Waste Isolation Safety Assessment Program

**Technical Progress Report
for FY-77**

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April 1979

Prepared for
Office of Nuclear Waste Isolation
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SUMMARY

The purpose of the Waste Isolation Safety Assessment Program (WISAP) is to develop a technology that can be used to evaluate the post-closure effectiveness of deep geologic nuclear waste repository systems. The work conducted by the Pacific Northwest Laboratory in FY77 centered in four subject areas: 1) the analysis of potential repository release scenarios, 2) the analysis of potential release consequences, 3) the measurement of waste form leaching rates, and 4) the measurement of the interactions of dissolved radionuclides with geologic media.

Progress during FY77 included:

- the evaluation of potentially applicable release scenario analysis methods
- the initiation of the development of a release scenario computer model
- the evaluation of potentially applicable release consequence analysis methods
- the initiation of the development of a release consequence analysis computing system
- the formulation of a mathematical model for transport of radionuclide decay chains in geomeia which considers multiple, chemically reacting species and irreversible mineralization
- the formulation of a mathematical model for the long-term accumulation of radionuclides in crop plants
- the preparation of sample glass waste forms doped with long-lived radionuclides
- the initiation of leaching studies on the doped glasses and on spent fuel
- the initial evaluation of sorption measurement methods
- the measurement of sorption characteristics for a generic data bank

- the development of correlations relating the empirical sorption distribution coefficients to the values of important system parameters
- the completion of studies to predict the maximum solution concentrations possible for geologic isolation environments
- the initiation of studies on the effect of solution ionic strength on nuclide sorption, controlled Eh-pH sorption for plutonium, and the solubility of plutonium compounds.

CONTENTS

SUMMARY	iii
LIST OF FIGURES	vii
LIST OF TABLES	viii
ACKNOWLEDGMENTS	xi
1. INTRODUCTION	1-1
2. ASSESSMENT METHODS DEVELOPMENT	2-1
2.1 RELEASE SCENARIO ANALYSIS	2-1
2.1.1 Identification of Potentially Disruptive Phenomena	2-1
2.1.2 Evaluation of Release Scenario Analysis Methods	2-2
2.1.3 Development of Repository Simulation Analysis	2-15
2.2 RELEASE CONSEQUENCE ANALYSIS	2-20
2.2.1 Evaluation of Release Consequence Analysis Methods	2-20
2.2.2 Development of Modeling System	2-29
2.2.3 Modeling System Refinements	2-34
3. DATA BASE DEVELOPMENT	3-1
3.1 WASTE FORM RELEASE RATE DATA	3-1
3.1.1 Preparation of Doped Glass Waste Forms	3-1
3.1.2 Leaching of Doped Waste Glass Forms	3-9
3.1.3 Leaching of Spent Fuel	3-13
3.2 RADIONUCLIDE GEOCHEMICAL INTERACTION DATA	3-18
3.2.1 Evaluation of Sorption Measurement Methods	3-18

CONTENTS (contd)

3.2.2	Generic Sorption Data Bank	3-28
3.2.3	Analysis of Generic Sorption Data	3-28
3.2.4	Validation Studies	3-34
3.2.5	Sorption Mechanism Studies	3-35
4.0	WORKSHOPS	4-1
4.1	SAFETY ASSESSMENT METHODS WORKSHOP	4-1
4.2	HYDROLOGIC AND CONTAMINANT TRANSPORT METHODS WORKSHOP	4-1
4.3	GEOLOGIC ANALYSIS WORKSHOP	4-3
4.4	GEOCHEMICAL INTERACTION DATA WORKSHOP	4-4
5.	REFERENCES	5-1
APPENDIX A:	DETAILS OF REPOSITORY SIMULATION MODEL DEVELOPMENT .	A-1
APPENDIX B:	DESCRIPTIONS OF POTENTIALLY APPLICABLE MODELS FOR RELEASE CONSEQUENCE ANALYSIS	B-1
APPENDIX C:	DETAILS OF GETOUT MODEL EXTENSION FOR IMPULSE RELEASE	C-1
APPENDIX D:	SORPTION DATA BASE DETAILS	D-1
DISTRIBUTION LIST		Dist-1

LIST OF FIGURES

1.1	WISAP Interfaces	1-3
2.1	Stratified Site Model	2-19
2.2	Two-Dimensional Surface Elements Used for DAVIS FE Model Verification with Long Island Hydrologic Data . .	2-32
2.3	Three-Dimensional Stratigraphic Elements Used for DAVIS FE Model Verification with Long Island Hydrologic Data	2-33
2.4	Schematic Diagram of a Two-Member, Two-Species Decay Chain with Chemical Reaction and Irreversible Mineralization	2-36
2.5	Radionuclide Exchange Processes for Irrigated Soil/Crop Plant Systems	2-38
3.1	X-ray Diffraction Patterns for Doped Glasses	3-7
3.2	X-ray Diffraction Patterns for Resistance and Induction Heated Melts	3-8
3.3	Micrographs of Doped Glasses	3-10
3.4	Radiograph and Micrograph of Curium Doped Beads	3-11
3.5	Schematic Diagram of Axial Filtration Apparatus	3-22
3.6	Schematic Diagram of High-Pressure Intact Core Flow-Through Column Apparatus	3-25

LIST OF TABLES

1.1	Waste Isolation Safety Assessment Program - FY77 Activities	1-6
2.1	Potentially Disruptive Phenomena for Nuclear Waste Repositories	2-3
2.2	Consultant Categories	2-17
2.3	Categorization Format for Hydrologic and Contaminant Transport Models	2-22
2.4	Hydrologic and Contaminant Transport Models Useful for Waste Isolation Safety Assessment	2-24
2.5	Water-Dose and Air-Dose Models Useful for Waste Isolation Safety Assessments	2-27
2.6	Characteristics of WISAP Release Consequence Analysis Models	2-30
2.7	Comparison Between Seed Concentrations Predicted by the 50-Year Accumulation Assumption and the Long-Term Accumulation Model	2-40
2.8	Health Effects Conversion Factors	2-41
3.1	Composition of Frit, Wastes and Doped Waste Glass Used for Actinide Release Studies	3-3
3.2	Doped Glass Bead Characteristics	3-6
3.3	Leaching Schedule for Doped Waste Glasses	3-12
3.4	Waste Form Leach Solutions	3-13
3.5	Chemical Composition of Salt Brine	3-14
3.6	Ionic Concentration of Salt Brine	3-15
3.7	Doped Glass Leach Solution Analyses	3-16
3.8	Leaching Studies for Doped and High-Level NFS Glasses and Spent Fuel	3-17

LIST OF TABLES (contd)

3.9	Comparison of K_d by the Batch, Low-Pressure Column, and Axial Filtration Methods	3-26
3.10	Comparison of K_d by the Batch and Soil Channel Chromatography Methods	3-26
3.11	Information Requirements for Generic Data Bank	3-30
3.12	Preliminary Empirical Sorption Correlations Using Linear Regression	3-30
3.13	Preliminary Distribution Coefficients for Strontium, Cesium, Americium and Plutonium with Basalt and Plagioclase Feldspars Similar to those Present in Basalt	3-31
3.14	Preliminary Distribution Coefficients for Cesium with Montmorillonite	3-32
3.15	Preliminary Distribution Coefficients for Plutonium and Americium with Tablets and Crushed Material	3-33

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1. INTRODUCTION

Commercial nuclear power production and utilization requires safe management of potentially hazardous radioactive waste materials. To meet this need, the U.S. Department of Energy (DOE) is sponsoring the National Waste Terminal Storage (NWTs) Program whose mission is to implement nuclear waste isolation repository systems that prevent the waste radionuclides from causing adverse effects to present and future humans and their environments. Comprehensive analyses are needed to quantify the effectiveness of specific isolation systems in achieving that mission.

Under sponsorship of the NWTs Program the Waste Isolation Safety Assessment Program (WISAP) was begun at the Pacific Northwest Laboratory (PNL) on December 1, 1976. WISAP builds on studies of geologic isolation systems performed at PNL from 1972 to 1976 under the Advanced Waste Management and Waste Management Systems Studies Programs sponsored by the Atomic Energy Commission (AEC) and the Energy Research and Development Administration (ERDA). The mission of WISAP is to provide methods and data for evaluating the performance of nuclear waste repository systems. By direction of the program's manager, the Office of Waste Isolation (OWI), the scope of the WISAP mission is restricted to exclude consideration of: 1) the repository performance prior to sealing (i.e., short-term effects) and 2) phenomena caused by presence of the waste on or in the materials or phases present in the repository system (i.e., near-field effects). Thus the WISAP scope includes only long-term, far-field considerations. Although not a comprehensive performance assessment program, WISAP does provide technology useful during many stages of the development and operation of repositories.

The process of establishing and operating a geologic nuclear waste repository can be divided into eight steps: 1) site reconnaissance, 2) site exploratory evaluations, 3) repository design, 4) site environmental impact statement procedures, 5) repository construction, 6) repository licensing procedures, 7) licensed repository operation, and

8) filled repository maintenance. These steps are shown in approximate time sequence on the upper half of Figure 1.1. During Steps 2, 3, 4, 6, and 8 major decisions (i.e., What site? What design? Environmental impacts acceptable? Safe enough?, and Make irretrievable?) must be made by DOE and the Nuclear Regulatory Commission (NRC). For each of these decisions, comprehensive assessments must be made to provide the necessary supporting information. WISAP starts with the basic understanding of long-term, far-field repository system phenomena provided by man's scientific and technological experience and organizes that understanding into a system model. WISAP then obtains the data necessary to exercise the system model (with help from other parts of the NWTs Program) and performs the assessments shown by the labeled arrows. To properly perform comprehensive assessments for all of the repository development steps shown in Figure 1.1, short-term and near-field assessments are necessary to complement the WISAP results and in the best of circumstances these assessments would precede those of WISAP in order to provide the boundary conditions for long-term, far-field assessments. There are four kinds of assessments which can be performed using WISAP technology (at least in part):

1. alternative site comparisons for site selection
2. long-term radiological impact assessments for environmental impact procedures
3. long-term safety assessments for repository licensing procedures
4. long-term safety assessments for repository closure procedures.

These assessments are briefly described in the paragraphs that follow.

When site options are available, choices must be made between the alternative sites. WISAP release scenario analysis methods are intended to provide a rationale for these decisions by considering simultaneously the effects of the natural and man-caused phenomena on the sites' abilities to prevent potential radioactivity transport agents from contacting the waste. The parameters or factors necessary to describe these phenomena are measurable properties of the sites, and the result of

FIGURE 1.1. WISAP Interfaces

the assessment will be influenced by their numerical value. However, some factors may not be completely quantifiable, and if the nonquantifiable factors are of dominant importance to the site selection decision, a technically objective choice between sites will not be possible. The procedure for choosing between alternative sites has the following steps:

1. Measure the site selection factors (e.g., rock permeabilities) during the exploratory evaluations at all alternative sites
2. Exercise the WISAP release scenario and release consequence analysis methods for the sets of measured factor values and reference waste package and repository design specifications
3. Compare the results between sites and select the sites with the lowest dose results that also meet available NRC/EPA standards.

