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SITE SUITABILITY CRITERIA FOR SOLIDIFIED HIGH LEVEL WASTE REPOSITORIES

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ABSTRACT AND FOREWORD

NOTICE
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The Nuclear Regulatory Commission (NRC) is responsible for the management and disposal of nuclear wastes from licensed facilities. The agency also has licensing responsibility for long-term storage and disposal of high-level radioactive wastes from commercial operations and the Department of Energy.

In discharging its responsibilities, the NRC is developing a framework of regulations, criteria, and standards. Lawrence Livermore Laboratory (LLL) provides broad technical support to the NRC for developing this regulatory framework, part of which involves site suitability criteria for solidified high-level wastes (SHLW).

Both the regulatory framework and the technical base on which it rests have evolved in time. This document is the second report of the technical support project. It was issued as a draft working paper for a programmatic review held at LLL from August 16 to 18, 1977. It was printed and distributed solely as a briefing document on preliminary methodology and initial findings for the purpose of critical review by those in attendance. An earlier draft was generated as a briefing document for meetings with the NRC at LLL on March 22 and 23, 1977.

These briefing documents are being reprinted now in their original formats as UCID-series reports for the sake of the historical record. The LLL program has evolved rapidly and extensively. Some approaches that merited consideration during the initial stage of investigation have been discarded. New approaches have been tested. The models have been continuously refined and the data base updated with the accumulation of new information. Analysis results have evolved as both the models and data base have changed. As a result, the methodology, models, and data base in this document are severely outmoded.

In addition to these evolutionary programmatic changes, major shift in program direction was mandated during FY 78 as a result of the Presidential

decision to defer the reprocessing of spent reactor fuel. Emphasis was shifted from SHLW disposal to the study of spent-fuel disposal and retrieval in the environment of a deep geologic repository.

For current (1979) information, the reader is referred to the most recent publications of the LLL technical support project, in particular, "High-Level Waste Repository Site Suitability" (UCRL 52633, JRE6/CR 0578), which has its genesis in the two 1977 briefing documents.

**SITE SUITABILITY CRITERIA
FOR SOLIDIFIED HIGH LEVEL WASTE REPOSITORIES**

A Preliminary Report Prepared for
The Waste Management Program
Division of Fuel Cycle and Material Safety
Office of Nuclear Material Safety and Safeguards
U.S. Nuclear Regulatory Commission

**SITE SUITABILITY CRITERIA
FOR SOLIDIFIED HIGH LEVEL WASTE REPOSITORIES**

August 16, 17, and 18, 1977

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This preliminary report summarizes the results of the LLL study on "Site Suitability Criteria for Solidified High Level Waste" performed under the direction of William M. Hewitt of Waste Management Program of the Nuclear Regulatory Commission.

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1. INTRODUCTION

1.1 Purpose of Study

DEVELOPMENT OF REPOSITORY SITE SUITABILITY CRITERIA IS AN
ESSENTIAL STEP TOWARD CLOSING THE NUCLEAR FUEL CYCLE.

THE NRC MUST ISSUE EFFECTIVE AND REALISTIC REGULATIONS FOR THE DISPOSAL OF NUCLEAR WASTES IN ORDER TO BE RESPONSIVE TO ITS MANDATE TO PROTECT THE PUBLIC HEALTH AND SAFETY. THE TECHNICAL BASIS FOR THESE REGULATIONS IS PROVIDED BY THE STUDY BEING CONDUCTED BY LLL. TIMELY DEVELOPMENT OF SSC IS ESSENTIAL PORTION OF THE WM EFFORT.

The development of regulations for the safe management of nuclear waste must have a sound technical basis both to provide for the protection of the public health and safety and to renew public assurance in the ability of the federal government to wisely regulate the nuclear industry. This basis is provided by a complex, inter-disciplinary study of the components of the waste management system and their associated risks.

LLL is presently conducting this study for each of the components

illustrated on the opposite page. The post-sealing history presently considers repository site suitability criteria and will incorporate the development of design, performance criteria in the future.

The analysis of the factors involved in site suitability is being conducted with both timeliness and technical completeness in mind. This report will describe the analytical methods being used, preliminary results, and the areas to be emphasized in future cycles of the study.

SPENT FUEL

PROCESSING PLANT

PROCESSED WASTE

INTERIM STORAGE

HIGH-LEVEL
WASTE

Scope of
Site Suitability
Study

REPOSITORY SITE

1. INTRODUCTION

1.2 Systems Analysis Approach

THE POST-SEALING HISTORY OF A REPOSITORY IS EFFECTIVELY ANALYZED USING A SYSTEM ANALYSIS APPROACH.

SYSTEMS ANALYSIS IS AN EFFECTIVE MEANS FOR DEFINING AND ANALYZING THE COMPONENTS OF THE WASTE MANAGEMENT SYSTEM. THE SYSTEM CAN BE DECOMPOSED INTO INDEPENDENT COMPONENTS TO FACILITATE ANALYSIS. THE POST-SEALING HISTORY CAN THEN BE DESCRIBED BY APPROPRIATE GEOLOGIC, HYDROLOGIC, AND RISK ASSESSMENT MODELS.

The high-level waste management system has been defined as: solidification of the high-level waste and interim storage; transportation to the repository site; handling and emplacement of the repository until the repository is sealed; and the future history of the sealed repository. This system is shown diagrammatically on the opposite page.

Each component can be analyzed separately when the interfaces are understood and correctly modeled with a consistent set of assumptions. The risks associated with each component can then be minimized by identifying the critical factors. Thus, the overall risk from the waste management processes can be minimized.

Modeling of the post-sealing history of a repository will result in the identification of the critical factors related to site suitability. This requires the analysis of reasonable geologic events, and their effect on geohydrologic parameters, the modeling of waste transport through the hydrologic system and the calculation of the associated radiologic risk. Some events that must be considered are shown on the diagram to the right.

A multicycle systems analysis approach is being used. Each cycle serves to more clearly define the parameters and their uncertainties, to further refine the models developed and to validate assumptions and approximations used.

Nuclear Fuel Cycle Operation
spent fuel reprocessing

WASTE MANAGEMENT SYSTEM

Components of the Nuclear Waste Management System

1. INTRODUCTION

1.3 Fuel Cycle Assumption

ONLY THE URANIUM - PLUTONIUM RECYCLE FUEL CYCLE HAS BEEN ANALYZED IN THE INITIAL PHASES OF THE STUDY.

THE ANALYSIS HAS BEEN BASED UPON RADIONUCLIDE INVENTORIES CONSISTENT WITH SOLIDIFIED LIQUID WASTE RESULTING FROM THE REPROCESSING OF LWR FUEL. ALTERNATE WASTE TYPES, INCLUDING SPENT FUEL, WILL BE STUDIED IN THE NEXT CYCLES.

The assumption used thus far has been that the waste to be disposed of in a deep geologic repository is that resulting from the reprocessing of light water reactor fuel 150 days after removal from the reactor. The reprocessing removes 99.5% of the uranium and plutonium and a portion of the volatiles.

The alternate waste forms to be studied include other forms of solidified HLW, spent fuel, military high level wastes, and other commercial high level wastes.

The wastes that eventually will be disposed of in a repository will depend upon the waste classification system chosen by NRC.

**Present Fuel Cycle Assumed
in Radionuclide Inventory
Calculations:**

URANIUM-PLUTONIUM RECYCLE

**Fuel Cycles and Waste
Forms to be Analyzed:**

URANIUM-ONLY RECYCLE

NO RECYCLE

TRU WASTES

MILITARY HIGH LEVEL WASTES

OTHER HIGH LEVEL WASTES

FUEL CYCLE ASSUMPTIONS

1. INTRODUCTION

1.4 Review of Cycle I Analysis

THE FIRST CYCLE SCOPED THE PROBLEM, ANALYZED RELATIVE
PARAMETER AND EVENT IMPORTANCE, AND DEFINED FUTURE
ANALYTIC STRUCTURE.

THE STRUCTURE OF THE SYSTEM AND THE ANALYTIC METHODS TO BE USED WERE
DEFINED IN THE FIRST CYCLE. THE PRELIMINARY DETERMINISTIC ANALYSES
NECESSARY TO PROVIDE AN ADEQUATE SCOPING OF THE PROBLEM WERE OUTLINED
AND INITIATED. THE UNDERSTANDING GAINED FROM THESE PRELIMINARY
ANALYSES WILL FACILITATE THE USE OF MORE COMPLEX, PROBABILISTIC
MODELS IN THE FUTURE.

Assessing the suitability of a site for the location of a high level repository forms a system of many interrelated, and not always well-defined factors. The nature of this problem lends itself to a multi-cycle systems analysis approach. The study is proceeding with parallel efforts in data development and model development.

In the first cycle, an exhaustive list of the parameters likely to affect the performance of a repository site was compiled. At this point some parameters that would have little effect on the system and had high inherent uncertainties were deferred for later study. The rest were separated into groups of similar parameters, i.e., lumped quantified via discussion and consensus of engineers, geologists, and hydrologists familiar with the problem.

A macroscopic model was developed. This model incorporated a one-dimensional hydrologic model, waste concentration calculation, and a human-uptake (radiological risk) model.

Some performance measures likely to be used in the definition of acceptable risk were used.

A typical repository site was modeled. Geologic events were described deterministically (i.e., state and time were specified) rather than probabilistically. Some very low probability events were deferred for later study.

A preliminary parameteric sensitivity analysis was performed using these models and the estimated parameters. This analysis served to indicate which factors needed further study with more well-defined quantification of the parameters and a more realistic repository model.

A Markov chain model was chosen for use in incorporating the probabilistic nature of the events occurring at a repository. This model will be used in the future when further deterministic studies have served to more clearly define the impact of geologic events on groundwater parameters.

CYCLE I ANALYSIS

2. SUMMARY

2.1 Regulatory Philosophy

THE MULTIBARRIER CONCEPT AND THE TEMPORAL NATURE OF THE RISK IMPACT REGULATORY PHILOSOPHY.

THE NATURE OF THE REPOSITORY SYSTEM REQUIRES THE INCORPORATION OF MANY TRADE-OFFS IN THE REGULATIONS. ASSURING THE INTEGRITY OF A REPOSITORY IS NOT ANALOGOUS TO ASSURING THE SAFETY OF A REACTOR OR OTHER ENGINEERED FACILITIES. THE DEPENDENCE UPON NATURAL BARRIERS REQUIRES THERE TO BE REDUNDANCY IN THE EXISTING SYSTEM. THE INTERPLAY OF THE NATURAL FACTORS IS THUS THE CONCERN OF THE REGULATOR RATHER THAN THE REQUIREMENT OF ADDED ENGINEERED SAFETY FEATURES TO ASSURE ADEQUATE REDUNDANCY IN A SUITABLE SITE.

The classical approach to nuclear facility has been to identify the components of the facility whose failure could endanger the public health and safety and to require redundancy, stricter quality control or other measures intended to reduce the risk associated with that failure.

The suitability of a site for the disposal of high-level nuclear waste is a different problem. In this case, due to the time frame involved, reliance must be placed upon the natural conditions existing at the site rather than on engineered safety features. Therefore, redundancy must be provided by the formation the waste is emplaced in.

A suitable site can, in fact, provide this redundancy, or in

other words, multibarrier protection. The regulator must now assure that the combined effect of the critical factors acting at a repository system is to provide protection to the public. This protection is assured by providing sufficient additional barriers so that the probability of release is decreased and so that the risk in the event of a release is minimized.

The temporal behavior of the hazard associated with the waste inventory may also have an impact on the regulatory philosophy. Two sets of regulations may be necessary. One for the near term emphasizing the minimization of the probability of major disturbances and one for the long term emphasizing the reduction of the consequences given that such an event occurs.

BIOSPHERE

2. SUMMARY

2.2 Multibarrier Concept

THE REPOSITORY SYSTEM IS COMPOSED OF GEOCHEMICAL,
HYDROLOGICAL, AND GEOMETRICAL BARRIERS.

THE MULTITUDE OF FACTORS OPERATING IN THE REPOSITORY SYSTEM PROVIDES A NATURAL REDUNDANCY, I.E., MULTIPLE BARRIERS TO RADIONUCLIDE RELEASE TO THE BIOSPHERE. THE MOST SIGNIFICANT OF THESE APPEARS TO BE THE GEOCHEMICAL RETARDATION OF RADIONUCLIDES. THE SYSTEM HYDROLOGICAL FACTORS AND GEOMETRY ALSO SERVE AS BARRIERS. IF ANY ONE BARRIER IS DEFICIENT, WASTE ISOLATION AT A SUITABLE REPOSITORY SITE IS STILL ASSURED.

The single parameter sensitivity analyses have been performed on three sets of repository characteristics: hydrologic, geochemical, and geometric factors. The preliminary results seem to indicate that deficiency in one of these areas does not significantly effect the risk. Validation of the assumptions that the study is based on, will add confidence to this result.

The system appears to be most sensitive to geochemistry. Geochemical waste/rock interaction: serve to retard radionuclide transport in the groundwater. Actinide and fission product sorption is the major mechanism in this retardation. Even when the geochemical interactions are taken to retard waste less than is expected the length of

time taken to reach the biosphere (due to hydrologic and geometric considerations) and dilution at the aquifer discharge serve to reduce the consequence of the release to acceptable levels.

When these parameters are varied together in the direction of increasing nuclide release the dose is significantly affected.

These results are preliminary. More multiple parameter analyses will be performed in the next cycle as well as a complete analysis of the results of the single parameter analyses. This study will provide a clearer understanding of which factors, in combination, provide the multibarrier system.

2. SUMMARY

2.3 Temporal Behavior of Risk

RADIOLOGICAL HAZARD ASSOCIATED WITH THE WASTE INVENTORY DECREASES SIGNIFICANTLY WITHIN 400 YEARS.

THE FIRST 400 YEARS AFTER SEALING OF THE REPOSITORY REPRESENTS A PERIOD OF HIGH CONSEQUENCE GIVEN A SIGNIFICANT RELEASE OF RADIONUCLIDES OCCURS BUT A CORRESPONDENTLY HIGH CONFIDENCE THAT THE PROBABILITY OF A RELEASE OCCURRING IS SMALL. CONVERSELY THE CONFIDENCE THAT ALL RELEASES CAN BE PREVENTED OVER VERY LONG TIMES IS QUITE SMALL; HOWEVER, THE CONSEQUENCE OF A GIVEN RELEASE IS ALSO SMALL. HENCE, ALTHOUGH THE TOTAL RISK CAN BE CONFIDENTLY HELD BELOW REASONABLE LEVELS, TWO DISTINCTIVELY DIFFERENT PHILOSOPHIES OF SUITABILITY CRITERIA MUST BE IMPLEMENTED,

Radiological risk is a function of probability of release and consequence. To minimize risk, one can limit probability or consequence or both. The indication of the study thus far has been that during the first 400 years after sealing of the repository, the consequence of a significant release is high due to the concentrations of ^{90}Sr and ^{137}Cs in the waste. After this time the hazard associated with the waste inventory has decreased several orders of magnitude.

This suggests that during the first 400 years where consequence domin-

ates the risk, regulations should be aimed at reducing the probability of release. This would require good containment and a geologically stable region, for example. After

this period ^{90}Sr and ^{137}Cs have

decayed away and the remaining nuclides are long-lived. Also, by this time the confidence in the ability to contain the waste has decreased significantly. Therefore, the long range emphasis should be upon retarding radionuclide transport through the geohydrologic system. This might require good actinide sorption capabilities and slow ground water movement, for example.

50 yr BODY DOSE TO AVERAGE INDIVIDUAL PER MW-yr PER yr OF WASTE ENTERING RIVER, ESTUARY, OCEAN SYSTEM - CONSTANT INPUT

3. ANALYTIC STRUCTURE

3.1 Cycle II Analysis Overview

CYCLE II ANALYSES EXTENDED AND REFINED THE SENSITIVITY ANALYSIS EXECUTED IN CYCLE 1.

THE SENSITIVITY ANALYSES IN CYCLE II WERE PERFORMED USING MORE JUSTIFIABLE DATA INPUTS, A MORE CLEARLY DEFINED MODEL AND REVISED RADIOLOGICAL RISK PARAMETERS. THESE REVISIONS ALLOW MORE CONFIDENCE TO BE PLACED IN THE RESULTS. THIS ANALYSIS SERVES AS A BASIS FOR PROBABILISTIC MODELS TO BE USED IN THE FUTURE.

The major emphases in Cycle II were upon data base development and extensive single parameter sensitivity analyses.

The data were essentially regenerated. Studies were made of major salt and shale basins in the U.S. Preferred values for the parameters and their generic ranges and uncertainties were then derived.

The repository model was revised to include the permeable fracture zones around the repository shaft and tunnel.

Radiological risk was calculated and stored in terms of individual and population doses and radionuclide concentrations. These values will be available when the acceptable risk criteria study is complete.

Single parameter sensitivity analyses were performed on the parameters identified for study in the first cycle using the new data. The parameters were varied from the preferred values to the "worst limit" of the generic range to determine the sensitivity of the system to each parameter.

A multiparameter analysis was initiated. Groups of parameters were varied simultaneously in the direction of increased radionuclide flow.

The increased understanding of the relative sensitivities of the system to each parameter and of which factors the system is essentially insensitive to will facilitate use of a probabilistic model in future cycles of the study.

CYCLE II ANALYSIS

3. ANALYTIC STRUCTURE

3.2 Model Description

THE GEOLOGY-HYDROLOGY MODEL IS DESIGNED TO FACILITATE SENSITIVITY ANALYSES.

THE CALCULATION OF RISK FROM RADIONUCLIDE RELEASE TO THE BIOSPHERE INVOLVES THE MODELING OF RADIONUCLIDE TRANSPORT IN GROUNDWATER, HUMAN WATER USE SYSTEMS AND PATHWAYS AND THE PROBABILITY OF FUTURE EVENTS AND THEIR EFFECT ON RADIONUCLIDE RELEASE. THE FUTURE EVENTS CAN BE TAKEN INTO ACCOUNT EITHER BY SPECIFYING WHEN THEY OCCUR OR BY USING A PROBABILISTIC MODEL AND CALCULATING EXPECTED VALUES OF CONSEQUENCE. BOTH METHODS ARE BEING USED. THE MODEL IS DESIGNED TO FACILITATE SENSITIVITY ANALYSES.

The geology-hydrology model and computer program calculates the release of radioactive waste to the biosphere due to transport in groundwater. The model incorporates the effects of mass transport, chemical interactions between waste components and soil, and hydrodynamic dispersion.

Future events may affect the movement of groundwater and dissolved radionuclides. The model can take these future events into account by either of two methods.

- Doses can be calculated for scenarios in which events occur at specified times.
- The events can be taken to occur at random times with given probability of occurrence per year and expected values of consequence calculated.

Presently the first method is being used. The statistical method which makes possible the second type of analysis has been developed.

Calculations for the geology-hydrology model are carried out by a central computer program in conjunction with a number of other computer codes. The information flow between these codes is shown in the illustration on the opposite page.

flow of waste without consideration of radioactive decay. The results of its calculations are in units of fractions of the total inventory of each nuclide. In order to provide numbers which directly measure risk, these results must be multiplied by the inventories of the nuclides. These inventories are provided by the ORIGEN code, which was originally developed at Oak Ridge National Laboratory.

Doses to humans will depend on the movement of waste through surface waters, concentration in the ecosystem, human diets and living habits and the biochemistry of the waste nuclides in the human body. These factors are modeled in the human uptake program.

Outputs of the different programs are multiplied together and final data manipulations are performed by the waste concentration and dose programs.

Because the characteristics of possible waste repository sites and engineering designs are not well defined at this time, the model is constructed so as to facilitate sensitivity studies. The groundwater flow pattern is approximated by a network of one-dimensional flow paths, which need not be straight. The justification for this procedure is discussed in Appendix 3.2.

3. ANALYTIC STRUCTURE

3.3 Radiological Risk Calculations

RELATIVE RADIOLOGICAL RISK IS MOST EASILY EVALUATED WHEN
EXPRESSED IN TERMS OF DOSE AND RADIONUCLIDE CONCENTRATIONS.

AQUIFER CONCENTRATIONS ALLOW THE EVALUATION OF THE INTEGRITY OF THE REPOSITORY INDEPENDENT OF UNCERTAINTIES IN WATER USE SYSTEMS AND DEMOGRAPHY. DOSE CALCULATIONS ARE MORE EASILY UNDERSTANDABLE IN THE ASSESSMENT OF RISK TO THE PUBLIC. UNTIL THE RESULTS OF THE ACCEPTABLE RISK STUDY INDICATE WHICH EXPRESSION OF RISK IS MORE DESIRABLE BOTH WILL CALCULATED AND STORED TO ALLOW FUTURE ACCESS FOR THE CALCULATION AND COMPARISON OF PERFORMANCE MEASURES.

Radiological risk is presently being calculated in terms of dose and radionuclide concentrations. The dose calculations are for peak 50 year maximum and average individuals and then integrated over population and over population and repository lifetime. These six values of risk are being stored. The peak average individual dose and integrated population dose are printed out in the tables in the appendix.

The individual dose has been insensitive to changes in the baseline parameters, thus the population dose serves as a better means of comparison. A major uncertainty in the population dose calculation is the number to be used for the affected population. The confidence in that value decreases significantly with time - especially when conditions leading to loss of administrative control are considered. Also, an existing water use system must be assumed. The assumption is made that a river is 10 miles from

the repository and that the radionuclides are diluted in it.

The other expression of risk being calculated is groundwater radionuclide concentrations. The concentrations at various points in the flow path are being calculated and stored. The aquifer concentrations referred to in the tables in the appendix refer to concentrations in the aquifer above the repository and diluted by that volume of water. These concentrations are independent of the local water use system and demography and therefore may have less uncertainty associated with them.

The results of the acceptable risk criteria study should indicate which expression of risk is most reasonable. At that time, the necessary calculations will be made with the existing values to present the risk in a manner consistent with the results of the study.

DOSES

- (1) Peak 50-year dose to average individual
- (2) Integrated average population dose
(integrated over population of average individuals)
- (3) Integrated average population dose
(integrated over population of average individuals
and over repository lifetime)
- (4) Peak 50-year dose to maximum individual
- (5) Integrated maximum population dose
(integrated over population of maximum individuals)
- (6) Integrated maximum population dose
(integrated over population of maximum individuals
and over repository lifetime)

CONCENTRATIONS

- (7) In aquifer directly above repository
- (8) In escape pathways from repository to biosphere

RADIOLOGICAL RISK - PERFORMANCE MEASURES

3. ANALYTIC STRUCTURE

3.4 Data Base Refinement

NECESSARY DATA BASE IMPROVEMENTS WERE IMPLEMENTED TO PROVIDE MORE ACCURATE INPUT TO THE MODEL.

THE DATA USED IN CYCLE I WERE APPROXIMATIONS DERIVED THROUGH THE CONSENSUS OF ENGINEERING JUDGMENT. AN ANALYSIS OF MAJOR SALT AND SHALE FORMATIONS IN THE U.S. PROVIDED PREFERRED VALUES AND GENERIC RANGES FOR THOSE CRITICAL FACTORS IDENTIFIED IN CYCLE I. PROBABLE UNCERTAINTIES IN MEASUREMENTS AT A SPECIFIC SITE WERE ALSO DELINEATED.

The data input to the analysis in Cycle I were approximations based upon the consensus of the judgement of engineers, geologists, and hydrologists familiar with the problem. The sensitivity analysis was performed by varying the parameters one order of magnitude from the baseline values.

To provide more accuracy, the data input for Cycle II was completely regenerated. Studies were made of major salt and shale basins in the U.S. to quantify hydrology, geology, and rock mechanics/mining parameters. The parameter values were compiled

and preferred values were derived from the information available. Generic ranges covering the range of values that were found in those basins were assigned to each parameter.

The necessity to make approximations of regional parameters using a finite number of measurements give rise to uncertainties in the values. Uncertainties also arise from inefficiencies in the measuring techniques, etc. The range of uncertainty was derived for each parameter.

Reference: Pierce and Rich, USGS Bull 1140

SALT AND SHALE BASINS
STUDIED FOR CYCLE II
DATA REGENERATION

3. ANALYTIC STRUCTURE

3.5 Repository Model

ITERATIONS IN THE REPOSITORY MODEL LEND REALISM TO THE STUDY.

REVISIONS WERE MADE IN THE CYCLE I REPOSITORY MODEL TO CORRELATE IT MORE CLOSELY WITH CONDITIONS THAT MIGHT EXIST AT AN ACTUAL REPOSITORY SITE. THE REPOSITORY MODEL WAS BASED UPON GEOLOGIC PROPERTIES EXPECTED IN A TYPICAL BASIN STRUCTURE IN THE U.S. RATHER THAN THE "IDEAL" SITE.

The basic repository model used in both cycles I and II is a six-layer model. The layers are numbered from the surface down. Layer 4 is the emplacement layer composed of either salt or shale. Layers 2 and 6 are sandstone aquifers. Layers 3 and 5 are sandstone, siltstone, shale sequences. (See illustration on opposite page.)

Layer 6 is assumed to be under a greater hydraulic head than layer 2, thus water flows up through the repository into the upper aquifer and then flows through this aquifer to a larger river 10 miles away.

Since it is difficult to generalize whether ground water flow will be through fractures or interstitial pore spaces, values for both were

input to the model for layers 3, 4, and 5.

The Cycle II repository model was revised to include the more permeable fracture zone around the repository shaft and tunnel.

It is also assumed that no ground flows out of the repository zone until the ground water regime is re-established and the mine is saturated. The preferred value for recharge time is 100 years. After 100 years ground water flow will begin.

In the future cycles, more revisions will be made to the repository model to more closely represent what might actually occur.

REPOSITORY MODEL

3. ANALYTIC STRUCTURE

3.6 Use of Markov Chain

A SIMPLE MARKOV CHAIN WAS USED IN CALCULATING EXPECTED VALUES OF RISK FOR FAULTING IN SHALE AND BRECCIA PIPE FORMATION IN SALT.

THE MARKOV CHAIN IS EFFECTIVE IN CALCULATING THE EXPECTED VALUE OF RISK WHEN FAILURE MODES ARE SEQUENCES OF RANDOM EVENTS. THE SELECTION AND APPLICATION OF THE MARKOV CHAIN IN THIS STUDY HAS BEEN VALIDATED. ITS USE IN OUR ANALYSIS WAS INITIATED IN THIS CYCLE BY APPLYING IT TO TWO SINGLE NODE CHAINS FOR SALT AND SHALE. A MORE COMPLEX MARKOV CHAIN CAN BE USED EFFICIENTLY WHEN THE RELATIVE IMPORTANCE OF THE FACTORS OPERATING IN THE REPOSITORY SYSTEM IS MORE WELL-DEFINED.

Unlike events leading to reactor failures, which are deterministic and which can only occur once, the events causing the breaching of a repository system are stochastic, i.e., they are random in time and frequency. Therefore, consequences depend upon the sequence and timing of the events as well as the events themselves. This type of process is most efficiently analyzed using a Markov chain.

The Markov chain describes the time history of the geologic states of the repository system. Using this description expected values of risk can be calculated. The expected value is essentially the risk averaged over a large number of repositories.

The model that has been developed describes the repository/waste

system as two parts: the geologic state of the repository and escape pathways and the waste distribution throughout the system. Geologic states are defined independent of waste distribution, but waste distribution depends not only on the present state, but also upon the history of states. The model has been developed to handle this complication (See Appendix 3.6).

The Markov chain model was used in this cycle in two simple cases: formation of a breccia pipe in salt and the opening and closing of a faucet in shale. The expected values of risk for these events are shown in the tables in the Appendix. They indicate that transition from the initial state directly to those states have negligible effect on the risk given the assumptions used in the model.

$\lambda_{\beta} \equiv$ transition rate
for formation
of breccia pipe

SALT

$\lambda_o \equiv$ transition rate
for fault
opening

$\lambda_c \equiv$ transition rate
for fault
closing

SHALE

MARKOV CHAIN SEQUENCES USED IN CYCLE II

4. CONTINUED EFFORT

4.1 Hydrology Model

THE VERIFICATION AND EXTENSION OF THE HYDROLOGY MODEL IS VITAL TO THE DEVELOPMENT OF SITE SUITABILITY CRITERIA.

THE ACCURACY OF THE RESULTS FROM THE ONE-DIMENSIONAL PIPE MODEL BEING USED MUST BE EVALUATED. ONE FACTOR IN THIS VALIDATION IS ASSESSING THE EFFECT THE ASSUMPTIONS USED IN THE 1-D MODEL HAVE ON THE RESULTS. ANOTHER ISSUE TO BE ADDRESSED IS WHETHER ADDITIONAL DIMENSIONS WILL SIGNIFICANTLY INCREASE THE ACCURACY OF THE RESULTS AND WHETHER THE INCREASED PROGRAM OPERATING TIME AND COST IS JUSTIFIED BY THE INCREASE IN ACCURACY. TWO-DIMENSIONAL, AND IF NECESSARY THREE-DIMENSIONAL, HYDROLOGIC MODELS WILL BE ADOPTED TO GENERATE 1-D ALGORITHMS FOR INCLUSION IN THE RISK ASSESSMENT MODEL.

A survey of existing simple and complex hydrology codes has been done to identify one suitable for use in validation of our codes (See Appendix 4.1). A simple model will be used to both validate our existing algorithms and to create new algorithms.

The hydrology code will be expanded to include these and other features:

- comparison of assumed vs. calculated flow.
- the simulation of 3-D features

- consideration of fluid/rock compressibility.
- consideration of the direct and indirect effects other non-linear phenomena such as temperature.

For further verification, a comparison to other major programs will be carried out to identify differences in analytic structure and data development. These differences will be studied to assure that they did not arise from errors in our study.

VERIFICATION AND EXPANSION OF HYDROLOGY MODEL

4. CONTINUED EFFORT

4.2 Climatology

MAJOR CLIMATOLOGICAL CHANGES WILL EFFECT GROUND WATER PARAMETERS

VARIATIONS IN GLOBAL TEMPERATURE WHICH LEAD TO VARIATIONS IN GLOBAL ICE COVERING AND RAINFALL HAVE BEEN CLOSELY CORRELATED WITH CHANGES IN THE EARTH'S ORBITAL PARAMETERS. BY PREDICTING THOSE CHANGES IN THE EARTH'S ORBIT AND CORRESPONDING TEMPERATURE CHANGES THE FUTURE REGIONAL CLIMATES CAN BE PREDICTED. A MODEL IS BEING DEVELOPED TO DO THIS PREDICTION AND TO CALCULATE THE EFFECTS OF CLIMATIC CHANGES (E.G., INCREASED RAINFALL) ON GROUND WATER PARAMETERS.

Providing data for the hydrologic input of the site suitability criteria requires prediction of long term climate change.

The climatic and subsequent hydrologic parameters for various regions (sites) may be estimated by the following procedure.

Step 1. The high degree of correlation of past δO^{18} ratios with earth orbital variations suggests that future global ice volumes may be predicted.

Hayes et al. (1976) presented temperature and ice volume data showing correspondence between earth orbital parameters and global ice volumes which may be extrapolated into future times. The figure opposite shows more detailed structure of one sea core from which temperature data can be extracted.

We are preparing a smoothed statistical equation for this prediction of ice volume/temperature based on earth orbital variations given some time in the future.

Step 2. Numerous "typical" climatic regimes (full glacial, interglacial, warm, dry, wet, cool, etc.) can be identified to have occurred over the past 10^6 years. No evidence exists that suggests these "patterns"

will not be repeated in some sequence in the future.

