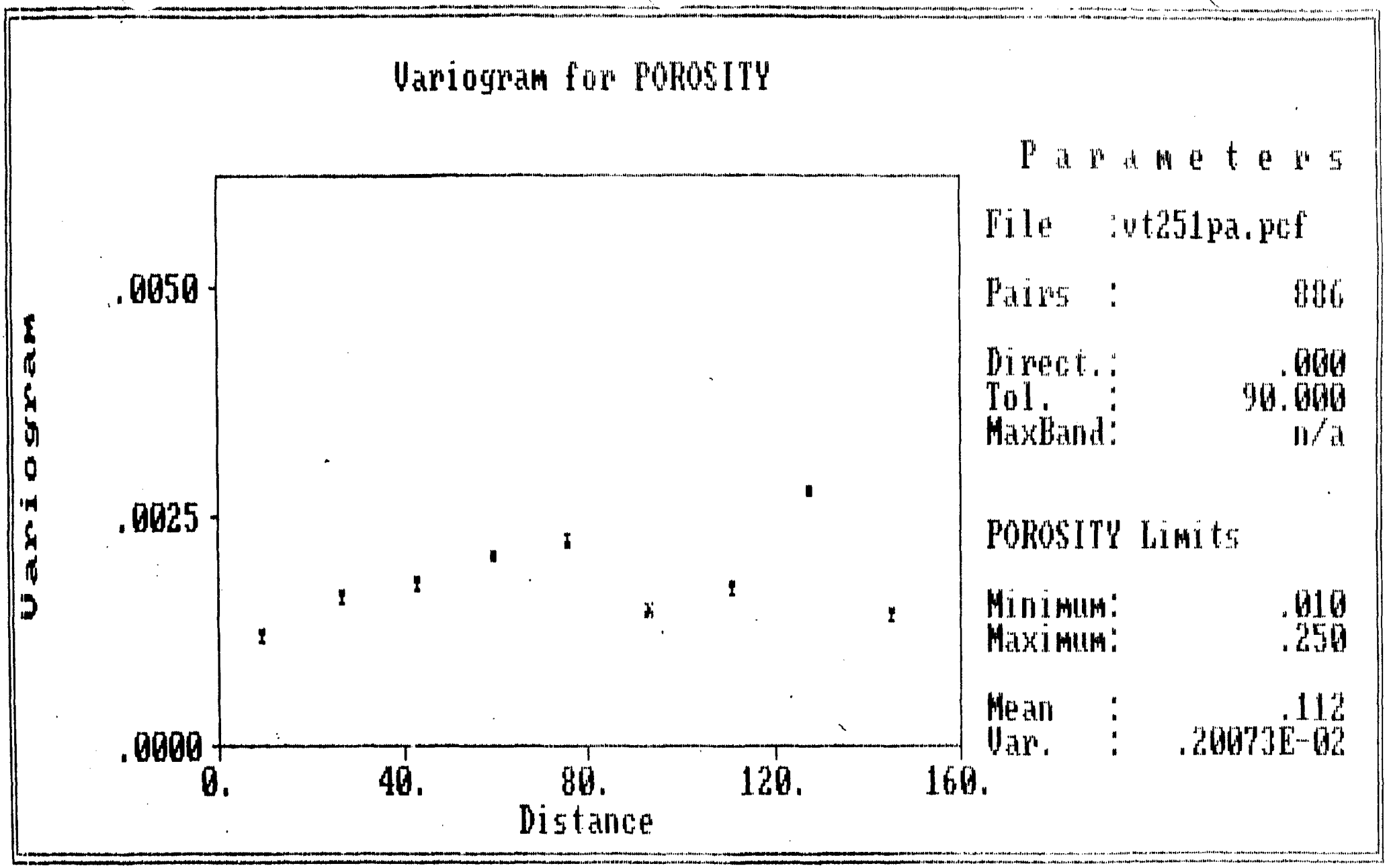



Figure F-7 Porosity Variogram, Hole UE25a-1, Topopah Springs Unit

Document Name:
MOUA2.4

Requestor's ID:
NICHOLSO

Author's Name:
tjm

Document Comments:
appendix 2.4

App. G

# APPENDIX G - TWO-DIMENSIONAL (CROSS SECTION) FLOW MODEL

## G.1 Introduction

The Yucca Mountain site is comprised of a number of layers which vary over a large range (approximately four orders of magnitude) of hydraulic conductivity. Due to contrasts in properties at unit interfaces and a dip (average dip of 6 degrees) of the units it could be expected that water would perch or preferentially move down-gradient in the horizontal direction rather than the typical vertical flow expected in the unsaturated zone.

The degree of horizontal flow is an important consideration because: 1) above the repository flow diversion could lead to a reduction in flux through the repository, and 2) below the repository horizontal flow would lead to a shorter travel time to the water table. Hydrologic modeling can be useful in identifying the conditions (i.e., flux rate) that lead to horizontal flow and the influence these conditions have on flux and travel time.

## G.2 Purpose

Hydrologic modeling of unsaturated fractured tuff currently is limited to a dual-porosity approach for the treatment of fracture-matrix interaction and is computationally intensive. However, some relatively simple modelling of Yucca Mountain could be done to: 1) gain insights into the flow diversion issue and how this affects the fluid flux through the repository and the validity of the vertical flow path assumption, and 2) better understand the numerical limitations.

## G.3 Problem Set-up

This initial analysis will assume matrix flow only and will use the description of Yucca Mountain defined by DOE in the HYDROCOIN Project (Prindle, 1987) and use the VAM2D computer program to simulate the matrix flow problem (a newer version of the program will be able to simulate partially the influence of fractures via characteristic curves which define suction and hydraulic conductivity as a function of the degree of saturation). The analysis will involve a steady state simulation using the layering and parametric values presented in Figure G-1 and Table G-1, respectively. The steady state conditions involved applying a constant infiltration rate on the upper surface, a constant head at the lower (water table) boundary, and noflow conditions on the sides.

## G.4 Results and Conclusions

The diversion of flow at the interfaces was investigated by simulating the HYDROCOIN Yucca Mountain description with three different infiltration rates (.1, .2, and .5 mm/yr - for the .5 mm/yr simulation the low conductivity Tiva Canyon was not included due to the fact that fracture flow would be needed to accomodate this magnitude of flux). The results of the simulations, presented as the ratio of horizontal to vertical flow

immediately above an interface, are presented in Table G-2. Vertical flow dominates in all units when the infiltration is .1mm/yr. When infiltration is .2 mm/yr or more, horizontal flow is at least an order of magnitude higher than vertical flow above the low conductivity Topopah Springs #1 unit. Although the Calico hills unit shows a large component of horizontal flow, this result is due to the water table at the base of the Calico Hills unit.

These simulations indicate that infiltration rates greater than .2 mm/yr combined with the six degree slope in unit bedding could produce a significant amount of horizontal flow. These flows could result in perched zones or localized fracture flow. It is very important to note, that this analysis did take in to account the presence of fractures and heterogeneities and anisotropy in hydraulic parameters. Future modeling efforts should examine the influence of these additional complications.

## G.5 References

Prindle, R.W., 1987, Specification of a Test Problem for HYDROCOIN Level 3 Case 2: Sensitivity Analysis for Deep Disposal in Partially Saturated, Fractured Tuff, Sandia National Laboratories, SAND86-1264, Albuquerque, New Mexico.