After the repository sites have been selected but before beginning final repository design and construction, an environmental report must be completed. WISAP methods are intended to provide the means to estimate the long-term radiological portion of those environmental impacts in a consistent manner for all candidate sites. The long-term radiological impact estimation procedure has the following steps:

1. Determine values of the repository system parameters from the continuing site evaluations and the reference waste package and repository design specifications.
2. Exercise WISAP release consequence analysis methods for typical release scenarios.

The outputs from these calculations are dose-to-man estimates and contamination boundaries.

Before repositories for commercial waste can be operated, a license must be granted by the NRC. During the licensing procedures, a safety report must be completed for the repository system. WISAP methods are intended to analyze the far-field potentially disruptive human and natural phenomena which are important to the long-term safety performance of the repository system. Technology outside of WISAP will be required to assess short-term and near-field safety. Analyses in all of these areas will be

necessary to perform a comprehensive safety assessment. The procedure for the WISAP portion of these assessments has the following steps:

1. Update the values for the site properties and organize the results of the short-term and near-field assessments into appropriate boundary conditions for long-term far-field analysis.
2. Exercise WISAP release scenario analysis methods to define the probability weighted distribution of release scenarios which are possible.
3. Exercise WISAP release consequences analysis methods to estimate the consequences of those release scenarios.

The primary outputs of these analyses are dose commitments to individuals living at various future times. Secondary outputs can be population doses and health effects.

Safety analyses of a similar kind are also expected to be required to support the decision to close the repository when the ability to retrieve the waste is no longer desired.

This document reports progress made in FY77 toward accomplishing the WISAP mission. Where a topical report has been or is about to be issued, the information is summarized without going into the technical details. Where a topical report is not imminent, detailed technical information is included. Where appropriate, supporting information is given in the Appendices. A summary of this report was issued earlier in PNL-2451, "Waste Isolation Safety Assessment Program - Summary of FY77 Progress."

Work in FY77 can be conveniently classed according to whether it supported the development of assessment methods or the development of the data base required for method application. Table 1.1 lists the FY77 activities in each of these classifications. The discussion in the remainder of this document is organized in a manner consistent with Table 1.1.

TABLE 1.1. Waste Isolation Safety Assessment Program - FY77 Activities

<u>Assessment Methods Development</u>	<u>Data Base Development</u>
Analysis of Potential Release Scenarios:	Waste Form Release Data:
Assemble a geophysics research team for development of applicable predictive geology	Preparation of sample glass waste forms doped with long-lived radionuclides
Identification of natural and man-caused disruptive events and processes	Leaching of doped glass waste forms
Evaluation of potentially applicable analysis methods	Leaching of spent fuels
Development of repository simulation analysis	Radionuclide Geochemical Interaction Data:
Analysis of Potential Release Consequences:	Evaluation of sorption measurement methods
Evaluation of potentially applicable analysis methods	Sorption measurements for generic data bank
Development of computational modeling system using methods selected	Analysis of generic sorption data
Refinement of the component models of the system	Validation studies
	Sorption mechanism studies

2. ASSESSMENT METHODS DEVELOPMENT

Performance assessments for geologic isolation repositories have six elements:

1. identification of the events and processes which could potentially cause breach of containment at the repository cavity
2. analysis of the ways these phenomena could combine to cause containment breaches
3. quantitative description of the radioactivity release scenarios
4. prediction of radionuclide release rates from the repository cavity
5. prediction of the transport of released radionuclides to man
6. prediction of radionuclide interaction with man.

Assessment method development activities related to the first three elements can be considered together under the term "Release Scenario Analysis," while those related to the last three elements can be considered together under the term "Release Consequence Analysis."

2.1 RELEASE SCENARIO ANALYSIS

2.1.1 Identification of Potentially Disruptive Phenomena

The first step in predicting repository release scenarios is the identification of potentially disruptive phenomena. There have been several previous attempts to identify these phenomena.^(1,2) Schneider and Platt⁽¹⁾ reported a preliminary fault tree for geologic disposal which contained a number of these phenomena as initiating events. Logan⁽²⁾ reported a list of phenomena obtained during the course of a workshop attended by geoscientists and safety analysts. Using this prior work as a basis, a new and expanded list of phenomena was developed. The phenomena were grouped into three classes:

1. natural geologic phenomena
2. man-caused phenomena
3. waste-induced phenomena.

Phenomena in these groups are listed in Table 2.1. These phenomena include events (e.g., drilling into repository) and processes (e.g., glaciation). The events occur over relatively short time periods and are described by probability distributions. The processes occur over relatively long time periods and are described by initiation probability distributions and phenomena rate, duration, and lag time distributions. Many of these phenomena are interrelated, and thus the classification shown in Table 2.1 is somewhat arbitrary. Furthermore, the list is not all-inclusive.

2.1.2 Evaluation of Release Scenario Analysis Methods

Once the disruptive phenomena have been identified, a method or combination of methods must be developed to analyze the ways these phenomena could combine to cause breaches in containment at the repository cavity. The method(s) must also describe the repository release scenarios. In this study, prior to method development, available release scenario analysis methods were analyzed. This section summarizes the results of that evaluation. A more detailed discussion of this evaluation is presented in PNL-2643, "Scenario Analysis Methods for Use in Assessing the Safety of the Geologic Isolation of Nuclear Waste."

Many criteria can be developed to guide the evaluation, but three are more important than the others. The first of these follows from the products which can be obtained by application of a release scenario analysis method or methods (together with the release consequence analysis methods discussed in Section 2.2). The products are:

1. alternative site comparisons
2. long-term safety assessments.

Both of these applications require quantitative prediction of: 1) the probability weighted distribution of possible containment breaches at the repository cavity and 2) the conditions of the repository system during and after the breach using the logic and principles of the scientific method. The first is necessary in order that the analyses are not biased toward the low probability - high consequence release scenarios. The second is necessary in order to determine the boundary conditions for

TABLE 2.1. Potentially Disruptive Phenomena for Nuclear Waste Repositories

Natural Phenomena	Man-Caused Phenomena	Waste-Induced Phenomena
Climatic Fluctuations	Improper Design/Operation	Thermal Effects
Glaciation	• Shaft Seal Failure	• Differential Elastic Response
Denudation and Stream Erosion	• Improper Waste Emplacement	• Non-Elastic Response
Magmatic Activity	Undetected Past Intrusion	• Fluid Pressure Changes
• Extrusive	• Undiscovered Boreholes	• Fluid Migration
• Intrusive	• Mine Shafts	• Canister Migration
Epeirogenic Displacement	Inadvertent Future Intrusion	Chemical Effects
• Igneous Emplacement	• Archeological Exhumation	• Geochemical Alterations
• Isostasy	• Weapons Testing	• Corrosion
Orogenic Diastrophism	• Non-Nuclear Waste Disposal	• Waste Package - Geology Interactions
• Near-Field Faulting	• Resource Mining (Mineral, Hydrocarbon, Geothermal, Salt)	• Gas Generation
• Far-Field Faulting	• Storage of Hydrocarbons or Compressed Air	Mechanical Effects
• Diapirism		• Local Fracturing
• Diagenesis		• Canister Movement
Static Fracturing	Intentional Intrusion	Radiation Effects
• Surficial Fissuring	• War	• Material Property Changes
• Impact Fracturing	• Sabotage	• Radiolysis
• Hydraulic Fracturing	• Waste Recovery	• Criticality
Meteorites	Perturbation of Groundwater System	• Decay Product Gas Generation
Dissolutioning	• Irrigation	
Sedimentation	• Reservoirs	
Flooding	• Intentional Artificial Recharge or Withdrawal	
Undetected Features	• Establishment of Population Center	
• Faults, Shear Zones		
• Breccia Pipes		
• Lava Tubes		
• Gas or Brine Pockets		

subsequent release consequence analysis. As a result of the criterion that the method be quantitative and based on the principles of science, method applications will be amenable to both sensitivity and uncertainty analyses.

The second and third criteria follow from unique features of this assessment problem. A deep geologic nuclear waste repository may be affected by a large number of potentially disruptive phenomena. The effect of a given phenomenon is often a function of its interaction and timing with respect to other phenomena. Since analytical representations of the many complex situations are not possible with the present state of our knowledge, at least a portion of the assessment method should be stochastic (i.e., our understanding and data availability at the level of resolution required preclude a completely deterministic analysis). Furthermore, since a list of potentially disruptive phenomena includes both events (e.g., meteoritic impact) and processes (e.g., erosion), the method should be capable of treating both discrete and continuous perturbations of the repository system.

In summary, the evaluation of the release scenario analysis methods was based on the following criteria:

1. The method should yield quantitative information about potential release scenarios and be based on the principles of science.
2. The method should be compatible with system knowledge and data.
3. The method should analyze discrete events and continuous processes and their complex interactions.

The release scenario analysis methods identified included: expert opinion/Delphi, classical systems analysis, fault/event trees, and Monte Carlo/Markov chain analysis. These methods are described in the next four sections.

2.1.2.1 Expert Opinion/Delphi

Expert opinion is a qualitative assessment technique in which a recognized body of experts determines whether an activity is acceptably safe or not. This was the original waste isolation safety assessment

method applied in 1957 by the National Academy of Sciences in recommending that high-level wastes be stored in bedded salt formations.⁽³⁾

An important feature of expert opinion is credibility, and difficulties often arise over the individual qualifications of an expert. This is particularly true where the experts are perceived to be associated with special interest groups. Furthermore, the experts commonly disagree. Reasons for disagreement include: stepping beyond the bounds of real expertise, operating from different (but unstated) premises, differing personal values, selected use of technical knowledge, and an emotional desire to win the argument.^(4,5,6) When views of experts conflict and credibility is questioned, the decision must rely on the completeness of data and analyses which support the conflicting opinions.

Biases in opinion are common and subtle. In developing an opinion, experts rely on methods that simplify the assessment process but that can lead to error. Examples of these are summarized below:

1. representativeness - the prediction of a condition based on representative data and general relationships which hold in most (but not all) cases
2. availability - the prediction of conditions according to the ease with which those conditions are brought to mind from the expert's past experience
3. adjustment - the prediction of some condition by starting with a parameter value from a known system and adjusting it for differing characteristics of the new system
4. anchoring - the prediction of some condition by referring to a parameter value of a known system without adjusting that value for the differing characteristics of the new system.