We have prepared a first approximation of various climatic regimes that appear to be typical of various climates in the past. (See Appendix 4.2 - Table 1)

Step 3. Various climatic reconstruction schemes show the changes in the hydrologic parameters (of interest to the SSC) in the past. Figure 1 (in the Appendix) shows the global precipitation change between the maximum glacial period and the present climatic as calculated by a three dimensional general circulation models. More detailed of the continental U.S. reconstructions are in preparation. Figure 3 and 4 (in the Appendix) show another of the climatic regimes from Table I of the Appendix, the "Little Ice Age" for both January and July.

Step 4. Given the changes in precipitation and sea level over various regions of the U.S. the changes in precipitation will then be used as input to a hydrology model. The changes in general hydrology in each region will be calculated in terms of change in precipitation, geology, soils, and hydrologic gradient (sea level variations).

Figure 1

TEMPERATURE DATA EXTRACTION FROM SEA CORE SAMPLE

4. CONTINUED EFFORT

4.3 Uncertainty Analysis

UNCERTAINTIES DUE TO DATA INPUT UNCERTAINTIES AND MODEL ASSUMPTIONS MUST BE EVALUATED.

UNCERTAINTIES IN THE RISK CALCULATION OUTPUTS ARISE FROM TWO SOURCES: UNCERTAINTIES IN THE DATA INPUT AND UNCERTAINTIES CAUSED BY APPROXIMATIONS AND ASSUMPTIONS USED IN THE MODELS. THE EFFECTS OF BOTH WILL BE ASSESSED. A MONTE CARLO MODEL HAS BEEN DEVELOPED FOR THE EVALUATION OF THE EFFECT OF DATA UNCERTAINTIES. METHODS FOR THE EVALUATION OF THE EFFECT OF MODELING APPROXIMATIONS ARE BEING DEVELOPED.

The uncertainty inherent in the data input has an effect on the accuracy of the model output. The magnitude of the uncertainty in the calculated output will be estimated using a Monte Carlo method. A Monte Carlo random generator will be used to generate data input. These data are assumed to follow a Gaussian distribution where the 1σ limits will correspond to the uncertainty limits on the actual input data. The random data will be input to the model and a statistical analysis will be performed on the output. This will define the mean of the output and the variance.

The Monte Carlo routine has been written. In some cases factors are correlated, (e.g. porosity/permeability). The random generator incorporates these correlations to

make the input reasonable.

The model approximations and assumptions have been identified and methods to quantify the uncertainties associated with them are being developed. These approximations range from the simple to evaluate effect of the number of time steps to the complex problem of the effect of the assumption used in the Markov chain that the effects of a change in state on the waste transport are not "felt" during the transition from state to state.

The evaluation of the effect of the time steps was initiated in this cycle by varying the number to half and twice the number presently used. This seems to have little effect on the output. A more complete analysis is planned.

DATA INDUCED UNCERTAINTIES

uncertainty in input data
leads to uncertainty in
results

Generate random data within
probability distribution
function using Monte Carlo
method

Perform statistical analysis
on results using "random"
data

MODEL INDUCED UNCERTAINTIES

approximations and assump-
tions incorporated in model
lead to uncertainty in
accuracy of results

Identify factors that may
lead to uncertainties

Develop methodology to assess
level of uncertainty

STRUCTURE OF UNCERTAINTY ANALYSIS

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DRAFT SITE SUITABILITY CRITERIA FOR HIGH-LEVEL WASTE REPOSITORIES

Applicants for a license to construct and operate a HLW repository in deep geological media shall demonstrate that the characteristics of the proposed site meet the following minimum requirements in order to assure the safe and environmentally acceptable long-term containment of the HLW materials. In determining the extent to which a proposed site meets these criteria it should be recognized that it is the overall repository system optimization which is of overriding importance rather than the optimization of any single criterion.

Ownership and Control

- (a) The repository site shall be owned and controlled by the United States Government. This ownership shall include the ownership and control of all mineral and exploration rights and shall include any other such controls that are required to ensure the integrity of the site.
- (b) The applicant shall provide for the ownership and control of the site area to the boundary of the buffer zone.

Barriers to Waste Transport

- (c) The repository site shall provide a system of multiple, naturally occurring barriers to waste transport.
- (d) The potential for radiological releases to the environment shall be reduced to the lowest level which is reasonably achievable considering the entire spectrum of expected and unplanned credible events over the required life of the repository.
- (e) Radionuclide concentrations in any pathway to man, at the first point of reasonable accessibility, shall be as low as is reasonably

achievable and in any case shall not exceed a small fraction of the limits specified 10 CFR Part 20, Appendix B, Table 11, Column 2, considering the failure of any single barrier in the system.

Suitability of Geological Medium

- (f) The geological medium shall be such that the use of state-of-the-art techniques for site exploration, subterranean construction, and depository decommissioning will not significantly compromise the long-term effectiveness of the repository.
- (g) The geological medium shall be such that chemical, radiological, and thermal effects of the waste on the repository will not significantly compromise the long-term effectiveness of the repository.
- (h) The repository site shall be shown to be geologically stable, i.e., it shall not have experienced geologic events during the past 10^7 year period of a type and magnitude such that the long-term effectiveness of the repository could be significantly compromised were such events to occur at some future time.
- (i) The repository site shall have characteristics such that the likelihood of unplanned intrusions caused by either natural events or by acts of man will be as low as reasonably achievable.

Testing and Exploration

- (j) The repository site shall not have been subjected to mining or extensive deep drilling due to prior land usage or exploration.
- (k) Testing and exploration techniques used in the selection and/or development of the repository site shall have been such that their potential effects on the long-term effectiveness of the repository will be as low as reasonably achievable.---Such testing and explora-

tion shall have overall lesser effects on the repository site performance than the actual mining and waste emplacement.

- (l) Determinations of site suitability shall be based on the best data obtainable, consistent with preserving the integrity of the potential repository site. Data shall be obtained in accordance with NRC approved quality assurance procedures.
- (m) Determinations of site suitability shall consider the results of geological investigations extending to a minimum radius of 200 miles from the repository.

Socio-Economic Considerations

- (n) The actual or potential resource value of the repository site shall be such that it will neither invite future exploration nor deprive this or future generations of valuable resources to the greatest extent that this is reasonably achievable.
- (o) The repository site shall provide adequate natural barriers to radionuclide release and have an inherently low resource value such that surveillance and administrative controls after decommissioning shall not be prerequisite to assuring that the public health and safety will be preserved.
- (p) The site shall be located so as to reduce risks from the transportation of wastes to the site to the lowest reasonably achievable level.

DEFINITION OF TERMS

barrier: one component in the multicomponent system for waste containment and isolation provided by the repository system. The components include, but shall not be limited to:

1. Isolation of waste from potential transport mechanisms
2. Limiting waste mobility within the depository

3. Limiting waste transport through barrier and buffer zones

4. Limiting transport to man through environmental pathways

barrier zone: The subterranean region which will provide the system of natural barriers against transport of the waste from the depository. The barrier zone will be centered at the depository and have a radius which will be determined by the specific site characteristics.

biosphere: For the purpose of this regulation the biosphere is any actual or potential surface or subsurface, life supporting air or water system.

buffer zone: Annular region beginning at outer boundary of the barrier zone to a distance adequate to protect against the disruption of the repository system by man induced activities, e.g., drilling, deep excavations. The extent of the buffer zone will be determined by the site specific characteristics.

containment: The prevention or retardation of waste transport through the geohydrological system surrounding the depository.

deep geological media: Naturally occurring media in the earth's crust at a depth below the land surface sufficient to ensure that the effects of geologic processes active at or near the surface and acts of man resulting from loss of administrative control will not compromise the integrity of the repository.

depository: A subterranean cavern excavated in a deep geological medium for the disposal of nuclear waste.

depository decommissioning: Final backfilling, sealing, and isolation of the depository after which time re-entry is not anticipated.

effective sealing: The sealing of penetrations in the repository site in a manner which will maximize the period of performance of the seal such that the integrity of the repository system shall be maintained.

emplacement medium: The geological medium in which the depository will be excavated.

isolation: The emplacement of wastes in such a way as to isolate them from potential transport mechanisms.

long-term: That which is consistent with the required period for waste containment.

reasonably achievable: That which is capable of being achieved based on balancing the state of technology, the economics of improvements and the overall system effectiveness in relation to benefits to the public health and safety and environmental, societal, socioeconomic factors.

repository site: The entire region, subterranean and surface, extending to the outer boundary of the buffer zone, which will be owned and controlled by the Federal government for the purpose of HLW disposal.

surrounding strata: The geologic strata above, below, and adjacent to the stratum which contains the emplacement medium.

Appendix 3.1 - Results of Sensitivity Analyses

FOR YOUR INFORMATION and review of work in the
The materials and methods may be modified or supplemented
work proceeds. We will welcome comments and suggestions.

ASSUMPTIONS OF TABLES 1 AND 2

Tables 1 and 2 describe a shale repository with flow paths to the aquifer through a fracture zone surrounding the tunnel and shaft and through the two overlying layers of shale. It is assumed that the flow through the shale is interstitial flow. Baseline parameter values are given in Table A. Changes in parameters varied in sensitivity analysis, when not shown, are listed in Tables H and I.

ASSUMPTIONS OF TABLES 3 AND 4

Tables 3 and 4 describe a bedded salt repository with flow paths to the aquifer through a fracture zone surrounding the tunnel and shaft and through the overlying salt and shale layers. It is assumed that the flow through both the salt and a shale barrier layer is interstitial flow. Baseline parameter values are given in Table B. Changes in parameters varied in sensitivity analysis, when not shown, are listed in Tables J and K.

ASSUMPTIONS OF TABLE 5

Table 5 describes a shale repository with flow paths to the aquifer through a fracture zone surrounding the tunnel and shaft and through the overlying layers of shale. It is assumed the flow through both shale layers is fracture flow. Baseline parameter values are as given in Table A, except for flow through the two shale layers, which is described by the values given in Table C. Changes in parameters varied in sensitivity analysis, when not shown, as listed in Table L.

ASSUMPTIONS OF TABLE 6

Table 6 describes a bedded salt repository with flow paths to the aquifer through a fracture zone surrounding the tunnel and shaft and through the overlying salt and shale layers. It is assumed that the flow through the shale barrier layer is fracture flow, and the flow through the salt layer is interstitial flow. Baseline parameter values are as given in Table B, except for flow through the shale barrier layer, which is described by the values given in the "barrier layer" row of Table C.

ASSUMPTIONS OF TABLES 7 AND 8

Tables 7 and 8 assume the same flow paths as in the shale and salt repositories of Tables 1 and 3 respectively. An additional flow path to the aquifer exists through the deteriorated backfill in the tunnel and shaft. Partial mixing between the backfill and the surrounding fracture zone is assumed. Baseline parameter values for the deteriorated backfill are given in Table D; baselines for other pathways are given in Table A for Table 7 and in Table C for Table 8. Changes in parameters varied in sensitivity analysis are listed in Tables M and N respectively.

ASSUMPTIONS OF TABLES 9 AND 10

Tables 9 and 10 assume the same flow paths as in the baseline shale and salt repositories of Tables 1 and 3 respectively. An additional flow path to the aquifer exists through borings on which the seal has failed. It is assumed that initially 10% of the borings have failed. After 500 yrs. 30% have failed, and after 1000 yrs. 50% have failed. Baseline parameter values for the failed borings are given in Table E; baselines for other

pathways are given in Table A for Table 9 and in Table B for Table 10.

ASSUMPTIONS OF TABLE 11

Table 11 describes a shale repository with the possibility of the occurrence of a fault. The probability of the occurrence of a fault in any given yr is assumed to be 5×10^{-7} . It is further assumed that when a fault does occur it will close almost completely after 70 yrs. The opening is assumed to be along an existing fault. Baseline parameter values are as given in Table A, with the additions and changes in Table F.

ASSUMPTIONS OF TABLE 12

Table 12 describes a salt repository with some probability of a breccia pipe forming between the repository and the aquifer. The probability that a breccia pipe will open in a given year is assumed to be 5×10^{-7} . Baseline parameter values are as given in Table B, with the additions and changes in Table G.

BASELINE PARAMETERS FOR TUNNEL 1 AND 2

TABLE A

PATHWAY	LENGTH (M)	CROSS SECTION (m ²)	PEROSITY	PERMEABILITY (cm/sec)	SORPTION	DEGRADATION (M)
1ST SEGMENT OF TUNNEL	1200	310	0.1	0.1	120, 90% OTHER FISSION PRODUCTS ACTINIDES	1, 2 10 ² 10 ¹
2ND SEGMENT OF TUNNEL	440	18.00	0.1	0.1	120, 90% OTHER FISSION PRODUCTS ACTINIDES	1, 2 10 ² 10 ¹
SHAFT IN DEPOSITION LAYER	100	10	10 ⁻³	10 ⁻⁴	120, 90% OTHER FISSION PRODUCTS ACTINIDES	1, 2 10 ² 10 ¹
SHAFT IN GRAVE SANDIER LAYER	200	5	10 ⁻³	10 ⁻⁴	120, 90% OTHER FISSION PRODUCTS ACTINIDES	1, 2 10 ² 10 ¹
DEPOSITION LAYER	200	5 x 10 ⁶	0.05	10 ⁻⁵	120, 90% OTHER FISSION PRODUCTS ACTINIDES	1, 2 10 ² 10 ¹
SANDIER LAYER	200	5 x 10 ⁶	0.05	10 ⁻⁷	120, 90% OTHER FISSION PRODUCTS ACTINIDES	1, 2 10 ² 10 ¹
ACTIVATOR	1.0 x 10 ¹	4 x 10 ⁵	0.1	10 ⁻¹	120, 90% OTHER FISSION PRODUCTS ACTINIDES	1, 2 10 ² 10 ¹

A.3.1

A3.1

TABLE II

TABLE OF PARAMETERS VARIED IN TABLE 1

RUN INDEX NUMBER	VARIED PARAMETER	BASELINE VALUE	NEW VALUE
(1)	SORPTION PRODUCT OF FISSION PRODUCTS OTHER THAN I AND Tc SORPTION PRODUCT OF ACTINIDES	10^2 10^4	10^2 10^2
(2)	POROSITY OF THE TUNNEL POROSITY OF THE SHAFT POROSITY OF THE REPOSITORY LAYER POROSITY OF THE BARRIER LAYER POROSITY OF THE AQUIFER	10^{-1} 10^{-3} 5×10^{-2} 5×10^{-2} 10^{-1}	10^{-3} 10^{-4} 10^{-2} 10^{-2} 2×10^{-2}
(3)	POROSITY OF THE TUNNEL POROSITY OF THE SHAFT	10^{-1} 10^{-3}	10^{-2} 10^{-4}
(4)	CROSS SECTION OF THE 1ST SEGMENT OF THE TUNNEL (m^2) CROSS SECTION OF THE 2ND SEGMENT OF THE TUNNEL (m^2) PERMEABILITY OF THE TUNNEL (cm/sec)	316 18.91 10^{-1}	580 34.8 10^{-4}
(5)	CROSS SECTION OF THE 1ST SEGMENT OF THE TUNNEL (m^2) CROSS SECTION OF THE 2ND SEGMENT OF THE TUNNEL (m^2) CROSS SECTION OF THE 1ST SEGMENT OF THE SHAFT (m^2) CROSS SECTION OF THE 2ND SEGMENT OF THE SHAFT (m^2)	316 18.91 10 5	785 47.1 100 100
(6)	PERMEABILITY OF THE REPOSITORY LAYER (cm/sec) PERMEABILITY OF THE BARRIER LAYER (cm/sec)	10^{-9} 10^{-7}	10^{-7} 10^{-5}
(7)	PERMEABILITY OF THE TUNNEL (cm/sec) PERMEABILITY OF THE SHAFT (cm/sec)	10^{-1} 10^{-4}	10^{-3} 10^{-3}

TABLE I

TABLE OF PARAMETERS VARIED IN TABLE 2

RUN INDEX NUMBER	VARIED PARAMETER	BASELINE VALUE	NEW VALUE
(1)	PERMEABILITY OF THE TUNNEL (cm/sec) PERMEABILITY OF THE SHAFT (cm/sec) PERMEABILITY OF THE AQUIFER (cm/sec)	10^{-1} 10^{-4} 10^{-4}	10^{-3} 10^{-3} 10^{-2}
(2)	PERMEABILITY OF THE TUNNEL (cm/sec) PERMEABILITY OF THE SHAFT (cm/sec) PERMEABILITY OF THE AQUIFER (cm/sec) ACTINIDE SORPTION FACTOR	10^{-1} 10^{-4} 10^{-4} 10^4	10^{-3} 10^{-3} 10^{-2} 10^2
(3)	PERMEABILITY OF AQUIFER (cm/sec) PERMEABILITY OF REPOSITORY LAYER (cm/sec) PERMEABILITY OF BARRIER LAYER (cm/sec)	10^{-4} 10^{-9} 10^{-7}	10^{-2} 10^{-7} 10^{-5}
(4)	PERMEABILITY OF THE TUNNEL (cm/sec) PERMEABILITY OF THE SHAFT (cm/sec) PERMEABILITY OF THE AQUIFER (cm/sec) PERMEABILITY OF THE REPOSITORY LAYER (cm/sec) PERMEABILITY OF THE BARRIER LAYER (cm/sec)	10^{-1} 10^{-4} 10^{-4} 10^{-9} 10^{-7}	10^{-3} 10^{-3} 10^{-2} 10^{-7} 10^{-5}
(5)	PERMEABILITY OF THE SHAFT (cm/sec) PERMEABILITY OF THE AQUIFER (cm/sec) POROSITY OF THE TUNNEL	10^{-4} 10^{-4} 10^{-1}	10^{-3} 10^{-2} 10^{-2}
(6)	PERMEABILITY OF THE AQUIFER (cm/sec) PERMEABILITY OF THE REPOSITORY LAYER (cm/sec) PERMEABILITY OF THE BARRIER LAYER (cm/sec)	10^{-4} 10^{-9} 10^{-7}	10^{-2} 10^{-11} 10^{-9}

A.31

A.3.1

TABLE 1

SHALE DEPOSITION SENSITIVITY ANALYSIS
LIFE-Span Model

VARIABLE PARAMETER	BASELINE VALUE	NEW VALUE	INTEGRATED POPULATION DOSE (MAR-KI%/MW-YR)			PEAK INDIVIDUAL DOSE (REM/1000-YR)				
			WHOLE BODY DOSE	CRITICAL ORGAN DOSE	CRITICAL ORGAN	WHOLE BODY DOSE	TIME	CRITICAL ORGAN DOSE	TIME	CRITICAL ORGAN
BASISLINE	-	-	1.39 E -3	1.6 E -1	GI-LLI	8.10 E -14	1.44 E 4	7.49 E -12	1.44 E 4	GI-LLI
ACTINIDE & FISSION PRODUCT ADSORPTION FACTORS	(1)		8.98 E -2	3.56 E 1	GI-LLI	2.78 E -12	1.24 E 5	2.31 E -11	1.44 E 4	GI-LLI
DISPERSION	50	10	1.51 E -3	1.88 E -1	GI-LLI	1.07 E -13	1.74 E 5	1.3 E -13	1.74 E 5	GI-LLI
LOW POROSITY EVERYWHERE	(2)		2.36 E -3	2.80 E -1	GI-LLI	2.91 E -12	4.32 E 4	3.56 E -11	4.32 E 4	GI-LLI
LOW POROSITY IN AQUIFER	0.1	0.02	1.75 E -1	1.65 E -1	GI-LLI	8.55 E -12	5.99 E 3	7.93 E -12	5.99 E 3	GI-LLI
POROSITY IN ROCK	0.95	0.91	2.23 E -3	2.74 E -1	GI-LLI	2.04 E -13	5.85 E 4	3.58 E -11	7.83 E 4	GI-LLI
LOW POROSITY IN SHAFT & TRAVEL FRACTURE ZONE	(3)		1.36 E -3	1.69 E -1	GI-LLI	8.53 E -14	1.17 E 4	7.01 E -12	1.17 E 4	GI-LLI
FAST SATURATION	100	20	1.30 E -3	1.0 E -1	GI-LLI	8.19 E -14	1.44 E 4	7.49 E -12	1.44 E 4	GI-LLI
MIN. AREA FRACTURE ZONE IN TUNNEL	(4)		1.29 E -3	1.59 E -1	GI-LLI	5.8 E -13	1.17 E 4	7.01 E -12	1.17 E 4	GI-LLI
MAX. AREA FRACTURE ZONE IN SHAFT AND TUNNEL	(5)		1.72 E -3	2.47 E -1	GI-LLI	7.48 E -13	1.17 E 4	9.05 E -11	1.17 E 4	GI-LLI
SHALE PERMEABILITY	(6)		2.73 E -3	4.14 E -1	GI-LLI	1.59 E -12	1.52 E 4	1.93 E -10	1.52 E 4	GI-LLI
ARTESIAN HEAD	60	150	1.93 E -3	2.37 E -1	GI-LLI	1.42 E -13	8.86 E 4	1.71 E -11	8.86 E 4	GI-LLI
AQUIFER PERMEABILITY	10 ⁻⁴	10 ⁻²	1.39 E -3	1.67 E -1	GI-LLI	6.57 E -14	3.96 E 3	7.05 E -12	3.96 E 3	GI-LLI
FRACTURE ZONE PERMEABILITY	(7)		1.60 E -3	2.23 E -1	GI-LLI	5.62 E -13	1.17 E 4	6.60 E -11	1.17 E 4	GI-LLI
HEAD GRADIENT IN AQUIFER	0.005	0.05	1.37 E -3	1.66 E -1	GI-LLI	6.64 E -14	4.87 E 3	8.04 E -12	4.87 E 3	GI-LLI
THICKNESS OF DEPOSITIONARY LAYER	200	20	2.44 E -3	3.12 E -1	GI-LLI	5.35 E -13	9.31 E 4	6.48 E -11	9.31 E 4	GI-LLI
THICKNESS OF BARRIER LAYER	200	20	1.76 E -3	2.24 E -1	GI-LLI	2.43 E -13	1.24 E 4	2.91 E -11	1.24 E 4	GI-LLI
LENGTH OF TUNNEL (INCREASE)	400	6000	1.30 E -3	1.60 E -1	GI-LLI	6.32 E -14	1.52 E 4	7.53 E -12	1.52 E 4	GI-LLI
LENGTH OF TUNNEL	440	200	1.30 E -3	1.60 E -1	GI-LLI	6.19 E -14	1.45 E 4	7.49 E -12	1.45 E 4	GI-LLI
DISSOLUTION RATE OF WASTE	10 ⁻⁴	0.1	1.34 E -3	1.65 E -1	GI-LLI	2.95 E -13	1.29 E 4	3.57 E -11	1.29 E 4	GI-LLI
FISSION PRODUCT ADSORPTION FACTORS	10 ²	1	3.39 E -3	3.09 E -1	GI-LLI	6.52 E -13	1.12 E 4	8.30 E -11	1.12 E 4	GI-LLI
ACTINIDE ADSORPTION FACTORS	10 ⁴	10 ²	8.78 E -2	8.78 E -2	WHOLE BODY	2.76 E -12	1.24 E 5	3.91 E -11	1.24 E 5	WHOLE
AQUIFER LENGTH	1.0 E 4	1.8 E 2	1.37 E -3	1.66 E -1	GI-LLI	8.52 E -14	5.13 E 3	7.89 E -12	5.13 E 3	GI-LLI

A3.1

SHALE RESERVOIR SENSITIVITY ANALYSIS
(INTERESTIVE, T, M)

VARIABLE PARAMETER	PEAK AQUIFER CONCENTRATION (G/M ³ - MG/L)								COMPUTER JOB#
	OR CONCENTRATION	TIME	126 CONCENTRATION	TIME	226 CONCENTRATION	TIME	237 CONCENTRATION	TIME	
BASILINE	2.02 E -11	4.0 E 3	1.31 E -14	2.14 E 5	1.09 E -24	3.0 E 6	1.44 E -38	3.0 E 6	ZBR 1033
ACTIVELY & FISSTON PRODUCT SORPTION FACTORS	2.0 E -11	4.0 E 3	7.5 E -13	3.75 E 3	2.3 E -15	2.25 E 5	1.3 E -14	1.7 E 5	ZBR 1034
DISPERSTION	3.44 E -12	3.65 E 5	2.6 E -14	2.37 E 5	0		0		ZBR 1555
LOW POROSITY EVERYWHERE	8.13 E -11	4.12 E 4	7.1 E -13	2.83 E 4	2.07 E -17	1.70 E 6	8.25 E -18	1.20 E 6	ZBR 1620
LOW POROSITY IN AQUIFER	2.02 E -11	3.9 E 3	1.35 E -14	2.14 E 5	1.04 E -34	3.00 E 6	1.44 E -38	3.00 E 6	ZBR 1621
POROSITY IN POCK	8.13 E -11	4.29 E 4	1.35 E -14	2.14 E 5	1.09 E -34	3.00 E 6	1.44 E -38	3.00 E 6	ZBR 1622
LOW POROSITY IN SHAFT & TUNNEL FRACTURE ZONE	2.37 E -11	8.2 E 3	7.07 E -13	2.83 E 4	2.07 E -17	1.70 E 6	2.44 E -37	2.20 E 6	ZBR 1623
FAST SATURATION	2.02 E -11	2.85 E 3	1.31 E -14	2.14 E 5	1.09 E -31	3.00 E 6	1.41 E -38	3.00 E 6	ZBR 1602
WIN AREA FRACTURE ZONE IN TUNNEL	2.15 E -11	2.18 E 2	5.67 E -13	7.37 E 3	8.22 E -16	4.05 E 5	4.81 E -10	3.78 E 5	ZBR 1631
WIN AREA FRACTURE ZONE IN SHAFT AND TUNNEL	2.69 E -10	9.24 E 2	2.13 E -12	4.52 E 4	7.92 E -17	3.00 E 6	1.65 E -20	3.00 E 6	ZBR 1031
SHALE PERMEABILITY	5.04 E -10	4.62 E 3	3.45 E -13	1.41 E 5	8.56 E -20	3.00 E 6	1.13 E -23	3.00 E 6	ZBR 1638
ADITION OF AQUIFER PERMEABILITY	4.45 E -11	7.89 E 4	7.1 E -14	9.33 E 4	1.03 E -21	3.00 E 6	1.83 E -22	3.00 E 6	ZBR 0930
PERMEABLE ZONE PERMEABILITY	2.02 E -11	3.8 E 3	1.34 E -16	2.14 E 5	1.88 E -30	3.00 E 6	1.11 E -40	3.00 E 6	ZBR 1632
PERMEABLE ZONE PERMEABILITY	2.04 E -10	5.51 E 2	2.65 E -12	2.83 E 4	1.73 E -18	1.79 E 1	8.84 E -18	1.88 E 6	ZBR 1631
PERMEABLE ZONE PERMEABILITY	2.02 E -12	3.96 E 3	1.30 E -15	2.14 E 5	1.09 E -35	3.00 E 6	1.41 E -39	3.00 E 6	ZBR 0551
THICKNESS OF PLUGGERS LAYER	1.74 E -10	2.43 E 4	1.71 E -15	2.25 E 5	4.02 E -25	3.00 E 6	5.31 E -37	3.00 E 6	ZBR 0953
THICKNESS OF BARRIER LAYER	8.58 E -11	1.20 E 3	4.91 E -13	6.16 E 1	2.24 E -18	3.00 E 6	2.88 E -22	3.00 E 6	ZBR 0955
LENGTH OF TUNNEL (INCREASE)	2.05 E -11	4.87 E 3	1.06 E -14	2.77 E 5	0		0		ZBR 0935
LENGTH OF TUNNEL	2.02 E -11	3.96 E 3	1.32 E -14	2.14 E 5	1.42 E -33	3.00 E 6	1.88 E -37	3.00 E 6	ZBR 1000
DISSOLUTION RATE OF WASTE	1.46 E -10	2.21 E 3	1.40 E -14	1.83 E 5	1.20 E -31	3.00 E 6	1.65 E -38	3.00 E 6	ZBR 1001
FISSTON PRODUCT SORPTION FACTORS	2.02 E -11	3.8 E 3	7.50 E -13	3.75 E 3	1.00 E -31	3.00 E 6	1.11 E -38	3.00 E 6	ZBR 1000
ACTIVELY SORPTION FACTORS	2.02 E -11	3.8 E 3	1.30 E -14	2.14 E 5	2.23 E -15	2.25 E 5	1.26 E -14	1.65 E 5	ZBR 1007
AQUIFER LENGTH	2.02 E -11	3.96 E 3	1.30 E -14	2.14 E 5	1.09 E -34	3.00 E 6	1.43 E -38	3.00 E 6	ZBR 1008

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TABLE 2

SHALE DEPOSITION SENSITIVITY ANALYSIS - MULTI-PARAMETER
(TABLE 2 OF 12)

VARIABLE PARAMETER	INFORMATION PRODUCTION LOSS (% - PER HOUR)			PEAK INDIVIDUAL LOSS (% - PER HOUR)			CRITICAL ORGAN
	WHOLE BODY (WS)	CRITICAL ORGAN LOSS	CRITICAL ORGAN	WHOLE BODY (WS)	TIME	CRITICAL ORGAN LOSS	
PERMEABILITY OF FRACTURE ZONE AND AQUIFER (1)	1.30 E -1	1.0 E -1	GI-LLI	6.09 E -11	1.41 E -4	2.50 E -12	GI-LLI
PERMEABILITY OF FRACTURE ZONE AND AQUIFER AND AQUICLUD SORPTION FACTOR (2)	1.07 E -1	3.4 E -1	GI-LLI	2.12 E -12	1.67 E -4	8.54 E -11	GI-LLI
SHALE AND AQUIFER PERMEABILITY (3)	1.72	1.72	WHOLE BODY	4.49 E -10	4.07 E -3	4.49 E -10	WHOLE BODY
PERMEABILITY EVERYWHERE (4)	4.60 E -3	4.79 E -1	GI-LLI	1.83 E -12	2.59 E -2	1.59 E -10	GI-LLI
SHALT FRACTURE ZONE AND AQUIFER PERMEABILITY AND TUNNEL FRACTURE ZONE POROSITY (5)	6.55 E -3	3.81 E -1	GI-LLI	1.41 E -12	4.82 E -3	1.08 E -10	GI-LLI
REDUCED SHALE PERMEABILITY AND INCREASED AQUIFER POROSITY (6)	2.42 E -3	3.60 E -1	GI-LLI	1.27 E -12	4.61 E -3	1.22 E -10	GI-LLI

VARIABLE PARAMETER	PEAK AQUIFER CONCENTRATION (% - PER HOUR)							
	100% CONCENTRATION	TIME	10% CONCENTRATION	TIME	1% CONCENTRATION	TIME	0.1% CONCENTRATION	TIME
PERMEABILITY OF FRACTURE ZONE AND AQUIFER	2.02 E -11	1.0 E 3	1.31 E -14	2.44 E 6	6.81 E -11	3.0 E 2	1.11 E -14	3.0 E 6
PERMEABILITY OF FRACTURE ZONE AND AQUIFER AND AQUICLUD SORPTION FACTOR	2.04 E -12	5.82 E 2	2.61 E -14	2.83 E 4	1.23 E -14	1.70 E 6	2.21 E -27	1.98 E 6
SHALE AND AQUIFER PERMEABILITY	5.04 E -12	1.67 E 3	3.45 E -15	1.41 E 5	8.56 E -22	3.0 E 3	1.13 E -25	3.0 E 8
PERMEABILITY EVERYWHERE	5.02 E -12	4.87 E 3	3.29 E -15	1.41 E 5	3.44 E -20	1.61 E 6	3.04 E -	1.08 E 6
SHALT FRACTURE ZONE AND AQUIFER PERMEABILITY AND TUNNEL FRACTURE ZONE POROSITY	1.87 E -12	5.25 E 2	5.85 E -14	4.17 E 5	1.58 E -16	2.5 E 5	5.13 E -16	1.83 E 5
REDUCED SHALE PERMEABILITY AND INCREASED AQUIFER POROSITY	3.0 E -12	8.6 E 3	2.72 E -15	4.19 E 5	0	-	0	-