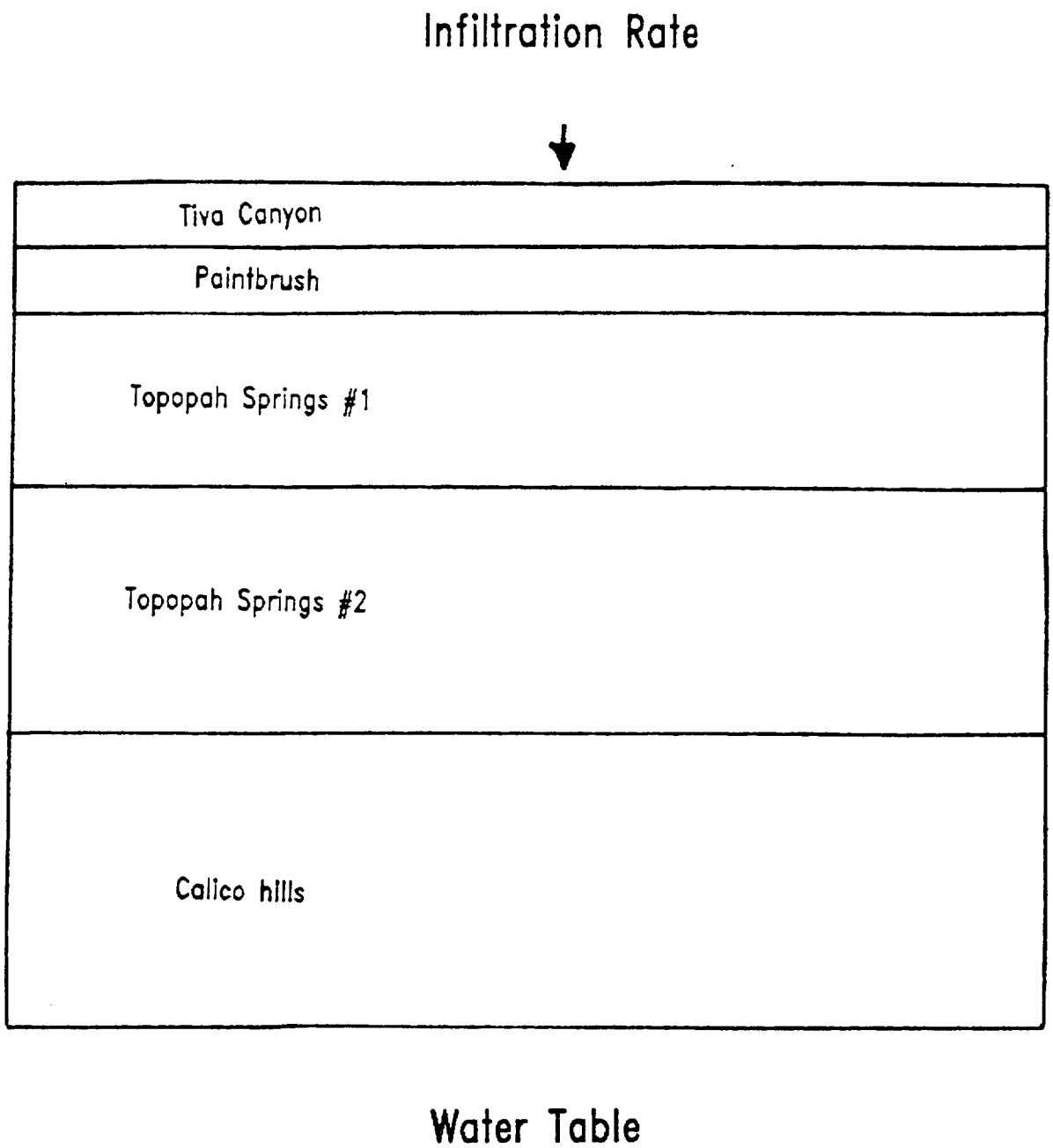



Figure G.1 Hydrogeologic units and boundary conditions used in the two-dimensional simulation of Yucca Mountain using the VAM2D computer model (note: the figure does not show the six degree incline that was included in the simulation).

Table G.1 Hydraulic properties used in the two-dimensional simulation of Yucca Mountain.

| Properties | Tiva Canyon | Paintbrush | Topopah Springs #1 | Topopah Springs #2 | Calico Hills |
|---|---|---|---|---|---|
| Saturated Conductivity (mm/yr) | .3 | 10,000. | .6 | .6 | 8,000. |
| Porosity | .08 | .40 | .11 | .11 | .28 |
| Thickness (m) | 26.8 | 38.1 | 130.1 | 205.1 | 130.3 |
| van Genuchten Parameters: | | | | | |
| Alpha (1/m) | .00821 | .015 | .00567 | .00567 | .016 |
| Beta | 1.558 | 6.872 | 1.798 | 1.798 | 3.872 |

Table G.2 Ratio of horizontal to vertical flow at the interfaces between different hydrologic units over differing infiltration rates.

RATIO OF HORIZONTAL TO VERTICAL FLOW

| Interface | Infiltration Rates (mm/year) .1 | .2 | .5 |
|---|---|---|---|
| Tiva Canyon (Ksat = .3 mm/yr)<br>Paintbrush (Ksat = 10,000. mm/yr) | .05 | .07 | -- |
| Paintbrush (Ksat = 10,000. mm/yr)<br>Topopah Springs #1 (Ksat = .6 mm/yr) | .07 | 15. | 19. |
| Topopah Springs #1 (Ksat = .6 mm/yr)<br>Topopah Springs #2 (Ksat = .6 mm/yr) | .005 | .005 | .005 |
| Topopah Springs #2 (Ksat = .6 mm/yr)<br>Calico Hills (Ksat = 8,000. mm/yr) | .010 | .010 | .010 |
| Calico Hills (Ksat = 8,000. mm/yr)<br>water table | 19. | 19. | 19. |

Document Name:
DRILLTEXT/1

Requestor's ID:
LAMBERTH

Author's Name:
N. Eisenberg

Document Comments:
Test of appendix on drilling analysis

## APPENDIX H - ANALYSIS FOR DRILLING SCENARIO

The analysis for the drilling scenario largely follows the concepts discussed in the DOE SCP, used to make an estimate of the Expected Partial Performance Measure, EPPM, (which is key to formulating the DOE Site Characterization Program) (DOE, 1988); however the analysis in the SCP is expanded upon and modified is some significant ways. The drillling scenario is in some ways the archetypical direct release scenario and it is anticipated that many of the approaches to analyzing both the probabilities and the consequences of this scenario can be extended to similar scenarios, with appropriate modifications.

Scenario Probability.

To analyze this scenario many of the concepts used in formulating Appendix B of 40 CFR 191 are used. Although this part of the regulation is offered as guidance and is not binding on either the DOE or the NRC, the concepts expressed are a useful starting point for this initial analysis. Two fundamental ideas behind the drilling analysis are: (1)that the institutional memory and control preventing disturbance of the repository fail after some period of time, (2)that the permanent markers at the site fail in their function after some time period, After the greater of these time periods, it is assumed that drilling for economic resources commences. It is assumed that this drilling occurs at the same rate of drilling as today for the type of rock involved. Because of these assumptions, a natural approach to the analysis is to assume that drilling occurs as a random function of space and time and that it can be effectively described as a Poisson process. Although these are rather sweeping assumptions, viable competing hypotheses appear to be at least as speculative or arbitrary. Furthermore, the purpose of the analysis is to reveal any weaknesses in the design or siting of the repository, so if these assumptions preserve important relationships between the important variables affecting the performance of the repository, then their inherent verissimilitude may not be important.

To begin the analysis assume that exploratory drilling takes place at a constant rate, r [per year per kilometer]; then the rate of drilling over the repository is:

$$R=rA_r \qquad (1)$$

where,

$R$ is the rate of drilling into the repository,

$A_r$ is the area of the repository.

If we assume that this drilling occurs in a random fashion, with no memory of previous drilling, then a Poisson distribution may be used to describe the probability of N boreholes being drilled into the repository over a period of

time, $\delta t$:

$$P(N) = \frac{(R\delta t)^N \exp(-R\delta t)}{N!} \qquad (2)$$

where,

$\delta t$ is the time period over which drilling occurs,

N is the number of boreholes.

In general, under this set of assumptions, there can be any number of boreholes over a particular period of time; however, the form of the distribution given in equation (2) assures that the expected value of number of boreholes, $\bar{N}$, is equal to $R\delta t$. Without too much difficulty at this stage of the analysis, a somewhat more general approach to drilling probability can be taken by assuming a Weibull distribution instead of the Poisson distribution. For the Weibull distribution we have,

$$F(x) = \begin{cases} \frac{\beta}{\delta} \{(x-\Gamma)/\delta\} \exp\{-[(x-\Gamma)/\delta]^{\beta}\} & x \geq \Gamma \\ 0 & x < \Gamma \end{cases}$$

For this analysis the location parameter, $\Gamma$, would be taken to be the time at which drilling is assumed to commence, $T_d$. The scale parameter, $\delta$, would be taken to be $1/R\delta T$. The shape parameter, $\beta$, could be chosen to represent a gradual change from a zero rate of drilling to the constant value R used in the Poisson distribution, (2), above. Of course the distribution would need to be suitably modified to account for the finite number of boreholes, N.