An effort to minimize opinion biasing is part of all well-performed expert opinion solicitations.

Expert opinion can be solicited in three ways:

1. workshops - A decision is reached by collective examination of the issues. Individual contributions can be diluted or suppressed by

three factors: (a) dominant individuals overly influence results; (b) the information is filtered or scrambled by the use of imprecise descriptions (semantic noise); and (c) group pressure for conformity may minimize input from participants with different views.

2. individual interviews - Individual decisions are reached by individual examination of the issues. However, it is not easy to obtain a collective decision because the maintenance of consistent interview procedures is difficult.
3. Delphi method - A consensus decision is reached by individual examination of the issues with collective feedback. This method attempts to combine the best features of workshops and individual interviews.

Delphi is a structured method of obtaining expert opinion which produces an estimate of the certainty of the safety conclusion. The method originated at the Rand Corporation in 1948.^(7,8,9) It has not been applied to the waste isolation repository assessment problem. The classic Delphi approach consists of a series of questionnaires given individually to a group of experts. The first questionnaire elicits the opinions of the experts based on only their own knowledge and experience. Subsequent questionnaires feed back results from the previous questionnaires, which then allows the experts to comment on the group consensus. The process occurs until there is convergence of opinion or it becomes obvious that additional results will not be produced. The Delphi procedure consists of the following steps:

1. selection of a group of qualified experts
2. preparation of a questionnaire by the study directors that requires the respondent to address study objectives with scaled or numerical input
3. issuance of instructions and ground rules
4. answering the questionnaire (by the experts)
5. incorporation of the statistical results of the first questionnaire into the questions of the second questionnaire
6. repetitive answering of the questionnaire until convergence.

Respondents at the ends of the distribution of results from any questionnaire can be asked to provide written justification for their opinion. Three or four administrations of the questionnaire are usually sufficient to obtain convergence.

The expert opinion and Delphi methods have the advantage of simplicity but the disadvantage of subjectivity. Subjectivity has become increasingly significant in the last decade with the growth of distrust of technology and technologists. However, these methods will be essential in release scenario analysis to provide input to the assessment in areas where the state of knowledge is incomplete or data cannot be obtained.

2.1.2.2 Classical Systems Analysis

Classical systems analysis is the completely deterministic prediction of system behavior using the laws of science and engineering. This technique requires that explicit relationships exist between all processes at work on and within the system. This kind of analysis has two parts, the determination of whether certain occurrences are possible and the prediction of the resulting conditions of the system subsequent to those occurrences. The usual method of accomplishing the first part is stability analysis; the method for accomplishing the second part can be termed science and engineering analysis.

Stability analysis is a deterministic technique for analyzing whether important properties of the system of interest remain unchanged if the system is disturbed. Applications of the technique, which began appearing in the middle of the nineteenth century, span the entire range of science and engineering disciplines.⁽¹⁰⁻¹⁴⁾

The analysis procedure begins by developing an idealized conceptual model of the system and specifying the system property whose stability is to be analyzed. Mathematical models are then made of the important processes at work within the model system. This modeling activity produces a set of coupled differential equations (along with mathematical expressions for the appropriate boundary conditions) which describes not only the individual processes but also their interaction. Linear and

nonlinear stability analyses are then performed on the model system. The linear analysis determines the system's response to mathematically imposed small arbitrary disturbances. Such small disturbances are present in all real systems. When performing the linear analysis the descriptive equations and the boundary conditions are linearized (if they were initially nonlinear). Thus, an analytical solution to the descriptive equations is often possible. The nonlinear analysis determines the system's response to large arbitrary disturbances. Such large disturbances are occasionally present in real systems as a result of rapidly occurring events. A numerical solution to the nonlinear equations is normally required. If the model system damps the imposed disturbances and the property of interest returns to its predisturbance state, the system is said to be stable; if the system allows the disturbance to grow in amplitude, the system is said to be unstable, and the analysis proceeds by determining the rate of approach to system breakdown. Breakdown occurs when the unstable property has changed to such an extent that the modeled system can no longer be described by the original set of descriptive equations.

To apply stability analysis techniques, the processes of the system must be expressed in quantitative mathematical form and the data must exist to evaluate the physical constants and boundary conditions. This requires that the system of interest be well characterized. The output of this analysis is either a conclusion that the system is stable or that the system is unstable and approaching breakdown at a predicted rate. By varying the range of the input parameters, the region of instability can be bounded, and this is useful in system design.

To date there have been no applications of stability analysis to the assessment of geologic isolation safety although the use of the technique for this purpose has been proposed.⁽¹⁵⁾ Although beyond the scope of WISAP, stability analysis may be useful in determining whether the combination of the natural geologic processes and the processes induced by the presence of the waste (i.e., processes caused by chemical potential, radiation, thermal and/or mechanical force gradients) cause instability of

one or more of the properties of the repository system. The results of this instability could be manifest in occurrences such as local fracturing, metamorphosis of the local geology with subsequent repository collapse, movement of the repository as a whole, or movement of individual canisters with subsequent meltdown and/or criticality. These occurrences in turn could cause radionuclides to be released from containment at the repository cavity. Both the linear and the nonlinear analysis techniques may be useful; in particular, nonlinear analysis could be used to evaluate whether the occurrence of large disturbances such as earthquakes could initiate instability in the system.

Stability analysis seems well suited to analyzing whether certain processes or combinations of processes at work on and in a geologic isolation repository could cause changes in system properties that lead to unwanted occurrences. However, the technique is not well suited to analyzing events because these are difficult to model by continuum mathematics. Furthermore, since stability analysis requires a well-characterized system, it may not be useful for the natural geologic processes. Thus, stability analysis is not a comprehensive technique for geologic isolation safety assessments but rather may be a specialized method for analyzing a portion of the safety assessment problem.

Science and engineering analysis investigates the instability scenarios identified in the first part of the analysis to determine the effect of their occurrence on the system (e.g., determine the effect of canister movement on the repository after a stability analysis showed that such movement was possible). There are an extremely large number of references to this kind of analysis.

The analysis uses the same system model developed for the stability analysis and simultaneously solves the resulting set of differential equations subject to the boundary conditions. If the system equations are linear or can be accurately approximated as linear, analytical solutions are possible. However, if the equations are nonlinear, numerical solution of the equations is usually required.

The critique of stability analysis made above holds for science and engineering analysis as well. Together these techniques can deterministically describe the behavior of the repository system for those disruptive phenomena which are well characterized. However, since our knowledge of some of the potentially disruptive phenomena is insufficient to permit deterministic analysis, classical systems analysis does not seem sufficient to assess geologic isolation safety when used alone.

2.1.2.3 Fault/Event Tree Analysis

The fault tree and event tree analysis techniques are the conventional methods for system reliability and probabilistic safety analysis. These methods were used to analyze the safety of nuclear reactors and have been used extensively elsewhere in the nuclear industry.⁽¹⁶⁾ In this approach, system failure logic is graphically displayed in tree-like structures. Computer-aided methods are available for analyzing these structures to determine both qualitative and quantitative aspects of system reliability and probabilistic safety performance.

Steps in fault or event tree analysis can include:

1. system definition
2. logic model construction
3. qualitative analysis
4. common cause failure analysis
5. quantitative evaluation
6. uncertainty analysis
7. formulation of conclusions and recommendations.

System definition is often the most time consuming aspect of the analysis. The following must be established:

1. system physical bounds
2. the failure event of interest
3. the initial state of all system components
4. events with an occurrence probability of zero
5. events with an occurrence probability of unity

6. the limit of resolution of the analysis
7. a detailed understanding of the system functions and interrelationships.

Qualitative analysis consists of the study of the logic models. Computer programs⁽¹⁷⁻¹⁹⁾ are available to determine the minimal cut sets for the logic model. (A cut set is a collection of basic events that, if they all exist, means the main failure of interest will exist.) A minimal cut set means that if any event is removed the cut set no longer exists. The minimal cut sets are suitable input for a common failure analysis.

The common cause failure analysis is a search for dependencies among basic events. Conventionally, only dependencies among the events in one of the minimal cut sets are sought; i.e., only dependencies that cause system failures are considered. Extensive computer-aided methods exist for common cause failure analysis.^(20,21)

Quantitative evaluations involve determining reliability characteristics of the main event of interest (e.g., release of radioactive material). These reliability characteristics include:

1. the reliability - the probability the event has not occurred
2. the availability - the probability the event does not exist at the specified time
3. the expected number of events during a time interval
4. the mean time to the event.

Not all of these characteristics are meaningful for every analysis. Computer programs exist to aid in determining these characteristics.⁽¹⁹⁻²³⁾

Uncertainty analysis is concerned with establishing an interval estimate of the reliability characteristic of interest based on uncertainty in the input data for the basic events. No uncertainty is reflected in this interval for errors or omissions in the logic model. Computer programs for uncertainty analysis exist.⁽¹⁶⁾

Fault tree analysis is a deductive probabilistic technique by which the component failures leading to system failure can be logically

deduced. It was developed by the aerospace industry in the early 1960s.⁽²⁴⁾ Application of the technique yields combinations of basic events whose occurrence causes the undesired system failure events. The application of fault trees requires a detailed knowledge of the system under study and explicit interrelationships between the various components which make up the system. Fault tree analysis starts with careful definition of the failure event and systematically diagrams backward in time to identify the events or combinations of events that could cause the failure event to occur. The logic is displayed graphically using Boolean logic in a tree-like structure. The process stops when the analyst defines events that are either not amenable to further resolution or where it appears there is no need for additional definition. These latter events are termed basic events. This tree is then analyzed to determine the set of cut sets which can lead to the occurrence of the failure event. The failure rates and repair rates for each component of the fault tree are inputs for probabilistic evaluation. The fault tree can be evaluated in terms of the probability of the failure event and/or the probabilities of the individual cut sets. Consequence analysis is then performed on the identified system failures. For small fault trees the calculations can be made by hand. For larger trees computer analysis is required. Many computer programs exist to analyze fault trees.^(17-19,25,26) Traditional fault tree analysis considers just the probability of the failure event or the cut sets. Methods are now available to estimate the risk characteristics of fault trees where risk is defined as the product of probability and consequences.^(22,23,28,29)

Schneider and Platt⁽¹⁾ reported a preliminary fault tree for the geologic disposal of high-level waste which analyzed the relationships of 77 basic events. This fault tree was never evaluated.⁽¹⁾ Logan⁽²⁾ applied the fault tree approach to a hypothetical high-level waste repository in salt in southeastern New Mexico.⁽³⁰⁾ Fault trees were constructed to describe the relationships between various geologic and man-caused events. The trees were evaluated and failure event probabilities for exhumation, upheaval, and ground-water transport scenarios were estimated. Consequence analyses were then performed for

the identified releases from containment. Proske developed fault trees for a geologic repository in salt for three time periods: operational, 1000 years, and 1,000,000 years.⁽³¹⁾ The failure event was release of radionuclides from the repository to the surrounding geologic strata. Consequence calculations were not performed. Bertozzi et al., used fault trees to evaluate the safety of a salt repository for the period from 1000 to 1,000,000 years after disposal.⁽³²⁾ The fault trees included 30 primary events. Consequence analyses were not performed.