BASELINE PARAMETERS FOR SHALE WITH FRACTURE FLOW
(TABLES B AND C)

TABLE C

(see also Table A)

PATHWAY	LENGTH	CROSS SECTION (μ^2)	POROSITY	PERMEABILITY (cm/sec)	SORPTION	DISPERSION (M)
DEPOSITARY LAYER	300	5×10^6	10^{-2}	10^{-8}	SAME	50
BARRIER LAYER	200	5×10^6	10^{-4}	10^{-3}	SAME	50

TABLE D

TABLE OF PARAMETERS VARIED IN TABLE 5

RUN INDEX NUMBER	VARIED PARAMETER	BASELINE VALUE	NEW VALUE
(1)	AQUIFER LENGTH (m) HEAD GRADIENT	1.6×10^4 5×10^{-3}	1.6×10^3 5×10^{-2}
(2)	PERMEABILITY OF THE AQUIFER (cm/sec) ACTINIDE SORPTION FACTOR	10^{-4} 10^{-4}	10^{-2} 10^{-2}
(3)	PERMEABILITY OF THE AQUIFER (cm/sec) ACTINIDE SORPTION FACTOR LEACH RATE (yr^{-1})	10^{-4} 10^{-4} 10^{-4}	10^{-2} 10^{-2} 10^{-1}

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TABLE 5

SMALL DEPOSITION SENSITIVITY ANALYSIS
(CHOCOLATE) (1000)

VARIABLE PARAMETER	BASELINE VALUE	NEW VALUE	INTEGRATED POPULATION DOSE (GAIN-REM/MG-KG-YR)			PEAK INDIVIDUAL DOSE (REM/1000-YR)				
			WHOLE BODY DOSE	CRITICAL ORGAN DOSE	CRITICAL UPPER	WHOLE BODY DOSE	TIME	CRITICAL ORGAN DOSE	TIME	CRITICAL ORGAN
BASALINE	-	-	2.77 E -3	4.32 E -3	01-LLI	1.86 E -12	1.17 E 4	2.28 E -10	1.17 E 4	01-LLI
AQUIFER LENGTH	1.6 E 4	1.8 E 3	6.76 E -3	5.15 E -2	01-LLI	2.09 E -12	1.92 E 3	2.53 E -10	1.92 E 3	01-LLI
DISPERSION DOWN	50	10	2.77 E -3	4.32 E -3	01-LLI	2.03 E -12	1.12 E 4	2.43 E -10	1.12 E 4	01-LLI
ACTINIDE SORPTION	10 ⁴	10 ³	3.14	3.14	WHOLE BODY	1.18 E -10	9.61 E 3	1.57 E -9	1.01 E 6	BORE
AQUIFER LENGTH AND GRADIENT, SIMULTANEOUSLY	(1)		2.32	2.32	WHOLE BODY	2.63 E -11	1.24 E 4	3.63 E -10	1.89 E 1	01-LLI
PERMEABILITY & ACTINIDE SORPTION SIMULTANEOUSLY	(2)		3.53	3.53	WHOLE BODY	1.47 E -9	1.40 E 4	1.47 E -9	1.60 E 4	WHOLE BODY
DISPERSION UP	50	100	2.77 E -3	4.31 E -3	01-LLI	1.71 E -12	1.28 E 4	2.11 E -10	1.28 E 4	01-LLI
ACTINIDE SORPTION, LEACH RATE & AQUIFER PERMEABILITY	(3)		2.40	2.40	WHOLE BODY	4.83 E -9	1.24 E 4	5.16 E -8	2.20 E 2	01-LLI

VARIABLE PARAMETER	PEAK AQUIFER CONCENTRATION (G/G-MG-YR)								COMPUTER JOB #
	50% CONCENTRATION	TIME	100% CONCENTRATION	TIME	228Ra CONCENTRATION	TIME	230Th CONCENTRATION	TIME	
BASALINE	6.84 E -10	2.3 E 2	1.65 E -11	5.89 E 3	2.02 E -14	1.03 E 5	4.14 E -13	1.27 E 5	ZBR 0912
AQUIFER LENGTH	6.84 E -10	2.29 E 2	1.65 E -11	5.89 E 3	2.02 E -14	1.03 E 5	4.14 E -13	1.27 E 5	ZBR 1643
DISPERSION DOWN	6.84 E -10	2.29 E 2	1.65 E -11	5.89 E 3	2.02 E -14	1.03 E 5	4.14 E -13	1.27 E 5	ZBR 1644
ACTINIDE SORPTION	6.84 E -10	2.29 E 2	1.05 E -11	0.89 E 3	7.50 E -14	1.17 E 4	1.12 E -10	7.37 E 3	ZBR 1647
AQUIFER LENGTH AND GRADIENT, SIMULTANEOUSLY	6.84 E -11	2.29 E 2	1.65 E -12	5.89 E 3	2.02 E -16	1.03 E 5	4.14 E -14	1.27 E 5	ZBR 1647
PERMEABILITY & ACTINIDE SORPTION SIMULTANEOUSLY	6.84 E -12	2.3 E 2	1.65 E -13	5.89 E 3	7.36 E -16	1.17 E 4	1.12 E -12	7.37 E 3	ZBR 1648
DISPERSION UP	6.84 E -10	2.29 E 2	1.65 E -11	5.89 E 3	2.02 E -14	1.03 E 5	4.14 E -13	1.27 E 5	ZBR 1645
ACTINIDE SORPTION, LEACH RATE & AQUIFER PERMEABILITY	1.46 E -9	1.23 E 2	7.33 E -13	2.02 E 3	5.70 E -14	5.57 E 3	3.36 E -12	2.13 E 3	ZBR 1033

BASELINE PARAMETERS FOR CASE

TABLE 8

	LENGTH (M)	CROSS SECTION (M ²)	POROSITY	PERMEABILITY (cm/sec)	SORPTION	DISPERSION (%)
SHIELD FROM TABLE A						
DEPOSITORY LAYER	200	4.0×10^6	0.05	10^{-6}	80%	50
BARRIER LAYER	200	1.0×10^6	0.05	10^{-7}	50%	50
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*FAULT OPEN IN BARRIER LAYER	200	1×10^5	10^{-3}	10^{-4}	120% DO OTHER FISSION PRODUCTS ACTINIDES	10^2 10^2 10^2
FAULT CLOSED IN DEPOSITORY LAYER	200	1×10^5	10^{-3}	10^{-6}	SAME	50
FAULT OPEN IN BARRIER LAYER	100	1×10^5	10^{-3}	10^{-5}	SAME	50
FAULT CLOSED IN DEPOSITORY LAYER	100	1×10^5	10^{-3}	10^{-7}	SAME	50

*THE PROBABILITY OF A FAULT IS 5×10^{-7} PER YEAR

TABLE 11

SHALE DEPOSITORY FAULTING - SENSITIVITY ANALYSIS
(INTERSTITIAL FLOW)

VARIABLE PARAMETER	BASELINE VALUE	NEW VALUE	INTEGRATED POPULATION DOSE (MAN-REM/10 ⁶ -YR)			PEAK INDIVIDUAL DOSE (REM/10 ⁶ -YR)			
			WHOLE BODY DOSE	CRITICAL ORGAN DOSE	CRITICAL ORGAN	WHOLE BODY DOSE	TIME	CRITICAL ORGAN DOSE	TIME
BASISLINE	-	-	$1.27 \text{ E } -3$	$1.57 \text{ E } -1$	GI-LLI	$6.67 \text{ E } -11$	$1.45 \text{ E } +4$	$7.32 \text{ E } -12$	$1.45 \text{ E } +4$
FAULT STAYS OPEN AND A HIGHER PROBABILITY OF OCCURRENCE	$5. \text{ E } -7$	$5. \text{ E } -5$	$1.27 \text{ E } -3$	$1.57 \text{ E } -1$	GI-LLI	$6.64 \text{ E } -11$	$1.45 \text{ E } +4$	$7.70 \text{ E } -12$	$1.45 \text{ E } +4$

ADDITIONAL BASELINE PARAMETERS FOR CASES WITH TAILED BORING BEALS
(TABLES 9 AND 10)

TABLE 9

PATHWAY	LENGTH (M)	CROSS SECTION (M ²)	POROSITY	PERMEABILITY (cm/sec)	SORPTION	DISPERSION (%)
BOREHOLE PATH LESS THAN 500 YEARS	300	0.1	10^{-2}	10^{-4}	100% DO OTHER FISSION PRODUCTS ACTINIDES	10^2 10^2 10^2
BOREHOLE PATH BETWEEN 500 AND 1000 YEARS	300	0.3	10^{-2}	10^{-4}	SAME	50
BOREHOLE PATH AFTER 1000 YEARS	300	0.5	10^{-2}	10^{-4}	SAME	50

TABLE 10

SHALE DEPOSITORY BORING SEAL DISSOLUTION - SENSITIVITY ANALYSIS
(INTERSTITIAL FLOW)

VARIABLE PARAMETER	BASELINE VALUE	NEW VALUE	INTEGRATED POPULATION DOSE (MAN-REM/10 ⁶ -YR)			PEAK INDIVIDUAL DOSE (REM/10 ⁶ -YR)			
			WHOLE BODY DOSE	CRITICAL ORGAN DOSE	CRITICAL ORGAN	WHOLE BODY DOSE	TIME	CRITICAL ORGAN DOSE	TIME
BASISLINE	-	-	$1.28 \text{ E } -3$	$1.58 \text{ E } -1$	GI-LLI	$6.11 \text{ E } -11$	$1.45 \text{ E } +4$	$7.30 \text{ E } -12$	$1.45 \text{ E } +4$
COMPLETE MIXING	-	-	$1.29 \text{ E } -3$	$1.58 \text{ E } -1$	GI-LLI	$6.09 \text{ E } -11$	$1.45 \text{ E } +4$	$7.37 \text{ E } -12$	$1.45 \text{ E } +4$
MAXIMUM PERMEABILITY IN BORING	10^{-4}	10^{-2}	$1.27 \text{ E } -3$	$1.78 \text{ E } -1$	GI-LLI	$2.46 \text{ E } -13$	$1.20 \text{ E } +5$	$8.98 \text{ E } -11$	$1.20 \text{ E } +1$

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ADDITIONAL BASELINE PARAMETERS FOR FILLED BACKFILL CASES
(TABLE 2 A3.1)

TABLE D

PATHWAY	LENGTH (M)	CROSS SECTION (M ²)	POROSIITY	PERMEABILITY (cm/sec)	DESORPTION	DISPERSION (%)
1ST SEGMENT OF TUNNEL BACKFILL	1200	33,600	10 ⁻²	10 ⁻¹	129, 99, 210 OTHER FISSION PRODUCTS 10 ³ 10 ¹	50
2ND SEGMENT OF TUNNEL BACKFILL	440	1,020	10 ⁻²	10 ⁻⁴	SAF	50
SHAFT BACKFILL	300	81	10 ⁻²	10 ⁻⁴	SAF	50

TABLE E

TABLE OF PARAMETERS VARIED IN TABLE 7

RUN INDEX NUMBER	VARIED PARAMETER	BASLINE VALUE	NEW VALUE
(1)	PERMEABILITY OF THE BACKFILL IN THE TUNNEL (cm/sec) PERMEABILITY OF THE BACKFILL IN THE SHAFT (cm/sec)	10 ⁻⁴ 10 ⁻⁴	10 ⁻³ 10 ⁻³
(2)	PERMEABILITY OF THE BACKFILL IN THE TUNNEL (cm/sec) PERMEABILITY OF THE BACKFILL IN THE SHAFT (cm/sec)	10 ⁻⁴ 10 ⁻⁴	10 ⁻³ 10 ⁻⁶
(3)	PERMEABILITY OF THE BACKFILL IN THE TUNNEL (cm/sec) PERMEABILITY OF THE BACKFILL IN THE SHAFT (cm/sec)	10 ⁻⁴ 10 ⁻⁴	10 ⁻³ 10 ⁻⁶

TABLE 7

SHALE REPOSITORY DETERIORATED BACKFILL - SENSITIVITY ANALYSIS
(INTERSTITIAL FLOW)

VARIED PARAMETER	INTEGRATED POPULATION DOSE (SAR-81.9/200-YR)			PEAK INDIVIDUAL DOSE (REM/100-YR)			
	WHOLE BODY DOSE	CRITICAL ORGAN DOSE	CRITICAL ORGAN	WHOLE BODY DOSE	CRITICAL ORGAN DOSE	TIME	CRITICAL ORGAN
BASLINE	1.50 E -3	2.21 E -1	GI-LLI	5.30 E -13	1.17 E -4	6.52 E -11	1.17 E -4
FURTHER DETERIORATED BACKFILL (1)	2.25 E -3	3.22 E -1	GI-LLI	8.01 E -13	1.17 E -4	9.73 E -11	1.17 E -4
IMPERMEABLE SHAFT (2)	1.30 E -3	1.50 E -1	GI-LLI	5.02 E -14	1.40 E -4	7.10 E -12	1.40 E -4
IMPERMEABLE SHAFT & HIGHLY PERMEABLE TUNNEL (3)	1.24 E -3	1.32 E -1	GI-LLI	4.70 E -14	1.05 E -4	8.80 E -12	1.05 E -4

VARIED PARAMETER	PEAK AQUIFER CONCENTRATION (Ci/m ³ -100-YR)							
	99 _{Tc} CONCENTRATION	TIME	137 _{Sr} CONCENTRATION	TIME	238 _{Pa} CONCENTRATION	TIME	238 _{Pa} CONCENTRATION	TIME
BASLINE	1.85 E -10	6.12 E +2	2.43 E -12	2.00 E +3	1.51 E -10	1.80 E +0	1.00 E -20	2.32 E +0
FURTHER DETERIORATED BACKFILL	2.05 E -10	3.48 E +2	5.87 E -12	1.37 E +3	1.65 E -10	9.12 E +5	2.13 E -10	4.85 E +0
IMPERMEABLE SHAFT	1.91 E -11	4.17 E +2	1.15 E -14	2.25 E +5	9.35 E -30	3.0 E +6	1.25 E -20	3.0 E +6
IMPERMEABLE SHAFT & HIGHLY PERMEABLE TUNNEL	1.55 E -11	1.57 E +5	1.00 E -23	1.80 E +0	0	-	0	-

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BASELINE PARAMETERS FOR TABLE 3 AND 4

TABLE B

PATHWAY	LENGTH (m)	CROSS SECTION (m ²)	POROSITY	PERMEABILITY (cm/sec)	SORPTION	DISPERSION (%)
1 ST SEGMENT OF TUNNEL	1200	140	10 ⁻³	10 ⁻⁶	1	50
2 ND SEGMENT OF TUNNEL	440	188	10 ⁻³	10 ⁻⁶	1	50
SHAFT IN SALT LAYER	100	60	10 ⁻³	10 ⁻⁶	1	50
SHAFT IN SHALE BARRIER LAYER	200	5	10 ⁻³	10 ⁻⁶	1	50
REPOSITORY LAYER	200	5 x 10 ⁶	10 ⁻²	10 ⁻⁶	1	50
BARRIER LAYER	200	5 x 10 ⁶	0.65	10 ⁻⁷	1	50
AQUIFER	1.6 x 10 ⁴	4 x 10 ⁹	0.1	10 ⁻⁴	1	50

TABLE 1

TABLE OF PARAMETERS VARIED IN TABLE 3

RUN INDEX NUMBER	VARIED PARAMETER	BASLINE VALUE	NEW VALUE
(1)	SORPTION PRODUCT OF FISSION PRODUCTS OTHER THAN I AND Tc SORPTION PRODUCT OF ACTINIDES IN AQUIFER	10 ² 10 ⁴	1 10 ²
(2)	POROSITY IN THE TUNNEL AND SHAFT POROSITY IN THE REPOSITORY LAYER POROSITY IN THE BARRIER LAYER	10 ⁻³ 10 ⁻² 5 x 10 ⁻²	10 ⁻⁴ 4 x 10 ⁻³ 10 ⁻¹
(3)	POROSITY IN THE REPOSITORY LAYER POROSITY IN THE BARRIER LAYER	10 ⁻² 5 x 10 ⁻²	4 x 10 ⁻³ 10 ⁻²
(4)	POROSITY IN THE TUNNEL AND SHAFT	10 ⁻³	10 ⁻⁴
(5)	CROSS SECTION IN THE 1 ST SEGMENT OF THE TUNNEL (m ²) CROSS SECTION IN THE 2 ND SEGMENT OF THE TUNNEL (m ²)	3.3 x 10 ³ 188	190 11.1
(6)	CROSS SECTION IN THE 1 ST SEGMENT OF THE TUNNEL (m ²) CROSS SECTION IN THE 2 ND SEGMENT OF THE TUNNEL (m ²) CROSS SECTION IN THE 1 ST SEGMENT OF THE SHAFT (m ²) CROSS SECTION IN THE 2 ND SEGMENT OF THE SHAFT (m ²)	3.3 x 10 ³ 188 60 5	6.4 x 10 ³ 384 110 100
(7)	PERMEABILITY OF THE REPOSITORY LAYER (cm/sec) PERMEABILITY OF THE BARRIER LAYER (cm/sec)	10 ⁻⁹ 10 ⁻⁷	10 ⁻⁷ 10 ⁻⁵
(8)	PERMEABILITY OF THE REPOSITORY LAYER (cm/sec) PERMEABILITY OF THE BARRIER LAYER (cm/sec)	10 ⁻⁹ 10 ⁻⁷	10 ⁻⁵ 10 ⁻⁵
(9)	PERMEABILITY OF THE SHAFT (cm/sec) PERMEABILITY OF THE TUNNEL (cm/sec)	10 ⁻⁶ 10 ⁻⁶	10 ⁻⁵ 10 ⁻⁵

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INPUT DATA			CALCULATED DATA				CHECKED DATA			
PARAMETER	INPUT VALUE	UNIT	WATER BODY	CRITICAL ORGANISM	CRITICAL CONCENTRATION	WATER BODY	TIME	CRITICAL ORGANISM	TIME	CRITICAL ORGANISM
BIOLOGICAL			1.00 E + 0	2.00 E + 1	GI-111	1.00 E + 0	1.00 E + 0	1.00 E + 0	1.00 E + 0	GI-111
ATMOSPHERIC DEPOSITION FACTOR	(1)		2.00	2.00	WATER BODY	2.00 E + 1	1.00 E + 0	2.00 E + 1	1.72 E + 0	WATER BODY
DISPERSED	50	10	1.00 E + 0	1.00 E + 1	GI-111	1.00 E + 0	1.00 E + 0	1.00 E + 0	1.00 E + 0	GI-111
LOW PERMEABILITY EVERYWHERE	(2)		1.00 E + 0	1.00 E + 1	GI-111	1.00 E + 0	1.00 E + 0	1.00 E + 0	1.00 E + 0	GI-111
LOW PERMEABILITY IN ROCK	(3)		1.00 E + 0	1.00 E + 1	GI-111	1.00 E + 0	1.00 E + 0	1.00 E + 0	1.00 E + 0	GI-111
LOW PERMEABILITY IN SAND & GRAVEL	(4)		1.00 E + 0	1.00 E + 1	GI-111	1.00 E + 0	1.00 E + 0	1.00 E + 0	1.00 E + 0	GI-111
MINIMUM AREA FRACTURE PERCENT IN TUNNEL	(5)		1.00 E + 0	1.00 E + 1	GI-111	1.00 E + 0	1.00 E + 0	1.00 E + 0	1.00 E + 0	GI-111
MAXIMUM AREA FRACTURE PERCENT IN SAND & GRAVEL	(6)		1.00 E + 0	1.00 E + 1	GI-111	1.00 E + 0	1.00 E + 0	1.00 E + 0	1.00 E + 0	GI-111
SALT PERMEABILITY	10 ⁻⁴	10 ⁻⁵	1.00 E + 0	1.00 E + 1	GI-111	1.00 E + 0	1.00 E + 0	1.00 E + 0	1.00 E + 0	GI-111
ROCK PERMEABILITY MODERATELY PERMEABLE	(7)		1.00 E + 0	1.00 E + 1	GI-111	1.00 E + 0	1.00 E + 0	1.00 E + 0	1.00 E + 0	GI-111
ROCK PERMEABILITY MODERATELY PERMEABLE	(8)		1.00 E + 0	1.00 E + 1	GI-111	1.00 E + 0	1.00 E + 0	1.00 E + 0	1.00 E + 0	GI-111
ARTESIAN AREA	50	150	1.00 E + 0	1.00 E + 1	GI-111	1.00 E + 0	1.00 E + 0	1.00 E + 0	1.00 E + 0	GI-111
ARTESIAN PERMEABILITY	10 ⁻³	10 ⁻²	1.00	2.00	WATER BODY	1.00 E + 1	1.00 E + 0	1.00 E + 1	1.00 E + 0	WATER BODY
FRACTURE ZONE PERMEABILITY	(9)		1.00 E + 0	1.00 E + 1	GI-111	1.00 E + 0	1.00 E + 0	1.00 E + 0	1.00 E + 0	GI-111
THICKNESS OF BARRIER LAYER	200	20	1.00 E + 0	1.00 E + 1	GI-111	1.00 E + 0	1.00 E + 0	1.00 E + 0	1.00 E + 0	GI-111
LENGTH OF TUNNEL (DISPERSED)	400	0000	1.00 E + 0	1.00 E + 1	GI-111	1.00 E + 0	1.00 E + 0	1.00 E + 0	1.00 E + 0	GI-111
LENGTH OF TUNNEL	400	200	1.00 E + 0	1.00 E + 1	GI-111	1.00 E + 0	1.00 E + 0	1.00 E + 0	1.00 E + 0	GI-111
DISSOLUTION RATE OF ASBESTE	10 ⁻⁴	0.1	1.00 E + 0	1.00 E + 1	GI-111	1.00 E + 0	1.00 E + 0	1.00 E + 0	1.00 E + 0	GI-111
FITNESS PROBABLY SORPTION FACTORS	10 ²	1	1.00 E + 0	1.00 E + 1	GI-111	1.00 E + 0	1.00 E + 0	1.00 E + 0	1.00 E + 0	GI-111
ACTIVATION FACTORS	10 ⁴	10 ²	1.00	2.00	WATER BODY	1.00 E + 1	1.00 E + 0	1.00 E + 1	1.00 E + 0	WATER BODY
ACTIVATION LENGTH	1.0 E 4	1.0 E 3	1.00 E + 0	1.00 E + 1	GI-111	1.00 E + 0	1.00 E + 0	1.00 E + 0	1.00 E + 0	GI-111

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SALT ACCUMULATION BEHAVIORAL ANALYSIS

VARIABLE PARAMETER	PLAK AQUIFER CONCENTRATION							
	10^{-11} CONCENTRATION	TIME	10^{-12} CONCENTRATION	TIME	10^{-13} CONCENTRATION	TIME	10^{-14} CONCENTRATION	TIME
BASIS LINE	2.58 E -11	1.09 E +5	7.04 E -13	1.04 E +5	5.67 E -14	1.15 E +5	1.61 E -12	8.41 E +4
ACTIVINE & FISSION PRODUCT SORPTION FACTOR	2.58 E -11	1.09 E +5	7.04 E -13	1.04 E +5	5.67 E -14	1.15 E +5	1.61 E -12	8.41 E +4
DISPERSION	5.4 E -11	1.21 E +5	1.42 E -12	1.15 E +5	9.22 E -13	1.21 E +5	2.82 E -12	1.15 E +5
LOW POROSITY EVERYWHERE	1.26 E -10	3.45 E +4	4.19 E -12	3.31 E +4	1.20 E -13	4.52 E +4	1.84 E -11	7.11 E +4
LOW POROSITY IN ROCK	1.26 E -10	3.45 E +4	4.19 E -12	3.31 E +4	1.20 E -12	4.52 E +4	1.84 E -11	7.11 E +4
LOW POROSITY IN SHAFT & TUNNEL FRACTURE ZONE	2.58 E -11	1.09 E +5	7.04 E -13	1.04 E +5	5.67 E -14	1.15 E +5	1.61 E -12	8.41 E +4
ARTISIAN AREA FRACTURE ZONE IN TUNNEL	2.60 E -11	1.09 E +5	7.08 E -13	1.04 E +5	5.70 E -14	1.15 E +5	1.61 E -12	8.41 E +4
ARTISIAN AREA FRACTURE ZONE IN SHAFT AND TUNNEL	2.56 E -11	1.09 E +5	6.97 E -13	1.04 E +5	5.62 E -14	1.15 E +5	1.62 E -12	8.41 E +4
SALT PERMEABILITY	1.57 E -10	5.99 E +3	1.66 E -11	5.69 E +3	7.51 E -11	1.24 E +4	1.13 E -10	7.37 E +3
ROCK PERMEABILITY MODERATELY PERMEABLE SALT	5.33 E -10	3.57 E +3	2.01 E -11	2.39 E +3	6.21 E -14	1.05 E +4	1.13 E -10	4.85 E +3
ROCK PERMEABILITY EXTREMELY PERMEABLE SALT	7.11 E -10	2.88 E +3	2.71 E -11	2.44 E +3	5.12 E -11	1.17 E +4	1.05 E -10	1.73 E +3
ARTISIAN HEAD	6.96 E -11	5.28 E +4	1.26 E -12	5.01 E +4	9.69 E -14	6.17 E +4	8.31 E -12	4.97 E +4
AQUIFER PERMEABILITY	2.56 E -11	1.09 E +5	7.04 E -13	1.04 E +5	5.67 E -14	1.15 E +5	1.61 E -12	8.41 E +4
FRACTURE ZONE PERMEABILITY	2.87 E -11	5.25 E +2	1.11 E -12	5.25 E +2	5.31 E -11	1.21 E +5	4.48 E -12	4.17 E +3
THICKNESS OF DEPOSITIONARY LAYER	2.12 E -10	1.87 E +5	7.23 E -12	1.97 E +4	1.11 E -12	2.03 E +4	4.48 E -11	1.52 E +3
THICKNESS OF BARRIER LAYER	6.33 E -11	3.31 E +4	2.11 E -12	3.31 E +4	6.87 E -14	3.01 E +4	1.02 E -11	2.63 E +4
LENGTH OF TUNNEL (INCREASE)	2.60 E -11	1.09 E +5	7.08 E -13	1.04 E +5	5.69 E -14	1.15 E +5	1.65 E -12	7.99 E +4
LENGTH OF TUNNEL	2.57 E -11	1.09 E +5	7.01 E -13	1.04 E +5	5.65 E -14	1.15 E +5	1.63 E -12	8.42 E +4
DISSOLUTION RATE OF WASTE	2.70 E -11	6.63 E +4	8.42 E -12	1.94 E +5	5.77 E -14	1.09 E +5	3.87 E -12	2.02 E +3
FISSION PRODUCT SORPTION FACTORS	2.58 E -11	1.09 E +5	7.04 E -13	1.04 E +5	5.66 E -14	1.15 E +5	1.61 E -12	8.41 E +4
ACTIVINE SORPTION FACTORS	2.58 E -11	1.09 E +5	7.04 E -13	1.04 E +5	5.67 E -14	1.15 E +5	1.64 E -12	8.41 E +4
AQUIFER LENGTH	2.58 E -11	1.09 E +5	7.04 E -13	1.04 E +5	5.67 E -14	1.15 E +5	1.64 E -12	8.41 E +4

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TABLE K

TABLE OF PARAMETERS VARIED IN TABLE 4

RUN INDEX NUMBER	VARIED PARAMETER	BASLINE VALUE	NEW VALUE
(1)	PERMEABILITY OF AQUIFER (cm/sec) PERMEABILITY OF REPOSITORY LAYER (cm/sec) PERMEABILITY OF BARRIER LAYER (cm/sec)	10^{-4} 10^{-9} 10^{-7}	10^{-2} 10^{-5} 10^{-5}
(2)	PERMEABILITY OF THE SHAFT (cm/sec) POROSITY OF THE TUNNEL PERMEABILITY OF THE AQUIFER (cm/sec)	10^{-6} 10^{-3} 10^{-4}	10^{-5} 10^{-4} 10^{-2}
(3)	PERMEABILITY OF THE SHAFT (cm/sec) PERMEABILITY OF THE TUNNEL (cm/sec) PERMEABILITY OF THE AQUIFER (cm/sec)	10^{-6} 10^{-6} 10^{-4}	10^{-5} 10^{-5} 10^{-2}
(4)	PERMEABILITY OF THE SHAFT (cm/sec) PERMEABILITY OF THE TUNNEL (cm/sec) PERMEABILITY OF THE REPOSITORY LAYER (cm/sec) PERMEABILITY OF THE BARRIER LAYER (cm/sec) PERMEABILITY OF THE AQUIFER (cm/sec)	10^{-6} 10^{-6} 10^{-9} 10^{-7} 10^{-4}	10^{-5} 10^{-5} 10^{-5} 10^{-5} 10^{-2}

TABLE L

SALT DEPOSITORY SENSITIVITY ANALYSIS - MULTIPLE PARAMETER
(INTENSIVE TEST)

VARIED PARAMETER	INITIAL DEPOSITATION DOSE			PEAK INDIVIDUAL DOSE				
	WHOLE BODY DOSE	CRITICAL ORGANS DOSE	CRITICAL ORGANS	WHOLE BODY DOSE	TIME	CRITICAL ORGANS DOSE	TIME	CRITICAL ORGANS
BASLINE	1.69×10^{-5}	2.41×10^{-1}	GI-LI	6.15×10^{-1}	1.15×10^5	0.46×10^{-2}	1.15×10^5	GI-LI
PERMEABILITY OF ROCK AND AQUIFER (1)	3.17	3.17	WHOLE BODY	1.32×10^{-10}	0.07×10^5	1.50×10^{-9}	1.02×10^5	BONE
PERMEABILITY OF SHAFT & AQUIFER POROSITY OF TUNNEL (2)	2.61	2.41	WHOLE BODY	7.10×10^{-1}	1.12×10^6	7.10×10^{-1}	1.12×10^6	WHOLE BODY
PERMEABILITY OF SHAFT TUNNEL & AQUIFER (3)	2.63	2.43	WHOLE BODY	7.20×10^{-1}	1.12×10^6	7.20×10^{-1}	1.12×10^6	WHOLE BODY
HIGH PERMEABILITY BARRIER LAYER (4)	3.17	3.17	WHOLE BODY	1.22×10^{-10}	0.01×10^5	1.50×10^{-9}	1.01×10^5	BONE

VARIED PARAMETER	PEAK AQUIFER CONCENTRATION (1) (2) (3) (4) (5) (6) (7) (8)							
	BB ₀ CONCENTRATION	TIME	BB ₀ CONCENTRATION	TIME	BB ₀ CONCENTRATION	TIME	BB ₀ CONCENTRATION	TIME
BASLINE	2.50×10^{-11}	1.09×10^5	2.91×10^{-13}	1.04×10^5	1.07×10^{-14}	1.15×10^5	1.07×10^{-14}	8.41×10^4
PERMEABILITY OF ROCK & AQUIFER	7.1×10^{-12}	2.65×10^5	2.71×10^{-13}	2.68×10^5	1.7×10^{-16}	1.17×10^5	1.7×10^{-16}	1.71×10^5
PERMEABILITY OF SHAFT & AQUIFER POROSITY OF TUNNEL	2.37×10^{-12}	1.03×10^5	7.0×10^{-15}	1.01×10^5	1.01×10^{-16}	1.15×10^5	1.01×10^{-16}	8.31×10^4
PERMEABILITY OF SHAFT TUNNEL & AQUIFER	2.47×10^{-12}	5.25×10^5	1.11×10^{-14}	1.25×10^5	1.01×10^{-16}	1.21×10^5	1.01×10^{-16}	1.17×10^5
HIGH PERMEABILITY BARRIER LAYER	7.1×10^{-12}	2.65×10^5	2.71×10^{-13}	2.67×10^5	1.7×10^{-16}	1.17×10^5	1.7×10^{-16}	1.71×10^5