For the purpose of this scenario the time period of interest is the time between the commencement of drilling, $T_d$, and the time duration of the simulation (the period of time over which the performance of the repository is to be estimated, e.g. 10,000 years), $T_p$. That is:

$$\delta t = T_p - T_d \qquad (3)$$

Then combining equations (2) and (3), the probability of N boreholes penetrating the site is given by,

$$P(N) = \frac{(R(T_p - T_d))^N \exp(-R(T_p - T_d))}{N!} \qquad (4)$$

and the probability that no boreholes penetrate the site is given by,

$$P(0) = \exp(-R(T_p - T_d)) \qquad (5)$$

Both of the above probabilities assume that $T_p > T_d$; that is that drilling starts sometime before the end of the period of consideration. If drilling starts at a later time, then equations (4) and (5) must be replaced by,

$$P(N) = 0 \qquad (4a)$$

and

$$P(0) = 1 \qquad (5a)$$

The probability of the drilling scenario, $P_s$, i.e. that some drilling into the repository occurs, is given by:

$$P_s = 1 - P(0)$$

or

$$P_s = 1 - \exp(-R(T_p - T_d)) \qquad (6)$$

For the assumptions used in the SCP ($r$ = .0003 boreholes per square km per year, $A_r$ = 5.1 square km, $T_p$ = 10,000 years, and $T_d$ = 0), $P(0)$ = 2.27 E-07, $P_s \equiv 1$, and $N$ = 15.3. This means that the likelihood of no drilling is very small and that, on average, at least 15 boreholes will be drilled at the site over the 10,000 year period of consideration.

The discussion above establishes the probability for the drilling scenario overall and the probability of N boreholes being drilled on the repository site. However, the analysis of this scenario is made more complex, because a borehole can either penetrate the emplaced waste or merely excavate some of the surrounding host rock. In effect, embedded in this scenario is a two-branch event tree:

```
                                |drill excavates
                                |     waste
                                |
drilling occurs ----------------|
on site                         |
                                |
                                |
                                |drill excavates
                                   host rock
```

In the event that host rock, rather than waste, is excavated, some radiological consequences may occur, because in general the host rock will be contaminated to some level by the movement of contaminated groundwater from the repository. The probabilities and consequences of these two event-tree branches need to be considered in the analysis.

First consider the probability of excavation of waste given that drilling occurs on the repository site, $P_e$. Assume:

$$P_e = \frac{\text{intercept area}}{\text{repository area}}$$

or

$$P_e = \frac{N_T A_p}{A_r} \qquad (7)$$

where $A_p$ is the projected intercept area of a waste package on a horizontal plane

and $N_T$ is the total number of waste packages.

For vertical emplacement the projected intercept area is a circle with a radius equal to the sum of the package radius and the drill radius (see Figure H-1). Thus for vertical emplacement:

$$A_p = \pi ( r_p + r_d )^2 \qquad (8a)$$

where $r_p$ is the radius of the waste package
and $r_d$ is the radius of the drill.

For horizontal emplacement, the projected intercept area is a rectangle with height equal to the sum of the package diameter and the drill diameter and width equal to the sum of the package length and drill diameter (see Figure H-2). Thus for horizontal emplacement:

$$A_p = [2(r_p + r_d)] [L + 2r_d] \qquad (8b)$$

where L is the length of the waste package.

For the current repository and waste package design ($r_p$ = .34 m, L = 4.3 m, $N_T$ = 18,000, $A_r$ = 5.1 square km, and assuming the drill diameter is 6 cm), we find for vertical emplacement:

$$P_e = .001518$$

and for horizontal emplacement:

$$Pe = .01139$$

Consequence Analysis.

With such small target-strike probabilities, the usual outcome will be to excavate contaminated host rock rather than waste. Therefore, it is important to estimate the consequences of excavating contaminated host rock.

First consider the volume of waste that would be excavated if a borehole penetrated a waste package. Considering the manner in which the probability of excavation was calculated, a conservative assumption is being used here; i.e., if the waste package is touched by the drill, then the entire cylinder of material excavated from the horizon of the waste package top to the horizon of the waste package bottom is assumed to be solid waste. For boreholes just tangent to the perimeter of the waste package or only partially overlapping it, this is clearly a conservative assumption. For this assumption the volume of excavated waste, $V_e$, for vertical emplacement is given by:

$$V_e = \pi r_d^2 L \qquad (9a)$$

For horizontal emplacement the situation is somewhat more complicated because the length of the column of excavated waste depends on the location on the package at which the drill impinges (see figure 2.). If we let h be the height

of the column of waste and x be the distance from the center of the drill to the midpoint of the waste package, then

$$h = 2\,(r_p^2 - x^2)^{\frac{1}{2}}$$

where $x = \langle 0,\ r_p \rangle$

and x is considered to be uniformly distributed over the indicated range. The average value of height, h, is:

$$\bar{h} = \frac{\pi r_p}{2}$$

whereas the maximum value of h is $2r_p$. Since the ratio of the maximum value of height to the average value is $4/\pi$, a slightly conservative assumption is to assume that the maximum height should be used in calculating the waste volume. But since the values are so close, either choice is reasonable. For a very detailed analysis, in which a great many simulations would be run, the location parameter, x, could be treated as a random variable selected from a uniform distribution; however, this seems to be an excessive level of analysis for this aspect. Therefore, we take as the average volume of waste excavated for each borehole penetrating a horizontally emplaced waste package:

$$V_e = \frac{r_p\,(\pi r_d)^2}{2} \qquad (9b)$$

Now the concentration of waste in the waste package can be considered to be:

$$C_w = \frac{A_s\,Q_w}{N_T\,V_p} \qquad (10a)$$

where $A_s$ is the specific activity of the emplaced waste (curies per MTHM)

$Q_w$ is the total quantity of emplaced waste (MTHM)

$N_T$ is the total number of waste packages

$V_p$ is the volume of a single waste package.

The concentration of waste in the host rock, assuming no sorption onto the rock, depends upon a number of factors including the solubility of the waste, how long the waste has been dissolving, how rapidly the waste is being dispersed in the groundwater system, the porosity of the rock, and the degree of saturation of the rock. As an upper limit (closely following the assumptions for waste leaching used in the groundwater release scenario) on the concentration of waste in the rock, assume that the water is at the saturation limit for the uranium matrix and that the rock is fully saturated. Then, neglecting sorption on the rock and accounting for waste only dissolved in groundwater, the concentration of waste in the host rock is given by:

$$C_r = A_s C_s \varepsilon F \qquad (10b)$$

where $C_r$ is the concentration of radionuclides in the host rock in curies per cubic meter

$A_s$ is the specific activity of the emplaced waste (curies per MTHM)

$C_s$ is the concentration limit for the uranium matrix in water (g $UO_2$ per g $H_2O$)

$\varepsilon$ is the porosity of the rock

and F is a conversion factor of 1.E-06 MT/g * 1.E+06 $cc/m^3$ * 1. g/cc of $H_2O$

Then the ratio of concentration in the rock to concentration in the waste is:

$$C_r/C_w = \frac{C_s \varepsilon F}{(Q_w / N_T V_p)} \qquad (11)$$

For the values assumed here ($\varepsilon$ = .36 - a high representative value, $C_s$ = .001 - the upper limit of the range sampled) the ratio indicated in (11) becomes 3.6 E-04 : 2.49. Thus for equivalent waste volumes the amount of radioactivity released by excavating host rock will be about .01 % of the amount released by excavating waste, given the assumptions used here which tend to overestimate the amount of contamination in the rock. However the rock could be contaminated in much of the space below the emplacement horizon. Given a single borehole, the length of a cylinder of contaminated rock could be as much as the distance from the emplacement horizon to the water table (assuming that the much larger quantities of water in the saturated zone will substantially reduce the concentration). According to the SCP Overview the static water table is 1300 to 2000 feet below ground surface and the repository is 1000 feet below ground surface. Therefore the length of a contaminated rock column could be from 100 to 330 meters. For vertical emplacement the length of the waste column is 4.3 m and for horizontal emplacement averages .53m. Thus the contaminated rock volume could be 77 or 630 times the volume of waste excavated for vertical and horizontal emplacement respecively. This corresponds to .011 and .091, for vertical and horizontal emplacement respectively, as the ratio of consequences between rock excavation and waste excavation. Since excavation of waste is approximately .0015 and .0114 times less likely than the excavation of contaminated rock, for vertical and horizontal emplacement respectively, excavation of contaminated rock could contribute in a significant way to the consequences of this scenario. That is, the incremental risk from excavation of rock could be 7.3 and 8.0 (vertical and horizontal emplacement respectively) times more than excavation of waste. If the sorption of radionuclides by the rock were accounted for, the significance of the excavation of rock could be greater than the above estimate; however, if radionuclides are sorbed, then the concentration of radionuclides in the groundwater would decrease. Of course for very long times and for radionuclides with long half lives, the entire rock column down to the water table could be at the concentration limit for that radionuclide and the rock

itself could be contaminated by sorption to several times that concentration limit. Such considerations, which were omitted from the above estimates, could dwarf the consequence of the other assumptions which may have overestimated the consequences of excavating host rock. For example, if a saturation condition of 0.2, on average, is assumed instead of a value of 1 (complete saturation), the consequences estimated above would be reduced by a factor of 0.2. Regardless, the result of this evaluation appears to be clear; consequences from the excavation of host rock should be included in the model.