Event tree analysis is an inductive probabilistic technique which reverses the fault tree approach by starting with the basic events and working forward in time to display their logical propagation to system failure events. The method evolved from formal analysis of business decisions. Event trees diagrammatically illustrate the alternative outcomes or consequences of a specified initiating event. In business applications the trees are termed decision trees and are used to evaluate the various outcomes of business and investment decisions.^(33,34) However, use of these trees in system safety has evolved into a discipline quite removed from the original theory.^(16,22,27) In safety assessment the trees provide a pictorial representation of outcomes and provide the basis for a quantitative risk assessment of the various sequences which arise from an initiating event. Consequence analyses are performed on the failures identified from the event tree analysis. There have been no applications of the event tree technique to the geologic isolation safety assessment problem.

Because of its "binary" logic the fault/event tree approach is well suited for quantitatively analyzing events which either occur or do not occur; however, it is not well suited for analyzing processes which occur continuously at some finite rate. Furthermore, because of their deterministic nature, fault/event trees are not well suited for analyzing the interaction of the many different possible sequences of the potentially disruptive phenomena. The state of knowledge about the events and processes affecting geologic isolation repositories does not permit deterministic relationships to be developed for all interactions of those phenomena.

2.1.2.4 Monte Carlo/Markov Chain Analysis

Monte Carlo and Markov chain techniques are stochastic methods of simulation analysis. These methods are generally used for systems that cannot be described in a deterministic manner either because the system is too complex to be described in abstract mathematical form or because the mathematical equations cannot be solved analytically.

A simulation analysis describes the time behavior of the system by a series of mathematical "experiments" which utilize known information about system processes. A number of "simulation languages" are available which simplify the task of writing computer simulation programs.⁽³⁵⁻⁴⁰⁾ These languages provide a generalized structure for designing simulation models and provide flexibility in the output formats.

Monte Carlo analysis (as applied in safety assessment) begins by listing the basic system events and estimating their probabilities of occurrence. The analysis then steps through time assuming occurrence of these events according to their estimated probability distributions until a system failure occurs. By performing the simulation a large number of times, a distribution of failures can be determined.⁽⁴¹⁾ Consequence analyses are then performed on this failure distribution.

Markov chain analysis begins by specifying the possible states of the system and determining the probabilities for transition between those states. Implicit in the analysis is the assumption that the transitional probability between two states is independent of earlier states of the system. The analysis then steps through time assuming probabilistic occurrence of the transitional events until a system failure occurs. Rather than simulate the system repetitively as in Monte Carlo analysis, Markov chain analysis uses extensive mathematical formalism to reduce the Markovian processes to analytical functional forms.⁽⁴²⁾

There have been no applications of either technique to geologic isolation safety assessments. Both techniques are well suited to quantitatively analyzing the discrete events, and because of their stochastic nature they are also well suited to analyzing the complex interactions of these events. A disadvantage of Monte Carlo analysis is

the large number of simulations expected to be necessary in order to obtain adequate failure distributions for low probability events and their combinations. Monte Carlo analysis can be generalized to consider the continuous processes present in geologic isolation systems by updating the state of the system for their effect at each time step. Markov chain analysis, on the other hand, does not appear applicable to the continuous processes because the states of the system must be specified a priori in order to apply the method. Furthermore, the transitions between states of a geologic system seem likely to be dependent on previous state transitions, in violation of the basic assumption of Markovian processes.

As described above, there are qualitative, deterministic, stochastic, and probabilistic methods available to assess the safety of geologic isolation repositories. Each type of method seems best applied to one or more, but not all, portions of the problem. However, when considered together the methods appear to provide the means to assess comprehensively and efficiently the safety of geologic isolation repositories. The least sophisticated (but most flexible) of the quantitative assessment methods, a generalized Monte Carlo analysis, appears to be the most desirable method for this problem, and it forms the base of the WISAP assessment method, hereafter called repository simulation analysis.

2.1.3 Development of Repository Simulation Analysis

Repository simulation analysis is a combination of expert opinion/Delphi, fault/event tree analysis, classical systems analysis, and Monte Carlo analysis. During FY77 the following steps for implementing the concept were defined:

1. Potentially disruptive natural and man-caused events and processes are identified (see Table 2.1).
2. The interdependencies of the phenomena are determined and their coupling relationships are quantified to the extent possible.
3. A stratified model of the site-specific geology is made.
4. Initiation probabilities and occurrence rates, durations, and lag times for the phenomena are determined.

5. Repository response curves (e.g., permeabilities, hydrologic potentials, flow path lengths) are derived by simulating the combined effects of the disruptive phenomena for the site-specified geologic model.
6. Containment breaches (i.e., transport agent crosses the boundary of the repository cavity) are noted and the failure times are combined with information from the repository response curves to determine the boundary conditions for subsequent consequence evaluation.

These steps (with the exception of Step 1 which was described previously) are discussed in more depth in the paragraphs that follow.

Basic to repository simulation is the understanding of how the potentially disruptive phenomena can combine to cause breaches of containment at the repository cavity. The first step in accomplishing the above is the development of a logic tree (fault or event) which relates the phenomena. An example of such a logic tree for some of the natural and man-caused events and some of the natural geologic processes is shown in Section 6.1. Next, the phenomena interrelationships are quantified using the present state of geologic knowledge. These interrelationships can be very complicated as the following example sequence shows:

1) rupture along an undetected fault in the crystalline basement beneath a bedded salt formation, 2) healing of the zone through the salt but not through the more brittle caprock material, 3) slow circulation of ground water at the caprock/salt interface, 4) salt dissolution, and 5) ultimate exposure of the waste to ground water. In WISAP this kind of information will be supplied by a team of geoscientists organized in FY77 and to be expanded in FY78. Table 2.2 is a list of the consultant categories. Examples of the kinds of specific questions which can be asked of these consultants are:

1. Given that the climate for the next million years will vary according to the Milankovitch theory, how will continental glaciation and mean sea level vary? What are the frequencies, rates, amplitudes, and phase relationships of these phenomena?

2. Given that the world climate supports continental glaciation, what are the consequences of such glaciation at a specific site? What is the potential magnitudes of ice and meltwater stream erosion, pressurized ground-water recharge, and fracturing at the periphery of the ice sheet?
3. What is the likelihood of tectonic uplift at a specific site and what are some of the related consequences? What are the erosion rates and extent of stress-induced fracturing?
4. If the in situ effective stress should change as a result of the addition or removal of overburden material or changing tectonic forces, how might the permeabilities of the geology be affected?
5. How can an increase in precipitation affect aquifer recharge or what is the impact on vertical recharge of a lake or ocean superimposed on the site?

TABLE 2.2. Consultant Categories

Climatology
Meteorites
Glaciology
Volcanology
Seismology
Man Caused
Geomorphology
Coastal
Pacific Northwest
Southwest
Structural Geology
Gulf Interior
Pacific Northwest
Southwest
Subsurface Hydrology
Gulf Interior
Pacific Northwest
Southwest

A preliminary computer model containing quantitative relationships between the potentially disruptive phenomena was developed in FY77 with minimal geoscience input to explore the repository simulation concept. The flow diagram for this model is shown in Appendix A.

The stratified model of the site-specific geology is based on site exploration data. This model should include such things as: surface relief and features, stratigraphy and rock types, aquifer locations, fault locations, hydraulic potentials, layer permeabilities, and the state of effective stress in the area. Additional information is needed about such things as: the stress-strain relationship of the rocks, fracture and fault character, rock properties, and ground-water properties. Figure 2.1 is an example of a stratified site model.

The data necessary to specify values for the natural and man-caused probabilities and natural geologic process parameters is obtained by expert opinion from the geoscience and social science communities. Since this activity involves the projection of incompletely understood past geologic and human behavior into the far future, considerable variance in the data is likely. The Delphi approach (discussed in Section 2.1.2.1) or one of its modifications (Subjective Probabilities) may be used to obtain this information.

Using the computer model and data distributions developed in the previous steps, the occurrence of the events and processes is simulated on the stratified site model. The values of important system parameters (e.g., vertical distance to biosphere, horizontal distance to ground-water discharge points, layer permeabilities and hydraulic gradients, etc.) are continuously updated during the simulation so that the occurrence of containment breaches at the repository cavity can be determined and the conditions of the system at the time of breach will be known. The simulations are performed repetitively until sufficient breaches have occurred to determine a statistically significant distribution. The

FIGURE 2.1. Stratified Site Model

distribution of breaches and distributions of repository system parameters are then combined into the boundary conditions necessary for subsequent consequence evaluation.

The development work on repository simulation performed during FY77, including initial contact with the geoscience community, suggests that the concept is feasible. However, no model, regardless of how well conceived, is any better than the data that are available to perform the calculations. Thus, it is possible that this analysis of repository release scenarios will yield breach and system parameter distributions with such large uncertainty levels that definitive safety conclusions cannot be made. However, should this be the case, the development and use of the model should make the reasons for this condition explicit and guide the gathering of higher quality data.

2.2 RELEASE CONSEQUENCE ANALYSIS

2.2.1 Evaluation of Release Consequence Analysis Methods

After the repository release scenarios have been described, the consequences to humans must be estimated. Consequence calculation requires the development of a computational system which models the transport of the radionuclides through the geosphere and biosphere to humans and calculates radiological doses. For this study, before beginning method development activities, an evaluation of available consequence analysis methods was performed. This section summarizes the results of that evaluation. A more detailed discussion of this evaluation will be presented in PNL-2708, "Safety Assessment Methods for the Geologic Isolation of Nuclear Waste - Release Consequence Analysis."

An extensive compilation of computer models potentially applicable to this task was first performed. Over 150 hydrologic, contaminant transport, water-dose, and air-dose models were identified. Information about the hydrologic and contaminant transport models was obtained from a broad international assessment of such models by the Holcomb Research Institute.⁽¹⁾ Information about the water-dose and air-dose models was obtained from recent compilations in the literature.^(2,3) Because of

the number and diversity of the hydrologic and contaminant transport models, a method for categorizing these models was devised. Table 2.3 shows the format for that categorization. The categorization facilitates comparing purely hydrologic models, purely contaminant transport models, and models which have characteristics of both types to be easily compared. The hydrologic model categories are shown as vertical columns, and the contaminant transport model categories are shown as horizontal rows. Models which simulate flow only are categorized in the first row, while those which simulate transport only are categorized in the first column. Combination models are categorized in the remainder of the boxes. The water-dose and air-dose models had considerable similarity and did not require a complex categorization.