A3.1

ADDITIONAL LABELING PARAMETERS FOR FAULTED BACKFILL CASES
(TABLES 7 AND 8)

TABLE 7

PATHWAY	LENGTH (M)	CROSS SECTION (M ²)	POROSITY	PERMEABILITY (cm/sec)	SORPTION	DISPERSION (M)
1ST SEGMENT OF TUNNEL BACKFILL	1200	33,000	10 ⁻²	10 ⁻⁴	120 ₂ D ₂ OTHER FISSION PRODUCTS 10 ⁻³ 10 ⁻⁴	50
2ND SEGMENT OF TUNNEL BACKFILL	400	1,620	10 ⁻²	10 ⁻⁴	SAME	50
SHAFT BACKFILL	300	64	10 ⁻²	10 ⁻⁴	SAME	50

TABLE 8

TABLE OF PARAMETERS VARIED IN TABLE 8

RUN INDEX NUMBER	VARIED PARAMETER	BASILINE VALUE	NEW VALUE
(1)	PERMEABILITY OF BACKFILL IN THE TUNNEL (cm/sec) PERMEABILITY OF BACKFILL IN THE SHAFT (cm/sec) POROSITY OF BACKFILL IN THE SHAFT AND TUNNEL	10 ⁻⁴ 10 ⁻⁴ 10 ⁻²	10 ⁻³ 10 ⁻³ 10 ⁻¹
(2)	PERMEABILITY OF BACKFILL IN THE TUNNEL (cm/sec) PERMEABILITY OF BACKFILL IN THE SHAFT (cm/sec) POROSITY OF BACKFILL IN THE SHAFT AND TUNNEL	10 ⁻⁴ 10 ⁻⁴ 10 ⁻²	10 ⁻³ 10 ⁻⁶ 10 ⁻¹
(3)	PERMEABILITY OF BACKFILL IN THE TUNNEL (cm/sec) PERMEABILITY OF BACKFILL IN THE SHAFT (cm/sec) POROSITY OF BACKFILL IN THE SHAFT AND TUNNEL	10 ⁻⁴ 10 ⁻⁴ 10 ⁻²	10 ⁻¹ 10 ⁻⁶ 10 ⁻¹
(4)	PERMEABILITY OF BACKFILL IN THE TUNNEL (cm/sec) PERMEABILITY OF BACKFILL IN THE SHAFT (cm/sec) POROSITY OF BACKFILL IN THE SHAFT AND TUNNEL	10 ⁻⁴ 10 ⁻⁴ 10 ⁻²	10 ⁻¹ 10 ⁻³ 10 ⁻¹

TABLE 9

SALT DEPOSITIVITY INTEGRATED BACKFILL - SENSITIVITY ANALYSIS
CONCENTRATION (M)

VARIED PARAMETER	INTEGRATED POPULATION DOSE (10 ⁻³ Sv/yr/10 ⁻⁵ Sv)			PEAK INDIVIDUAL DOSE (REV 200-10)				CRITICAL ORGAN
	WHOLE BODY DOSE	CRITICAL ORGAN DOSE	CRITICAL ORGAN	WHOLE BODY DOSE	TIME	CRITICAL ORGAN DOSE	TIME	
BASILINE	1.86 E -13	3.14 E -1	GI-LLI	3.06 E -13	1.44 E +4	6.15 E -11	1.44 E -1	GI-LLI
100% DETERIORATED BACKFILL (1)	2.33 E -13	3.73 E -1	GI-LLI	1.19 E -12	1.87 E +4	1.44 E -10	1.87 E +4	GI-LLI
100% PERMEABLE SHAFT (2)	1.62 E -13	2.83 E -1	GI-LLI	7.82 E -14	1.25 E +5	9.38 E -12	1.21 E +3	GI-LLI
100% PERMEABLE SHAFT HIGHLY PERMEABLE TUNNEL (3)	1.86 E -13	3.29 E -1	GI-LLI	3.58 E -13	3.14 E +4	4.23 E -11	3.14 E -1	GI-LLI
PERMEABLE TUNNEL & SHAFT (4)	2.73 E -13	4.27 E -1	GI-LLI	1.51 E -12	2.68 E +4	1.82 E -10	1.88 E +4	GI-LLI

VARIED PARAMETER	SOLUBLE CONCENTRATION (10 ⁻³ M/10 ⁻⁵ M)				226Ra CONCENTRATION				226Ra CONCENTRATION			
	CONCENTRATION	TIME	CONCENTRATION	TIME	CONCENTRATION	TIME	CONCENTRATION	TIME	CONCENTRATION	TIME	CONCENTRATION	TIME
BASILINE	1.63 E -10	4.16 E +3	6.10 E -12	4.10 E 3	1.35 E -14	1.41 E +3	3.62 E -11	4.85 E +3				
100% DETERIORATED BACKFILL (1)	3.74 E -10	9.55 E +3	1.38 E -11	9.55 E +3	6.33 E -14	1.33 E +4	1.11 E -10	1.0 E +4				
100% PERMEABLE SHAFT (2)	2.81 E -11	1.15 E +5	6.76 E -13	1.04 E +5	3.69 E -13	1.27 E +4	1.53 E -12	3.41 E +4				
100% PERMEABLE SHAFT HIGHLY PERMEABLE TUNNEL (3)	1.18 E -10	2.15 E +4	3.07 E -12	2.10 E +4	6.39 E -14	2.33 E +4	2.04 E -11	2.15 E +4				
PERMEABLE TUNNEL & SHAFT (4)	3.85 E -10	6.40 E +3	1.84 E -11	6.80 E +3	6.38 E -13	1.17 E +4	1.32 E -10	7.70 E +3				

PERMEABILITY (MD)	5.0	1×10^{-12}	0.5	10^{-12}	1	1
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**THE PROBABILITY OF A BRECCIA PIPE FORMATION IS 5×10^{-2} PER YEAR

TABLE 12

SALT REPOSITORY BRECCIA FORMATION - SENSITIVITY ANALYSIS
(CONTINGENCY FROM)

VARIABLE PARAMETER	BASELINE VALUE	NEW VALUE	INTEGRATED POPULATION DOSE (MAN-REVS/250-YR)			PEAK INDIVIDUAL DOSE (MICROSV/50-YR)			
			WHOLE BODY DOSE	CRITICAL ORGAN DOSE	CRITICAL ORGAN	WHOLE BODY DOSE	TIME	CRITICAL ORGAN DOSE	TIME
BASISLINE	-	-	$1.02 \text{ E } -3$	$2.84 \text{ E } -3$	GI-LLI	$8.05 \text{ E } -14$	$1.15 \text{ E } +5$	$9.74 \text{ E } -12$	$1.15 \text{ E } +5$
HIGH PROBABILITY OF BRECCIA FORMATION	$5. \text{ E } -7$	$5. \text{ E } -5$	$1.18 \text{ E } -3$	$3.01 \text{ E } -3$	GI-LLI	$1.72 \text{ E } -13$	$2.43 \text{ E } +4$	$2.48 \text{ E } -11$	$2.10 \text{ E } +4$

ADDITIONAL BASELINE PARAMETERS FOR CASES WITH FAILED BORING SEALS
(TABLES 8 AND 10)

TABLE 1

PATHWAY	LENGTH (M)	CROSS SECTION (M ²)	POROSITY	PERMEABILITY (cm/sec)	SORPTION	DISPERSION (M)
BORINGHOLE PATH LESS THAN 500 YEARS	300	0.1	10^{-2}	10^{-4}	$120 \text{ E } 90 \text{ Tc}$ OTHER FISSION PRODUCTS ACTINIDES	10^2 10^4
BORINGHOLE PATH BETWEEN 500 AND 1000 YEARS	300	0.3	10^{-2}	10^{-4}	SAME	50
BORINGHOLE PATH AFTER 1000 YEARS	300	0.5	10^{-2}	10^{-4}	SAME	50

SALT REPOSITORY BORING SEAL DISSOLUTION - SENSITIVITY ANALYSIS
(CONTINGENCY FROM)

VARIABLE PARAMETER	BASELINE VALUE	NEW VALUE	INTEGRATED POPULATION DOSE (MAN-REVS/250-YR)			PEAK INDIVIDUAL DOSE (MICROSV/50-YR)			
			WHOLE BODY DOSE	CRITICAL ORGAN DOSE	CRITICAL ORGAN	WHOLE BODY DOSE	TIME	CRITICAL ORGAN DOSE	TIME
BASISLINE	-	-	$1.02 \text{ E } -3$	$2.84 \text{ E } -3$	GI-LLI	$7.90 \text{ E } -14$	$1.21 \text{ E } +5$	$9.67 \text{ E } -12$	$1.21 \text{ E } +5$
DISSOLUTION	-	-	$1.02 \text{ E } -3$	$2.84 \text{ E } -3$	GI-LLI	$7.90 \text{ E } -14$	$1.21 \text{ E } +5$	$9.67 \text{ E } -12$	$1.21 \text{ E } +5$
DISSOLUTION IN DISSOLUTION	10^{-1}	10^{-2}	$1.02 \text{ E } -3$	$2.84 \text{ E } -3$	GI-LLI	$1.50 \text{ E } -13$	$1.21 \text{ E } +5$	$1.93 \text{ E } -11$	$1.21 \text{ E } +5$

A3.1

BASELINE PARAMETERS FOR SHALE WITH FRACTURE FLOW
(TABLES 3 AND 4)

TABLE 3

PARAMETER	LENGTH	CROSS SECTION (m ²)	PORE VOLUME	PERMEABILITY (cm/sec)	SORPTION	DESORPTION (%)
REPOSITORY LAYER	200	5×10^6	10^{-5}	10^{-8}	SAVE	50
BARRIER LAYER	200	5×10^6	10^{-6}	10^{-5}	SAVE	50

TABLE 4

SALT DEPOSITION SENSITIVITY ANALYSIS
(EXHAUSTIVE FLOOD)

VARIABLE PARAMETER	BASELINE VALUE	NEW VALUE	INTEGRATED POPULATION DOSE (MUS-RU/WHO-YR)			PEAK INDIVIDUAL DOSE (REM/MG-YR)				CRITICAL ORGAN
			WHOLE BODY DOSE	CRITICAL ORGAN DOSE	CRITICAL ORGAN	WHOLE BODY DOSE	TIME	CRITICAL ORGAN DOSE	TIME	
BASELINE	-	-	$2.56 \text{ E } -3$	$4.06 \text{ E } -3$	GI-LLI	$5.83 \text{ E } -13$	$2.56 \text{ E } +4$	$7.07 \text{ E } -11$	$2.56 \text{ E } +4$	GI-LLI
SALT PERMEABILITY	10^{-9}	10^{-5}	$2.77 \text{ E } -3$	$4.32 \text{ E } -3$	GI-LLI	$1.88 \text{ E } -12$	$1.17 \text{ E } +4$	$2.27 \text{ E } -10$	$1.17 \text{ E } +4$	GI-LLI
DESORPTION	50	10	$2.61 \text{ E } -3$	$4.18 \text{ E } -3$	GI-LLI	$1.00 \text{ E } -12$	$2.56 \text{ E } +4$	$1.12 \text{ E } -10$	$2.56 \text{ E } +4$	GI-LLI

VARIABLE PARAMETER	AQUIFER CONCENTRATION (C.I. = 10 ⁻⁶ MG/L-PP)							
	90% CONCENTRATION	TIME	120% CONCENTRATION	TIME	220% CONCENTRATION	TIME	230% CONCENTRATION	TIME
BASELINE	$1.86 \text{ E } -10$	$1.69 \text{ E } +1$	$6.5 \text{ E } -12$	$1.6 \text{ E } +4$	$8.08 \text{ E } -14$	$2.60 \text{ E } +4$	$4.07 \text{ E } -11$	$1.17 \text{ E } +4$
SALT PERMEABILITY	$6.82 \text{ E } -10$	$3.15 \text{ E } +2$	$2.61 \text{ E } -11$	$3.13 \text{ E } +2$	$5.17 \text{ E } -14$	$1.12 \text{ E } +4$	$1.12 \text{ E } -10$	$1.73 \text{ E } +3$
DESORPTION	$3.15 \text{ E } -10$	$1.6 \text{ E } +1$	$1.11 \text{ E } -11$	$1.52 \text{ E } +4$	$1.27 \text{ E } -13$	$1.02 \text{ E } +4$	$7.66 \text{ E } -11$	$1.57 \text{ E } +4$

APPENDIX 3.2

GEOLOGY-HYDROLOGY MODEL DESCRIPTION

1.

INTRODUCTION

The TASC geology-hydrology model and computer program calculates the release of radioactive waste to the biosphere due to transport in groundwater. The model incorporates the effects of mass transport, chemical interactions between waste components and soil, and hydrodynamic dispersion.

Because the characteristics of possible waste repository sites and engineering designs are not well defined at this time, the model is constructed so as to facilitate sensitivity studies. In order to make this possible, procedures which divide the region of interest into a lattice of cells, such as finite element and finite difference methods, are avoided. Instead, the groundwater flow pattern is approximated by a network of one-dimensional flow paths, which need not be straight. The justification for this procedure is discussed in Appendix A.

Future events, such as faulting or failure of engineered seals, may affect the movement of groundwater and dissolved radionuclides. The times at which such events will occur can usually be predicted only on a probabilistic basis. The model can take these future events into account by either of two methods.

- Doses can be calculated for scenarios in which events occur at specified times.
- The events can be taken to occur at random times with given probability of occurrence per year and expected values of consequence calculated.

The statistical method which makes possible the second type of analysis is derived in Appendix B.

Calculations for the TASC geology-hydrology model are carried out by a computer program called WASTE. The assessment of effects of repositories requires that WASTE be operated in conjunction with a number of other computer codes. The information flow between these codes is shown in Fig. 1-1.

The WASTE program calculates the flow of waste without consideration of radioactive decay. The results of its calculations are in units of fractions of the total inventory of each nuclide. In order to provide numbers which directly measure risk, these results must be multiplied by the inventories of the nuclides. These inventories are provided by the ORIGEN code, which was originally developed at Oak Ridge National Laboratory (Ref. 1).

Doses to humans will depend on the movement of waste through surface waters, concentration in the ecosystem, human diets and living habits and the biochemistry of the waste nuclides in the human body. These factors are modeled in the TASC-developed program SIG3.

Outputs of the different programs are multiplied together and final data manipulations are performed by the programs WSCONS (which is a subroutine of WASTE) and WSTPLOT.

Figure 1-1 Information flow among computer programs involved in assessment of post-emplacement risk from radioactive waste repositories. WSCONS is currently executed as a subroutine of WASTE.

GENERAL APPROACH

As discussed in Appendix A, the TASC model approximates the groundwater flow pattern around a repository by a network of one-dimensional flow paths, or "pipes". The variables which describe each pipe are listed in Table 2-1.

TABLE 2-1
VARIABLES DESCRIBING FLOW PATHWAYS

$B(j, m_1, m_2, n)$	The sorption factor for nuclides of type j in the pipe from node m_1 to node m_2 in state n (dimensionless)
$W(m_1, m_2, n)$	The cross-section of pipe m_1, m_2 in state n in square meters.
$\alpha(m_1, m_2)$	The dispersion constant in meters.
$K(m_1, m_2, n)$	The permeability in cm/sec.
$HEAD(m, n)$	The hydraulic head at node m in meters.
$z(m_1, m_2)$	The distance from m_1 to m_2 in meters.
$\epsilon(m_1, m_2, n)$	The effective porosity (dimensionless).

Each point in the network at which pipes branch, or at which any of the variables listed in Table 2-1 changes value, is defined as a node. The nodes are numbered in such a way that water flow is always from lower-numbered to higher-numbered nodes.*

*This would appear to preclude situations where flow reverses when state changes. But this restriction may be avoided by artificially placing more than one node at the same location.

The program begins by calculating how much waste leaves the repository (node 1) as a function of geologic state and time. (See Chapter 6.) Then the program considers each node in the system of pipes in sequence. The rate at which waste arrives at a given node is calculated from the amounts of waste which had earlier left lower-numbered nodes.

In order to carry out digital calculations, time must be divided into discrete intervals. The program then calculates a quantity $F(j, l, m, n)$, which is the amount of waste type j passing through node m during time interval l , given that the system is in state n , multiplied by the probability of the system being in state n . This quantity is analogous to $\phi_j(x; n, t)$ defined in Appendix B; F is related to the mass flux integrated over interval l in the same way as ϕ_j is related to the concentration.

The following equation is used to calculate F for nodes other than the repository itself

$$F(l, m, n) = \sum_{m' < m} \sum_{l' \leq l} \sum_{n'} F(l', m', n') \times SP(m', m, n') G(l', l, m', m, n') TP(l', l, n', n) \quad (2-1)$$

In this formula, one begins with $F(l', m', n')$, the amount of waste leaving node m' in state n' during interval l' . This is multiplied by SP , the fraction of the waste leaving m' which enters a pipe leading directly from m' to m . (If there is no such pipe, SP is zero.) G is the fraction of the waste entering the pipe during interval l' which reaches the end of the pipe (node m) during interval l . This is calculated under the assumption that the system is always in the same state, n' , as it was in when the waste entered the pipe. Thus the

waste does not react to the system's change of state until it reaches a node. The state changes are accounted for when the waste reaches node m by the factor TP ; TP is the probability that the system, having been in state n' during interval t' , will be in state n during interval t . The effect of multiplying by TP is to take the waste, which migrated through the pipe from m' to m on the assumption that the system was still in state n' , and distribute it among all the states (including n') in proportion to the probability that while the waste was in the pipe the system went from state n' to state n .

The mathematical approximation (as compared to an exact solution of Eq. B-13) of delaying the effect of state changes on waste until the waste reaches a node greatly simplifies calculations. Its effect may be reduced by inserting intermediate nodes in pipes. Waste will react to state changes when reaching these intermediate nodes and then proceed through the remainder of the pipe at a velocity appropriate to the new state. The overall effect of the approximation may be analyzed by measuring the effect of adding such intermediate nodes; such tests are planned as a part of model validation.

The assumptions and methods used to calculate the factors SP , G , and TP are described in the following sections.

The problem of radionuclide transport in a one dimensional pipe is solved explicitly using a Green's function approach. The resulting integral equation is integrated again so that a simple numerical quadrature technique may be applied. This approach avoids the inherent difficulties of numerical dispersion associated with finite difference schemes.

3.1 THE HYDROLOGICAL EQUATIONS

The fundamental equation governing transport and dispersion of ions in one-dimensional flow through porous media is

$$\frac{\partial C_r}{\partial t} + v \frac{\partial C_r}{\partial x} = \alpha v \frac{\partial^2 C_r}{\partial x^2} - \Gamma_r C_r + \sum_s \Gamma_s^r C_s - \frac{\partial m_r}{\partial t} \quad (3.1-1)$$

Here Γ_r is the radioactive decay constant of nuclide r (equal to $\ln 2$ divided by the half-life), Γ_s^r is the production rate of nuclide r from decay of nuclide s , v is the interstitial water flow velocity, C_r is the concentration of nuclide r in the interstitial water, α is the longitudinal dispersion constant, and m_r is the amount of ion r absorbed on the solid per unit volume. The following assumptions are now made.

- Ion exchange is instantaneous and the ion-exchange absorption isotherm is linear.

- The first term on the right side of equation (1) represents the rate of change of the concentration of the nuclide in the water phase, $\frac{dC_w}{dt}$.
- The second term on the right side of equation (1) represents the rate of change of the concentration of the nuclide in the sediment phase, $\frac{dC_s}{dt}$.
- The third term on the right side of equation (1) represents the rate of change of the concentration of the nuclide in the atmosphere, $\frac{dC_a}{dt}$.
- The fourth term on the right side of equation (1) represents the rate of change of the concentration of the nuclide in the food chain, $\frac{dC_f}{dt}$.

The first term on the right side of equation (1) is

$$Q \frac{dC_w}{dt} = Q \frac{dC_w}{dt} \quad (1-2)$$

where Q is the flow rate of water through the reservoir and C_w is the concentration of the nuclide in the water phase. The second term on the right side of equation (1) is

$$Q \frac{dC_s}{dt} = Q \frac{dC_s}{dt} \quad (1-3)$$

$$C_r = \frac{C_s}{C_w}$$

$$C_r = \frac{C_s}{C_w}$$

$$C_r = \frac{C_s}{C_w} \quad x = 0$$

where Q is the flow rate of water through the reservoir and $C_r = C_s/C_w$ is the retention factor. Since that $C_r = C_s/C_w$, the subscripts may be replaced with a single subscript r , denoting a group of nuclides which have the same retention factor. In the remainder of this chapter we will omit the subscript r . This simplification allows us to eliminate from our model a detailed analysis of nuclide decay chains. The assumption that the

retention factor is the same for all parent-daughter combinations is very reasonable in light of our imprecise knowledge of these parameters. That this causes only minor perturbations in our results will be discussed in a later document.

The final set of equations is,

$$\frac{\partial c}{\partial t} + \frac{V}{B} \frac{\partial c}{\partial x} = \frac{\alpha V}{B} \frac{\partial^2 c}{\partial x^2} \quad x > 0 \quad (3.1-4)$$

$$c = 0 \quad t = 0$$

$$c = 0 \quad x = \infty$$

$$c - 2D \frac{\partial c}{\partial x} = \frac{R(t)}{Q} \quad x = 0$$

For the next pipe in the network, at a distance z from the repository, we would have,

$$\frac{\partial c'}{\partial t} + \frac{V'}{B'} \frac{\partial c'}{\partial x} = \frac{\alpha' V'}{B'} \frac{\partial^2 c'}{\partial x^2} \quad x > z$$

$$c' = 0 \quad t = 0$$

$$c' = 0 \quad x = \infty$$

$$\left(c' - \alpha' \frac{\partial c'}{\partial x} \right) \Big|_{x=z+0} = \left(c - \alpha \frac{\partial c}{\partial x} \right) \Big|_{x=z-0} \quad (3.1-5)$$

3.2 FORMULAS FOR DISCRETE TIME INTERVALS

The solution of Eq. 3.1-4 can be written as,

$$c(x, t) = \frac{V}{BQ} \int_0^t R(\tau) G(x, t-\tau) d\tau \quad (3.2-1)$$

Figure 3.2-1 Procedure for calculating the output of a pipe.

where the Green's function is

$$G(x,t) = \frac{1}{\sqrt{4\pi\alpha\frac{V}{B}t}} \exp \left\{ -\frac{(x - \frac{V}{B}t)^2}{4\alpha\frac{V}{B}t} \right\} \quad (3.2-2)$$

In order to solve our problem on the computer, this continuous-time solution must be modified to be compatible with discrete time intervals. The means by which this is done is illustrated graphically in Fig. 3.2-1, this procedure will be developed mathematically in the remainder of this chapter.

We first define

$$F(l) = \int_{T(l)}^{T(l+1)} Qc(z,t) dt \quad (3.2-3)$$

Eq. 3.2-3 represents approximately the amount of waste leaving the pipe at $x = z$ during the time period $(T(l), T(l+1))$.

This can also be written as

$$\begin{aligned} F(l) = & \frac{V}{B} \int_0^{T(l)} \int_{T(l)}^{T(l+1)} R(\tau) G(z, t-\tau) dt d\tau \\ & + \frac{V}{B} \int_{T(l)}^{T(l+1)} \int_{\tau}^{T(l+1)} R(\tau) G(z, t-\tau) dt d\tau \end{aligned} \quad (3.2-4)$$

We now move $R(\tau)$ outside the τ integral and integrate the Green's function over a single time interval. Let

$$G_1(z, \tau, l) = \frac{V}{B} \int_{T(l)}^{T(l+1)} G(z, t-\tau) dt \quad \tau \leq T(l) \quad (3.2-5a)$$

and

$$G_2(z, \tau, l) = \frac{V}{B} \int_{\tau}^{T(l+1)} G(z, t-\tau) dt \quad T(l) < \tau < T(l+1) \quad (3.2-5b)$$

These functions give the fraction of an impulse of waste entering the pipe at time τ which would leave the pipe during the time interval $(T(l), T(l+1))$. $R(\tau)$ is the rate at which waste enters the pipe. The integrals of Eq. 3.2-5 can be carried out explicitly, giving

$$\frac{V}{B} \int_{T(l)}^{T(l+1)} G(z, t-\tau) dt = \frac{1}{2} e^{\frac{z}{2a}} \left[g(z, T(l+1) - \tau) - g(z, T(l) - \tau) \right]$$

and

$$\frac{V}{B} \int_{\tau}^{T(l+1)} G(z, t-\tau) dt = \frac{1}{2} e^{\frac{z}{2a}} g(z, T(l+1) - \tau)$$

where

$$g(z, t) = \operatorname{erfc} \left\{ \frac{z - \frac{V}{B} t}{\sqrt{\frac{4aVt}{B}}} \right\} e^{\frac{z}{2a}} - \operatorname{erfc} \left\{ \frac{z + \frac{V}{B} t}{\sqrt{\frac{4aVt}{B}}} \right\} e^{\frac{z}{2a}} \quad (3.2-6)$$

The quantity $F(l)$ can now be used as the input to the next pipe. A new set of integrated Green's functions will then tell us the fraction of waste leaving the second pipe. This procedure, as generalized to more complicated networks, is described by Eq. 2-1.

3.3 NUMERICAL TECHNIQUE

In order to calculate $F(l)$ we break time up into discrete steps. The step size has been chosen to be

$$TD(l) = T(l+1) - T(l)$$

where

$$T(l) = 10 \left(2 + \frac{4.5(l-1)}{l_{\max}} \right) - 100 \quad (3.3-1)$$

This choice of step size corresponds to our choice to display the output on a log-log scale. This also puts greater emphasis on earlier times when releases may be more critical. The equation for the output of a given pipe becomes,

$$\begin{aligned} F_O(l) \cong & \sum_{i=1}^{l-1} \int_{T(i)}^{T(i+1)} R(\tau) G_1(z, \tau, l) d\tau \\ & + \int_{T(l)}^{T(l+1)} R(\tau) G_2(z, \tau, l) d\tau \end{aligned} \quad (3.3-2)$$

where $R(\tau)$ is the rate at which waste enters the pipe.

The integrals are usually evaluated using the mid-point rule. The computer program takes each input, $R(\tau) d\tau$, to a pipe and computes the fraction that comes out of the pipe at all time intervals.

When the Green's function is narrower than the time steps, G may be approximated by a delta function

$$G(z,t) \cong \delta(z - \frac{V}{B} t) \quad (3.3-3)$$

If the midpoint rule were then used to integrate Eq. 3.3-2 with changing time steps, for some values of l the sum would contain two non-zero terms and for other values of l it would only contain one non-zero term. Numerical noise would result, as illustrated in Fig. 3.3-1. In such cases, it is more accurate to use Eq. 3.3-3 directly to solve Eq. 3.2-4. The precise conditions under which this is done are discussed in Appendix C.

An additional procedure is necessary to avoid round-off errors. Both $g(z,t)$ and $G_1(z,\tau,l)$ involve differences of complementary error functions. When these differences are small the error functions are expanded so that accuracy may be maintained. (See Appendix C.)

The program is written so that as few calls as possible are made to the complementary error function routine. The net result is an accurate and efficient calculation of nuclide migration.

a) ENTERING PIPE

TWO PULSES IN
ONE TIME INTERVAL

b) LEAVING PIPE

Figure 3.3-1 Numerical noise arises when the Green's function is narrower than the time interval and the duration of time intervals is not constant. In b, note the arrival of two pulses during the same time interval.

4. TREATMENT OF NODES WHERE FLOW PATHS BRANCH

At some nodes flow paths will branch and there will be more than one route by which waste can proceed from that point. For example, in our baseline models waste may leave the repository either through the fracture zone around the shaft and tunnel, through the bulk permeability of the surrounding rock, or sometimes by other pathways. In these cases it is necessary to determine how much of the waste enters each open pipe.

The model divides the waste in proportion to the volumetric flow of water in each pathway. The proportion of the waste leaving node m_1 in state n which proceeds toward node m_2 is given by

$$SP(m_1, m_2, n) = \frac{V(m_1, m_2, n) W(m_1, m_2, n) \epsilon(m_1, m_2, n)}{\sum_{m'} V(m_1, m', n) W(m_1, m', n) \epsilon(m_1, m', n)} \quad (4-1)$$

where V is the water velocity in each pathway, W is the cross-section of the pathway, and ϵ is the effective porosity.

It will be noted that sorption factors do not enter into this formula; the velocity used is the water velocity rather than the velocity of the waste. This requires some comment. In situations where streamlines branch in an area where rock chemistry, water impurities, etc. are homogeneous and sorption factors change only after the waste has been irrevocably committed to a particular pathway, the waste transport will simply be proportional to the water flow. This situation leads directly to Eq. 4-1.

The situation where streamlines branch in an area of inhomogeneous sorption is more complicated. The applicability of Eq. 4-1 to this case will be the subject of additional analysis in the future.

5. METHOD OF CALCULATING PROBABILITIES OF TRANSITION

The quantity $TP(l', l, n', n)$ used in Eq. 2-1 is defined as the conditional probability that the system, having been in state n' at time $T(l')$, is in state n at time $T(l)$. (n' may be equal to n .)

When the program is used to analyze deterministic scenarios TP is equal to unity if the system is in state n' at time $T(l')$ and is also in state n at time $T(l)$. Otherwise TP is equal to zero.

When the transitions among states are stochastic processes, more complicated formulas for TP must be used. The simplest case is when the transition rates λ (defined in Appendix B) are constant. For given l' and l , a matrix of $TP(n', n)$ may be calculated from the equation

$$TP = e^{-M[T(l) - T(l')]}$$

where M is a matrix whose elements are the transition rates.

When transition rates are not constant, formulas for TP must be derived by solving the appropriate differential equations.

6.

LEACHING CALCULATION

The model assumes that no waste leaves the repository until the void space left by mining operations has been re-saturated by groundwater. The interval required for this to occur (designated T_{fill}) is an input to the program.

Once the mine has resaturated, the rate at which waste leaves is assumed to be proportional to the amount remaining in the repository. The rate at which waste leaves the repository is therefore given by

$$R(t) = \lambda q(t) \quad (6-1)$$

where λ is the fractional dissolution rate (in yr^{-1}) of the waste and $q(t)$ is the amount of waste in the repository at time t in MWe-yr.

The quantity actually used by our model is the input to the first pipe, $F(l,1,n)$, which represents the expected amount of waste leaving the repository during time interval l if the system is in state n , multiplied by the probability of the system being in state n . Since Eq. 6-1 is linear in q , the expected rate of release will simply be the expected amount in the repository multiplied by λ . Integrating over a time interval, we have

$$F(l,1,n) = Q(l,n) \left\{ 1 - \exp(-\lambda(j,n)[T(l+1) - T(l)]) \right\} \quad (6-2)$$

Here $Q(l,n)$ is the expected amount of waste remaining in the repository at time $T(l)$ if the system is in state n , multiplied

by the probability of the system being in state n. The following equation for $Q(l,n)$ may be derived from Eq. B-13.

$$Q(l,n) = \sum_{n'} TP(l-1,l,n',n) \left[Q(l-1,n') - F(l-1,l,n') \right] \quad (6-3)$$

The initial values $Q(1,n)$ are inputs to the program. If the total amount of waste is normalized to one MWe-yr, then $Q(1,n)$ is the probability that the system is in state n at time T(1).