To begin a more precise consideration of the consequences from this scenario, consider first the consequences of excavating waste. The consequence of excavating waste by a single borehole at some time, t, is just the release of radionuclides at that time:

$$C_i(t) = \frac{V_e}{V_T} I_i(t) \qquad (12)$$

where,

$C_i(t)$ = is the incremental release of nuclide i at time t

$V_e$ is given by equations (9)

$V_T$ is the total volume of waste emplaced and as used in equation (10a) is given by the product, $N_T V_p$.

$I_i(t)$ is the inventory present in the repository as a function of time.

Now the inventory in the repository at any time depends on two factors: (1)how the inventory changes due to radioactive decay and, in some cases, production and (2)how the inventory changes due to dissolution and migration by groundwater (see Figure H-3). Factor (1) is relatively easy to handle and is conventionally treated in considering the release of radionuclides to the environment by groundwater migration. Factor (2) is very important to treat in this case because it provides the coupling between this scenario class and the groundwater transport scenario classes. That is, we would expect that a "tight" repository would be more vulnerable to releases by drilling, because more of the waste remains in place. Alternatively, a "loose" repository that releases a lot of radioactive material to the geosphere, beginning at an early time, would be less vulnerable to drilling because less waste remains in place. (in other words mother nature is a bitch!) The coupling is not precisely this clear, because, as discussed above, substantial consequences could result from excavating contaminated rock.

The two factors discussed above may be explicitly considered by writing:

$$I_i(t) = D_i(t)L(t) \qquad (13)$$

where,

$D_i(t)$ is the function of time describing radionuclide decay and production, which is radionuclide dependent

and

$L(t)$ is the function of time describing removal of inventory from the repository by dissolution and migration, which can be nuclide dependent, but was assumed to be the same for all nuclides here (in the groundwater migration analysis a simple leach time is calculated based on solubility of the uranium matrix, but for nuclides less solubel, releases from the repository compartment is dependent of the solubility of each nuclides.) and is also assumed).

Now for decay only,

$$D_i(t) = I_i(0)\exp(-\alpha_i t) \qquad (14)$$

where,

$I_i(0)$ is the emplaced inventory of nuclide i for the entire repository

and

$\alpha_i$ is the decay constant for the ith radionuclide because Displaywrite is such a piss poor wordprocessor that it doesn't have a lambda.

To consider decay and production the Bateman equations must be used instead of equation (14); however, for this stage of the analysis only decay is considered.

For the treatment of the source term used in the analysis of the groundwater release scenarios it has been assumed that releases begin from the engineered barrier system at some time after closure, $T_s$, and release of the uranium matrix occurs at a constant rate, until all the matrix is gone, after passage of the time period, $T_L$. This means that the function, $L(t)$, in equation (13) is given by (see Figure H-4):

$$L(t) = \begin{cases} 1 & t<T_s \\ 1 - \dfrac{(t - T_s)}{T_L} & T_s \leq t < (T_s+T_L) \\ 0 & t \geq (T_s+T_L) \end{cases} \qquad (15)$$

where,

$T_s$ is the time at which releases from the EBS start

and

$T_L$ is the time for the waste to move completely from the EBS to the geosphere.

The above equation assumes, implicitly, that the amount of waste excavated by drilling is small compared to the total amount of waste in the repository, since the inventory is reduced in time only by the amount of radionuclides removed by groundwater and not by the amount removed by drilling.

It is clear from equations (12) through (15) that the consequences of excavating waste by a single borehole depend significantly on the time at which such excavation occurs. One approach to treating this issue is to simulate a

number of realizations in which the number and timing of the boreholes are random variables. Another approach would be to divide the time interval of interest into subintervals and to use a representative consequence for each interval. The approach chosen here is to calculate the expected value of consequences over the entire interval of interest. Since equation (12) represents the consequence from a single borehole excavated at time, t, the consequence of N boreholes excavated at time, t, is just:

$$C_i^N(t) = N\, C_i(t) \qquad (16)$$

Let us take this value of the consequence of N boreholes as representative of the consequences that occur over some time increment, $\delta t$, where t is some time in the interval $\delta t$. Then the expected value of consequences, averaged over all possible values of number of boreholes, is:

$$\hat{C}_i(t) = \sum_{N=1}^{\infty} P(N)\, C_i^N(t)$$

$$= \sum_{N=1}^{\infty} P(N)\, N\, C_i(t)$$

Where P(N) is the probability of N boreholes over the time interval, $\delta t$. but since P(N) is given by equation (2), we find:

$$\hat{C}_i(t) = \sum_{N=1}^{\infty} \frac{(R\delta t)^N \exp(-R\delta t)}{N!}\, N\, C_i(t)$$

Since $C_i(t)$ and $\exp(-R\delta t)$ do not depend on the number of boreholes, N, these terms can be taken from under the summation to give:

$$\hat{C}_i(t) = C_i(t) \exp(-R\delta t) \sum_{N=1}^{\infty} \frac{(R\delta t)^N}{(N-1)!}$$

or

$$\hat{C}_i(t) = C_i(t) \exp(-R\delta t)\, (R\delta t) \sum_{N=1}^{\infty} \frac{(R\delta t)^{N-1}}{(N-1)!}$$

or

$$\hat{C}_i(t) = C_i(t) \exp(-R\delta t)\, (R\delta t) \sum_{N=0}^{\infty} \frac{(R\delta t)^N}{(N)!}$$

or

$$\hat{C}_i(t) = C_i(t) \exp(-R\delta t)\, (R\delta t) \exp(+R\delta t)$$

or

$$\hat{C}_i(t) = C_i(t)\, (R\delta t) \qquad (17)$$

Taking the limit of equation (17) as $\delta t$ approaches zero, we have:

$$d\hat{C}_i(t) = C_i(t)\ (Rdt) \qquad (18)$$

Then integrating this result over the time period of interest gives:

$$\hat{C}_i(t) = R \int_{T_d}^{T_p} C_i(t)\ dt \qquad (19)$$

Combining equations (12) and (13) with the above gives:

$$\hat{C}_i(t) = R \frac{V_e}{V_T} \int_{T_d}^{T_p} D_i(t)\ L(t)\ dt \qquad (20)$$

where $D_i(t)$ can be obtained from equation (14) and $L(t)$ can be obtained from equation (15).

To perform the integration indicated in equation (20), it is useful to note the following: (1)if $T_d \leq T_p$ then the integral in (20) is zero (no drilling during the time period of interest); (2)if $T_d > T_s + T_L$ then the integral in (20) is zero (drilling commences after all the waste has migrated from the EBS). Assuming that $T_d < T_p$ and that $T_d < T_s + T_L$, then we may write:

$$\hat{C}_i(t) = R \frac{V_e}{V_T} (I_\alpha + I_\beta) \qquad (21)$$

where,

$$I_\alpha = \begin{cases} 0 & \text{if } T_d > T_s \\ \dfrac{I_i(0)}{\alpha_i} [\exp(-\alpha_i T_d) - \exp(-\alpha_i T_s)] & \text{if } T_d \leq T_s \end{cases} \qquad (22)$$

and

$$I_\beta = \frac{I_i(0)}{T_L \alpha_i^2} [(1+\alpha_i\{T_b - T_s - T_L\})\exp(-\alpha_i T_b) - (1+\alpha_i\{T_a - T_s - T_L\})\exp(-\alpha_i T_a)] \qquad (23)$$

where,

$$T_a = \begin{cases} T_s & \text{if } T_d < T_s \\ T_d & \text{if } T_d \geq T_s \end{cases} \qquad (24a)$$

and

$$T_a = \begin{cases} T_s + T_L & \text{if } T_p > T_s + T_L \\ T_p & \text{if } T_p \leq T_s + T_L \end{cases} \qquad (24b)$$

The above formulas provide an estimate of the consequences of excavating waste. Since the previous analysis also shows that excavation of contaminated rock

could be significant and that the probability of excavating rock is much higher than excavating waste, the following analysis is developed to estimate the consequences of excavating contaminated rock.