2.2.1.1 Hydrologic and Contaminant Transport Models

The evaluation of the hydrologic and contaminant transport models for the WISAP release consequence analysis system was based on three criteria. First, a range of data sophistication can be accommodated so that many scoping calculations can be made quickly and cheaply and yet important scenarios can be analyzed in depth. The ability to efficiently perform scoping calculations seems particularly important because of the large numbers of calculations expected to be necessary in order to perform the many assessments which are anticipated. Secondly, the system should have the capability to model isothermal saturated flow through heterogeneous geologic media. This criterion follows directly from programmatic direction to exclude near-field effects from the scope of WISAP. Finally, the system should have the capability to model hydrodynamic dispersion, radioactive chain decay, and equilibrium sorption.

In summary the evaluation of the release consequence analysis methods was based on the following criteria:

1. The methods should have a range of modeling sophistication.

2. The methods should model isothermal saturated flow through heterogeneous media.
3. The methods should model hydrodynamic dispersion, radioactive chain decay, and equilibrium sorption.

Four levels of sophistication were defined for the hydrologic and contaminant transport part of the WISAP release consequence analysis system. For most of these levels a number of models were identified that met the criteria or could be made to meet the criteria with a reasonable amount of additional development. These models or model combinations are shown in Table 2.4 and are described in Appendix B. Because there were a number of models of essentially equal applicability, models were chosen for the WISAP release consequence analysis system that could be most efficiently adapted to our computing systems (UNIVAC 1100/44 and PDP 11/45). As a result three of the five codes selected were PNL-developed codes.

The first or simple level of hydrologic-contaminant transport model uses an analytic solution of the steady-state flow equation to obtain the ground-water flow velocity for the release scenario of interest. This velocity is then used as input to the GETOUT model.⁽⁴⁾ GETOUT assumes that the contents of the repository are released either as an impulse or at a constant rate to the ground water which flows at constant velocity through a one-dimensional column of the homogeneous geologic medium surrounding the repository and discharges to a surface-water body. The dissolved radionuclides are assumed to be in sorption equilibrium at all points in the flow path. Radioactive decay (including chain decay of the actinides) is modeled at the repository and during migration through the geologic medium. Trace concentrations of the dissolved nuclides are assumed and as a result the sorption factors are independent of concentration. A constant axial dispersion coefficient is assumed. GETOUT is applicable to particulate or fractured media provided the necessary sorption data are measured properly. The model can be applied to heterogeneous media if the relevant input parameters are averaged properly. The GETOUT code uses the analytical solution of the

TABLE 2.4. Hydrologic and Contaminant Transport Models Useful for Waste Isolation Safety Assessment

Level of Modeling Complexity	Hydrologic	Contaminant Transport	Additions Needed to Meet Selection Criteria
Simple	Analytic Solution of Steady State Flow Equation	GETOUT ⁽⁴⁾	None
Simple-Intermediate	PATHS ⁽⁵⁾	GETOUT	None
	PATHS	PATHS (EXTENDED)	Equilibrium Sorption and Chain Decay
	FLOP-1 ⁽⁶⁾	FLOP 1 (EXTENDED)	Equilibrium Sorption and Chain Decay
	FLOP-2 ⁽⁶⁾	FLOP 2 (EXTENDED)	Equilibrium Sorption and Chain Decay
	FRONT-N ⁽⁶⁾	FRONT-N (EXTENDED)	Equilibrium Sorption and Chain Decay
	RCPIGW ⁽⁷⁾	RCPIGW (EXTENDED)	Equilibrium Sorption and Chain Decay
Intermediate-Complex	HCTM*	MMT ⁽⁸⁾	None
	TRIGAT*	MMT	None
	(COOLEY) ⁽⁹⁾	MMT	None
	VTT ⁽¹⁰⁾	MMT	None
	MULTIAQUIFER ⁽¹¹⁾	MMT	None
	MOC ⁽¹²⁾	MMT	None
	BEWTA ⁽¹³⁾	MMT	None
	MTMVMC*	MMT	None
	ISQUAD2*	MMT	None
	NEWSAM*	NEWSAM (EXTENDED)	Equilibrium Sorption and Chain Decay
	MOC	MOC (EXTENDED)	Equilibrium Sorption and Chain Decay
	HCTM	HCTM (EXTENDED)	Equilibrium Sorption and Chain decay
	DAVIS FE ⁽¹⁴⁾	MMT	None
	DWDM (Newer Version)*	DWDM (Newer Version)	None
Complex	VCHFLD*	VCHFLD	Equilibrium Sorption and Chain Decay
	DAVIS FE	DAVIS FE (EXTENDED)	Equilibrium Sorption and Chain Decay

* Code either proprietary or undocumented or both

one-dimensional transport equation and is thus the most time and cost effective method of scoping the release consequences to individuals affected by a contaminated surface-water body. However, because of its one-dimensional nature it cannot be used to accurately calculate the release consequences to individuals using, for example, well water.

The second or simple-intermediate level uses the PATHS hydrologic code.⁽⁵⁾ PATHS assumes a homogeneous geologic medium and saturated steady-state flow and uses a two-dimensional analytic solution for the ground water potential distribution between the repository and a surface-water body. From the potential distribution, the pathline differential equations are solved numerically to give the paths of fluid particles and their position with time between the repository and a surface-water body. The GETOUT code is then used to calculate transport of the radionuclides along any or all paths of interest. The second-level system is less time and cost effective than the first-level system, but provides a more detailed representation of the contaminant transport. The first two levels of modeling complexity idealize the real system and do not require as much input data as the last two levels.

The third or intermediate-complex level uses the VTT hydrologic code.⁽¹⁰⁾ VTT models two-dimensional, saturated ground-water flow through heterogeneous media. The code is based on a Boussinesq approximation model and uses standard finite difference solution techniques. It has multiaquifer capability with variable thickness features for the unconfined strata and can solve both transient and steady-state problems. More detailed solution at a finer difference grid spacing is possible by a sequential solution process wherein the results of a large region simulation are used as boundary conditions for a smaller region. The MMT code uses the flow vectors from VTT as input to the nodes of a rectangular grid system and models the transport of contaminants.⁽⁸⁾ The MMT code models dispersion (using a random walk analogy), radionuclide chain decay, and equilibrium sorption. Because of its numerical nature all parameters of the model can be varied with position. Thus, data of considerable detail can be accommodated.

The fourth or complex level uses the DAVIS FE code.⁽¹⁴⁾ This model considers saturated ground-water flow (transient and steady state) in three dimensions through a heterogeneous geologic medium with both the fluid or geologic medium considered to be compressible. Because the differential equations are solved by finite element techniques, the code is able to satisfy irregular boundary conditions. The MMT code will again be used to model contaminant transport using flow vectors from the DAVIS FE code as input.

2.2.1.2 Water-Dose and Air-Dose Models

The evaluation of dose models for the WISAP release consequence analysis system was based on three criteria. First, the system should model drinking water, terrestrial food, water immersion, external shoreline, and aquatic food doses. These characteristics describe the important pathways by which humans received radiation doses from contaminated water. Secondly, the system should model chronic and acute air immersion and inhalation doses. Finally, the system should calculate both individual and population doses. In the water-dose case only one set of codes was available; in the air-dose case a number of models of essentially equal applicability according to the criteria were identified. These models are shown in Table 2.5. Appendix B contains a description of each of these models. In the air-dose case models were chosen which could be adapted most efficiently to the PNL computing system. All dose codes selected for the WISAP system were PNL-developed codes.

ARRRG calculates annual individual and population doses resulting from radionuclides released to surface-water bodies.⁽¹⁶⁾ Eight environmental pathways are modeled: eating fish, crustacea, molluscs, and algae; drinking surface water; direct external radiation from shoreline; water immersion (swimming), and direct external radiation from boating. Doses are calculated for skin, total body, gastrointestinal-lower large intestinal tract, thyroid, bone, liver, lung, and kidney. The output format specifies contributions to the dose by nuclide and by pathway.

TABLE 2.5. Water-Dose and Air-Dose Models Useful for Waste Isolation Safety Assessments

Water-Dose				Air-Dose			
Water Immersion	Water Ingestion	Terrestrial Food Ingestion	Aquatic Food Ingestion	Acute Immersion	Acute Inhalation	Chronic Immersion	Chronic Inhalation
HERMES ⁽¹⁵⁾	HERMES	HERMES	HERMES	ACRA II ⁽²³⁾	ACRA II	AIRDOS ⁽³¹⁾	AIRDOS
ARRRG ⁽¹⁶⁾	ARRRG	FOOD ⁽²⁰⁾	ARRG	COMRADEX ⁽²⁴⁾	CONRADEX	AIREM ⁽³²⁾	AIREM
EXREM III ⁽¹⁷⁾	CARDOCC ⁽¹⁹⁾	TERMOD ⁽²¹⁾	AQUAMOD ⁽²²⁾	EXREM III	DACRIN ⁽²⁹⁾	GRONK ⁽¹⁶⁾	DACRIN
VADOSCA ⁽¹⁸⁾	VADOSCA	VADOSCA	VADOSCA	FISSP/CLOUD ⁽²⁵⁾	EXREM III	KRONIC ⁽³³⁾	GRONK
				RACER ⁽²⁶⁾	FISSP/CLOUD		INREM
				RSAC II ⁽²⁷⁾	INREM ⁽³⁰⁾		
				SUBDOSA ⁽²⁸⁾	RSAC II		
				SUBPOPA			

FOOD is a companion code to ARRRG and calculates annual individual and population doses from eating garden foods and animal products contaminated by air deposition or water irrigation.⁽²⁰⁾ Doses are calculated for 14 foods. A key assumption in the code (which is discussed further in Section 2.2.3.2) is that the accumulation and dispersion processes in the biosphere are such that the local soils used for farming contain the accumulated radionuclides from a specified number of years of irrigation previous to the time of interest.

KRONIC calculates annual external total body tissue dose from chronic release of radionuclides to the atmosphere.⁽³³⁾ The dose is calculated as a function of the radionuclides released, the plume height, the plume size, the climatology for the site, and the physical properties. Atmospheric dispersion effects are estimated using data on joint frequency of wind speed, wind direction, and stability for the site. Each sector is considered to be a plume for which the centerline ground-level dose is calculated for specified downwind distances. The output format is a table of annual dose rates as a function of direction and distance from the release point.

SUBDOSa calculates external doses from acute release of radionuclides to the atmosphere.⁽²⁸⁾ Doses may be calculated as a function of depth in tissue and may be summed and reported as skin, eye, and genetic doses. The doses are calculated for six release periods with separate nuclide inventories and dispersion in each period. Nuclide decay is considered during release and/or transit using a chain decay scheme with branching to account for transitions between isomeric states.