It will be noted that in Eq. 6-2, the dissolution rate λ was written as a function of both nuclide type j and geologic state n. This notation gives the program the capability of handling dissolution rates which are affected by water flow, repository temperature, or other geologic state variables or by chemical properties of different nuclides. However, as noted in Section 3.1, parent and daughter nuclides in any single decay chain are represented as having the same dissolution rate if both are present in the waste at the time it is dissolving.

CALCULATION OF MAXIMUM CONCENTRATIONS

The maximum concentrations of selected radionuclides in the interstitial water at the entrance to each pipe are calculated by the subprogram WSCONS. These concentrations may be of interest for regulatory purposes. Also, they may be used to check the consistency of our physical assumptions as to the degree of ion solubility and the rate of ion-exchange reactions. These computations are made only for deterministic models, as for these purposes actual concentrations and not expected concentrations are required.

The formula used to compute the interstitial concentration at the entrance to pipe (m_1, m_2) at time $T(i)$ is

$$C_r(i, m_1, 1) = \frac{F(i, m_1, 1) \text{ INV}_r(T(i)) \text{ SP}(m_1, m_2, 1)}{(T(i+1) - T(i)) \text{ V}(m_1, m_2, 1) \text{ W}(m_1, m_2, 1) \text{ c}(m_1, m_2, 1)} \quad (7-1)$$

This formula is just the flow rate of waste, $F/(T(i+1) - T(i))$, multiplied by the inventory of nuclide r , INV_r , and the fraction of waste flowing into pipe (m_1, m_2) , SP , and divided by the flow rate of water in the pipe, VWc .

In order to calculate concentrations in the aquifer, mixing through an area equal to the height of the aquifer times the width of the repository was assumed. The capability of calculating explicitly the horizontal distribution of waste in the aquifer from both point and plane sources has been added to the program and will be described in a later document.

APPENDIX A
ONE-DIMENSIONAL APPROXIMATION TO
DISPERSIVE FLOW IN POROUS MEDIA

The basic TASC model of flow through porous media consists of a series of interconnected one-dimensional pipes. The complicated problem of solving two or three dimensional transport equations for a variety of changing parameters and geologic states is thus avoided. The simplification is justified on both pragmatic and mathematical grounds. It is not practical to do extensive sensitivity analysis on multi-state generic repository models without such simplification. Further there is considerable conceptual advantage to modeling flow as a series of linear pathways. The dynamics are decomposed into a fundamental form so that a physical understanding of the processes involved is facilitated.

Mathematically the pipes represent stream tubes and the complexity of the fluid flow defines the number and positioning of the pipes. For our initial models, fairly simple flow fields were chosen. More complicated and more realistic flow determined by two and three-dimensional hydrology programs is a matter for future consideration.

Under certain constraints the transport equation for dispersive flow reduces to our simple one-dimensional flow model in stream coordinates. Quite generally, transport of radionuclides in porous media is described by a diffusivity equation (Ref. 3). Hence if the concentration of nuclide r in the interstitial water is $C_r(\underline{x}, t)$ and the interstitial fluid velocity is $\underline{v}$ then

$$\frac{\partial C_r}{\partial t} = \frac{\partial}{\partial x_j} (D_{ij} \frac{\partial C_r}{\partial x_j}) - \lambda_r C_r + \sum_{i=1}^n \lambda_i C_i - \alpha_r C_r \quad (A-1)$$

Here D_{ij} is the coefficient of collective dispersion, λ_r is the radioactive decay constant, λ_i^r is the production rate of nuclide r from decay of nuclide i and α_r is the amount of α adsorbed on the solid per unit volume. This equation may be further simplified (Chapter 3) and we write, dropping the r subscript:

$$B \frac{\partial C}{\partial t} = \frac{\partial}{\partial x_j} (D_{ij} \frac{\partial C}{\partial x_j}) - \frac{\partial}{\partial x_j} (C_j C) \quad (A-2)$$

where B is the retention factor, and $C_j C$ is $C_j C_r$ divided by the amount of nuclide r from repository waste in existence at time t .

We now assume that D_{ij} reduces to a linear function of the flow velocity in the one-dimensional case (Ref. 2, 4, 5). This assumption requires some additional comment. We have implicitly assumed that flow due to diffusion is negligible when compared to dispersion. In this regime a linear relation between D_{ij} and $|v|$ is acceptable. If diffusion becomes important our equations become inapplicable. However for such a case no waste would ever have time to migrate to the biosphere.

The simplest form of D_{ij} must now be

$$D_{ij} = \frac{a_{ijim} v_i v_m}{v} \quad (A-3)$$

where $v = |v|$. (Ref. 3).

The tensor a_{ijk} is called the dispersivity tensor of the porous medium. If it is now assumed that a_{ijk} is an isotropic tensor then its most general form is

$$a_{ijk} = (\alpha - 2\mu) \frac{1}{3} \delta_{ijk} + \frac{2\mu}{3} (\delta_{ij} v_k + \delta_{ik} v_j + \delta_{jk} v_i) + \frac{2\mu}{3} (v_i v_j v_k + \text{cyclic permutations}) \quad (A-4)$$

Because of Onsager's relation (Ref. 6) D_{ij} can be postulated to be symmetric and the last term in the above equation is equal to zero. Hence

$$D_{ij} = (\alpha - 2\mu) \delta_{ij} V + \frac{2\mu v_i v_j}{V}$$

and

$$B \frac{\partial c}{\partial t} + \frac{\partial}{\partial x_i} (v_i c) = (\alpha - 2\mu) \frac{\partial}{\partial x_i} V \frac{\partial c}{\partial x_i} + 2\mu \frac{\partial}{\partial x_i} \frac{v_i v_j}{V} \frac{\partial c}{\partial x_j} \quad (A-5)$$

For steady incompressible flow $\nabla \cdot \underline{v} = 0$ and the above equation simplifies to

$$B \frac{\partial c}{\partial t} + \underline{v} \cdot \nabla c = (\alpha - 2\mu) \nabla \cdot (V \nabla c) + 2\mu (\underline{v} \cdot \nabla) \frac{1}{V} (\underline{v} \cdot \nabla) c \quad (A-6)$$

We now rewrite this equation in coordinates determined by the velocity field. The natural coordinates (S,N,T) are those where S represents the distance along a streamline in the direction of stream flow. The equation reduces to

$$B \frac{\partial c}{\partial t} + V \frac{\partial c}{\partial S} = \frac{1}{V} \frac{\partial}{\partial S} \left(\frac{\alpha - 2\mu}{h_1 h_3} (h_1 h_3 V) \frac{\partial c}{\partial S} \right) + \frac{(\alpha - 2\mu)}{h_1 h_2} \frac{\partial}{\partial T} (h_1 h_2 V) \frac{\partial c}{\partial T} \quad (A-7)$$

here h_1 , h_2 and h_3 are the scale factors. The similarity of this equation to the familiar result for $\lambda = 0$, and u constant is clear, i.e.

$$B \frac{\partial c}{\partial t} = D \left(\frac{\partial^2 c}{\partial x^2} + (b-2) \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2} \right) \quad (A-8)$$

We now wish to average Eq. A-7 across the stream tube. The area over which to integrate is determined by the rate at which the velocity and the concentration gradient drop off in the N and T directions. For example, if a source inputs an impulse at time zero into a pipe in which V is a constant then the concentration will fall off in the radial direction, r , as $\exp(-r^2/4l(b-2))$. Here l represents the distance the pulse has traveled. For a pipe 200 meters long and with $(b-2) = 10$ meters the pulse would spread about 180 meters by the time it exited the pipe.

Returning to Eq. A-7 we note that in this formulation S , N and T represent distances along coordinate axes. Hence the order of differentiation cannot in general be interchanged. Introducing coordinates (S^* , N^* , T^*) where $dS = h_1 dS^*$, $dN = h_2 dN^*$ and $dT = h_3 dT^*$ and integrating over the cross-sectional area of the pipe we have

$$\begin{aligned} B \frac{\partial}{\partial t} \iint_A c h_1 h_2 h_3 dN^* dT^* + \frac{\partial}{\partial S^*} \iint_A V c h_2 h_3 dN^* dT^* \\ = - \frac{\partial}{\partial S^*} \iint_A \frac{V}{h_1} \frac{\partial c}{\partial S^*} h_2 h_3 dN^* dT^* \end{aligned} \quad (A-9)$$

The area of the stream tube, the mean velocity and the mean concentrations can now be defined as

$$\begin{aligned}
 W &= \iint_A h_2 h_3 dN^* dT^* \\
 \bar{V} &= \iint_A V h_2 h_3 dN^* dT^* / W \\
 \bar{C} &= \iint_A V c h_2 h_3 dN^* dT^* / W \\
 \langle c \rangle &= \iint_A c h_2 h_3 dN^* dT^* / W
 \end{aligned}
 \tag{A-10}$$

If h_1 is, to first order, independent of N^* and T^* across the pipe then it may be taken outside of the integrals and we have approximately

$$B \frac{\partial^2 c}{\partial t^2} + V \frac{\partial c}{\partial S} = \alpha - V \frac{\partial^2 c}{\partial S^2}
 \tag{A-11}$$

The constraint on h_1 is equivalent to requiring the integral of the curvature across the stream to be not less than one.

There are several situations for which the averaged equation may not be a good representation of transport. Figure A-1 shows a situation where a stream tube branches into two parts. Since the concentration is averaged over the width of the stream the initial concentration in each branch is the same. In order to represent situations in which the mixing is not expected to be complete at a given node, mixing factors can be included in the program. For example, the concentration of waste entering a borehole at the repository may not be the same as the mean concentration of waste over the entire repository.

Figure A-2 illustrates a possible situation which is not currently handled by the WASTE program. Here the

majority of waste flows laterally in a layer which only partially leads to the biosphere. The upper faster-moving layer leads directly to a river or lake. Waste can migrate upwards from the lower layer due to dispersion and enter the biosphere. Since in this case the stream tube contains only of the lower layer, the amount of waste entering the river is underestimated. Furthermore since the upper layer is moving faster than the lower layer waste will reach the river more quickly. It can be seen that this situation occurs only when a large fraction of the waste in the lower layer does not go directly into the river. Therefore this mechanism for release is in general of less concern than one in which all the waste in the lower layer enter the river.

Figure A-1 Branching of a Stream Tube

Figure A-2 Dispersive Flow into a River

APPENDIX B

USE OF THE MARKOV CHAIN IN MODELING RELEASE OF HIGH LEVEL WASTE FROM AN UNDERGROUND REPOSITORY

1. OVERALL APPROACH

The primary means by which solidified radioactive waste can escape from a repository deep underground to enter the biosphere is transport in flowing groundwater. The prediction of radionuclide migration in groundwater is therefore essential to risk assessment of high level waste disposal.

Modeling of this migration in a given hydrologic setting is, in itself, not a simple problem. Moreover, the time periods during which radioactive wastes may remain dangerous are sufficiently long that the status of the repository might be altered. Such changes could be initiated as a result of creation of the repository, by subsequent human activity, or by geologic forces. Some examples of events which could affect release of radioactivity from a repository are faulting, dissolution of soluble rock and consequent collapse of the overburden, and failure of a bore-hole seal.

In a classical fault tree analysis, these events would be treated as independent failure modes. Their probabilities and consequences (as well as the probabilities and consequences of common mode failures) would be evaluated independently and summed. In the cases usually treated by this technique, severe failures lead to a cessation of normal operations until corrective action has been taken. A particular airplane can only crash once and a particular reactor core can only melt once -- such, at least, is the assumption made in fault tree analysis. The same does not hold for a waste repository. In the distant future which concerns us, there is no guarantee that men will be

able to detect and correct a failure. The risk analysis must therefore deal not only with the probabilities and consequences of individual failures, but also with multiple, sequential failures. In such cases, consequences will depend on the sequence and timing of events as well as the events themselves.

The radioactive waste hazard analysis introduces the element of time dependence into the problem. Because the nuclide in waste decay, the effects of a release will usually be lessened if the release occurs at a later time. Fault tree analyses of engineered systems, on the other hand, assume no explicit relationship between system age and the consequences of failures.

To address this complex situation, TASC has developed a model which analyzes waste repositories on two levels. A total system, composed of the repository, the waste, and the various pathways by which the waste might reach the biosphere, is described by a geologic state* and a waste distribution. The geologic state is defined by the condition of the strata in which the repository is located and of the escape pathways. For a given geologic state, the permeability and porosity of different rock layers, the velocity field of ground water, etc., will be uniquely defined. The waste distribution is a description of the concentration of radioactive waste in the repository and the different pathways at any given time.

The evolution of the waste distribution over time depends on the geologic state. The model assumes, however, that the geologic state evolves independently of changes in the waste distribution, and that the time history of the geologic state may be described as a Markov chain.

2. THE MAIN CHAIN

Any geological system is described by a large number of parameters which may, in general, either remain constant or change smoothly over time or make sudden discontinuous jumps. These geological parameters will, in turn, affect the movement of radioactive waste in rather complex ways. In the present state of geologic knowledge many of these changes can, at best, be predicted only in a probabilistic manner. In order to make the analysis of this extremely complex problem tractable, simplifying assumptions must be made.

In the approach developed by TASC, the nature of different geologic states is defined autonomously -- without reference to the location of waste. The movement of waste depends parametrically on the state of the geologic system. Unfortunately, the location of the waste at any time depends not only on the current geologic state, but also on what the geologic state was at all previous times. For example, waste will likely have moved further in a situation where an escape pathway opened just after it was emplaced and remained open t years than in a case where the same pathway has just opened t years after emplacement. In both cases the geologic state is the same -- the pathway is open.

A scenario-by-scenario study of waste transport would therefore require analysis not merely of the possible geologic states, but of the far greater number of possible histories which a repository might experience as it passes from state to state. However, this complexity can be greatly reduced by the method developed here. As shown below, one need not calculate the motion of waste for each particular history, but may instead study the transport of an aggregate quantity $\phi_r(\underline{x}; \alpha, t)$, which is defined

as the expected value of concentration of isotope r at point $\underline{x}$. Given that the system is in geologic state g , multiplied by the probability of the system being in state g . This quantity represents a sum over the various histories which could lead to state g at time t .

B.2 MATHEMATICAL DERIVATION

The derivation begins with the observation that the concentration of waste nuclides in groundwater at any point may depend on the whole history of the repository area from emplacement to the time being considered. Concentration at time t therefore depends not only on the current geologic state $g(t)$, but on the entire evolution of the geologic state from zero to t . The history of the geologic system will be denoted by h ; each value of h is an entire realization of the stochastic process whose value at time t is the random variable $g(t)$. The expected value of the concentration of any radionuclide r at point $\underline{x}$, $C_r(\underline{x};h,t)$ will be given by integrating over all histories

$$E(C_r(\underline{x},t)) = \int C_r(\underline{x};h,t) p(h) dh \quad (B-1)$$

where $p(h)$ is the probability density of history h .

We assume that waste transport is described by an equation of the form

$$\frac{\partial C_r(\underline{x};t)}{\partial t} = \lambda^{-1}(h) \left[\frac{\partial}{\partial x} (V_{10n} C_r(\underline{x};t)) + \alpha \frac{\partial^2}{\partial x^2} (C_r(\underline{x};t)) \right] - \Gamma_r C_r(\underline{x};t) \quad (B-2)$$

where, for any $\underline{x}$, $\lambda^{-1}(h)$ is an operator which operates on the spatial coordinates of C_r . Γ_s is the rate at which nuclide s decays into nuclide r . Γ_s is equal to $\ln 2$ divided by the half-life of nuclide s if nuclide r always decays into s . This assumption is consistent with the usual equation for flow of dissolved material in groundwater (Ref. 3), which in one dimension takes the form

$$\frac{\partial C_r}{\partial t} = \left[-V_{10n} \frac{\partial}{\partial x} + \alpha \frac{\partial^2}{\partial x^2} - \Gamma_r \right] C_r \quad (B-3)$$

where V_{10n} is the advection velocity of the ions, α is the dispersion constant and Γ_r is the decay rate of nuclide r .

We wish to obtain an equation for waste transport which does not involve the history h , but only the current state g . In order to do so, we define a quantity ϕ_r by integrating over all histories h which reach state g at time t

$$\phi_r(\underline{x};g,t) = \int_{\Omega: \{h(t)=g\}} C_r(\underline{x};h,t) p(h) dh \quad (B-4)$$

The integral is over all realizations h of the random process which take the value g at time t . In subsequent equations this integration will be understood and the $\int$ and brackets will

be omitted. ϕ_r may be interpreted physically as the expected value of concentration of nuclide r at point $\underline{x}$ given that the system is in state g , multiplied by the probability that the system is in g . By comparing Eq. B-4 and Eq. B-1, it is seen that expected concentrations may be calculated from the relationship.

$$E(C_r(\underline{x}, t)) = \sum_g \phi_r(\underline{x}; g, t) \quad (B-5)$$

In order for this definition to be useful, we must derive an equation for the evolution of ϕ_r which does not depend on h . We begin by taking the time derivative of Eq. B-4. In order to deal with the summation over histories, we must explicitly use the definition of the derivative.

$$\begin{aligned} \frac{\partial}{\partial t} \phi_r(\underline{x}; g, t) &= \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left\{ \int_{h(t+\Delta t)=g} C_r(\underline{x}; h, t+\Delta t) p(h) dh \right. \\ &\quad \left. - \int_{h(t)=g} C_r(\underline{x}; h, t) p(h) dh \right\} \end{aligned} \quad (B-6)$$

In order to separate out the time dependence of C_r , we add and subtract identical terms.

$$\begin{aligned} \frac{\partial}{\partial t} \phi_r(\underline{x}; g, t) &= \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left\{ \int_{h(t+\Delta t)=g} C_r(\underline{x}; h, t+\Delta t) p(h) dh \right. \\ &\quad - \int_{h(t+\Delta t)=g} C_r(\underline{x}; h, t) p(h) dh + \int_{h(t+\Delta t)=g} C_r(\underline{x}; h, t) p(h) dh \\ &\quad \left. - \int_{h(t)=g} C_r(\underline{x}; h, t) p(h) dh \right\} \end{aligned} \quad (B-7)$$

The first two terms are integrals over the same range of values of h and thus can be combined and simplified by using Eq. B-2.

$$\begin{aligned}
& \lim_{\Delta t \rightarrow 0} \int_{h(t+\Delta t)=g} p(h) \frac{C_r(\underline{x}; h, t+\Delta t) - C_r(\underline{x}; h, t)}{\Delta t} dh \\
&= \int_{h(t)=g} p(h) \frac{\partial}{\partial t} C_r(\underline{x}; h, t) dh \\
&= \int_{h(t)=g} p(h) L^{(h)} C_r(\underline{x}; h, t) dh \\
&+ \sum_{s \neq r} p(h) \Gamma_s^r C_s(\underline{x}; h, t) dh \quad (B-8)
\end{aligned}$$

In order to simplify the two remaining terms of Eq. B-7, we must assume the range of possible states g is countable. Canceling terms which appear in both integrals, we then obtain

$$\begin{aligned}
& \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left\{ \int_{\substack{h(t+\Delta t)=g \\ \text{and } h(t) \neq g}} C_r(\underline{x}; h, t) p(h) dh \right. \\
& \quad \left. - \int_{\substack{h(t)=g \text{ and} \\ h(t+\Delta t) \neq g}} C_r(\underline{x}; h, t) p(h) dh \right\} \\
&= \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left\{ \sum_{g' \neq g} \int_{\substack{h(t+\Delta t)=g \\ \text{and } h(t)=g'}} C_r(\underline{x}; h, t) p(h) dh \right. \\
& \quad \left. - \sum_{g' \neq g} \int_{\substack{h(t)=g \text{ and} \\ h(t+\Delta t)=g'}} C_r(\underline{x}; h, t) p(h) dh \right\} \quad (B-9)
\end{aligned}$$

In order to proceed further, we must examine more closely the role of h . The variable h represents the geologic history over the entire time period of concern in the analysis. We define two partial histories, e and f , as the histories from time zero through times t and $t+\Delta t$ respectively. If each value of h is thought of as a sequence of states, each value

of e or f will be a shorter sequence. Each sequence e or f will be included in many different h 's. Different partial histories f which are identical through time t and then reach different states at time $t+\Delta t$ will all include the same partial history e .

Now, it is reasonable to assume causality; i.e., that the concentration of waste at a given time will depend only on the previous geologic states of the system and not on what happens at subsequent times. For all histories h which include the same partial history f , $C_r(\underline{x};h,t)$ are then identical. All the terms in Eq. B-8 which correspond to the same f can be grouped together, and the right hand side of that equation can be written as:

$$\lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left\{ \sum_{g' \neq g} \int_{S_{g',g}} C_r(\underline{x};f,t) p(f) df \right. \\ \left. - \sum_{g' \neq g} \int_{S_{gg'}} C_r(\underline{x};f,t) p(f) df \right\}$$

We have denoted the space of partial histories f which pass through state a at time t and through b at time $t+\Delta t$ as S_{ab} . The membership of S_{ab} will, of course, change when the value of Δt is varied.

Each space S_{ab} may be partitioned into subspaces S_{ab}^e . Each subspace S_{ab}^e is composed of all those partial histories f which follow a particular partial history e from time zero to t , at which time they have reached state a , and then reach state b at time $t+\Delta t$. Since S_{ab} is equal to the union of all the S_{ab}^e corresponding to e which reach state a at time t , we may rewrite our integrals to obtain

$$\lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left\{ \sum_{g' \neq g} \int_{e(t)=g'} de \int_{S_{g'g}^e} df C_r(\underline{x}; f, t) p(f) \right. \\ \left. - \sum_{g' \neq g} \int_{e(t)=g} de \int_{S_{gg'}^e} df C_r(\underline{x}; f, t) p(f) \right\}$$

We now invoke causality again to make concentration C_r at time t a function only of e and not of f . Since only the integral over f depends on Δt , the order of operations can be altered to obtain

$$\sum_{g' \neq g} \int_{e(t)=g'} de C_r(\underline{x}; e, t) \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \int_{S_{g'g}^e} p(f) df \\ - \sum_{g' \neq g} \int_{e(t)=g} de C_r(\underline{x}; e, t) \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \int_{S_{gg'}^e} p(f) df$$

Now the integral of $p(f)$ over S_{ab}^e is simply $p(e)$ multiplied by the conditional probability $P(b, t+\Delta t | e)$ that the system, having experienced partial history e and having reached state a at time t , will reach state b at time $t+\Delta t$. We therefore have

$$\sum_{g' \neq g} \int_{e(t)=g'} de C_r(\underline{x}; e, t) p(e) \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} P(g, t+\Delta t | e) \\ - \sum_{g' \neq g} \int_{e(t)=g} de C_r(\underline{x}; e, t) p(e) \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} P(g', t+\Delta t | e)$$

We may now define the transition rate from a to b, λ_{ba} , by

$$\lambda_{ba}(e) = \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} P(b, t + \Delta t) | a, t; e \quad (B-10)$$

In this definition the transition rate has been written so as to show that it may be a function of past history e ; in what follows we will not explicitly show this dependence. In the cases we are considering, the value of e at time t is defined by the restrictions on the integrals over e , and so we can substitute the definition directly to obtain

$$\begin{aligned} & \sum_{g' \neq g} \int_{e(t)=g'} C_r(\underline{x}; e, t) p(e) \lambda_{gs} de \\ & - \sum_{g' \neq g} \int_{e(t)=g} C_r(\underline{x}; e, t) p(e) \lambda_{g'g} de \end{aligned}$$

In order to restore simplicity of notation, the integrals over e may be expanded back into integrals over h . Substituting into Eq. 6 the values we have obtained for its terms, a formula for the derivative of ϕ_r is obtained.

$$\begin{aligned} \frac{\partial}{\partial t} \phi_r(\underline{x}; g, t) &= \int_{h(t)=g} p(h) L^{(h)} C_r(\underline{x}; h, t) dh \\ &+ \sum_{g' \neq g} \int_{h(t)=g'} \lambda_{gg'} p(h) C_r(\underline{x}; h, t) dh \\ &- \sum_{g' \neq g} \int_{h(t)=g} \lambda_{g'g} p(h) C_r(\underline{x}; h, t) dh \\ &+ \sum_{s \neq r} \int_{h(t)=g} \Gamma_s^r p(h) C_s(\underline{x}; h, t) dh \quad (B-11) \end{aligned}$$

The first term in this equation represents the flow through space and decay of radionuclide r . The second term represents the increase in ϕ_r due to transitions into g from other states, and the third term represents transitions out of state g . The fourth term describes the creation of nuclide r by the decay of parent nuclides.

We now make two assumptions about the transport operator L : that L depends only on g and not on h , and that it operates linearly on C_r . We may then move it outside the integral so that

$$\begin{aligned} & \int_{h(t)=g} p(h) L^{(h)} C_r(\underline{x};h,t) dh \\ &= L^{(g)} \int_{h(t)=g} p(h) C_r(\underline{x};h,t) dh \\ &= L^{(g)} C_r(\underline{x};g,t) \end{aligned} \quad (B-12)$$

We assume further that the system described by the geologic states is a Markov process. The transition rates λ will now be independent of the past history. They, like the decay rates Γ , also may be moved outside the sum. Eq. B-11 for the evolution of ϕ_r reduces to

$$\begin{aligned} \frac{\partial}{\partial t} \phi_r(\underline{x};g,t) &= L^{(g)} \phi_r(\underline{x};g,t) \\ &+ \sum_{g' \neq g} \lambda_{gg'} \phi_r(\underline{x};g',t) - \sum_{g' \neq g} \lambda_{g'g} \phi_r(\underline{x};g,t) \\ &+ \sum_{s \neq r} \Gamma_s^r \phi_s(\underline{x};g,t) \end{aligned} \quad (B-13)$$

Equation B-13 involves only the current state g and may be solved for the ϕ_r ; Eq. B-5 may then be used to calculate expected values of concentration.

With this result, one need not calculate the motion of waste for each history, but may instead solve for the quantities $\phi_r(\underline{x};g,t)$, which were defined as the expected value of concentration of radionuclide r at point $\underline{x}$, given that the system is in geologic state g , multiplied by the probability of the system being in state g . These quantities represent an aggregation of the various histories which could lead to state g at time t . It is not necessary to solve an infinite number of partial differential equations corresponding to an infinity of possible histories. Instead one need solve a system of as many equations as there are geologic states and radionuclides.

B.3 DISCUSSION

The principal assumptions made in the above derivation are as follows:

- The operator describing motion of waste must depend only on the current geologic state and not on past geologic states
- The operator describing waste motion in any given state must be linear in waste concentration
- The transition rates between geologic states cannot depend on the past history of the system
- The geologic system is restricted to a countable set of states.

The first two of these assumptions restrict waste transport to flows which can be described by linear instantaneous operators. These assumptions are satisfied by the most commonly used transport equation, as described above in the discussion of Eq. B-3.

The other two assumptions govern the geologic states. They require that the system of geologic states form a Markov chain. Whether this requirement is satisfied depends on the particular set of states used in a model.

APPENDIX C
FORMULAS USED TO CALCULATE G

As shown in Section 3.2, the fraction of waste entering a pipe at time τ which leaves the pipe between $\tau + t$ and $\tau + t + \Delta t$ is given by

$$G = g(t + \Delta t) - g(t) \quad (C-1)$$

where $g(t)$ represents the fraction of waste which passes through the pipe in less time than t . The formula for g derived in Section 3.2 is

$$g_A(t) = \frac{1}{2} \left[\operatorname{erfc}(\phi_-(t)) - e^{z^2/a} \operatorname{erfc}(\phi_+(t)) \right] \quad (C-2)$$

where

$$\phi_{\pm}(t) = \frac{z \pm \frac{v}{B} t}{\sqrt{4a \frac{v}{B} t}} \quad (C-3)$$

A number of numerical problems can arise if Eqs. C-1 and C-2 are used directly to calculate G . These problems may be resolved by judicious use of the asymptotic expansion of the complementary error function

$$\operatorname{erfc}(u) \xrightarrow{u \rightarrow \infty} \frac{e^{-u^2}}{\sqrt{\pi} u} \left(1 - \frac{1}{2u^2} + \frac{3}{4u^4} - \dots \right) \quad (C-4)$$

This expansion possesses the useful property that the error is always less than the first excluded term.

Consider first the case $z/a \gg 1$. If z/a is sufficiently large, the exponentiation in Eq. C-2 will yield a number that exceeds the machine's storage capacity. (The actual criterion used is $z/a > 144$). By expanding $\text{erfc}(\phi_+(t))$, we obtain

$$g_B(t) = \frac{1}{2} \left[\text{erfc}(\phi_-(t)) - \frac{e^{-\phi_-^2(t)}}{\sqrt{\pi} \phi_+(t)} \right] \quad (C-5)$$

The fractional error introduced by dropping terms of order ϵ_+^{-2} and higher will always be less than $a/2z$.

Roundoff errors can occur in the subtraction operation of either Eq. C-2 or Eq. C-5. Both complementary error functions must then be expanded and large terms occurring in both expansions canceled. The formula which results is

$$g_C(t) = \frac{e^{-\phi_-^2(t)}}{\sqrt{4\pi a B/(Vt)}} \frac{1}{\phi_+(t) \phi_-(t)} \times \left[1 - \frac{1}{2} \left(\frac{1}{\phi_+^2(t)} + \frac{1}{\phi_+(t)\phi_-(t)} + \frac{1}{\phi_-^2(t)} \right) \right] \quad (C-6)$$

Round off errors will exceed 1% when the computer calculates using six-digit numbers and

$$\frac{g(t)}{\text{erfc} \phi_-(t)} < 10^{-5}$$

When Eqs. C-4 and C-6 are substituted into this relation, one finds

$$\frac{1}{1 + \frac{2B}{Vt}} \left[\frac{1 - \frac{1}{2} \phi_+^{-2}(t) + \phi_+^{-1}(t) \phi_-^{-1}(t) + \phi_-^{-2}(t) + \dots}{1 - \frac{1}{2} \phi_-^{-2}(t) + \dots} \right] < 10^{-5}$$

Finally, we have the case discussed in Section 3.3 when the dispersion time $\frac{B}{V} \sqrt{4\alpha z}$ is much less than the time interval $T(l+1) - T(l)$. In this case, G is calculated ignoring dispersion altogether, but taking account of the width of the input pulse. The formulas used are:

where $T(l') + T_f < T(l)$ and $T(l'+1) + T_f > T(l)$:

$$G(l', l) = \frac{T(l'+1) + T_f - T(l)}{T(l'+1) - T(l')}$$

$$G(l', l-1) = 1 - G(l', l)$$

where $T(l') + T_f > T(l)$ and $T(l'+1) + T_f < T(l+1)$:

$$G(l', l) = 1$$

otherwise $G = 0$

These formulas are used whenever, from an impulse input into the pipe, 95% of the output will emerge during a single time interval. This will occur when the time interval is longer than four times the variance of the Gaussian output pulse i.e., when

$$4 \frac{B}{V} \sqrt{2\alpha z} > T(l+1) - T(l)$$

However, dispersion cannot be neglected when the input pulse is narrower than the Green's function. For that reason, these formulas are not used when

$$\frac{F(l', m', n')}{F(l'+1, m', n')} < 0.05$$

or

$$\frac{F(l'+1, m', n')}{F(l', m', n')} < 0.05$$

As long as $\phi_-(t) > 1$, this can only be satisfied when $Vt/zB \geq 10^{-5}$. For $z \geq \alpha$, this implies $\phi_+ \geq 10^2$ and the error in Eq. C-6 due to dropping additional terms will be much less than 1%.