We proceed in a manner very similar to that used for estimating the consequences of excavating waste. We rewrite equation (12) for the excavation of rock:

$$C'_i(t) = \frac{V'_e}{V'_T} I'_i(t) \qquad (25)$$

where,

$C'_i(t)$ is the incremental release from excavated rock of nuclide i at time t

$V'_e$ is the volume of rock excavated by a single borehole

$V'_T$ is the total volume of rock that is potentially contaminated by waste from the repository

$I'_i(t)$ is the inventory present in the contaminated rock as a function of time.

As an approximation to the total volume of contaminated rock we use:

$$V'_T = A_r \, d_r \qquad (26)$$

where,

$A_r$ has been defined previously as the area of the repository

and

$d_r$ is the depth of rock underlying the repository subject to contamination

As discussed above, a reasonable assumption is that the concentration of waste in the rock is reduced substantially below the water table, because more flow is available to dilute and disperse the contamination entering from the unsaturated zone. For the Yucca Mountain repository, the water table is at different depths below the repository horizon depending on the lateral location in the repository. This variation in depth is shown in Table 1 of Chapter 3. Based on the information in this Table and taking the weighted average of these depths one obtains an average depth of 249.1 m.

A consistent approximation to the volume of rock excavated is then given by:

$$V'_e = \pi \, r_d^2 \, d_r \qquad (27)$$

Then

$$V'_e/V'_T = \pi \, r_d^2/A_r \qquad (28)$$

As in the analysis for the excavation of waste we can divide the time dependence of inventory into a term related to radioactive decay, $D'(t)$, and a

term related to migration of radionuclides from the repository into the geosphere, $L'(t)$. In an analogue to equation (13) we have:

$$I'_i(t) = D'_i(t)L'(t) \qquad (29)$$

where,

$D'_i(t)$ is the function of time describing radionuclide decay and production, which is radionuclide dependent

and

$L'(t)$ is the function of time describing movement of inventory from the repository to the host rock by dissolution and migration, which can be nuclide dependent, but was assumed to be the same for all nuclides in the groundwater migration scenario and is also assumed here.

To be consistent with the analysis for excavation of waste we assume that the decay function for waste in the geosphere is the same as for waste in the repository and that the removal function for the geosphere, $L'(t)$, is the complement of the removal function for the repository. That is:

$$D'_i(t) = D_i(t) \qquad (30a)$$

and

$$L'(t) = 1 - L(t) \qquad (30b)$$

where $D_i(t)$ is given by equation (14) and $L(t)$ is given by equation (15). These assumptions comprise a tidy compartmental analysis for the waste. Whatever waste does not decay must be either in the repository or in the geosphere. Further undecayed waste moving out of the repository must be in the geosphere. This is a conservative estimate of waste excavated, because the waste transported by groundwater, gas movement, or other means to the accessible environment is not removed from the compartments subject to excavation.

Combining (15) and (30b) we obtain (see Figure H-4):

$$L'(t) = \begin{cases} 0 & t<T_s \\ \dfrac{(t-T_s)}{T_L} & T_s \leq t < (T_s+T_L) \\ 1 & t \geq (T_s+T_L) \end{cases} \qquad (31)$$

In a manner similar to the derivation of equations (16) through (20) we obtain the analogous result for excavation of contaminated rock:

$$\bar{C}'_i(t) = R \frac{V'_e}{V'_T} \int_{Td}^{T_p} D_i(t)\, L'(t)\, dt \qquad (32)$$

As in the previous analysis, to perform the integration indicated in equation (32), it is useful to note the following: (1)if $T_d \geq T_p$ then the integral in (20) is zero (no drilling during the time period of interest); (2)if $T_p < T_s$ then the integral in (20) is zero (leaching commences after the time period of

interest, so all the waste is in the EBS). Assuming that $T_d < T_p$ and that $T_p > T_s$, then we may write:

$$\hat{C}_i'(t) = R \frac{V_e'}{V_T'} (I_\alpha' + I_\beta') \tag{33}$$

If $T_s+T_L > T_p$ then $T_d < T_s+T_L$ and:

$$I_\beta = 0$$

and

$$I_\alpha = \frac{I_i(0)}{T_L \alpha_i^2} [(1+\alpha_i\{T_a-T_s\})\exp(-\alpha_i T_a) - (1+\alpha_i\{T_p-T_s\})\exp(-\alpha_i T_p)] \tag{34a}$$

where

$$T_a = \begin{cases} T_s & \text{if } T_d < T_s \\ T_d & \text{if } T_d \geq T_s \end{cases} \tag{34b}$$

If $T_s+T_L < T_p$ then:

$$I_\beta = \frac{I_i(0)}{\alpha_i} [\exp(-\alpha_i T_p) - \exp(-\alpha_i T_c)] \tag{35a}$$

where,

$$T_c = \begin{cases} T_s + T_L & \text{if } T_d < T_s + T_L \\ T_d & \text{if } T_d \geq T_s + T_L \end{cases} \tag{35b}$$

and

$$I_\alpha = \begin{cases} 0 & \text{if } T_d \geq T_s + T_L \\ \frac{I_i(0)}{T_L \alpha_i^2} [(1+\alpha_i\{T_a-T_s\})\exp(-\alpha_i T_a) - (1+\alpha_i T_L)\exp(-\alpha_i\{T_s+T_L\})] & \text{if } T_d < T_s + T_L \end{cases} \tag{35c}$$

$$T_a = \begin{cases} T_s & \text{if } Td < T_s \\ T_d & \text{if } T_d \geq T_s \end{cases} \tag{35d}$$

If the events of excavating rock and waste were mutually exclusive, then one could just multiply each consequence by its probability of occurence and sum to find the average consequence. However, since every time waste is excavated there is nothing to prevent the column of host rock from also being excavated (unless we assume that if waste were brought to the surface then drilling would stop). Therefore here we will assume that the consequences given by equations

(33 to 35) occur with conditional probability 1.0 (i.e. if drilling occurs with probability given by equation (6)). To find the average consequences, the consequences of excavating waste, as given by equations (21 to 24), must be multiplied by the conditional probability of such excavation, $P_e$, as given by equation (7), and summed with the average consequence of excavating host rock. That is,

$$\hat{C}_f(t) = P_e \, C_f(t) + \hat{C}_f(t) \qquad (36)$$

where,

$\hat{C}_f(t)$ is the overall average consequence

and the other terms have been defined previously.

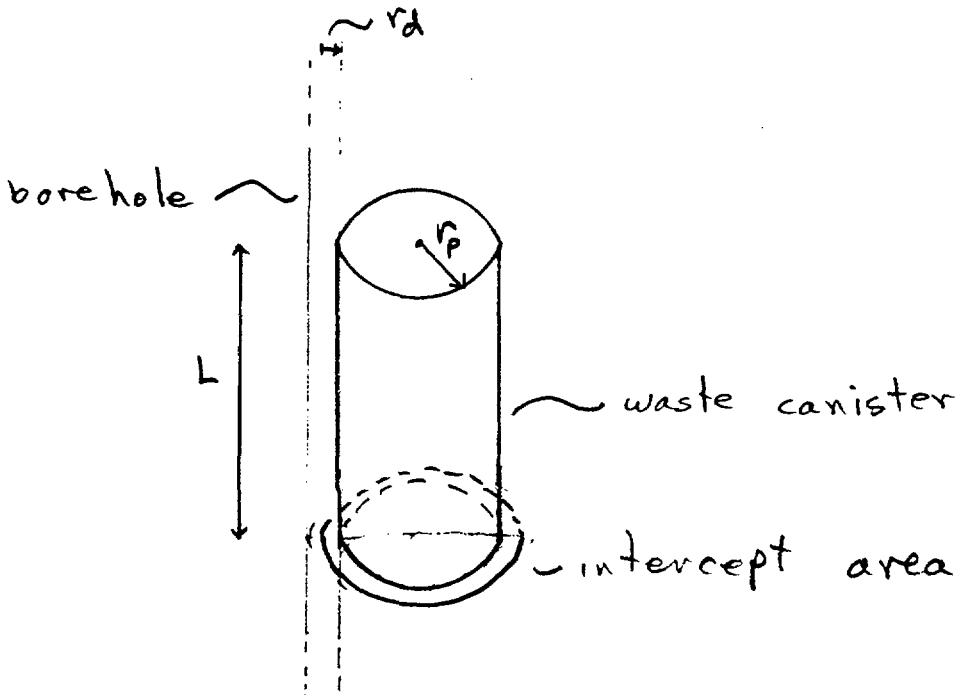



Figure H-1a. Emplacement geometry for vertical emplacement.