DACRIN calculates the effective radiation dose to the human respiratory tract and other organs from the inhalation of radioactive aerosols.⁽²⁹⁾ The program follows the basic precepts the International Committee on Radiation Protection Task Group on Lung Dynamics and a simple exponential model for retention by the organ of interest. As an adjunct to the organ dose model, mathematical models of atmospheric dispersion are included in order to model transport to humans from either acute or chronic

releases. The code calculates the effective radiation dose to any of 18 organs and tissues from inhalation of any one or combination of the radionuclides.

2.2.2 Development of Modeling System

The evaluation of the consequence analysis models listed in Section 2.2.1 resulted in the selection of 10 models to form the base of the WISAP release consequence analysis system. The characteristics of these models are summarized in Table 2.6. To enhance the usefulness of these models, work was initiated in FY77 to integrate these models so that input and output formats were compatible (GETOUT and ARRRG/FOOD were already compatible when WISAP was initiated). Work was also initiated to verify the predictive capability of the models using existing field data. The major effort in this area during FY77 was focused on making the DAVIS FE model operational on one of the PNL computing systems and in verifying its predictability using a data set which describes the multilayered ground-water system beneath Long Island, New York.

The DAVIS FE model uses a finite element solution method (irregular grid size) which makes it somewhat more powerful for space and boundary definition of real sites (which have irregular features) than finite difference methods (uniform square or rectangular grid size). The spacing of nodes near locations of interest (repository, pumping wells, boreholes, or surface-water bodies) can be conveniently decreased, and the hydraulic conductivities can change abruptly from element to element thus allowing representation of fault zones and confining layers. Some complex site-specific geologic configurations consist of multiaquifer systems separated by semiconfining layers, and these aquifers respond conjunctively to stress imposed on either aquifer. Such coupling of aquifers requires modeling all of the layers simultaneously, and the three-dimensional DAVIS FE model provides the means to describe this situation realistically.

The logic procedure for describing a given ground-water system for the DAVIS FE code has the following steps:

TABLE 2.6. Characteristics of WISAP Release Consequence Analysis Models

HYDROLOGIC

- PATHS - Two-dimensional, analytical/numerical method, homogeneous geology, saturated flow
- VTT - Two-dimensional, finite difference numerical method, heterogeneous geology, saturated flow
- DAVIS FE - Three-dimensional, finite element numerical method, heterogeneous geology, saturated flow

CONTAMINANT TRANSPORT

- GETOUT - One-dimensional, analytical method, chain decay, single speciation, equilibrium sorption, constant leach rate, dispersion
- MMT - Three-dimensional, numerical method, chain decay, single speciation, equilibrium sorption, time variant leach rate, dispersion

WATER DOSE

- ARRRG - Drinking water, immersion, external shoreline, and aquatic food doses
- FOOD - Terrestrial food dose

AIR DOSE

- KRONIC - Chronic external dose
- SUBDOSA - Acute external dose
- DACRIN - Chronic or acute inhalation dose

1. Contour maps are prepared showing the elevation and thickness of major hydrogeologic units using the geologic logs of bench mark wells.
2. Discontinuities, major breaks in slopes, fault zones, or other important features are noted and are identified as discrete nodes on the contour maps.
3. Additional nodes are placed along surface-water bodies (lakes, rivers, seashore, etc.), at recharge or discharge wells, at boreholes, and in regions of significant surface-water infiltration.
4. All nodes are joined by straight or curved (quadratic or cubic) lines according to the geologic and surface-water boundaries to create the surface elements.
5. Using these two-dimensional surface elements and the vertical log details at each node, the code generates the three-dimensional stratigraphic elements.

Using the above procedure the multilayered aquifer system beneath Long Island was successfully modeled, and the accuracy of the present version of the DAVIS FE model was thus verified. The two-dimensional surface elements and three-dimensional stratigraphic elements used in this verification are shown in Figures 2.2 and 2.3.

A disadvantage of former versions of the DAVIS FE code were the extensive core storage requirements needed for simulating even small problems. However, by using an efficient disk accessing method, the model verification using the Long Island data set was performed with the present code using a core of less than 32,000, 16-bit words. The improved version of the DAVIS FE code is under development.

FIGURE 2.2. Two-Dimensional Surface Elements Used for DAVIS FE Model Verification with Long Island Hydrologic Data

FIGURE 2.3. Three-Dimensional Stratigraphic Elements Used for DAVIS FE Model Verification with Long Island Hydrologic Data

2.2.3 Modeling System Refinements

The development of the WISAP release consequence analysis system in FY77 emphasized the modeling of the most common repository release situations using available modeling technology. Thus, the modeling system does not presently contain models to describe water flow in partially saturated, or multiphase systems. Such models will be added later if situations are identified where the use of these models would lead to a substantially better prediction of ground-water flow. Non-isothermal hydrologic models are excluded by programmatic direction to ignore near-field effects.

The contaminant transport models of the WISAP system do not presently consider phenomena such as finite rate sorption, multiple chemical species of the same nuclide, chemical reactions between these multiple species, reversible precipitation, colloid filtration, and irreversible mineralization. GETOUT and MMT will be extended to model these and other phenomena if the geochemical interaction data gathering activities of WISAP show that these phenomena are important for conditions of interest to geologic isolation safety assessments. A small amount of work in this area was performed during FY77 and is reported in Section 2.2.3.1.

The dose models of the WISAP system (and all other dose models as well) make some assumptions about the dynamics of the accumulation and dispersion processes of radionuclides in the biosphere when radionuclides are released chronically over long time periods. Studies to improve the modeling of this situation were begun in FY77 with support from the Waste Management Systems Studies Program. The work is described in Section 2.2.3.2 of this report because of its relevance to the WISAP mission. WISAP dose models do not estimate health effects from the calculated doses. Because health effects projections may communicate repository safety better than dose projections, a brief study to determine how the health effects conversion should be done was completed in FY77. The results are presented in Section 2.2.3.3.

2.2.3.1 GETOUT Model Extension

The theory of the GETOUT code described in Section 2.2.1 assumes that each radionuclide migrates as one chemical species and that all of its interactions with the geologic medium are completely reversible (i.e., ignores irreversible mineralization).⁽⁴⁾ However, recent experimental evidence suggests that neither of these assumptions is universally correct.^(34,35) The first assumption may be nonconservative (i.e., causing the predicted discharges to the biosphere to be smaller than reality in situations where a slower moving chemical species of a given nuclide reacts to form a faster moving species as it moves downstream from a water intruded geologic repository. The second assumption is always conservative but may be very conservative in some situations leading to conclusions of site unacceptability where those conclusions are not justified.

To explore the importance of these assumptions, the GETOUT theory was extended to consider the migration of multiple chemically reacting species which could become irreversibly bound to the geologic material. One of the many such situations that can be considered is a two-member decay chain with each member present as two different reacting chemical species. This situation is shown schematically in Figure 2.4. Each square represents a particular chemical species of a particular radionuclide. The vertical arrows between squares represent the radioactive decay of one nuclide to another. The horizontal arrows represent chemical reaction of one chemical species to another. The diagonal arrows represent irreversible mineralization reactions. The theoretical analysis for this simple system can be straightforwardly extended to systems of arbitrary complexity provided all phenomena can be described as linear processes and the chemical and mineralization reactions are irreversible. The details of the analysis are presented in Appendix C. Work to develop a computer code to implement the results is under way.

$N_{i,j}$ = "i"th nuclide, "j"th species

λ_i = radioactive decay rate coefficient

$\lambda_{i,j}$ = chemical reaction rate coefficient

$\lambda_{i,j}^m$ = irreversible mineralization rate coefficient

FIGURE 2.4. Schematic Diagram of a Two-Member, Two-Species Decay Chain with Chemical Reaction and Irreversible Mineralization

2.2.3.2 Long-Term Accumulation of Radionuclides in Crop Plants

Previous estimations of the consequences of ground-water intrusion into a geologic isolation repository have shown that the consumption of crop plants grown using contaminated irrigation water is an important contributor to human dose.^(36,37) When estimating these doses in situations where the radionuclides have been discharging from the repository to the irrigation water source chronically over long time periods, an assumption must be made about the extent to which nuclides accumulate in soils used for agriculture. Burkholder et al.,⁽³⁷⁾ for example, assumed that the quantities of radionuclides in the surface soils at any given time were equal to the total deposited on the soils during the previous 50 years.^(16,20,37) Because of this assumption the doses from many of the long lived nuclides in that study were found to be linearly proportional to the number of years assumed for the accumulation, and some of these nuclides were predicted to discharge to the biosphere over millions of years. Thus, the long-term accumulation phenomena are potentially very important, and a study was begun in FY77 to improve the way they are modeled.

Figure 2.5 is a flow diagram showing the processes of radionuclide exchange between soil/plant systems. As shown, radionuclides enter the system by deposition of irrigation water on the plant surfaces and on the ground and leave the system by harvestation and percolation below the root zone. The nuclides deposited on the plant surfaces are either absorbed or deposited on the ground as runoff. The nuclides deposited on the ground are carried into the soil by the percolating water and may sorb on soil. A portion of these radionuclides is taken up by the plants. The portion of the plants that are not harvested (and their contained radionuclides) are plowed into the soil and eventually decompose thereby releasing the contained radionuclides for loss by percolation or equilibration with soil mineral and reuptake by subsequent crops.

FIGURE 2.5. Radionuclide Exchange Processes for Irrigated Soil/Crop Plant Systems

The fate of nuclides released from the decomposed unharvested plant materials is crucial to the long-term accumulation process. Fortunately, a series of classic experiments have been conducted at the Rothamsted Experimental Station in the United Kingdom for the past 100 years and these experiments provide the needed data for the modeling of the processes in the soil organic matter compartment.⁽³⁸⁾ Using these data and data about typical farming practices in the United States, a model was developed and evaluated subject to a number of assumptions to make preliminary comparisons of the model results with the 50-year accumulation assumption. The results of the evaluation are shown in Table 2.7. These results show that the 50-year accumulation assumption is in general agreement with the long-term accumulation model. However, the 50 year accumulation assumption tends to produce conservative results (higher concentrations in the edible plant material) for radionuclides which are weakly retarded from percolating through the soil and strongly taken up by the plants (e.g., ⁹⁹Tc) and non-conservative results for nuclides which are strongly retarded and weakly taken up by the plants (e.g., the actinides).