For large times when $Vt/Bz \gg 1$, on the other hand round-off errors can arise in Eq. C-1. To deal with this, we rewrite Eq. 3.2-6 as follows.

$$\begin{aligned} G &= g_A(T(l+1)-\tau) - g_A(T(l)-\tau) \\ &= \frac{1}{2} \left\{ \operatorname{erfc}(\phi_-(T(l+1)-\tau)) - \operatorname{erfc}(\phi_-(T(l)-\tau)) \right. \\ &\quad \left. + e^{z/\alpha} [\operatorname{erfc}(\phi_+(T(l)-\tau)) - \operatorname{erfc}(\phi_+(T(l+1)-\tau))] \right\} \\ &= g'_A(T(l+1)-\tau) - g'_A(T(l)-\tau) \end{aligned}$$

where

$$g'_A(t) = \frac{1}{2} [-\operatorname{erfc}(-\phi_-(t)) - e^{z/\alpha} \operatorname{erfc}(\phi_+(t))]$$

In the limit $\frac{Vt}{zB} \rightarrow \infty$, one has $\phi_- \rightarrow -\infty$ and $\phi_+ \rightarrow +\infty$, and use of the asymptotic expansion yields Eq. C-6 as the formula for $g'_A(t)$. This formula is used when

$$\frac{G}{g_A(T(l)-\tau)} < 10^{-5}$$

and its precision will be governed by considerations similar to those of the preceding case

When $l=l'$, this problem cannot arise because the subtraction of Eq. C-1 is not carried out. Eq. C-2 or C-5 is then used as appropriate.

The different cases discussed in this appendix, their defining conditions, and the formulas used in them, are summarized in Table C-1.

TABLE C-1
FORMULAS FOR G

CASE NO.	CONDITIONS	FORMULA
0.1	$l = 1'$ $z/a < 144$ not Case 5	$G = E_A(T(l'-1) - T(l'))$
0.2	$l = 1'$ $z/a \geq 144$ not Case 5	$G = E_B(T(l'-1) - T(l'))$
1	$l = 1'$ $E_A(T(l'-1) - T(l')) \geq 1$ $\frac{E_A(T(l'-1) - T(l'))}{E_C(T(l'-1) - T(l'))} < 10^{-2}$ not Case 5	$G = E_C(T(l'-1) - T(l'))$ $- E_C(T(l') - T(l'-1))$
2	$l = 1'$ $E_C(T(l') - T(l'-1)) < -2$ $\frac{G}{E_A(T(l') - T(l'-1))} < 10^{-2}$ not Case 5	$G = E_C(T(l'-1) - T(l'))$ $- E_C(T(l') - T(l'-1))$
3	$l = 1'$ $z/a \geq 144$ not Cases 1, 2, or 5	$G = E_B(T(l'-1) - T(l'))$ $- E_B(T(l') - T(l'-1))$
4	$l = 1'$ $z/a < 144$ not Cases 1, 2, or 5	$G = E_A(T(l'-1) - T(l'))$ $- E_A(T(l') - T(l'-1))$
5.1	$4 \frac{E}{\sqrt{2a\pi}} < T(l_{opt}') - T(l_{opt}-1)$	$G(l_{opt}-1, l_{opt}-2) = \frac{T(l_{opt}-1) - T(l') - T_2}{T(l_{opt}-1) - T(l')}$ $G(l_{opt}-1, l_{opt}-1) = \frac{T(l_{opt}-1) - T_2 - T(l_{opt}-2)}{T(l_{opt}-1) - T(l')}$
5.2	$\frac{F(l'+1, m', n')}{F(l', m', n')} > 0.05$ $\frac{F(l'+1, m', n')}{F(l'+1, m', n')} > 0.05$	$G(l_{opt}', l_{opt}') = \frac{T(l_{opt}-1) - T_2 - T(l_{opt}')}{T(l_{opt}-1) - T(l')}$ $G(l_{opt}', l_{opt}-1) = \frac{T(l_{opt}') - T(l_{opt}-1) - T_2}{T(l_{opt}-1) - T(l')}$
5.5	$T_1 + T_2 > T(l_{opt}-1)$ $T(l_{opt}-1) - T_2 < T(l_{opt}')$	$G(l_{opt}-1, l_{opt}-1) = 1$

$\epsilon_{\pm}$, E_A , E_B , E_C , T_f and l_{opt} are defined on the next page.

In this table:

$$g_A(t) = \frac{1}{2} \left[\operatorname{erfc} \phi_-(t) - e^{z/a} \operatorname{erfc} \phi_+(t) \right]$$

$$g_B(t) = \frac{1}{2} \left[\operatorname{erfc} \phi_-(t) - \frac{e^{-\phi_-^2(t)}}{\sqrt{\pi} \phi_+(t)} \right]$$

$$g_C(t) = \frac{e^{-\phi_-^2(t)}}{\sqrt{\frac{4\pi a B}{Vt}} \phi_+(t) \phi_-(t)} \left[1 - \frac{1}{2} \left(\frac{1}{\phi_+^2(t)} + \frac{1}{\phi_+(t)\phi_-(t)} + \frac{1}{\phi_-^2(t)} \right) \right]$$

$$\phi_{\pm}(t) = \frac{z \pm \frac{V}{B} t}{\sqrt{4a \frac{V}{B} t}}$$

and k_{opt} is defined by $T(k_{\text{opt}}-1) < T(k) + T_f \leq T(k_{\text{opt}})$

where $T_f = \frac{zB}{V}$

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APPENDIX 3.3

RADIOLOGICAL RISK - DOSE CONVERSION FACTORS

TASC has evaluated the impact of the long-term contamination of surface waters including the dosages from ingestion of water, aquatic foods, and products from irrigated fields, and from exposures while at the shoreline and while immersed in water. They have extended the analysis described in Appendix C of LLL-NUREG-1002 Draft (October 29, 1977) and developed a steady-state model for river, estuary and ocean sources. They have adopted the dose-conversion constants of Appendix F of BNWL-1927 (H. C. Burkholder, M. D. Cloninger, D. A. Baker, and G. Jansen, Incentives for Partitioning High-Level Waste, Battelle Pacific Northwest Laboratories, Report BNWL-1927, 1975) which are one-year dose commitments from a single 50-year dose commitments for chronic ingestion. The effective half lives for calculation of the 50-year dose accumulation factors were supplied by Joe K. Soldat, Battelle Pacific Northwest Laboratories. These one-year dose commitments and effective half-lives are evidently those represented in the HERMES computer code, which has been used in the Year 2000 Studies of the Upper Mississippi River Basin and the Tennessee River Valley. In contrast to the internal dosages for inhalation and deposition, which have been computed as the critical organ and whole body (and whole body equivalent) dose, the internal dose for each pathway leading from contaminated surface water has been computed for each of eight organs.

It is reasonable not to require a common source for the dose conversion factors. Frank Congel and Keith Eckerman of the Radiological Assessment Branch of NRC state that NRC commonly develops its regulatory guides with dose

conversion factors from more than one source. On the other hand, it seems desirable that there be uniformity in the reporting of internal dosages and that the dosages for the same organs be evaluated for the different modes of internal exposure. This practice lends itself to a straightforward summing of the doses for a given organ and minimizes the likelihood of overlooking a potentially significant contribution to the dose.

Certain options in the reporting of dose are available that seem reasonable and that are compatible with the goal of adequately reporting the results of the SSC assessment:

I. Present plan:

Surface waters: uses NUREG data for drinking water, shoreline and swimming pathways; considers 8 organs and uses BNWL-based (chronic) dose factors for ingestion of foods.

Possible modifications in present plan:

Use BNWL-based (acute) ingestion dose factors in place of those derived by Y. Ng. (All the ingestion dose factors will then have a common basis that is compatible with NUREG guides.)

Exclude or reevaluate the whole body equivalent dose (see discussion in Section 2).

Sum the critical organ doses for each nuclide without regard to organ identity.

II. Alternative to present plan:

Surface waters: Follow present scheme

Comments:

Use of BNWL-based ingestion dose factors throughout facilitates documentation and renders the dosimetry compatible with NUREG guides.

Consideration of each of eight reference organs rather than just the critical organ and the whole-body is a more rigorous approach to dosimetry.

In case the dose to an organ can't be estimated because retention data are lacking, assign the whole-body dose to that organ.

The final reporting of dose estimates may be simplified by using the appropriate whole-body equivalent dose in summing the organ doses for each nuclide by each pathway.

2. Derivation and Proposed Use of the Whole-Body Equivalent Dose

The concept of the whole-body equivalent dose has been developed to facilitate assessment of the biological impacts from internal exposures to radionuclides following release to the environment (Appendix B, LLL-NUREG-1002 Draft, October 29, 1977). The whole-body equivalent dose can be regarded as the whole-body dose that is associated with the same biological risk as a given dose to a specified organ, which may be the "critical" organ. In the initial formulation the whole-body-equivalent dose-conversion factor was derived as the

critical-organ dose-conversion factor times the ratio of the annual dose limit for the whole body and the annual dose limit for the critical organ (see Appendix B, LLL-NUREG-7002 Draft, October 29, 1977). The intention has been to derive a weighting factor such that one can estimate the whole-body dosage that would result in the same biological risk as given dose to the critical organ. In this initial formulation, it is tacitly assumed that the annual dose limits that have been established for various organs are inversely proportional to the risk per unit dose. Reporting of organ doses in terms of the whole-body or whole-body equivalent dose could simplify the assessment of risk if one could justify reporting only one kind of dose rather than separate doses to various organs.

An alternative formulation of the whole body equivalent dose is based on BEIR Committee estimates of the risk of excess deaths from cancer in the U. S. population from exposure to ionizing radiation (NAS-NRC Advisory Committee on the Biological Effects of Ionizing Radiations, The Effects on Populations of Exposure to Low Levels of Ionizing Radiation, National Academy of Science, National Research Council, Washington, D.C., 1972). If one accepts the cancer risk factors derived by Strom and Watson from the BEIR Committee Report (P. O. Strom and E. C. Watson, "Calculated Doses from Inhaled Transuranium Radionuclides and Potential Risk Equivalence to Whole-Body Radiation," in Transuranium Nuclides in the Environment, pp. 603-626, IAEA, Vienna, 1976), which are shown in Table A-1 of the attached sheet. The whole body equivalent of a 1-rem dose to the kidneys would be

$$\frac{5 \times 10^{-7}}{2.5 \times 10^{-6}} = 0.2 \text{ rem.}$$

APPENDIX

EQUIVALENT RISK MODEL

A method has been developed to estimate the intake in microcuries (via inhalation) to yield the same risk of cancer as one rem to the whole body. The resulting values are referred to as "intake equivalents" (I_e). For a given set of exposure conditions the intake equivalent is calculated as

$$I_e = \frac{R_{WB}}{\sum R_i D_i}$$

where I_e is intake equivalent to yield same risk of cancer as one rem of whole-body dose ($\mu\text{Ci/rem}$)

R_{WB} is whole-body cancer risk factor (deaths/a/rem)

R_i is cancer risk factor for organ i (deaths/a/rem)

D_i is dose to organ i per μCi intake (rem/ μCi)

The above method has been used to calculate intake equivalents for a large number of radionuclides. The computer program DACRIN (6) can be used to calculate the organ dose factors, D_i , as a function of exposure conditions. These factors are then used to calculate the corresponding intake equivalents. The organs considered and the assumed risk factors are listed in Table A1.

TABLE A1. CANCER RISK FACTORS

Organ of reference	Cancer risk factor (deaths/a/rem)
Whole body	2.5×10^{-4}
Kidneys	5.0×10^{-7}
Liver	5.0×10^{-7}
Stomach	2.0×10^{-7}
Lungs	2.5×10^{-4}
GI tract ^a	1.0×10^{-6}

^a Calculated as the sum of the dose to each of the four compartments.

In actual fact, an exposure that results in a given internal dose to a "critical" organ, will deliver a dose to other organs besides. Let us assume that an exposure that leads to an internal kidney dose of 1 rem also results in liver and bone doses of 0.2 rem each. The whole body equivalent of a 1-rem dose to the kidneys would be (see Table A-1)

$$\frac{5 \times 10^{-7} + (0.2) (5 \times 10^{-7}) + (0.2) (2 \times 10^{-7})}{2.5 \times 10^{-6}} = 0.26$$

The 0.2 rem first calculated for the whole-body equivalent dose would underestimate the whole-body dose that is associated with the same risk as 1 rem to the kidneys. Estimation of the whole-body dose based solely on the dose to the critical organ is meaningful only if the critical organs stand alone, i.e., if the critical organ is the only organ in the body that is irradiated.

The simple exercise above demonstrates clearly that a complete and meaningful evaluation of the whole body equivalent dose for a nuclide requires estimates of the doses delivered to each of the organs in the body. To be sure, in many instances an estimate of the whole-body equivalent dose that is based on one or relatively few organs will not grossly underestimate the true whole-body equivalent dose.

In the case of the TASC internal dose estimates for atmospheric sources, a sound approach would be to make dose estimates for the same organs considered for surface-water sources. The whole-body equivalent dose for each nuclide can then be computed taking into account all the organs irradiated. Final summation over nuclides and pathways would yield a single dose estimate

expressed in terms of the whole-body equivalent dose. In this manner relatively few tables would be needed to effectively summarize the results of the study.

Appendix 3.41- Data Base Refinement/Geochemistry
Interdepartmental Letterhead

W. Stewart 224

EL 4124

EG 77-9

MEMORANDUM - July 20, 1977

TO: Don Towse and Dick Heckman

FROM: Dana Isherwood

I. Solubility Controls on Radionuclide Concentrations

A number of the biologically important radionuclides have maximum groundwater concentrations at node 1 (i.e., leaving the repository) which exceed their theoretical solubility (Table 1). I'd originally thought that we could adjust the concentrations at node 1 to reflect the low solubilities, thus decreasing the population dose. This may still be true for the actinides; however, recent data show that concentrations in natural waters (at least for Zr, Sn, and Th) commonly exceed their solubility limits (Table 2). For example, the solubility of Sn at pH 6.8 (a common value for fresh water) is 4×10^{-18} M. Yet, the values given for the Saale River in Germany are 2×10^{-9} M. No doubt, the major cause for the differences is the formation of soluble organic or inorganic complexes. Until we can identify the actual species likely to exist in natural water systems, solubility limits as a way to control radionuclide concentrations should be used with caution.

II. Effect of Delayed Dissolution

The amount of ^{226}Ra and ^{229}Th present in the waste increases with time. Therefore, the maximum concentration of these nuclides in the groundwater depends on the time dissolution takes place. We can study the effect of delayed dissolution by comparing TASC's maximum concentrations where dissolution begins at 100 years to maximum concentrations that might occur if dissolution took place at some later time when ^{226}Ra or ^{229}Th is present in the greatest amount (i.e., 10^5 and 10^6 years).

1. If dissolution begins at 100 years, the maximum concentration of ^{226}Ra ($4 \times 10^{-5} \frac{\text{Ci}}{\text{m}^3}$) is reached at 11,700 years. If dissolution is delayed for 100,000 years, the maximum concentration is $9 \times 10^{-4} \frac{\text{Ci}}{\text{m}^3}$. This represents only a 20-fold increase.

EG 77-9
7-20-77
Page 2

2. If dissolution begins at 100 years, the maximum concentration of ^{229}Th ($9 \times 10^{-5} \frac{\text{Ci}}{\text{m}^3}$) is reached at 14,400 years. If dissolution is delayed for a million years, the maximum concentration is $1 \times 10^{-2} \frac{\text{Ci}}{\text{m}^3}$. Considering the high retardation factor predicted for Th, even this 100-fold increase is probably not important.

1000

DJl:ky
Attachments

TABLE 1

RADIONUCLIDE CONCENTRATIONS EXCEEDING SOLUBILITY

	MPC _w ($\frac{\text{Ci}}{\text{m}^3}$)	Groundwater* ($\frac{\text{Ci}}{\text{m}^3}$)	Solubility** ($\frac{\text{Ci}}{\text{m}^3}$)
^{126}Sn	2×10^{-5}	2×10^{-2}	4×10^{-12}
^{229}Th	7×10^{-6}	9×10^{-5}	1×10^{-8}
^{239}Pu	3×10^{-10}	8×10^{-2}	1×10^{-7}
^{240}Pu	9×10^{-11}	3×10^{-1}	5×10^{-7}
^{241}Am	5×10^{-12}	6.6	4.5
^{243}Am	8×10^{-11}	6×10^{-1}	3×10^{-1}

* Maximum groundwater concentration at node 1 (i.e., leaving a repository of 6×10^6 MWeyr)

** Maximum theoretical solubility in groundwater (pH = 5-8, Eh=0)

TABLE 2

COMPARISON OF THEORETICAL SOLUBILITY AND
CONCENTRATIONS IN NATURAL WATERS

	Solubility (M) (pH = 8.15)	Sea Water (M)	Solubility (M) (pH = 6.8)	Fresh Water (M)
Sn	2×10^{-15}	8×10^{-9} (1)	4×10^{-18}	2×10^{-9} (2)
Th	7×10^{-26}	2×10^{-8} (3)	2×10^{-20}	?

1. Heide and Reichardt, 1975
2. Hamabuchi, et al., 1964
3. Bernat and Goldberg, 1969

May 16, 1977

Mr. Ben Ross
The Analytic Sciences Corp.
6 Jacob Way
Reading, Massachusetts 01867

Dear Ben:

The following are revised parameter values for second cycle.

1. Transition rates.

Rate of faulting ($\text{yr}^{-1}\text{km}^{-2}$)Minimum: 10^{-10} Preferred: 10^{-7} Maximum: 10^{-5}

(Minimum value has been reduced 3 orders of magnitude to include well-selected sites. Values need to be multiplied by area of the repository being considered.)

Variation with time: None.

2. Sorbtion factors.

Iodine: Minimum, Preferred, Maximum: all 1.

Other Fission products: Minimum: 1; Preferred: 10^2 ; Maximum: 10^3
(Maximum increased one order of magnitude to cover some good sorbtion materials.)

Actinides in fresh water: Minimum: 10^3 ; Preferred: 10^4 ; Maximum: 10^5
(Maximum increased one order of magnitude to include Thorium and to simulate very low solubilities.)

Actinides in saline water: Minimum: 1; Preferred: 10^2 ; Maximum: 10^3

(No change.)

3. Dispersion constant: 10, 50, 100 m. (No change.)

4. Waste Dissolution Time: $10, 10^4, 10^4$ yr. (No change.)

Mr. Ben Ross

May 16, 1977

5. Thickness of repository layer: 26,200,1000 m. (No change.)
6. Thickness of barrier layer: 20,200,1000 m. (No change.)
7. Distance to aquifer discharge: $1.6 \times 10^3, 1.6 \times 10^4, 8 \times 10^4$ m. (No change.)

Variation (uncertainties) with time

We may assume initially that proper in situ values of these parameters are known to an accuracy of $\pm 10\%$. In most geologic systems these are not expected to vary beyond 10% for 10^4 years. From that point on natural processes may cause changes. For items #2 through #7, above, I show an estimate of the possible change (uncertainty) from the initial value at 10^6 years. I would vary this linearly from 10^4 years, in the absence of any better information.

Variation at 10^6 years

#2 Sorbtion factor:	$\pm$ order-of-magnitude
#3 Dispersion constant:	$\pm$ percent
#4 Waste dissolution time:	—
#5, #6 Thicknesses:	No change without major event
#7 Distance to Discharge:	No change without major event

Sincerely,

Don

Don Towse

DT:ky

cc: Peter Davies (GEI)
 Bob Plum (Golder)
 Dick Heckman
 Tom Holdsworth
 Dana Isherwood

A.B.41

LAWRENCE LIVERMORE LABORATORY

May 31, 1977

Mr. Ben Ross
The Analytic Sciences Corp.
6 Jacob Way
Reading, Massachusetts 01867

Dear Ben,

Regarding retardation factors for the 2nd cycle; Don and I would like you to disregard our previous instructions of May 16th and use the following values:

Shale Repository

	<u>Minimum</u>	<u>Preferred</u>	<u>Maximum</u>
Iodine and Technetium	1	10^2	10^3
Other Fission Products	10^2	10^4	10^5
Actinides			

Salt Repository

Iodine and Technetium	1	1	1
Other Fission Products			
Salt Repository and barrier bed:	1	10^2	10^3
Aquifer:	1	10^2	10^3
Actinides			
Salt Repository and barrier bed:	10^2	10^4	10^5
Aquifer:	10^2	10^4	10^5

Uncertainties with time for retardation factors will remain the same (i.e., $\pm$ order of magnitude).

Sincerely,

Alana

Gina Isherwood
K Division L-227

cc: Peter Davies (GEI)
Bob Plum (Golder)
Dick Beckman
Tom Holdsworth
Don Towse

MEMO: REVISED HYDROLOGIC PARAMETERS
TASC BASIC MODEL - SECOND GENERATION
SHALE AND SALT REPOSITORY

TO: TASC LLL DATE: May 31, 1977
Attention: B. Ross ATTN: D. JOB NO.: S77300
TOWSE

1. General: This information relates to the basic six-layer model with layers 2 and 6 being a sandstone aquifer; layers 3 and 5 being a sandstone, siltstone, shale sequence; and layer 4 either shale or salt. Layer 6 is under a greater hydraulic head than layer 2; thus, water flows from layer 6 up through layers 5, 4, 3 to layer 2. The water in layer 2 then flows horizontally to a lake or river. This model is identical to the first generation model. Although useful in indicating trends, in our opinion it does not adequately reflect realistic geologic or hydrologic conditions. We understand that the third generation model will represent more realistic conditions.

2. Formation, Permeability and Porosity: It is not feasible to generalize for a generic model whether groundwater flow will be through fractures, interstitial pore space or both. Thus, the model should be run with two sets of values for layers 3, 4, 5. Parameters for layer 4 applies only to shale; salt data is provided by Geotechnical Engineers.

a. Values for Interstitial Flow

Layer	Horizontal Permeability (cm/sec)		Porosity	
	Preferred	Range	Preferred	Range
2	10^{-4}	10^{-2} to 10^{-6}	0.10	0.02-0.20
3	10^{-6}	10^{-4} to 10^{-8}	0.05	0.01-0.10
4	10^{-8}	10^{-6} to 10^{-10}	0.05	0.01-0.10
5	10^{-6}	10^{-4} to 10^{-8}	0.05	0.01-0.10
6	10^{-4}	10^{-2} to 10^{-6}	0.10	0.02-0.20

b. Values for Fracture Flow

Layer	Horizontal Permeability (cm/sec)		Porosity *	
	Preferred	Range	Preferred	Range
2	10^{-4}	10^{-2} to 10^{-6}	0.10	0.02-0.20
3	10^{-5}	10^{-3} to 10^{-7}	5×10^{-5}	10^{-3} - 10^{-6}
4	10^{-7}	10^{-5} to 10^{-9}	5×10^{-5}	10^{-3} - 10^{-6}
5	10^{-5}	10^{-3} to 10^{-7}	5×10^{-5}	10^{-3} - 10^{-6}
6	10^{-4}	10^{-2} to 10^{-6}	0.10	0.02-0.20

* NOTE: When performing combined permeability and porosity sensitivity analyses on layers 3, 4, 5 for fractured flow, the following porosity values should be used:

Preferred Permeability Value:
 Preferred Porosity: 5×10^{-5}
 Range: $10^{-5} - 10^{-4}$
 Maximum Permeability Value:
 Preferred Porosity: 5×10^{-4}
 Range: $10^{-4} - 10^{-3}$
 Minimum Permeability Value:
 Preferred Porosity: 5×10^{-5}
 Range: $10^{-6} - 10^{-5}$

c. Vertical Permeability

Preferred: $K_v = 0.1 K_H$; Range $K_v = K_H$ to $0.01 K_H$

NOTE: For purposes of the model analysis use $K_v = 0.1 K_H$ for all cases. The range in vertical permeability values is effectively modeled by the given ranges in horizontal permeabilities.

3. Gradients

a. Horizontal

Layers 2,6 $i = 0.005$ (preferred)
 $i = 0.0005$ to 0.05 (range)
 Layers 3,4,5 $i = 0$

b. Vertical Head Between Layers 2,6

Preferred = 200 ft (excess in layer 6)
 Range = 10 to 500 feet

4. Fracture Zone Around Shafts & Tunnels

a. General

For our evaluation it was necessary to assume some general mine layout; these parameters relate to a mine layout similar to the preliminary design presented in the "Waste Isolation Facility Description" by Parsons, Brinckerhoff, Quake & Douglas dated September 1976. The underlying assumption for the stress analysis is that the openings are sufficiently spaced so that there is minimal stress interaction between openings.

b. Parameters

The following table indicates the guesstimated radius of anticipated fracture zone around shafts (vertical) and tunnels (horizontal). The maximum fracture zone relates to a repository constructed in low strength rock with a high in-situ stress field and a poorly placed and/or non-rigid backfill. The minimum fracture zone relates to a repository in high strength rock with a low stress field and an ideal rigid backfill placed under pressure. Since the permeability within the general fracture zone decreases exponentially with distance from the tunnel or shaft face, the effective size of the fracture zone (using the peak permeability at the face) is only about 20% of the actual fracture zone.

Fracture Zone	Layers 3, 4 (shale)		Layer 4 (salt)	
	Shaft	Tunnel	Shaft	Tunnel
	Deep	Shallow		
<u>Intensely Fractured Zone</u>				
1. <u>Width</u>				
Preferred	--		1.05R	--
Minimum	--		0	--
Maximum	--		1.12R	--
2. <u>Properties</u>				
Perm.	--		$10^{-1}(10^0-10^{-2})$	--
Porosity	--		0.1(0.01-0.2)	--
<u>General Fracture Zone</u>				
1. <u>Width</u>				
Preferred	1.25(R+1m)	2(R+1m)	2.7(R+1)	2.7(R+1)
	1.1(R+1m)			
Minimum	R	1.45R	1.15R	1.15R
Maximum	3.3(R+1m)	4(R+1m)	3.5(R+1)	3.5(R+1)
	3.3(R+1m)			
2. <u>Properties</u>				
Perm.	-- + 10^{-4}	$(10^{-3} \text{ to } 10^{-6})$		+
Porosity	-- + 10^{-3}	$(10^{-2} \text{ to } 10^{-4})$		+

NOTE: R = radius or $\frac{1}{2}$ width of opening; thus, area of fracture zone would be $\pi R_2^2 - \pi R_1^2$ (R_2 : radius of fracture zone, R_1 : radius of opening).

c. Transition Times:

The above values relate to the maximum size of fracture zone which will develop in less than 50 to 100 years after repository backfilling. We estimate that the fracture zone in shale will not change significantly with time. In salt, we estimate that with time much of the fracture zone may heal. For this model, assume that the permeability of the fracture zone will decrease to 1% of its original value in 50 years (preferred); 20 to 200 years (range).

FOR YOUR INFORMATION and review of work in progress
The methods and limits may be subject to change as work proceeds.

d. Hydrologic Model - see Figure A

- Path a-b: Length = layer 5
Perm & Por = layer 5
Area - horizontal area of repository
use $5 \times 10^6 \text{ m}^2$
- Path b-c: Length - half thickness L-4
Perm & Por = L-4
Area - $5 \times 10^6 \text{ m}^2$
- Path c-d: Ditto above (b-c)
- Path d-e: Length - L-3
Perm & Por - L-3
Area - $5 \times 10^6 \text{ m}^2$
- Path c-f: Length - 1200m ($\frac{1}{2}$ length of HLW)
Perm & Porosity - See fracture zone table for tunnels; if a highly fractured zone exists (preferred and maximum in shale) ignore the negligible flow increase contribution from the general fracture zone.
- Areas (shale highly fractured) for tunnels
 - Preferred - 316 m^2
 - Min - 0 Max - 785 m^2
 - Areas (shale - general effective)
 - Preferred - 1900 m^2
 - Min - 580 m^2
 - Max - 7950 m^2
 - Areas (salt effective)
 - Preferred - 3300 m^2
 - Min - 190 m^2
 - Max - 6400 m^2
- Path f-g: Length - 440m (preferred)
200m - 6000m (range)
Perm & Por - see fracture zone table for tunnels
Areas - use 6% of above areas
- Path g-h: Length - $\frac{1}{2}$ L-4
Perm & Por - see fracture zone table for shafts
- Areas (shale effective)
 - Preferred - 10 m^2
 - Min - 0
 - Max - 100 m^2
 - Areas (salt effective)
 - Preferred - 60 m^2
 - Min - 4 m^2
 - Max - 110 m^2

FOR YOUR INFORMATION AND REVIEW OF WORK IN PROGRESS.
This is a preliminary report and is subject to change.
Work is being done on this project.

Path h-i: Length - L-5

Perm & Porosity - see fracture zone table for shafts

Area - Preferred: 5 m²

- min, max - ditto g-h (shale)

5. Mine Backfill Deterioration

a. Utilized Preliminary Parson design to estimate area of tunnels & shafts.

b. Occurrence of Deterioration:

Deterioration will be a function of host rock type, ground water flow, backfill type, placement methods and time. It is clearly impossible to project such an occurrence without some knowledge of backfill type and placement method. Thus, the parameters and transition rates presented below are only educated guesses. Preliminary backfill concept (OWI) for the salt repository is to use salt. Suitable backfill material for shale has not been evaluated at this time. Due to mechanical creep combined with precipitation and recrystallization, a properly placed salt backfill may result in a very low risk of deterioration.

c. Parameters

Assume that initially backfill has the same hydrologic characteristics of parent rock. With time there is a given probability that the fill may deteriorate with time.

Layer	Probability of Deterioration		Transition Rate		Final Properties			
	Preferred	Range	Preferred	Range	Perm.		Porosity	
					Pref.	Range	Pref.	Range
L-3	50%	20%-80%	500	50-5000	10 ⁻⁴	10 ⁻⁵ -10 ⁻³	10 ⁻²	10 ⁻¹ -10 ⁻⁴
L-4 (shale)	40%	20%-50%	500	50-5000	10 ⁻⁴	10 ⁻⁵ -10 ⁻³	10 ⁻²	10 ⁻¹ -10 ⁻⁴
L-4 (salt)	10%	5%-60%	500	50-5000	10 ⁻⁴	10 ⁻⁵ -10 ⁻³	10 ⁻²	10 ⁻¹ -10 ⁻⁴

d. Hydrologic Model - see Figure A

Identical pathways to fracture zone model except permeability and porosity are given above and areas as follows:

Path c-f: Area 33,000 m²

Path f-g: Area 1,620 m²

Path g-h, h-i: Area 64 m²

6. Boring Seal Dissolution (Borings taken for repository investigation only)

a. Geometry: Assume 50 borings (preferred) with 5 to 100 borings (range). Assume an effective diameter of 6 inches, 20% of the holes extend from the surface through layer 6; 80% extend from the surface to just below the repository zone.

b. Occurrence of Seal Dissolution: As with the backfill dissolution, it is clearly impossible to project the seal dissolution

FOR YOUR INFORMATION and review of work in progress. The methods and findings are, to be used as a guide as work proceeds. We will welcome comments and suggestions.

characteristics without some knowledge of sealing method. Although OWI has funded several research contracts to develop sealing procedures, no one method has been chosen. Thus, the parameters and probabilities presented below are only educated guesses. There is a certain probability that any boring seal will be improperly installed and effectively fail immediately. There is also a probable transition time in which the borehole seals will deteriorate. Obviously this transition rate depends on sealing procedure and quality of work.

c. Parameters

Assume, as with the backfill, that initially the borehole seal is effective and with time there is a given probability the seal may deteriorate.