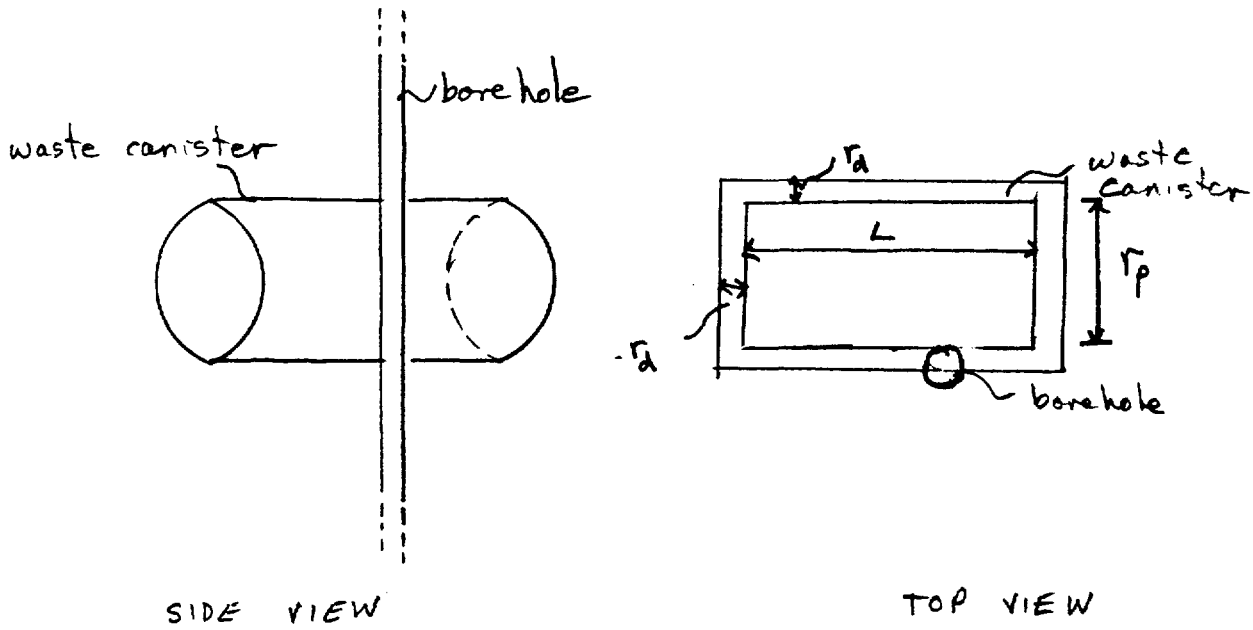
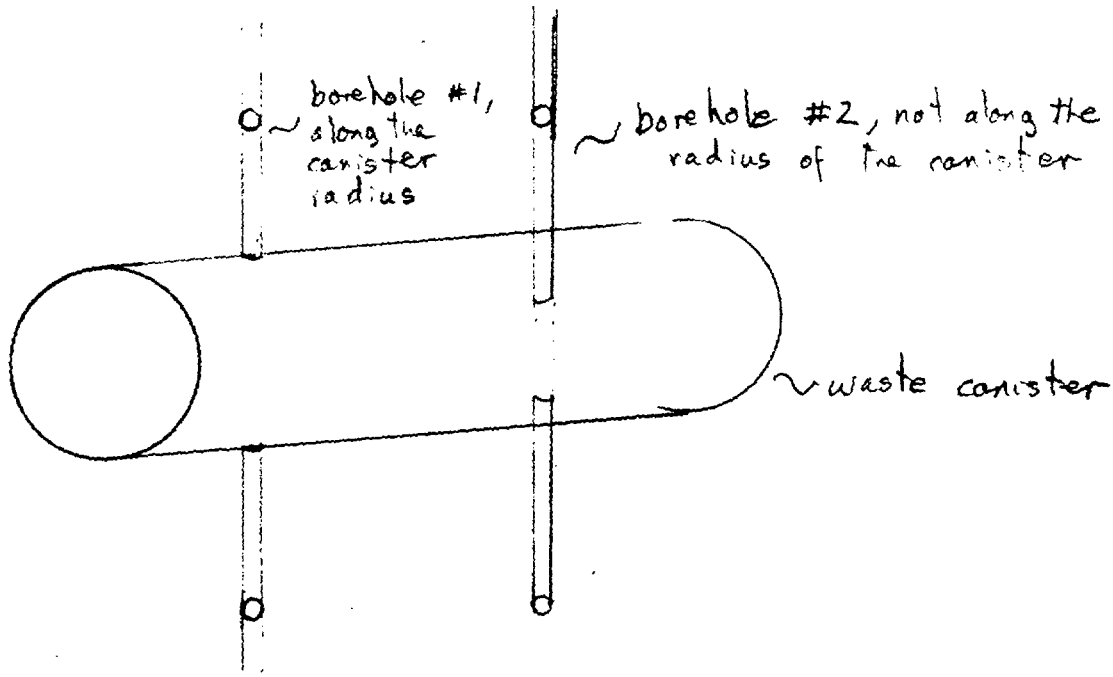



Figure H-1b. Intercept geometry for horizontal emplacement.



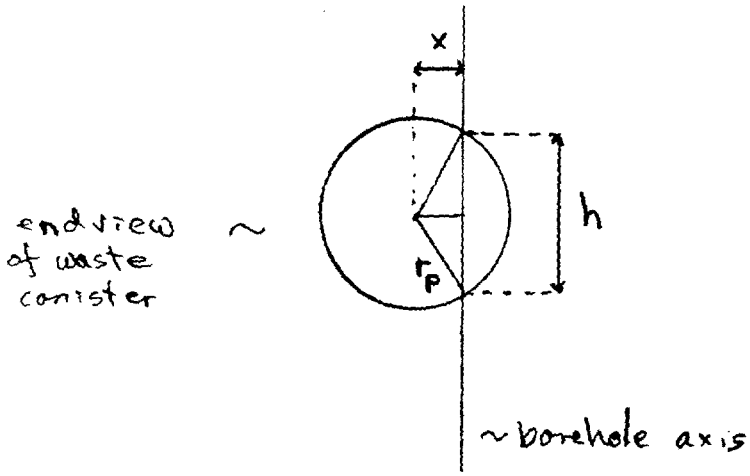




Figure H-2. Geometry for volume excavated by a bore-hole through a horizontally emplaced waste canister.