2.2.3.3 Health Effects Conversion

Significant uncertainties are involved in the calculation of radiation dose to far-future generations from potential repository release scenarios, and the meaningfulness of such doses can be questioned. Additional uncertainties are introduced because of limits on our ability to experimentally determine health effects from very low radiation doses (such as those expected for repository release scenarios). Thus, the meaningfulness of health effects estimates is even more subject to dispute than dose estimates, and individual doses may be a better technical basis for decision-making than health effects. However, health effects estimates to the general public may communicate risk better than radiological dose, and thus WISAP will be prepared to make such conversions. An additional conversion problem with health effects is the conservatism introduced into the conversion factors to assure that the

TABLE 2.7. Comparison Between Seed Concentrations Predicted by the 50-Year Accumulation Assumption and the Long-Term Accumulation Model

Nuclide	Plant to Soil Concentration Ratio (CR)	Retardation Factor (K)	Seed Concentration (Units of Activity/kg)	
			50-Year Accumulation	Maximum Accumulation Model Value
¹⁰ Be	0.0004	330	2.0	2.2
⁴¹ Ca	0.036	100	5.9	9.0
⁵⁹ Ni	0.019	500	4.0	14
⁶³ Ni	0.019	500	3.1	2.7
⁷⁹ Ce	1.34	100	150	180
⁸⁷ Rb	0.13	500	16	110
⁹⁰ Sr	0.2	100	13	5.8
⁹³ Zr	0.00017	10000	2.0	5.0
⁹³ Mo	0.13	25	16	8
⁹⁹ Tc	80	1	8800	120
¹⁰⁷ Pd	5	1100	550	550
¹¹³ Cd	0.3	2500	12	4.8
¹²⁶ Sn	0.0025	1100	2.2	7.1
¹²⁹ I	0.02	1	4.1	2.0
¹³⁵ Cs	0.003	1000	2.3	7.8
¹⁶⁶ Ho	0.0026	2500	2.2	3.5
²¹⁰ Pb	0.068	17000	3.9	2.3
²²⁶ Ra	0.00031	500	1.9	2.0
²³¹ Pa	0.0025	1700	2.2	8.7
²³² Th	0.0042	50000	2.4	160
²³³ U	0.0025	14000	2.2	52
²³⁷ Np	0.0025	100	2.2	2.4
²³⁸ Pu	0.00025	10000	1.3	1.9
²⁴³ Am	0.00025	10000	2.0	2.5
²⁴⁴ Pu	0.00025	10000	2.0	15
²⁴⁷ Cm	0.0025	3300	2.2	18

health effects are not underestimated. More realistic estimates are needed to keep these conservative estimates in perspective.

To address the concerns discussed above the WISAP release consequence analysis system will be prepared to provide output in three formats.

1. dose and dose rate comparisons
2. health effects conversions by Biological Effects of Ionizing Radiation (BEIR) report estimates
3. health effects conversions by PNL's best estimate

Dose and dose rate estimates would be the primary output of WISAP consequence analyses and the health effects estimates would be secondary outputs, perhaps in the appendices of reports.

Table 2.8 contains the health effects conversion factors for both the BEIR and PNL estimates. The BEIR report employs several different approaches to cancer risk estimation and arrives at dose-risk conversion factors ranging from about 100 to 450 cancer deaths per million person-rem depending on the assumptions employed.⁽³⁹⁾ The U.S. Environmental Protection Agency (EPA) has chosen a single value of 200 deaths per million person-rem as an appropriate mean risk number, and this number is suggested for WISAP-BEIR cancer risk estimates.⁽⁴⁰⁾

TABLE 2.8. Health Effects Conversion Factors

	<u>BEIR</u>	<u>PNL</u>
Somatic ^(a)	200	50 (low LET) 200 (high LET)
Genetic ^(b)	300	50

(a) deaths per million person-rem annual exposure

(b) serious genetic defects per million person-rem annual exposure

The BEIR cancer risk estimates assume a linear relationship between dose and health effects. There is abundant experimental evidence that this overestimates the effects of low LET (linear energy transfer)

radiation delivered at very low dose rates. The NRC Reactor Safety Study took this into account and arrived at a central estimate of about 50 cancer deaths per million person-rem. This value is suggested as the PNL best estimate. It is applied only to low LET (beta-gamma) radiation. The BEIR factor of 200 cancer deaths per million person-rem will be used for high LET (alpha) radiation.

The BEIR report estimates an incidence of serious genetic effects (congenital abnormalities, constitutional and degenerative diseases, etc.) ranging from 1800 to 45,000 per generation per rem continuous exposure (60 - 1500 genetic effects per year for a 30-year generation) to the U.S. population (3.6×10^6 births annually) depending upon the assumptions used. This level of effect is approached only after several generations of exposure; the risk to the first offspring generation is estimated to be about a factor of 5 less. Based on these BEIR estimates, the EPA adopted a single factor of 300 effects per million person-rem over all subsequent generations.⁽⁴⁰⁾

PNL's genetic effects conversion factor is based on data more recent than that employed in the BEIR report. These data suggest that previous estimates of the contribution of mutations to human ill health were too high and lead to estimates of equilibrium genetic effects of 10 per million person-rem (2 per million person-rem for the first offspring generation).^(41,42) A compromise conversion factor of 50 serious genetic effects to all generations per million person-rem is suggested as the PNL best estimate.

3. DATA BASE DEVELOPMENT

Performance assessments for geologic isolation repositories require data of six general types:

1. geologic and geophysical data for estimating disruptive event frequencies and disruptive process rates and durations
2. waste form and container property data for estimating radionuclide release rates under the conditions of potential repository release scenarios
3. geohydrologic data for estimating the origin, direction, and velocity of ground-water flow for potentially disruptive scenarios
4. geochemical data for estimating the degree to which radionuclides are retarded during ground-water transport through geologic media
5. geographic and demographic information about the repository sites
6. biologic, biochemical, and biophysical data concerning radionuclide transport processes in the biosphere.

Data base development activities in FY77 concentrated on measuring radionuclide leach rates for glass waste forms and sorption properties for geologic media of interest to the NWTs Program. Preliminary data base development activities were also carried out in conjunction with the geologic analysis workshop but these results are too preliminary to be reported in detail at present. The workshop is described in Section 4.3.

3.1 WASTE FORM RELEASE RATE DATA

3.1.1 Preparation of Doped Glass Waste Forms

For WISAP safety assessments, release rate data are needed for spent fuel, high-level, and TRU-contaminated waste forms. Because of difficulties in obtaining spent fuel for study, the initial work in FY77 focused on preparing actinide and fission product doped waste glasses. Since the formulations of Allied General Nuclear Services (AGNS) and Exxon

waste glasses were not completed, the Nuclear Fuels Services (NFS) glass composition was chosen. In order to study isotopes of long-term potential hazard without the high radiation fields of actual high-level waste, sample waste forms were made using these isotopes alone. Four glasses were made based on the NFS composition:

1. ^{99}Tc
2. ^{244}Cm
3. $^{233}\text{U} + ^{243}\text{Am}$
4. $^{237}\text{Np} + ^{239}\text{Pu}$

These isotopes were doped into the waste glass to the extent normally present in high level waste. The assumptions for this reference waste were:

1. burnup = 33,000 MWD/MTU
2. reactor type = reference PWR, 3.3% enriched
3. age of waste = 2 yr old
4. reprocessing loss = 0.5% U + Pu
5. specific power = 26.4 MW

The doped glasses, except for the ^{233}U series, contained the expected amount of uranium as ^{238}U . Table 3.1 gives the detailed composition for the frit, waste, and final glass product assuming a waste (fission products, actinide oxides, and reprocessing chemicals) loading of 33 wt %. The composition shown in Table 3.1 is specific for the glass doped with Np and Pu.

As a compromise between the reality of cracked glass monoliths and the powdered glass frequently studied in accelerated leach testing, glass beads were chosen as the sample waste form for study. Two methods of preparing these samples were developed. A resistance heated unit was installed in a glove box for preparation of doped glasses, and an induction heated system was set up for preparation of actual high-level waste glasses. Both units involve heating a comparatively large volume of glass to the melt temperature, continuously forming droplets at the end of a nozzle, and collecting the solid beads on a heated metal plate.

**TABLE 3.1. Composition of Frit, Wastes and Doped Waste Glass
Used for Actinide Release Studies**

Frit Composition, (a) wt%		Waste Calcine Composition, (b) wt%		Glass Composition, (c) wt%	
59.7	SiO ₂	29.2	Fe ₂ O ₃	40.0	SiO ₂
14.2	B ₂ O ₃	15.0	Na ₂ O	12.5	Na ₂ O
11.2	Na ₂ O	12.6	²³⁸ U ₃ O ₈	9.6	Fe ₂ O ₃
7.45	ZnO	6.8	MoO ₃ (d)	9.5	B ₂ O ₃
4.45	TiO ₂	5.3	ZrO ₂	5.0	ZnO
3.0	CaO	5.0	Nd ₂ O ₃ (e)	4.2	²³⁸ UO ₂
		3.6	CeO ₂	3.0	TiO ₂
		3.2	RuO ₂	2.2	MoO ₃
		3.1	Cs ₂ O	2.0	CaO
		1.7	BaO	1.7	ZrO ₂
		1.6	PdO	1.65	Nd ₂ O ₃
		1.6	La ₂ O ₃	1.19	CeO ₂
		1.6	Pr ₆ O ₁₁	1.07	RuO ₂
		1.41	²³⁷ NpO ₂	1.03	Cs ₂ O
		1.4	P ₂ O ₅	0.56	BaO
		1.2	Cr ₂ O ₃	0.53	PdO
		1.1	SrO	0.53	La ₂ O ₃
		0.98	Sm ₂ O ₃	0.53	Pr ₆ O ₁₁
		0.78	TeO ₂	0.46	²³⁷ NpO ₂
		0.64	Y ₂ O ₃	0.46	P ₂ O ₅
		0.60	NiO	0.40	Cr ₂ O ₃
		0.52	Rh ₂ O ₃	0.37	SrO
		0.38	Rb ₂ O	0.32	Sm ₂ O ₃
		0.21	Eu ₂ O ₃	0.26	TeO ₂
		0.15	Gd ₂ O ₃	0.21	Y ₂ O ₃
		0.140	²³⁹ PuO ₂	0.20	NiO
		0.10	CdO	0.17	Rh ₂ O ₃
		0.090	Ag ₂ O	0.13	Rb ₂ O
				0.070	Eu ₂ O ₃
				0.050	Gd ₂ O ₃
				0.046	²³⁹ PuO ₂
				0.033	CdO
				0.031	Ag ₂ O

(a) 76-101 Frit

(b) PW-8a-3 Calcine PNL Waste

(c) 76068 Glass Form Identifiers

(d) Chemical Stand-In for Mo + TC

(e) Chemical Stand-In for Nd, Am and Cm

As a result of numerous trial runs with both units, standard procedures for making glass beads were developed. The procedure for making doped glass beads using the resistance heated unit has the following steps:

1. Frit and calcine (33% calcine for NFS glass) are placed in a platinum crucible and melted (1050°C for NFS glass), the melt is cooled to form undoped solid glass.
2. The weighed dopant is dissolved in 6N HNO_3 . This is done with a minimum of liquid and heating. HNO_3 with 5% HF is used to dissolve NpO_2 and PuO_2 . A clear solution is obtained. Aliquots of the solutions are retained for future analysis.
3. The preformed NFS glass is crushed to -40+60 mesh, weighed, and thoroughly "wetted" with the dopant solution.
4. The wetted glass is vacuum dried and preheated to 500°C to reduce nitrate concentration (causes glass frothing).
5. The glass is melted in stainless steel crucibles for 2 hr at 1050°C, water quenched, and broken out of the crucible.
6. The glass is placed in a quartz bead making tube, the temperature adjusted to 1050-1100°C, and the beads collected on steel pans maintained at 400°C.
7. The beads are annealed for 2 hr at 500°C and cooled to ambient temperature at 100°C/hr.