BOREHOLE SEALS - PER BOREHOLE

	Immediately	0-500 yrs.	500-1000 yrs.	Never
Probability of Deterioration	10%	20%	20%	50%
Transition Time	0	200 yrs.	200 yrs.	
Final Perm:				
Preferred	10^{-4}			
Range	10^{-6} - 10^{-2}			
Final Porosity:				
Preferred	10^{-2}			
Range	10^{-4} - 10^{-1}			

d. Hydrologic Models - Figure B

The hydrologic affect of the boreholes cannot be generalized since it is a function of the vertical gradient distribution within layers 3,4,5 and within the borehole itself. For boreholes which extend through to layer 6 water may flow from the borehole into the repository, from the repository into the borehole, or there may be no flow at all between the boring and the repository. Thus, the models presented below are grossly simplified solutions intended to represent upper and lower bound approximations. The areas of the flow paths are 0.2 m^2 times the number of failed boreholes. The permeabilities and porosities are given above.

Worst Case (complete mixing)

Path j-c (deep boring): Length L-5, $\frac{1}{2}$ L-4

Point c: complete mixing

Path c-k (deep boring): Length $\frac{1}{2}$ L-4, L-5

Path c-l (shallow boring): ditto

Best Case and Preferred

(1) Repository not affected by borings (reduce total area)

Preferred: 100% - 0.5% N

Minimum: 100% - 0.05% N

FOR YOUR INFORMATION and review of work in progress
The methods and findings may be modified or supplemented as
work proceeds. We will welcome comments and suggestions.

- (2) Repository affected by borings
 Preferred: 0.5% N
 Minimum: 0.05% N
 Where: N = number of failed borings

Path a-b-c-d-e: ditto base case but with area equal to .5% N or 0.05% N of total area.

Path i-c (deep borings): length - L-5, $\frac{1}{2}$ L-4

Point c: (Complete mixing

Path c-k (deep boring): $\frac{1}{2}$ L-4, L-3

Path c-l (shallow boring): ditto

7. Event-Induced Faults

a. Occurrence:

This section applies to new faults or recurrent movement along old faults caused by a major seismic event. The probability of occurrence of the event is given by LLL. For a given seismic event, we estimate a 90% probability it will be caused by movement along a pre-existing fault zone and a 10% probability it will be caused by a new fault unrelated to any previous faulting.

b. Transition Rates:

The increasing stress field leading up to an event will open fractures within a zone around the fault and increase the permeability. The event itself will result in a release of stress with a subsequent closing of many of these fractures. Thus, the permeability of the zone affected by the event will increase with time to some maximum value, then decrease with time after the actual event to some residual value.

c. Parameters:

The following table indicates the permeability, porosity, width and transition rates for both new faults and movement along old faults. The maximum residual salt permeability relates to a solution opening along the fault zone and has a very low probability due to the creep behavior of the salt and the high salinity of the underlying L-6 aquifer.

d. Hydrologic Model - See Figure C:

The hydrologic effect of a fault has many of the same uncertainties as the affect of borehole seal deterioration. In fact, a very large fault could depressurize the lower aquifer and effectively stop upward flow of the waste. The models presented below are gross simplified solutions intended to represent upper and lower bound approximations. The area of the affected zone should be taken as 2500m times the width of affected area. The width, permeability and porosity is given on Tables 1 and 2. As shown on Figure 3, the repository should be subdivided into two general regimes as follows:

- (1) Repository not affected by the fault
Preferred: 98%
Range: 100% to 75%
(reduce total area)
- (2) Repository affected by the fault
Preferred: 2%
Range: 0% to 25%

Path a-b-c-d-e: ditto base case but reduced area
 Path f-g: fault in L-5
 Path g-c: fault in L-4
 Point c: complete mixing
 Path c-h: fault in L-4
 Path h-i: fault in L-3

e. Preliminary Modeling Recommendations:

Due to the complexity of the above faulting parameters combined with the anticipated sensitivity of these refinements, we recommend several simplifications for the actual model evaluation. These recommendations include:

1. Assume that any new fault movement will be along an existing fault (Table 1).
2. To assess the effect of faulting, a base case with an existing fault with initial properties shown in Table 1 should be evaluated.
3. The change in fault permeability with time can be simulated by a simple step function. The time the fault is open should be taken as total transition time, while the permeability of the fault should be conservatively assumed equal to the peak permeability.
4. For all cases use a porosity of 10^{-3} .

8. Ground Water Recharge

After mine abandonment time will be required to re-establish the original ground water regime and saturate the mine area. Until this occurs, no ground water will flow out of the repository zone. The length of time required for recharge depends on the nature of the original ground water regime, the effectiveness of the shaft seal, and the porosity and permeability of the back-fill and tunnel fracture zones. This affect should be incorporated into the model by not allowing any waste release after repository abandonment for the following delay periods:

Preferred: 100 years
 Range: 20-1000 years

9. Recommended Base Case

The general base case should include the fracture zone around the shafts and tunnels and the ground water recharge.

TABLE 1

FAULTS IN PLASTIC AND SEMI-PLASTIC MEDIA
SHALE AND SALT

RECURRENT FAULTING ALONG EXISTING MOVEMENT PLANES

Layer	Width of Hydraulically Affected Zone Preferred Range		Permeability Initial Peak % of Peak Range		Pref.	Residual % of Peak Pref. Peak		Transition Times Increase Decrease Range Pref. Range Pref. Years Years			
#3 400-600M Siltstone	30m	.6-50M	1	10^{-6} - 10^{-3}	10^{-4}	2	0-100	10-1000	50	1-500	20
#4 600-800M Shale	20m	.3-30M	1	10^{-7} - 10^{-4}	10^{-5}	2	0-100	10-1000	50	1-500	20
#4 * 600-800M Salt	3m	.01-10M	0	10^{-5} - 10^{-2}	10^{-3}	0	0	.01-10	1	.01-1	.5
#5 800-1000M Siltstone	20m	.3-30M	1	10^{-6} - 10^{-3}	10^{-4}	2	0-100	10-1000	50	1-500	20

Porosity 10^{-4} - 10^{-1}

Preferred value 10^{-3}

* NOTE: The probability and associated characteristics of new breccia pipe formation should be incorporated into the fault model.

FOR YOUR INFORMATION and review of work in progress.
The methods and findings may be modified or supplemented as
work proceeds. We will welcome comments and suggestions.

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TABLE 2

FAULTS IN PLASTIC AND SEMI-PLASTIC MEDIA
SHALE AND SALT

NEW FAULTS UNRELATED TO PREVIOUS FAULT MOVEMENT

Layer	Width of Hydraulically Effected Zone		Permeability		Pref.	Residual % of Peak		Transition Times			
	Preferred	Range	Initial % of Peak	Peak Range		Pref.	Peak	Increase Range Years	Pref.	Decrease Range Years	Pref.
#3 400-600M Siltstone	4m	.3-7M	0	10^{-6} - 10^{-3}	10^{-4}	1	0-100	100- 10,000	1,000	1-500	20
#4 * 600-800M Shale	2m	.15-3M	0	10^{-7} - 10^{-4}	10^{-5}	1	0-100	100- 10,000	1,000	1-500	50
#4 600-800M Salt	1m	.03-1M	0	10^{-5} - 10^{-2}	10^{-3}	0	0	.01-10	1	.01-1	.5
#5 800-1000M Siltstone	2m	.15-3M	0	10^{-6} - 10^{-3}	10^{-4}	1	0-100	100- 10,000	1,000	1-500	20

Porosity 10^{-4} - 10^{-1} Preferred value 10^{-3}

* NOTE: The probability and associated characteristics of new breccia pipe formation should be incorporated into the fault model.

FOR YOUR INFORMATION and review of work in progress.
The methods and findings may be modified or superseded as
work proceeds. We will welcome comments and suggestions.

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MODELS

Figure A

Figure B

Best and Preferred

Figure C

FOR YOUR INFORMATION and review of work in progress.
The methods and findings may be modified or improved.
work proceeds. We will send you a final report.

June 22, 1977

Dr. Don Towse
Lawrence Livermore Laboratory
University of California
P.O. Box 808
Livermore, California 94550

RE: TASC CYCLE II UNCERTAINTY PARAMETERS

Dear Don:

Enclosed are our recommended parameter uncertainty values to be used for the TASC Cycle II analysis. Some revised Cycle II parameters, which have been verbally presented to you and Ben Ross, are also included.

UNCERTAINTY VALUES

Given a specific site and assuming a certain level of exploration and instrumentation, there would be an uncertainty or confidence level associated with any parameter. This uncertainty arises from geologic variations, errors and limitations of testing techniques, and limitations in the evaluations of the tests or explorations. Since it is important to evaluate the merits of exploration vs. their harm (creating new pathways), we have developed uncertainty values for several different levels of information including both the pre-construction phase and for the post-construction phase. The levels considered appropriate are:

- a. Pre-construction Phase:
 - Minimal: No bore holes but research of available regional information and surface mapping.
 - Moderate: Approximately 40 shallow holes to level of repository and 10 deep holes through to underlying aquifers.
 - Maximum: Extensive explorations with hydrologic testing.
- b. Post-construction Phase:
 - After shaft and main corridors; both with major instrumentation and testing and with only instrumentation.
 - Just prior to backfilling; both with major instrumentation and testing; and with only instrumentation.

Dr. Don Towse
June 22, 1977
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The uncertainty values are expressed in terms of confidence limits on the mean value. Such as when you say that the ninety percent confidence limits on a parameter are A and B, it is meant that if the parameter was repeatedly sampled then ninety percent of the time the value obtained would lie between A and B. The geotechnical parameters are assumed to fit a log-normal distribution, which is commonly used in geologic and hydrologic studies. The standard unit for defining the uncertainty, U, of a parameter would correspond to one standard deviation in the logarithm of the parameter. Thus, if the parameter's value is V, the definition of its uncertainty, U, is "two thirds (approximately) of the sample population of the parameter lies between $\frac{V}{U}$ and VU ",

or alternatively, "ninety five percent of the sample population lies between $\frac{V}{U^2}$ and VU^2 ". All our values are given in terms of the value U.

Porosity and Permeability

The uncertainty attached to the parameters of permeability and porosity will be strongly dependent upon the degree of exploration. Maximum exploration will reduce uncertainties but may also create more pathways which, upon failure, can cause release of contaminants. In general, hydrologic testing can be conducted during the pre-mining phase, primarily through bore holes, and during the mining and waste emplacement phase by instrumentation within the mine.

The recommended values of U are as follows:

a. Permeability

Layer	Minimal	<u>Pre-Mine Phase</u>		<u>Nine Phase</u>	
		<u>Explorations</u>		<u>Main</u>	<u>After</u>
		<u>Moderate</u>	<u>Extensive</u>	<u>Shaft & Corridors</u>	<u>30 Years</u>
2	100	10	5	5 (4)*	5 (3)
3	100	10	5	5 (4)	5 (3)
4	100	10	5	5 (4)	4 (2)
5	100	10	5	5	5 (3)
6	100	10	5	5	5 (4)

* Numbers in parenthesis represent uncertainties if extensive explorations conducted in the mine.

Dr. Don Towse
June 22, 1977
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b. Interstitial Porosity

Layer	Minimal	Pre-Mine Phase Explorations		Main Shaft & Corridors	Mine Phase After 30 Years	
		Moderate	Extensive			
2	3	2	1.5	1.5		1.5
3	5	3	2	2		2
4	5	3	2	2		2
5	5	3	2	2		2
6	3	2	1.5	1.5		1.5

c. Fracture Porosity

3	10	8	5	5 (4)	5 (4)
4	10	8	5	4	4
5	10	8	5	5	5

Heads and Gradients

The capability exists to measure heads and compute horizontal and vertical flow gradients with a high degree of accuracy. The affects of salinity complicate this measurement and thus introduce uncertainty. Additional gradients do to osmotic potential, thermal potential, threshold phenomenon, etc., are not included in these uncertainties. The U values are:

	Layer	Pre-Mine Phase Explor.			Mine Phase Expl.	
		Minimal	Moderate	Extensive	Shaft & Cor.	30 Y
Horizontal	2	5	1.3	1.2	1.2	1.2
Gradients	6	10	1.3	1.2	1.2	1.2
Vertical Head between 2, 6		5	1.3	1.2	1.2	1.2

Other Parameters

We provided data on fault sizes and properties, bore hole seal dissolution and backfill dissolution, and size and properties of mine opening fracture zones. These are not measured values; rather they are computed values based on the analyses of many measured parameters. To credibly evaluate the uncertainty related to these computed parameters would involve a parametric sensitivity analysis. In our opinion, this complexity is inappropriate at this time. Rather than provide any guesstimates of uncertainties, we would recommend that the full range of values given be assumed to be the uncertainty for the 2nd cycle model. As we learn more about the uncertainty analysis concept to be used by TASC, we would develop uncertainties for future models.

Dr. Don Towse
June 22, 1977
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Enclosed is a discussion of the problems associated with uncertainties of fracture zone prediction.

Revised 2nd Cycle Data

The following revisions are recommended, as discussed with you and Ben Ross, to our original 2nd cycle data:

2. Fracture Flow Porosity:

<u>Layer</u>	<u>Preferred</u>	<u>Porosity</u> <u>Range</u>
3	10^{-4}	$10^{-3} - 10^{-5}$
4	10^{-5}	$10^{-4} - 10^{-6}$
5	10^{-4}	$10^{-3} - 10^{-5}$

b. Mine Backfill Deterioration

In addition to the original values which represented a effectively impervious backfill, we recommend the following case also be evaluated. This represents the case of impervious backfill techniques not being developed.

Permeability: 10^{-3} , range 10^{-1} to 10^{-6}
Porosity: 10^{-1} , range 2×10^{-1} to 10^{-3}

Consider at least the following:

- Tunnel backfill perm.: 10^{-3}
- Shaft backfill perm.: 10^{-3}
- Tunnel backfill perm.: 10^{-3}
- Shaft backfill perm.: 10^{-6}
- Tunnel backfill perm.: 10^{-1}
- Shaft Backfill perm.: 10^{-6}

c. Event Induced Faults:

Assume a fault in salt either seals immediately or develops into a breccia pipe. This would incorporate the breccia pipe data developed by GEI.

d. Bore Hole Seals:

The correct bore hole area is 0.02 m^2 times the number of failed bore holes (not 0.2 m^2).

If you have any questions about this information, please contact us.

RP:mm
cc: Ben Ross, TASC
P. Davies, GEI
77303
Encl.

PREFERRED PARAMETER VALUES FOR CYCLE II

I. Permeability and Porosity of Salt

A. Permeability

1. Vertical - 10^{-9} cm/sec (no change)
2. Horizontal - 5×10^{-8} cm/sec (revised)

B. Porosity - 0.01 (no change)

II. Rate of Breccia Pipe Formation (no changes)

- A. 200 m (Layer 4) - 4×10^6 years required to produce one critical cavity/sq mile
- B. 1000 m (Layer 4) - 9×10^7 years required to produce one critical cavity/sq mile
- C. 20 m (Layer 4) - 6×10^5 years required to produce one critical cavity/sq mile
- D. Note: All values assume other layers to be 200 m.

III. Permeability and Porosity of Collapse Breccia

- A. Permeability - 10^{-2} cm/sec (revised)
- B. Porosity - 0.3 (revised)
- C. Area - 10^4 m² (no change)

CALCULATIONS TO ESTIMATE THE EFFECTS OF NON-SALT INTERBEDS
ON THE PERMEABILITY OF SALT FORMATIONS

- I. Calculations were made to estimate the effects of non-salt interbeds on the overall permeability of salt formations. Terzaghi and Peck (1967) equations for the permeability of stratified masses were used. The equations are as follows:

$k_1, k_2, \dots, k_n$ = coefficients of permeability of the individual strata

$H_1, H_2, \dots, H_n$ = thicknesses of the corresponding strata

$H = H_1 + H_2 + \dots + H_n$ = total thickness

k_I = average coefficient of permeability parallel to bedding planes (usually horizontal)

k_{II} = average coefficient of permeability perpendicular to bedding planes (usually vertical)

$$k_I = \frac{1}{H} (k_1 H_1 + k_2 H_2 + \dots + k_n H_n)$$

$$k_{II} = \frac{H}{\frac{H_1}{k_1} + \frac{H_2}{k_2} + \dots + \frac{H_n}{k_n}}$$

- II. Data on the detailed lithology of salt bearing formations came from published logs:

A. Salado Formation (Delaware Basin) - Figure 6, Jones, 1973:

560 ft total section

- 18 ft claystone seams
- 4 ft clayey sandstone
- 510 ft halite, clayey halite and polyhalite
- 28 ft anhydrite

B. San Andreas Formation (north of Delaware Basin) - Figure 4, Jones, 1974:

1100 ft total section

- 80 ft shale
- 325 ft dolomite
- 410 ft salt
- 285 ft anhydrite

III. Results

A. Salado Formation:

Strata	Assumed Permeability*(horizontal and vertical)	Overall Permeability cm/sec
Case 1: Claystone	10^{-8} cm/sec	
Clayey sandstone	10^{-6} cm/sec	
Halite, clayey halite, polyhalite	10^{-9} cm/sec	
Anhydrite	10^{-9} cm/sec	
		8.4×10^{-9} (horizontal)
		1.0×10^{-9} (vertical)
Case 2: Claystone	10^{-6} cm/sec	
Clayey sandstone	10^{-4} cm/sec	
Halite, clayey halite, polyhalite	10^{-9} cm/sec	
Anhydrite	10^{-9} cm/sec	
		7.5×10^{-7} (horizontal)
		1.0×10^{-9} (vertical)

B. San Andreas Formation:

Strata	Assumed Permeability*(horizontal and vertical)	Overall Permeability
Case 1: Shale	10^{-8} cm/sec	
Dolomite	10^{-8} cm/sec	
Salt	10^{-9} cm/sec	
Anhydrite	10^{-9} cm/sec	
		4.3×10^{-9} (horizontal)
		1.5×10^{-9} (vertical)
Case 2: Shale	10^{-6} cm/sec	
Dolomite	10^{-6} cm/sec	
Salt	10^{-9} cm/sec	
Anhydrite	10^{-9} cm/sec	
		3.7×10^{-7} (horizontal)
		1.6×10^{-9} (vertical)

*Permeabilities of specific lithologies estimated utilizing data from GEI's January 6, 1977 report and from considerations of the permeability values used in Cycle I.

IV. Recommendations

- A. The effect of interstratified higher permeability layers on the vertical permeabilities in the sample formations is minimal. Therefore, no change in the vertical permeabilities is recommended.
- B. The potential effect of interstratified higher permeability layers on the horizontal permeability in the sample formations is significant: the overall horizontal permeability values range from 4.3×10^{-9} to 7.5×10^{-7} cm/sec, whereas the value for the permeability of salt presently used in the TASC model is 1×10^{-9} cm/sec. It is important to note that these increased values were calculated using permeability values for the interstratified layers which are (1) either equal to previously established mean values or (2) are values which represent only one order of magnitude difference (greater or smaller) than the mean values, a much smaller spread than the range of permeabilities previously given for the interstratified lithologies. (For example, the range for shale previously given was 2×10^{-4} to 5×10^{-10} cm/sec, which has a geometric mean of about 3×10^{-7} cm/sec. The two values used in the calculation of overall permeability for the permeability of the interstratified shale are 10^{-8} and 10^{-6} cm/sec.)

Therefore, it is recommended that the value of horizontal permeability of salt for use in the next cycle of the TASC model be 5×10^{-8} cm/sec, which is approximately the geometric mean of 4.3×10^{-9} and 7.5×10^{-7} .

REVISED PERMEABILITY AND POROSITY OF COLLAPSE BRECCIA

Computations of the permeability of collapse breccias formed in chimneys above underground nuclear detonation tests, which are based on measurements of atmospheric pressure and underground gas pressure, have yielded permeability measurements for chimneys in alluvium and tuff which ranges from 7×10^{-3} to 6×10^{-2} cm/sec.

These values suggest that the Cycle I preferred value of 10^{-1} cm/sec for permeability of a collapse breccia (which was based on a clean sand and gravel mix) is too conservative. Therefore, a revised value of 10^{-2} cm/sec is recommended for Cycle II.

The calculations of nuclear chimney breccias assume a porosity 0.3. Therefore, it is recommended that this value be used for Cycle II. However, as the actual data on which this assumption was made had not been reviewed to date, this revised porosity value will continue to be re-evaluated as new data is obtained.

WATER FLOW INTO BRECCIA PIPE
24 JUNE 1977

Case 1: Model water flow into breccia pipe* as a fault through Layer 5, connecting the base of the breccia pipe with the aquifer (Layer 6). This fault should be given the characteristics of "Recurrent Faulting Along Existing Movement Planes" as outlined by GAI memo, May 31, 1977. The characteristics for a fault through Layer 5 are given as follows:

	Preferred	Range
1. Width of hydraulically effected zone (fault) Area of Discharge = width of fault x diameter of breccia pipe (400 m)	20 m	0.3-30 m
2. Permeability (peak) (initial % of peak) (residual % of peak)	10^{-4} cm/sec 1 2	10^{-6} - 10^{-3} cm/sec 0-100
3. Porosity	10^{-3}	10^{-4} - 10^{-1}
4. Transition times (increase) (decrease)	50 years 20 years	10-1000 years 1-500 years
5. Gradient (excess head between Layer 2 and Layer 6)	200 ft	10-500 ft

Schematic Sketch

* Cross-section area of breccia pipe = 10^5 m^2

FOR YOUR INFORMATION and review of progress. The methods and findings may be modified as work proceeds. We will welcome comments and suggestions.

Project 77336
June 27, 1977

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PARAMETER RANGES AND UNCERTAINTY OF PREFERRED VALUES
FOR CYCLE II - SUMMARY

- I. Permeability and Porosity of Salt*
 - A. Permeability (Preferred: 10^{-9} cm/sec)
 1. Range: 10^{-10} to 10^{-5} cm/sec
 2. Uncertainty of Preferred Value: $\pm$ two orders of magnitude
 - B. Porosity (Preferred: 0.01)
 1. Range: 0.004 to 0.07
 2. Uncertainty Range Around Preferred Value: 0.005 to 0.02
- II. Rate of Breccia Pipe Formation
 - A. Ranges (no changes)
 1. 200 m (Layer 4) - 4×10^4 to 5×10^8 years required to produce one critical cavity/sq mile (Preferred: 4×10^6)
 2. 1000 m (Layer 4) - 1×10^6 to 1×10^{10} years required to produce one critical cavity/sq mile (Preferred: 9×10^7)
 3. 20 m (Layer 4) - 7×10^3 to 9×10^7 years required to produce one critical cavity/sq mile (Preferred: 6×10^5)
 4. Note: All values assume other layers to be 200 m. New values must be calculated to run other thicknesses.
 - B. Uncertainty of Preferred Value: $\pm$ one order of magnitude
- III. Permeability and Porosity of Collapse Breccia
 - A. Permeability (Preferred: 10^{-2} cm/sec)
 1. Range: 10^{-3} to 10
 2. Uncertainty of Preferred Value: $\pm$ one order of magnitude
 - B. Porosity (Preferred: 0.3)
 1. Range: 0.10 to 0.40
 2. Uncertainty of Preferred Value: $\pm$ 0.10

*See Background Information I.C.2. (page 3)

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PARAMETER RANGES AND UNCERTAINTY OF PREFERRED
VALUES FOR CYCLE II - BACKGROUND INFORMATION

1. Permeability and Porosity of Salt

A. Permeability

1. Range: 10^{-10} to 10^{-5} cm/sec

- a. Based on published test values for salt permeability. These are predominantly laboratory values.
- b. The low end of the range represents the minimum measured value excluding zero.
- c. The high end of the range excludes a few 10^{-4} cm/sec test values from tests performed with zero confining pressure (representing no overburden).

2. Uncertainty of Preferred Value: $\pm$ two orders of magnitude, based on the following factors:

- a. With proper calibration, the accuracy of in-situ pressure testing is $\pm$ one order of magnitude (Dick, 1975). Factors which can induce error in such testing are:
 - (1) Improperly sealed packers
 - (2) Joint patterns which by-pass packer
 - (3) Improper calibration of frictional losses on sides of pipe, fittings and flexible hose
 - (4) Flow gauge accuracy
 - (5) Drill cuttings along joints which cause a reduction of the measured permeability
 - (6) Expansion of rubber tubing under high pressures
 - (7) High head pressure causing hydraulic fracturing

- b. Laboratory testing error may be introduced in many areas, especially difficult is the preservation of the in-situ characteristics of the test sample when it has come from a substantial depth.
 - c. For salt, as with all other rock types, there is always some question as to how representative the testing is of the entire hydrogeologic framework of an area, considering the small fraction of that area which has actually been tested.
 - d. Uncertainty of the measurement values is higher for the extremes of the permeability spectrum.
3. Range over time - no input at this date, assume constant. (Further consideration to be given under Cycle III).

B. Porosity

1. Range: 0.004 to 0.07 (no change)
2. Uncertainty range around preferred value: 0.005 to 0.02
3. Range over time - no input at this date, assume constant (further consideration to be given under Cycle III).

C. Horizontal vs Vertical Permeability of Salt

1. All values for vertical permeability and porosity remain as indicated by GEI input for Cycle II (May 19, 1977 and this report).
2. The May 19, 1977 GEI input documented the important potential impact of flow in non-salt interbeds within a bedded salt formation. The results of the calculations of overall permeability based on selected sections of the Salado Fm. and the San Andreas Fm. using Terzaghi and Peck (1967) equations for the permeability of stratified masses may only be used for calculation of discharge. The actual flow velocity profile varies significantly between salt and non-salt beds.

Preliminary calculations of flow velocities and discharge from non-salt interbeds indicate these flow paths to be very important. Recommendations for representation of the non-salt interbeds as horizontal pipe(s) and parameter values will follow as part of GEI's input for Cycle III.

II. Rate of Breccia Pipe Formation

- A. Ranges (no changes)
- B. Uncertainty of preferred value: + one order of magnitude, based on consideration of the uncertainties of various inputs to the original calculations of preferred values.
- C. All values assume other layers to be 200 m. New values must be calculated to run other thicknesses.
- D. Uncertainty of range with time: Breccia pipe "window time" to be considered in Cycle III.

III. Permeability and Porosity of Collapse Breccia

- A. The ranges of permeability and porosity of collapse breccia have been broadened to encompass new input. Future study should address the question of the possible variations in permeability and porosity within a single breccia pipe due to:
 - 1. Breccia under high overburden pressures at the base of the breccia column may be more compacted than the breccia nearer the surface.
 - 2. If a breccia pipe has limited upward extent, an intensely fractured zone which is more permeable than the natural rock will extend upward (above) for some distance.

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DRAFT

UCID-

Lawrence Livermore Laboratory

PRELIMINARY REPORT ON RETARDATION FACTORS AND RADIONUCLIDE MIGRATION

Dana Islerwood

August 5, 1977

This is an informal report intended primarily for internal or limited external distribution. The opinions and conclusions stated are those of the author and may or may not be those of the laboratory.

Prepared for U.S. Energy Research & Development Administration under contract No. W-7405-Eng-48.

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INTRODUCTION

The primary geochemical control on radionuclide migration from a high-level waste repository is ion exchange. Other controls which constitute the geochemical barrier to radionuclide migration are ion filtration, hydrolysis and solubility.

The retention of radionuclides via ion exchange can be quantitatively expressed as a retardation factor; that is, the relative velocity of the groundwater to that expected for the individual radionuclide. The chief purpose of this report is documentation of the retardation factors used in Lawrence Livermore Laboratory's hydrologic modeling of radionuclide migration from a high-level waste repository. More detailed discussions on radionuclide chemistry, geochemical controls and how they influence waste/water/rock interactions are planned for future reports.

The mass transport hydrologic model referred to in this study was developed by The Analytic Sciences Corporation (TASC) for Lawrence Livermore Laboratory's high-level waste management program funded by NRC.

RETARDATION FACTORS

The retardation factor, $K_f = \frac{\text{water velocity}}{\text{nuclide velocity}} = 1 + rK_d$ where

K_d equals the ion exchange distribution coefficient, that is,

$$K_d = \frac{\left(\frac{\text{amount of nuclide}}{\text{in solid phase}} \right) / \left(\frac{\text{weight}}{\text{of solid}} \right)}{\left(\frac{\text{amount of nuclide}}{\text{in liquid phase}} \right) / \left(\frac{\text{volume of}}{\text{liquid}} \right)} = \left(\frac{\text{ml}}{\text{g}} \right)$$

and

$$r = \left(\frac{1 - \phi}{\phi} \right) \rho \quad \begin{array}{l} \rho = \text{rock density} \\ \phi = \text{effective porosity} \end{array}$$

When there is no sorption, $K_d = 0$ and the minimum value for the retardation factor is 1. Also note, as porosity increases, r decreases causing a decrease in K_f (Figure 1). For more complete discussions on sorption and the relative movement of radionuclides in groundwater, see Borg, et al, (1976) and Levy (1972).

Although the retardation factor is primarily defined as a function of the ion exchange distribution coefficient, retardation factors as used in the transport model represent the combined effects of ion exchange and adsorption of charged colloidal species on silica surfaces. Other processes which also affect radionuclide concentrations (e.g. low solubilities) are not accounted for in the retardation factor.

The retardation factors used in TASC's transport model originally came from Burkholder's estimated values for sorption in a western U.S. desert soil (Table 1). A recent evaluation of these retardation factors based on published K_d 's shows Burkholder's results are applicable to sedimentary rocks as well.

Figure 1: Retardation factor (K_F) as a function of the distribution coefficient (K_d).

TABLE I
RETARDATION FACTORS FOR WESTERN U.S. DESERT SOIL*

$K_f = 1$	Technetium		
	Iodine		
$K_f = 10^2$	Strontium	$K_f = 10^3$	Rubidium
	Antimony		Tin
	Polonium		Cesium
	Neptunium		Radium
$K_f = 10^4$	Yttrium	$K_f = 10^5$	Thorium
	Zirconium		
	Promethium		
	Niobium		
	Lead		
	Protactinium		
	Uranium		
	Plutonium		
	Americium		
	Curium		
	Europium		

*Burkholder, NR - CONF - 001, p. 456, values rounded to nearest order of magnitude.

As it was not practical to treat each radionuclide separately in the transport model, the 23 biologically significant nuclides in Table 2 were divided into three groups: fission products with no sorption properties, fission products with sorption, and the actinides and their daughter products. The fission product/actinide division separates the α emitters from the β and γ emitters. Maximum, minimum and preferred values were assigned for each group for both the shale and salt repositories. Values used in TASC's transport model are given in Table 3. Uncertainties with time for retardation factors are $\pm$ order of magnitude. Note that for the salt repository, sorption is modeled only in the aquifer (i.e., $K_f = 1$ in the salt layer and barrier bed). Salt has essentially no exchange capacity. In the barrier bed, it is assumed that the high salt content of the groundwater* will saturate the exchange sites to the extent that sorption will be severely limited. In the aquifer, it is assumed that dilution of the salty groundwater will decrease the salinity effect on ion exchange and sorption will take place as the radionuclides are transported through the aquifer.

The same retardation factors are used for both interstitial and fracture flow. This assumption is based on Fried and others (1977) Pu retardation experiments with artificial fissures in basalt.

Whether retardation factors are actually the same for both interstitial and fracture flow depends on the rate of ion exchange; that is, whether the passage time through the sorbing medium is sufficient for equilibrium to occur. Unfortunately, rates of reaction for radionuclide ion exchange are unknown. Because the flow rates for interstitial and fracture flow are low

*Data from the Salado and Castille Formations of the Delaware Basin show local groundwater concentrations of $> 300,000$ ppm TDS.