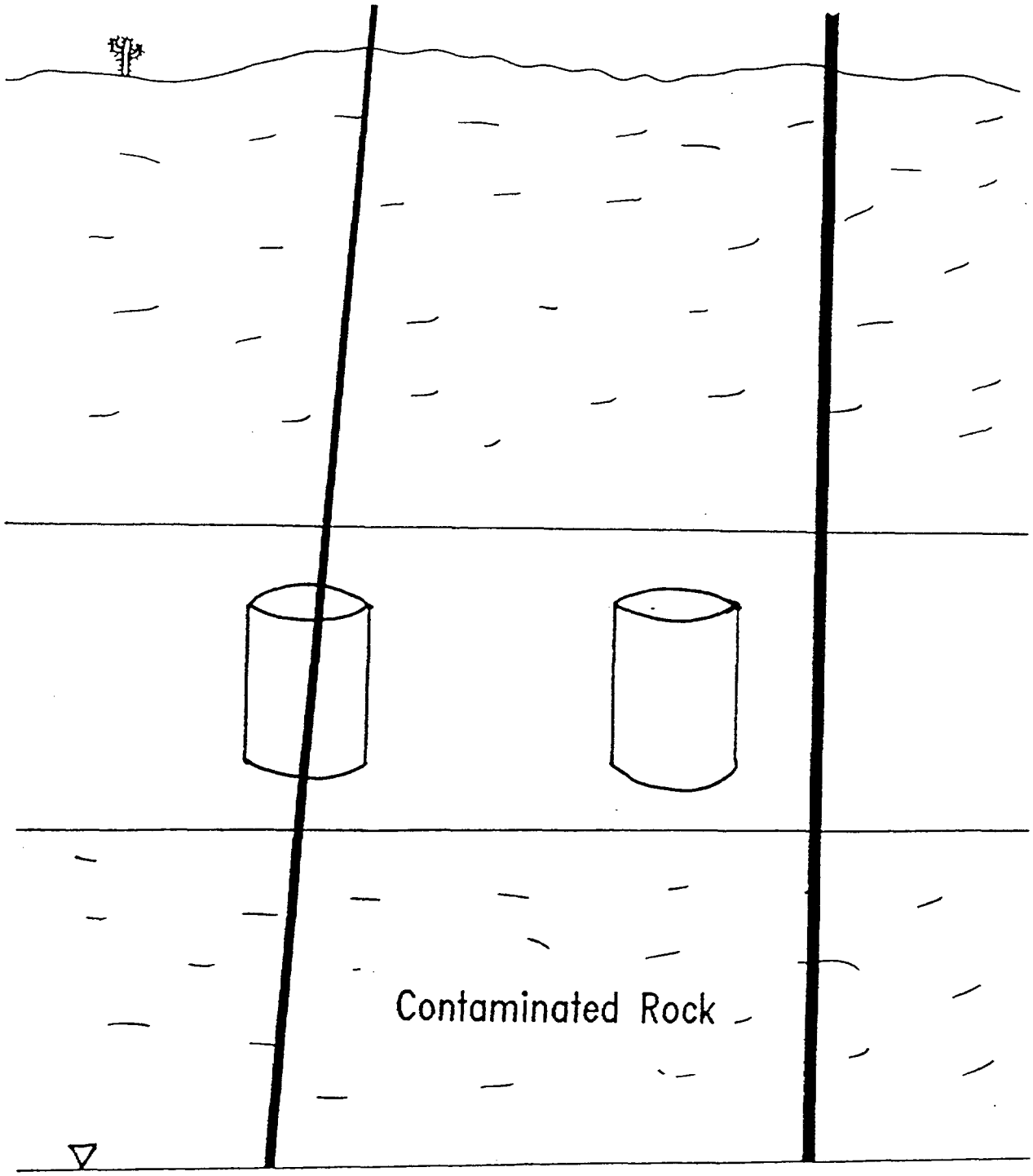



Figure H-3. Conceptual view of drilling through waste canister and contaminated rock below the repository and drilling into contaminated rock.

# Time Considerations

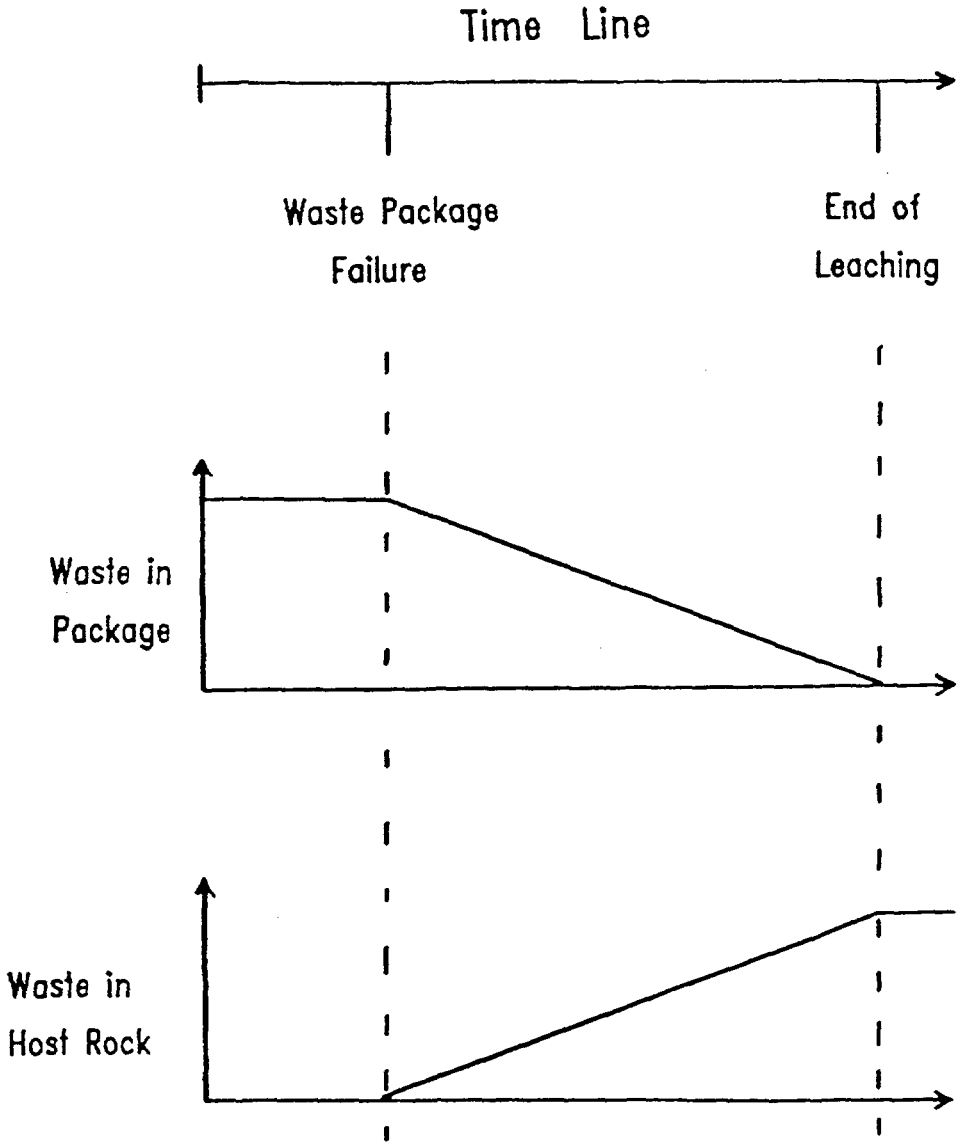



Figure H-4. Depiction of quantity of waste in packages and host rock from the time of waste emplacement till the end of leaching (all waste leached from waste package).

Appendix I

SYS. CODE STEPS

Document Name:
SYSSTEP

Requestor's ID:
FORD

Author's Name:
JAMES R PARK

Document Comments:
MOU APPENDIX ON SYSTEM CODE STEPS

## APPENDIX I - SYSTEM CODE STEPS

The following is a more detailed step-by-step outline of the system code operation than that provided in Section 4.4.4.

1. Set parameters and dimension the neccessary arrays

2. Open input and output files
   - A. EPALIM.DAT : file of EPA limits for 28 radionuclides based on an initial inventory of 10,000 Metric Tons Heavy Metal (MTHM)
   - B. SYS.INP : analyst-supplied input for a particular run, consisting of input/output flags, manner of execution, what scenarios and which release pathways to treat
   - C. SYS.DAT : file for more detailed output; amount placed here dependent on system code input values
   - D. SCENPROB.DAT : file of scenario probabilities
   - E. CCDF.DAT : file containing only that data needed to graph a CCDF

3. Read in input/output flags, simulation time, and fundamental events from SYS.INP

4. Write date and time of run to output file SYS.DAT

5. Read in EPA limits from EPALIM.DAT and calculate weighting factor for each radionuclide

6. Sequence thru scenarios
   - A Read in from SYS.INP scenario names, number of pathways, and pathway designators for the first scenario identified
   - B. Generate consequence model input vectors through LHS routine if run is internal
   - C. Check if groundwater pathway is accessed for radionuclide release
     if so, continue with 1) below
     if not, go to step 6D
     - 1a) run groundwater flow and transport model if run is internal
     - 1b) ask for name of groundwater model output file to access if run is external; read in file name from SYS.INP
     - 2) Open groundwater model output file
     - 3) Read in radionuclides and cumulative releases for each input vector until all data are input to the program
     - 4) Call ORDER subroutine
       - a. compare radionuclide names against names for which EPA limits are given
       - b. calculate normalized releases using EPA weighting factor corrected for initial inventory of 70,000 MTHM
       - c. places releases into four dimensional CUMREL array according to scenario, radionuclide, vector, and pathway