TABLE 2

BIOLOGICALLY SIGNIFICANT NUCLIDESFrom 10 yrs. to 10^6 After Irradiation

Nuclide	$T_{1/2}$	Specific Activity ($\frac{Ci}{g}$)	MPC_W ($\frac{Ci}{m^3}$)	MPC_W ($\frac{moles}{l}$)	Time Significant (yr)
^{90}Sr	28 yr	1.42×10^2	3×10^{-7}	2×10^{-14}	$10 - 100$
^{90}Y	64 hr	5.44×10^5	2×10^{-5}	4×10^{-16}	$10 - 100$
^{93}Zr	1.5×10^6 yr	2.56×10^{-3}	8×10^{-4}	3×10^{-6}	$10^3 - 10^6$
^{93m}Nb	14 yr	2.75×10^{-2}	3×10^{-4}	2×10^{-7}	$10^3 - 10^6$
^{99}Tc	2.1×10^5 yr	1.72×10^{-2}	3×10^{-4}	2×10^{-7}	$10^3 - 10^5$
^{126}Sn	1×10^5 yr	2.84×10^{-2}	2×10^{-5}	6×10^{-9}	$10^3 - 10^5$
^{129}I	1.7×10^7 yr	1.63×10^{-4}	6×10^{-8}	3×10^{-9}	$10^3 - 10^6$
^{134}Cs	2.0 yr.	1.33×10^3	9×10^{-6}	2×10^{-9}	10
^{137}Cs	30 yr	8.7×10	2×10^{-5}	2×10^{-12}	$10 - 100$
^{210}Pb	20 yr	8.52×10^1	1×10^{-7}	6×10^{-15}	$10^4 - 10^6$
^{210}Po	38 yr	4.49×10^3	7×10^{-7}	7×10^{-16}	$10^4 - 10^6$
^{226}Ra	1.6×10^3 yr	9.90×10^{-1}	3×10^{-8}	1×10^{-13}	$10^4 - 10^6$
^{229}Th	7.3×10^3 yr	2.0×10^{-1}	7×10^{-6}	2×10^{-10}	$10^5 - 10^6$
^{230}Th	8.0×10^4 yr	2.0×10^{-2}	2×10^{-6}	4×10^{-10}	$10^5 - 10^6$
^{231}Pa	3.3×10^4 yr	4.7×10^{-2}	9×10^{-7}	8×10^{-11}	10^6
^{233}U	1.6×10^5 yr	9.6×10^{-3}	3×10^{-5}	1×10^{-8}	$10^5 - 10^6$
^{237}Np	2.1×10^6 yr	7.19×10^{-4}	3×10^{-6}	2×10^{-8}	$10^3 - 10^6$

Continued

BIOLOGICALLY SIGNIFICANT NUCLIDES (continued)

From 10 yrs. to 10^6 After Irradiation

Nuclides	T $_{1/2}$	Specific Activity ($\frac{Ci}{g}$)	MPC _w ($\frac{Ci}{m^3}$)	MPC _w ($\frac{moles}{L}$)	Time Significant (yr)
^{239}Pu	86 yr	1.75×10^1	5×10^{-6}	1×10^{-12}	10 - 100
^{239}Pu	2.4×10^4 yr	6.2×10^{-2}	5×10^{-6}	3×10^{-10}	$10^3 - 10^5$
^{240}Pu	6.6×10^3 yr	2.26×10^{-1}	5×10^{-6}	9×10^{-11}	$10^3 - 10^4$
^{241}Am	4.6×10^2 yr	3.23	4×10^{-6}	5×10^{-12}	$10 - 10^4$
^{243}Am	8.0×10^3 yr	1.84×10^{-1}	4×10^{-6}	8×10^{-11}	$10 - 10^4$
^{244}Cm	18 yr	8.14×10^1	7×10^{-6}	4×10^{-13}	10 - 100

EQUATIONS:

$$\text{Specific Activity} = \frac{N \times 1.873 \times 10^{-11}}{t_{1/2} \text{ (sec)}}$$

$$N = \frac{\text{atoms}}{\text{mole}}$$

$$S.A. = \frac{1.12755 \times 10^1}{N \times t_{1/2} \text{ (sec)}} = \frac{Ci}{g}$$

$$N = g/\text{mole}$$

$$MPC_w \left(\frac{\text{moles}}{L} \right) = \frac{MPC_w \left(\frac{Ci}{g} \right)}{\text{Spec. Act.} \times 10^3 \times M}$$

TABLE 3
RETARDATION FACTORS FOR THE TRANSPORT MODEL

Shale Repository

	Minimum	Preferred	Maximum
Iodine and Technetium	1	1	1
Other Fission Products	1	² 10	³ 10
Actinides	² 10	⁴ 10	⁵ 10

Salt Repository

Iodine and Technetium	1	1	1
Other Fission Products			
Salt repository and barrier bed:	1	1	1
Aquifer:	1	² 10	³ 10
Actinides			
Salt repository and barrier bed:	1	1	1
Aquifer:	² 10	⁴ 10	⁵ 10

(10^{-3} to 10 m/yr) It is assumed that equilibrium conditions exist. However, the uncertainty in retardation factors for fracture pathways is greater than the uncertainty in retardation for interstitial flow.

Group I. IODINE AND TECHNETIUM

Assigning a zero sorption value for iodine and technetium is based on theoretical and experimental evidence. Both elements exist in natural waters as the negative ions, I^- and TcO_4^- . Since soils and rocks generally exhibit no anion exchange capacity except for that sometimes shown by soil organic matter, sorption should be zero.*

Soil experiments by Battelle at Hanford (BNWL 1950, Part 2) gave K_d 's for TcO_4^- of 2.8 and 0.007 (basically zero for our purposes). K_d 's for I^- were .08 - 52.5. The 52.6 value was attributed to Fe and Al oxide coatings on the soil particles, otherwise I^- showed no sorption. Gast and others at the University of Minnesota (COO - 2447-5) report similar K_d values for TcO_4^- in soils. In an earlier study of radionuclide migration at Hanford, Tc migrated at about the same rate as groundwater (i.e., $K_f = 1$) (Brown, 1976). K_d values for Tc were also zero over a wide range of $NaHCO_3$ concentrations for a South Carolina topsoil (Routson, et al., 1975).

*Natural anion exchange materials include kaolinite, apatite and hydrous aluminum oxide. All have low anion exchange capacities and are limited in their distribution in rocks and soils.

Group 2. OTHER FISSION PRODUCTS

Fission products with sorption characteristics include ^{90}Sr , ^{90}Y , ^{93}Zr , $^{93\text{m}}\text{Nb}$, ^{126}Sn , ^{134}Cs , and ^{137}Cs (see Table 2). The preferred retardation factor of 10^2 given this group is a conservative estimate based on the sorption characteristics of Sr and Cs, the only major contributors among the fission products to the waste inventory. ^{90}Y , in secular equilibrium with ^{90}Sr , has a half life of only 64 hours. The $^{93}\text{Zr} + ^{93\text{m}}\text{Nb}$ pair's inventory is 2×10^{-5} that of the combined inventory of ^{90}Sr plus ^{137}Cs in 10 year old waste. The ^{126}Sn inventory is even less than ^{93}Zr .

A compilation of Sr and Cs distribution coefficients shows a wide range of values (Table 4). For Sr, K_d 's vary from 0.19 in salt to 4000 in tuff. K_d 's for Cs show an even greater distribution: 0.027 in salt, 17,800 in tuff. With the exception of Amchitka basalts, Cs K_d 's are larger, often by an order of magnitude, than those for Sr. Of the 25 K_d 's for Sr and Cs in Table 4, only the following are applicable to the geology used in TASC's model (i.e., sedimentary rocks, excluding carbonates).

	K_d (Sr)	K_d (Cs)
Shaley siltstone	8	309
Sandstone	1.4	102
Sands	1.7-43	22-314
Sediments	50	300
Soils	9-282	250-1053

Based on the above K_d 's, 10 was chosen to represent an average Sr distribution coefficient. This gives a retardation factor of approximately 10^2 in sandstone (see Figure 1). Cs should have greater retardation than

TABLE 4

DISTRIBUTION COEFFICIENTS: Sr AND Cs*

Reference	K _d		Conditions
	Sr	Cs	
Angelo, et al., 1962	16-135	792-9520	Basalt, 32-80 mesh, prep. groundwater
Baetsle & Dejonghe, 1972	1.7-3.8	22-314	Quartz sand, Ph 7.7
Barten, et al., 1962	4-9	8-9	Granodiorite, 100-200 mesh, prep. groundwater.
	11-23	1030-1810	Granodiorite, 0.5-1 mm, prep. groundwater.
Brown, 1976	50	300	Hanford sediments.
Douhy, 1967	45-75	800-10 ³	Tuff
Essington & Nork, 1969	220	39	Basalt, 0.5-4 mm, 300 ppm TDS
	1220	280	Basalt, 0.5-4 mm, 300 ppm TDS
	1.1	6.5	Basalt, 0.5-4 mm, sea water
Godse, et al., 1962	143-282	617-1053	Soil, pH 6.8
Goldberg, et al., 1962	2070-3480	12,000-17,800	Tuff, 100-200 mesh, prep. groundwater
Hajek & Knoll, 1966	19-43	189-420	Soils
Hoffman, 1976	400	5000-8000	Tuff, chimney rubble, groundwater
Inoue, 1976	9.4-71	250-10 ³	Soils, Ca groundwater
Nork and Fenske, 1970	260	1020	Tuff, >0.4 mm, prep. water
	0.19	13.5	Carbonate, >4 mm, prep. water
	1.7	34.3	Granite, >4 mm, groundwater
	8.32	309	Shale siltstone, >4 mm, well water
	1.37	102	Sandstone, >4 mm, well water
	0.19	0.027	Salt, >4 mm, saturated salt water
Nork, et al., 1971	48-2454	121-3165	Alluvium, 0.5-4 mm, groundwater
Persons, 1961	13-43	100	Sands
Robertson, 1976	3	-	Basalt, in situ measurements
Stead, 1963	5-14	-	Dolomite, 4000 ppm TDS
	4000	-	Tuff

*Taken in part from Borg, et al., 1976, Table 23.

10^2 , but, to simplify calculations in the transport model, was included with Sr. The preferred value of 10^2 is used for both shale and sandstone units. The maximum and minimum values reflect the range of values commonly found for Sr in Table 4. The estimated uncertainty in the retardation factor as a function of time is $\pm$ an order of magnitude.

Group 3. ACTINIDES AND DAUGHTER PRODUCTS

The biologically important actinides in Table 2 are the products of 4 interrelated decay chains. Since the TASC transport model does not differentiate between parent nuclides and their daughters, all of the actinides are treated alike with regard to their retardation factors.

For example, ^{239}Pu is the daughter of ^{243}Am . Although there is evidence that Am migrates faster than Pu (Fried, et al., 1977; Hajek, 1966; Hajek and Knoll, 1966), in TASC's transport model both Pu and Am are treated alike. This is not unreasonable considering that the difference in retardation between them is probably less than the uncertainty in the combined estimated retardation factor of 10^4 (see below).

In the pH range of 5 to 8 for natural waters, the reported K_d 's for the actinides vary greatly (Table 5):

Americium	$2 \times 10^2 - 5 \times 10^4$
Neptunium	3.2×10^2

Plutonium	$2.5 \times 10^2 - 3.8 \times 10^5$
Thorium	$40 - >10^5$

Using the numbers above, an average K_d of 200-300 is a conservative estimate. From Figure 1, this gives a retardation factor of approximately 10^4 . Minimum and maximum K_d values of 10^2 and 10^5 represent possible K_d 's of 10 and 10^4 . Uncertainties as a function of time are estimated at $\pm$ an order of magnitude.

The literature suggests that the relative retardation factors could be:

$$\text{Th} \geq \text{Pu} > \text{Am} > \text{Np} > \text{Ra}^*$$

The actual differences between them will be a function of the repository characteristics (e.g., rock type, flow rates, groundwater composition, etc.). For the generic repository, treating the actinides as a group is justified. However, it should be remembered that Pu in particular may have a retardation factor as high as 10^7 -- an important consideration in modeling a repository for high-level waste from a throw-away cycle.

*As the daughter of ^{230}Th , the alkaline-earth element, ^{226}Ra , is included with the actinides. There is evidence from the deep sea cores that Ra migrates relative to Th by a factor of 10 to 100. Reconcentration effects (see Burkholder, 1976) caused by these differences are currently being evaluated.

TABLE 5

ACTINIDE DISTRIBUTION COEFFICIENTS

<u>Reference</u>	$K_d \left(\frac{\text{ml}}{\text{g}} \right)$	<u>Conditions</u>
<u>Americium</u>		
Hajek & Knoll, 1966	1	sand, 5 N NO_3^- , oil, org., pH 3
	2×10^2	sand, 5 N NO_3^- , oil, org., pH 7
	5×10^2	sand, sludge, pH 7
Van Dalen, et al., 1975	5×10^4	illite/kaolinite, 90% sat. NaCl, pH 7-8
	4×10^2	river sand, 90% sat. NaCl, pH 7-8
Routson, et al., 1975	$>1.2 \times 10^3$	desert sand, .002 M Ca, pH 2.5-3.1
	$>1.2 \times 10^3$	desert sand, 0.2 M Ca, pH 2.5-3.1
	67	sandy clay, .002 M Ca, pH 2.5-3.1
	1	sandy clay, .2 M Ca, pH 2.5-3.1
	1.6	sandy clay, 3 M Na, pH 2.5-3.1
	280	sandy clay, .015 M Na, pH 2.5-3.1
	$K_f = 10^4$	limestone, pH 6.7, pH 2.5-3.1
<u>Neptunium</u>		
Dahlman, et al., 1975	3.2×10^2	clay soil, pH 6.5, 5 mM $\text{Ca}(\text{NO}_3)_2$
Routson, et al., 1975	2.37	sand, .002M Ca, pH 2.5-3.1
	0.36	sand, .2M Ca, pH 2.5-3.1
	3.9	sand, .015M Na, pH 2.5-3.1
	3.2	sand, pH 2.5-3.1, 3.0M Na
	0.25	sandy clay, pH 2.5-3.1, .002 M Ca

TABLE 5 (Continued)

Reference	$K_d \left(\frac{\text{ml}}{\text{g}} \right)$	Conditions
	0.16	sandy clay, pH 2.5-3.1, .2M Ca
	0.7	sandy clay, pH 2.5-3.1, .015 M Na
	0.4	sandy clay, pH 2.5-3.1, 3.0 M Na
<u>Plutonium</u>		
Bondietti, et al., 1975	$1-1.7 \times 10^5$	soil clays, pH 6.5, Pu(IV), 5 ml Ca
	7.5×10^4	soil clays, pH 6.5, Pu(VI), 5 mM Ca
	2.1×10^4	montmorillonite, pH 6.5, Pu(IV), 5 mM Ca
	2.5×10^2	montmorillonite, pH 6.5, Pu(VI), 5 mM Ca
Dahlman, et al., 1975	3×10^5	clay soil, pH 6.5, Pu(IV), 5 mM Ca
Örsum and Parsi, 1974	$1-9 \times 10^4$	Mediterranean sediment
Glover, et al., 1976	35 to 1.4×10^4	17 soil samples, Pu(10^{-6} , 10^{-7} , 10^{-8} M)
Hajek, 1966	$K_f = 10^4$	surface soil, groundwater
Hetherington, et al., 1975	$2-4.8 \times 10^4$	5% clay, 50% silt, 45% sand
Miner, et al., 1974	$>4.3 \times 10^2$	soils
Mo and Lowman, 1975	$.16-3.8 \times 10^5$	clacareous sediment
Noshkin, et al., 1976	2.5×10^5	Ave. value for Enewitak groundwater particulates
Noshkin, 1977 unpub. data	1.1×10^5	coral soil and sediment
	8×10^4	clay silt particulates
Pillai & Mathew, 1976	9×10^4	Ave. value for suspended silt
Wahlgren, 1976	3×10^5	Lake Michigan particulates
Woodhead, 1976	5×10^4	sediments
Fried & Friedman, 1976	$K_f = 10^4$	tuff, Pu(IV), pH 6.7
	$K_f = 3 \times 10^2$	tuff, Pu(VI), pH 6.7

TABLE 5 (Continued)

Reference	$K_d \left(\frac{ml}{g} \right)$	Conditions
<u>Plutonium (Cont'd.)</u>		
Fried, et al., 1977	$K_f = 3 \times 10^4$	limestone, pH 6.7, Pu(IV)
	$K_f = 2 \times 10^4$	basalt "fissure", pH 6.7, Pu(IV)
<u>Thorium</u>		
Nishiwaki, et al., 1972	40-130	med. sand, pH 8.15
	310-470	v. f. sand, pH 8.15
	$2700-10^4$	silt/clay, pH 8.15
Rancon, 1973	8	schist soil, pH 3.2, 1g/1 Th.
	60	schist soil, pH 3.2, 1g/1 Th.
	120	illite, pH 3.2, 1 g/1 Th.
	10^3	illite, pH 3.2, 1 g/1 Th.
	$>10^5$	illite, pH >6, 1g/1 Th.
Dahlman, et al., 1975	1.6×10^5	clay soil, pH 6.5, 5 mM $Ca(NO_3)_2$
Bondietti, et al., 1976	1.6×10^5	silt loam, pH 6.5, Ca sat. clay
	4×10^5	montmorillonite, pH 6.5, Ca sat. clay
<u>Uranium</u>		
Rancon, 1975	3×10^2	clay soil, pH 5.5, 1ppm UO_2^{+2}
	2×10^3	clay soil, pH 10, 1 ppm UO_2^{+2}
	2.7×10^2	clay soil, pH 12, 1 ppm UO_2^{+2}
Dahlman, et al., 1975	4.4×10^3	clay soil, pH 6.5, U(VI), 5 mM $Ca(NO_3)_2$
Bondietti, et al., 1975	6.2×10^4	silt loam, pH 6.5, U(VI), Ca sat.

Future Work

For the purposes of examining the geochemical barrier to radionuclide migration, the estimated retardation factors described above are adequate for TASC's model. However, future improvements to the transport model will require more selective grouping of the radionuclides based on their retardation behavior. Instead of 3 groups we may want 6, or more, depending on how the actinide decay chains are handled. These refinements will be severely limited by the available data.

Our basic knowledge of waste/water/rock interactions is inadequate. The effect of the geochemical environment on retardation can be estimated -- but with much uncertainty. Assumptions need testing. For example, the assumption that ion exchange is zero in shale beds above a salt repository should be questioned. The decision on whether a salt repository can offer acceptable protection may depend on the answer.

Recommendations for research currently needed to answer questions related to ion exchange and retardation include:

1. An evaluation of K_d measurement techniques; i.e., static vs dynamic.
2. The effect on radionuclide retardation by changes in Eh, pH, groundwater composition and rock type.
3. A study of the rates of ion exchange and the question of flow rate vs equilibrium time.

SUMMARY

The available data on distribution coefficients for the biologically important radionuclides present in high level-waste were used to estimate retardation factors (K_f) for a mass transport hydrologic model. The radionuclides were divided into 3 groups: fission products with no sorption ($K_f = 1$), fission products with sorption ($K_f = 10^2$), and the actinides and their daughter products ($K_f = 10^4$). Minimum and maximum values were assigned the latter two groups. Uncertainties as a function of time were estimated at $\pm$ an order of magnitude.

NOTICE

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APPENDIX 3.5

FUTURE REPOSITORY MODEL CYCLES

1. Groundwater Flow Modeling

The present TASC model considers one-dimensional groundwater flow and does not consider other potentially important factors including non-linear factors (e.g., compressibility, some thermal effects, etc.) and lateral dispersion. The general modeling concept has involved an analytical dispersion. The general modeling concept has involved an analytical and/or numerical groundwater analysis performed exterior to the TASC model. Due to the hydrologic simplicity of the initial models, the analog evaluations have been relatively simple being adequately derived from basic analytical flow relationships. However, as more complex models are developed, more sophisticated two-dimensional (or as necessary three-dimensional) methods will be required to develop the flow algorithms and validate the basic TASC model simulations. Including consideration of non-linear factors (i.e., compressibility, some thermal affects, etc.)

The results of these models would then be incorporated into the future cycle TASC models. The resulting TASC model analog might be similar to a suggested third cycle format presented below in item 11. Should this future work indicate that significant errors may be introduced through the present TASC model, these problems would have to be resolved and/or the model altered.

2. Existing Mines and Wells

The effect of both existing and possible future mines and wells may prove to be of major significance to site suitability. In order to perform any credible evaluation of their effects, it is imperative that the nature and occurrence of

existing mines and wells be properly understood. Development of any models which are not consistent with known resource uses and their hydrologic effects will have little meaning and be an obvious weakness which may discredit the model.

The hydrologic effects of existing and future mines and wells must be evaluated in order to be properly incorporated into the TASC model. These effects can be divided into two general categories: the direct effect on the groundwater regime and pathways to the biosphere resulting from well operation and mine dewatering; and the permanent secondary alterations to the strata caused by deformation, stress changes, leaky seals, etc.

3. Heads and Gradients (Including Salinity Variations)

In normal shallow freshwater aquifer systems, the movement of the groundwater is usually controlled by hydrostatic pressure and elevation potentials. However, in deep multi-aquifer systems other potentials can be significant. These potentials may include osmotic potential, thermal potential, chemical potential, and density potential. In the deep sedimentary basins considered for the repository, most of the deep groundwaters are saline and often brine (more than 35,000 ppm dissolved solids). The basic TASC model concept of these high density, saltwaters migrating upward into lighter, fresh groundwaters must be reviewed with respect to these other potentials. The temperature gradients produced by the canisters may also alter the groundwater flow pattern. In addition, the concept of a minimum (threshold) gradient, which is known to be significant in certain clay soils, should be examined. Due to physiochemical interactions, groundwater flow may not occur in certain rocks until a threshold gradient is surpassed. In addition the future climatology model results must be incorporated in the determination of heads and gradients.

4. The Effects of Exploration vs. Undetected Anomalies

Since test borings themselves may represent a significant threat to the integrity of the repository, it is important to assess the relative merit of the information obtained from borings versus their liability. The general approach would involve evaluation of the negative effects of borings and the negative effects and probability of occurrence of undetected anomalies. Properly integrated into the TASC model, the results should provide significant information for site suitability and design performance. An effort is currently underway at San Jose State to provide useful information.

The undetected anomaly problem should also be considered for at least two stages after the repository construction has begun. These recommended stages would include: after the main shafts and corridors are constructed and monitored, and just prior to backfill after completion of the repository when some 30 years of monitoring information is available.

5. Mine Saturation

After mine abandonment, time will be required to re-establish the original groundwater regime and saturate the mine area. Until this occurs, no groundwater will probably flow out of the repository zone. The time required for re-saturation depends on the nature of the original groundwater regime, the effectiveness of seals, and the porosity and permeability of the backfill and mine fracture zones. A preliminary assessment of this effect for the second cycle TASC model has been performed. This work should be continued to refine the data for future cycles.

6. Gas Pathways

The TASC model only considers potential groundwater pathways to the biosphere.

Since the radiation decay of the high level waste canister will produce gas, potential gas pathways should also be evaluated. Other gas sources might include existing natural gas, the entrapped air after mine abandonment, and steam produced from the canister heat. Potential steam pathways may be very significant during the period prior to complete mine saturation.

7. Thermal Effects

The heat from the high level waste canisters will result in a significant temperature gradient around the repository. This temperature gradient may affect various phases of the repository including groundwater flow, gas flow, mechanical behavior of the host rock and backfill material, dissolution behavior, inducement of ground heave, and other effects. This problem is quite complex and has not yet been clearly delineated. Clearly, substantial work is required in this area in order to adequately consider the thermal affects. Many researchers feel that thermal affects may be the single most significant problem in the repository concept.

8. Tectonic Effects

All potential tectonic effects were evaluated using a criteria of a seismic effect of intensity VIII on the modified Mercalli Scale. Although this approach was reasonable for the initial TASC model cycles, the entire approach must be reconsidered for future models. Clearly, the subject of tectonic related changes incorporates a wide range of geologic phenomena including those caused by lower intensity seismic events and those not associated with seismic events.

9. Refined Model Geometry

The initial TASC models represented a relatively specific, geologic and

hydrologic situation. Future models should begin to incorporate more detailed geologic and hydrologic conditions based on the results of detailed regional analyses of actual known conditions. The generic shale and salt basin models that have been developed represent the results of such studies and will be incorporated into future models along with other types of basins. A suggested format for a third cycle and TASC model reflecting a generic shale basin model might include the following (see TASC Analog sketch and Figure 8):

1. Large sedimentary basin; repository in thick shale sequence.
2. Layers (from surface).
 - A-1: Upper non-indurated sediments.
 - A-2: Lower non-indurated sediments.
 - B-1: Sandstone aquifer.
 - B-2: Thick shale deposit (repository zone).
 - B-3: Sandstone aquifer.
 - C: Thick evaporite sequence.
3. Groundwater Regime
 - A-1: Groundwater aquifer, hydraulically continuous with surface waters.
 - A-2: Aquitard.
 - B-1: Artesian aquifer, generally higher pressure than A-1, fresh to saline, may include wells, locally connected to A-1 where A-2 is absent or at anomalies.
 - B-2: Aquitard.
 - B-3: Artesian aquifer, higher pressure than B-1, saline, may include oil or gas wells.
 - C: Aquifer-aquitard sequence, saline to brine, may include oil or gas wells.

Basin recharged along one end and discharged at the other.

4. Unflawed Repository: Multi-Pathways (see sketch).

a-b-c: Upward flow from B-3, through repository to B-1.

c-d-e: Ultimate discharge from basin at discharge area, c-d through B-1, d-e in A-1 to surface water, pathway large (over 50-100 miles) with considerable dilution.

$c_n-d_n-e_n$: (Multi-pathways) Various pathways out of B-1 to A-1 (c_n-d_n); hence to local surface waters (d_n-e_n). Pathways caused by local anomalies (faults, strata change, reefs, etc.), pinching out of A-2, minor leakage through A-2, and/or lateral (vertical) dispersion.

Due to dilution and dispersion, the concentration decreases with distance from the repository. However, the probability of the pathway existing would increase with distance. The final distance d_n-e_n would be a function of surface water environment (arid, wet, etc.). The number and characteristics of these pathways could be made relatively complex to simulate real geologic conditions.

TASC ANALOG SKETCH

5. Flaws

- a. Drinking water wells: A-1, B-1 (layers).
- b. Oil and gas wells: B-3, C (layers).
- c. Mines: C (layers).
- d. Fracture zone around shaft and tunnels.
- e. Borings
- f. Faults

6. Other shale configurations may be required to simulate different overall groundwater flow regimes.

10. Other Rock Types

The initial TASC models reflect only shale and bedded salt. Clearly other rock types will also have to be considered in detail. Of particular interest would be massive crystalline rock and domed salt.

Appendix 4.1 - Future Effort in Hydrology Modeling

PRELIMINARY REVIEW OF NUMERICAL CODES FOR SOLUTE TRANSPORT MODELING

This memo briefly reviews hydrologic and geologic factors which should be included in site suitability analyses and discusses available numerical codes for solute transport modeling of a repository site.

The environment of the repository site can be described by a set of interrelated parameters as follows:

- 1) Geometry
- 2) Properties of the geologic materials
 - a) Permeability
 - b) Porosity
 - c) Degree of saturation
 - d) Chemical composition
 - e) Compressibility
- 3) Properties of the transporting fluid
 - a) Viscosity
 - b) Density
 - c) Compressibility
 - d) Chemical composition
 - e) Temperature

- 4) Characteristics of the transported material and its interaction with the transporting fluid and geologic media
 - a) Source production rate
 - b) Concentration
 - c) Dispersion coefficient
 - d) Radioactive decay constant
 - e) Daughter product production rate
 - f) Sorption/Retardation coefficient
- 5) Hydrologic setting
 - a) Hydraulic gradients
 - b) Hydrologic boundary conditions

In most groundwater applications where temperature and salinity effects are not considered, the chemical composition and compressibility of the geologic medium, and the viscosity and compressibility of the transporting fluid may be neglected or need not be treated individually.

Solute transport problems are in practice composed of two separate parts--a groundwater flow problem and a mass transport problem. The numerical techniques usually applied are: finite differences (FD); finite elements (FE); or method of characteristics (MOC). Comparable results can be obtained using any of these methods. Finite element methods, however, are preferable if complex geometries or higher order approximations must be considered.

The following computer codes are suitable for solute transport modeling. Other programs are available but are less well documented for transport problems than those discussed below.

1. "Simple" models. These codes solve a maximum of two dimensions. The effects of variable temperature and salinity are not considered.

- a) "USGS" program - written by D. Grove at U.S. Geological Survey in Denver. This model interfaces a finite difference flow model by Pinder and Bredehoft with transport solutions using finite elements, finite differences, or method of characteristics as desired. Documentation is poor and input inefficient. Porosity is considered constant.
- b) "Waterloo" program - written by J. Pickens at the University of Waterloo, Canada. This model solves transient transport in a steady state flow field by finite element methods. Quality of documentation is unknown.
- c) ISOQUAD - developed at Princeton University. The program solves transient transport in a steady state flow field by finite element methods. The quality of documentation is unknown.
- d) "Oakridge" model - written by J. Duguid and M. Reeves at Oakridge National Laboratory. This model solves transient solute transport in cross-section using finite element methods. It can be coupled with a saturated--unsaturated flow model. The documentation is poor.

2. "Complex" models. These codes can solve the transport problem in one, two, and three dimensions.

- a) TRUMP - written by A. Edwards at LLL. This code solves a set of simultaneous partial differential transport equations with four independent variables and three primary dependent variables using integrated finite difference techniques. Originally developed for geothermal applications, the program can be used to solve both flow and transport problems. Complex boundaries are easily handled but permeability and dispersion coefficients are treated as scalars. TRUMP is currently being used on the NRC project by H. Cheung to model thermal gradients near the repository site.
- b) BIFED - developed primarily by C. Voss at Princeton University. This code uses block iterative, finite element methods to solve coupled non-linear second order partial differential equations.
- c) DAVIS/3FE - written by S. K. Gupta jointly at UC-Davis and Princeton University. This program computes transient flow and salt transport in large multiaquifer basins using finite element methods.
- d) INTERCOMP - developed by Intercomp and U.S. Geological Survey for Sandia. This code is a transient, finite difference solution for deep-well waste-disposal systems. Viscosity and density are allowed to be functions of

pressure, temperature, and composition. Decay rates may be calculated at each time change or at the end of the program.

Criteria for evaluating these codes for our purposes should be based on:

- (1) Degree of complexity required. All of the models listed above will solve a transient transport problem in a steady state flow field. As far as I know, only INTERCOMP is capable of including both temperature and salinity effects. TRUMP and BIFED may be able to handle these effects or can be modified to do so. Also any of the two dimensional models could be modified to deal with the temperature and salinity effects.
- (2) Documentation and operator requirements. Implementation and modification of the "complex" models requires personnel with modeling expertise and a familiarity with the code to be used. That expertise is available at LLL for the TRUMP code but would have to be developed for the other "complex" models.
- (3) Data availability.
- (4) Cost and computer storage limitations.

APPENDIX 4.2

CLIMATOLOGY EFFECTS ON HYDROLOGY PARAMETERS

TABLE I

Time of Representative Patterns From Past Climate Regimes	Characteristic	Location on Time Line
20,000 - 17,000 BC .	Full Glacial	Minimum eccentricity
7,000 - 6,000 BC	"Boreal" Early Warm	Few thousand years before peak in procession
4,000 BC	"Atlantic" moist post glacial-warm	Maximum in procession
2,000 BC	"Sub-Boreal" dry post glacial-warm	Maximum in procession
500 BC alas 1550-1700	"Little Ice Age"	Post maximum in procession

Figure 1

101 PREC EXP. 19-18 - ICE AGE EXP.-SUMMER CONTROL WLG RAND N/A
 TOTAL PRECIPITATION (MM/DAY)
 GLOBAL MEAN = -0.605
 DASHED LINE 0.00
 TIME = 1 JUL TO 1 AUG
 INTERVAL 5.00

FIGURE 2

* Based on Data from 1901-1950

FIGURE 3