D. Check if groundgas pathway is accessed for radionuclide release
if so, repeat steps C1 to C4 above
if not, go to step 6E
Note: no consequence model is installed at the present time for the groundgas pathway

E. Check if direct release pathway is accessed for radionuclide release
if so, repeat steps C1 to C4 above
if not, go to step 6F
Note: only release via drilling is installed at this time

F. Go to step 6A and check if more scenarios are to be modeled
if so, continue at step 6A
if not, continue with step 7 below

Summing Calculations

7. Sum normalized releases in CUMREL over release pathway into three dimensional PEPASUM array

8. Sum normalized releases in CUMREL by radionuclide into three dimensional REPASUM array

9. Sum REPASUM over release pathway into two dimensional SEPASUM array

10. Sum PEPASUM by radionuclide into two dimensional FEPASUM array

11. Compare SEPASUM against FEPASUM for errors

Calculations for CCDF

12. For each scenario treated, sort summed normalized releases in SEPASUM in ascending order top to bottom using the ASORT subroutine

13. Place ordered releases into EPASUM by scenario and vector, along with the probability of each consequence given that each vector in a scenario is equally probable, i.e., $P(R) = (\text{number of vectors})^{-1}$

14. Compress EPASUM by comparing each release with all other releases within the same scenario; if a match is found, the probabilities are combined and duplicate release values are deleted

15. Read in scenario probabilities

16. Calculate the total CCDF
    A. Place releases and their associated likelihoods for all scenarios from EPASUM into TSDF, a three dimensional array
    B. Sort TSDF from top to bottom in ascending order
    C. Compress TSDF array and recalculate probabilities as in step 14
    D. Create a running cumulative probability in the third dimension of TSDF

17. Generate system code output files
    A. SYS.DAT filled according to flags set in SYS.INP
    B. Place TSDF array into CCDF.DAT file

Document Name:
MOU APP J/

Requestor's ID:
MCCARTIN

Author's Name:
codell

Document Comments:
documentation of transport and source term models

App J

# APPENDIX J - DOCUMENTATION OF FILES AND PROGRAMS ON INEL CRAY XMP/24 FOR REPOSITORY PERFROMANCE CALCULATIONS

## J.1 Introduction

This appendix documents briefly the more significant computer programs, data files and output files used to generate and manipulate the results on source term and transport presented in this report.

## J.2 FORTRAN Programs

### J.2.1 NEFTRAN6

This is the modified version of NEFTRAN for the Yucca Mountain demonstration. It has the following modifications from the standard version in NUREG/CR-4766:

a. All calculations having to do with the determination of the flow through saturated flow tubes using Darcy's law are removed. Flux is now an input variable based on infiltration and fracture flow as determined by saturated hydraulic conductivity.

b. Most input variables needed for unsaturated flow and transport are contained in subroutine GETRV. This subroutine reads the random input vectors on TAPE10 generated by program LHSVAX, and generates an output vector file of radionuclide releases cumulated over time (either 10,000 or 100,000 years) and written to TAPE20.

c. There are minor changes to the output format of TAPE20 to include the scenario number on each record.

### J.2.2 CCDFLIM

This program takes the TAPE20 output files generated by NEFTRAN6 for the 4 columns and generates a CCDF for each scenario. It multiplies the output cumulative releases for each radionuclide by their respective EPA release limit factors to get an EPA ratio for each vector. The vectors are then combined for the four columns, sorted and written to a file for transmission to NRC and plotted with the commercial program GRAPHER on a PC. The CCDFLIM program also calculates the average contribution to the EPA ratios by radionuclides and sorts them in descending order. CCDFLIM allows the compiled output results to include or reject output vectors on the basis of limits on the input parameters or combinations of parameters read into NEFTRAN. For example, the program can screen out all vectors for which the groundwater travel time exceeds 1000 years, with the groundwater travel time determined from a combination of input parameters.

### J.2.3 COMBINE

This program combines the four TAPE20 output files from NEFTRAN for the four columns into a single combined TAPE20 output file. The main reason for this is to avoid having to send four lengthy files from the Cray system to the NIH system on BITNET, and to avoid a problem on BITNET which was causing some of the long lines of output to get clipped at 79 columns. The new output file is identical to the old TAPE20 output, except that the long lines are no longer written in list-directed form, but in formatted form with a line length of 68 characters. If the output for a particular chain is all zeros, then list-directed output is still used in order to take advantage of the compact structure.

J.2.4 LHSVAX

This program generates the Latin Hypercube sample for input to NEFTRAN6. The staff has modified it in the following way:

a. It now contains its own random number generator, RAN1 from Numerical Recipes.

b. It reads the names of the inputs and output files.

J.2.5 STEP

This program performs the stepwise linear regression and rank regression on the outputs of NEFTRAN6 for each scenario in order to determine sensitivities and uncertainties. The main modification to this program was to take the TAPE20 output from the four columns generated by NEFTRAN6 and combine them into EPA ratios for each vector using the EPA release limit factors. The combined EPA ratios are written to a temporary file and read into the STEP program to generate the regressions.

J.2.6 C14B

This program calculates the carbon-14 release from the waste packages as a function of time. The program assumes that the canisters fail with a normal probability distribution. Once failed, oxygen attacks the fuel matrix and releases its inventory according to a rate based on the spallation time, randomly picked from a uniform probability distribution bounded by two lines that are functions of temperature. To the release rate is added the prompt release at the time of canister failure.

J.3 Batch Script Files

The following batch files execute programs in the batch mode on the Cray using the batch queue function QSUB:

J.3.1 STATCON.SUB

This batch file executes in sequence the program LHSVAX and NEFTRAN6 for all four columns and then the program CCDFLIM, to generate a CCDF. The main purpose of this script file is to simplify the multistep operation for generating the CCDF, particularly for the statistical convergence exercise that demonstrated the sensitivity of the CCDF to the number of Latin Hypercube vectors samples chosen (either 100 or 500). We chose a new seed for each of the runs with 100 vectors.

## J.4 Data Files

J4.1 ympyuc2.dat - This file was used in every case to generate the Latin Hypercube samples for NEFTRAN6 based on the distribution and ranges specified for 47 variables. When used in the statistical convergence test, we chose a new random input seed specified in this file, for each CCDF run.

J4.2 epalim.dat - the EPA release limits by radionuclide in terms of permissible releases per 10,000 metric tons heavy metal.

J4.3 t51nl - This is the NEFTRAN6 card image input file for the basic parameters in column A, 10,000 year base case scenario, 500 vectors

J4.4 t52nl - same as above, but column B.

J4.5 t53nl - same as above, but column C.

J4.6 t54nl - same as above, but column D.

J4.7 t51100 - same as t51nl, but 100,000 years

J4.8 t52100 - same as t52nl, but 100,000 years

J4.9 t53100 - same as t53nl, but 100,000 years

J4.10 t54100 - same as t54nl, but 100,000 years

J4.11 TAPE10 - The random vectors produced by LHSVAX for the input file ympyuc2.dat

## J.5 Output files

J5.1 tape2051.10, tape2052.10, tape2053.10, tape2054.10 - These are the TAPE20 output files from NEFTRAN6 for the base case, 10,000 year cumulative releases for the four columns referred to in the text as columns A, B, C and D, respectively.

J5.2 tape201.500, tape202.500, tape203.500, tape204.500 - These are the TAPE20 output files from NEFTRAN6 for the base case, 100,000 year cumulative releases for the four columns refereed to in the text as columns A, B, C and D, respectively.

J5.3 tape20cmb.10 - This is the combined output for tape2051.10, tape2052.10, tape2053.10 and tape2054.10 produced by program COMBINE.

J5.4 ccdf10.out - This is the output file for plotting the CCDF for the 10,000 year base case scenario.

J5.5 ccdf100.out - This is the output file for plotting the CCDF for the 100,000 year base case scenario.

J5.6 TAPE6 - The normal printed output file for each NEFTRAN run.