The procedure for making high-level waste glass beads using the induction heated unit has the following steps:

1. Frit and high-level waste calcine are combined.
2. The frit/calcine mixture is melted and blended in a 1 in. OD stainless steel cylinder (304L) for 2 hr at 1050°C.
3. The cylinder and contained glass is air cooled.
4. The top and bottom of the cylinder are cut off with a diamond saw.
5. The stainless steel cylinder is placed inside a mild steel cylinder and placed in the induction unit.

6. The glass is melted at 1050°C and the beads are dropped on a stainless steel surface heated by a hot plate.
7. The beads are annealed for 2 hr at 500°C and cooled to ambient at 100°C/hr.

Approximately 1.5 kg of doped glass beads were prepared in four separate runs with the resistance unit. Table 3.2 summarizes the bead characteristics. The confidence limits shown are at one standard deviation. Thus, the beads had constant properties to within a few percent. This illustrates that a major value of this approach is reproducibility of sample preparation.

Random samples of the beads were examined by X-ray diffraction, metallography, and α -radiography. X-ray diffraction traces of the various glass preparations are shown in Figures 3.1 and 3.2. A comparison of the four traces in Figure 3.1 with the top trace in Figure 3.2 shows that little change in the crystalline properties of the glass occurred during the doping process. Weak reflections from a spinel type oxide (M_3O_4 ; $M = Fe, Cr, Ni, \text{ and } Zn$) and a fluorite type oxide (MO_2 ; $M = U, Ce$) are observed in the 1-3 wt% range.

The actual concentration varies somewhat from sample to sample because these "difficult to dissolve" phases tend to form clusters. Small concentrations of Pd metal and RuO_2 are also present in the glass but ≤ 1 wt%. All of these phases are common to waste glass compositions. At this relatively low concentration level and small crystal size (mainly $\leq 1\mu m$) they do not appear to adversely affect any of the properties of the glass, at least with regard to dispersibility.

Figure 3.2 also shows the X-ray patterns of glass beads produced in the induction heated system. No crystalline phases are detectable perhaps because direct electrical coupling assists the vitrification process in this very complex glass.

TABLE 3.2. Doped Glass Bead Characteristics

	Dopants			
	^{244}Cm	^{99}Tc	$^{237}\text{Np}/^{239}\text{Pu}$	$^{233}\text{U}/^{243}\text{Am}$
Beads Produced	400	450	2400	650
Mass (g/bead)	$.459 \pm .024$	$.362 \pm .006$	$.353 \pm .013$	$0.381 \pm .005$
Density (g/cm ³)	$3.040 \pm .004$	$3.042 \pm .025$	$3.028 \pm .038$	$2.974 \pm .015$
Diameter (cm)	$0.759 \pm .010$	$0.683 \pm .008$	$0.681 \pm .008$	$0.696 \pm .005$
Eccentricity (%)	0.7	0.3	0.5	0.3
Height (cm)	$0.455 \pm .005$	$0.437 \pm .008$	$0.437 \pm .005$	$0.442 \pm .003$
Amount of Isotope g/g glass	2.44×10^{-4}	Being Analyzed	$^{237}\text{Np} \ 4.08 \times 10^{-3}$ $^{239}\text{Pu} \ 4.13 \times 10^{-4}$	$^{243}\text{Am} \ 8.62 \times 10^{-4}$ $^{233}\text{U} \ 2.46 \times 10^{-2}$

Average "second" phase concentrations - for all beads.

1-3% M_3O_4 - spinel, M = Fe, Cr, Ni, Zn

1% MO_2 - fluorite, M = U, Ce

0-3% porosity

FIGURE 3.1. X-ray Diffraction Patterns for Doped Glasses

FIGURE 3.2. X-ray Diffraction Patterns for Resistance and Induction Heated Melts

Micrographs of the four doped glass preparations are shown in Figure 3.3. The porosity of all of the beads was less than 3%, which is lower than that measured in a full-scale canister of glass produced by the in-can melting (ICM) process.⁽¹⁾ In any case, the porosity will not affect the leaching studies now under way. Even after 2 years at a leach rate of $1 \times 10^{-5} \text{ g/cm}^2\text{-day}$, the depth of glass penetrated would only be $\sim 20 \mu\text{m}$. However, after high temperature autoclave work is completed, corrections for the internal area may be necessary if extensive dissolution of the glass occurs. Figure 3.4 shows a micrograph and α -radiograph of the ^{244}Cm doped glass. The α -radiograph shows that ^{244}Cm is uniformly distributed in the glass.

Large spinel phase inclusions which form by corrosion of the steel melting crucible (and also occur in full-scale ICM glasses) are seen to be highly depleted in actinides, as expected. The porosity in the glass tends to give a false impression of irregular α -tracking and some dark spots seen are anomalies of the film processing and radiography technique. Thus, the beads appear to be homogeneously doped with no significant changes in properties from the starting NFS glass. They are representative of the large scale canisters produced by the in-can melting process.

Complementing the work on NFS glass being conducted by WISAP, a variety of studies on this same glass composition have been undertaken by the Waste Fixation Program (WFP). These other studies include radiation damage effects and thermal stability.⁽²⁾

3.1.2 Leaching of Doped Waste Glass Forms

Leaching experiments were started on all of the doped glass forms using the International Atomic Energy Agency (IAEA) leach procedure. The IAEA procedure leaching and analysis schedule is given in Table 3.3. The leaching solutions used for the doped waste glasses are shown in Table 3.4. The salt brine is based on analysis after dissolving a salt rock core in deionized water. The core was taken at the 2725-ft level of AEC Well #8 at the Waste Isolation Pilot Plant (WIPP) facility. This corresponds to the intermediate level-high level waste horizon.

FIGURE 3.3. Micrographs of Doped Glasses

Alpha Radiograph - Cm Doped Beads

FIGURE 3.4. Radiograph and Micrograph of Curium Doped Beads

TABLE 3.3. Leaching Schedule for Doped Waste Glasses

<u>Cumulative Time</u>	<u>Leach Solution Changed</u>	<u>Series Number</u>	<u>Leach Solutions Analyzed</u>
Days	1	1	1
	2	2	2
	3	3	3
	4	4	4
Weeks	2	5	5
	3	6	6
	4	7	7
	5	8	8
	6	9	
	7	10	9
	8	11	
	9	12	10
Months	3	13	11
	4	14	
	5	15	12
	6	16	
	7	17	13
	8	18	
	9	19	14
	10	20	
	11	21	15
	12	22	

TABLE 3.4. Waste Form Leach Solutions

- WIPP site natural salt brine, 80% saturated
- Synthetic calcium ground water (30 meq/l CaCl_2)
- Synthetic bicarbonate ground water (30 meq/l NaHCO_3)
- Synthetic sodium ground water (30 meq/l NaCl)
- Deionized water

Tables 3.5 and 3.6 give the composition of the salt brine. Table 3.7 details the leach solution analysis before and after contacting the waste form. Prior to beginning the leaching procedure, the beads were washed in ethyl alcohol, weighed, and put in vials of 20 each. Each leach experiment used 20 beads suspended in a nylon basket centered in 300 ml of solution, giving a volume to surface area ratio of 10. The leach containers were polypropylene-jars with O-rings fitted into the lids to assure a good seal. Table 3.8 outlines the experimental program planned for the NFS doped glasses.

The limited experimental information obtained during FY77 shows that the leach rates of all nuclide dopants are decreasing with time presumably as the resistance to diffusion of the radionuclides through the waste depleted glass matrix near the surface of the beads becomes increasingly dominant. The high pH bicarbonate solution (pH = 9) shows higher leach rates for all nuclides than the low pH solutions. This is presumably caused by an increased dissolution rate of the glass matrix itself. Analytical measurements are being started to account for the effect of actinide plate-out on the leaching container. If actinide plate-out is verified, the leach rate calculations will be corrected.

3.1.3 Leaching of Spent Fuel

Spent fuel from the H. B. Robinson reactor is being used for the spent fuel leach studies as shown in Table 3.7. Approximately 2000 g of fuel chunks of from 1/8 in. to 3/8 in. diameter have been separated out

TABLE 3.5. Chemical Compositon of Salt Brine

<u>Compound</u>	<u>Concentration (g/l)</u>
NaCl	287.0
Na ₂ SO ₄	0.0062
Na ₂ B ₄ O ₇ ·10H ₂ O	0.0160
NaHCO ₃	0.0140
NaBr	0.5200
KCl	0.0290
KI	0.0130
MgCl ₂	0.0400
CaCl ₂ ·2H ₂ O	0.0033
FeCl ₃	0.0060
SrCl ₂ ·2H ₂ O	0.0330
Rb ₂ SO ₄	0.0016
CsCl	0.0013
Total Dissolved	297.2 g/l
pH (adjusted)	6.5

TABLE 3.6. Ionic Concentration of Salt Brine

<u>Ion</u>	<u>Concentration (g-mole/l)</u>
Na ⁺	5.0
K ⁺	0.00038
Rb ⁺	0.000012
Cs ⁺	0.000008
Mg ⁺⁺	0.00041
Ca ⁺⁺	0.022
Sr ⁺⁺	0.00017
Fe ⁺⁺⁺	0.000036
Cl ⁻	4.94
Br ⁻	0.0050
I ⁻	0.000079
HCO ₃ ⁻	0.00016
SO ₄ ⁻⁻	0.036
B (BO ₃ ⁻⁻⁻)	0.00017

TABLE 3.7. Doped Glass Leach Solution Analyses

<u>Prior to Contact with Waste Form</u>	<u>After Contact with Waste Form</u>
<ul style="list-style-type: none"> • Temperature • Conductivity • pH • Eh • Spark Source Mass Spectrometry • Si 	<ul style="list-style-type: none"> • Temperature • Conductivity • pH • Eh • ^{99}Tc, ^{233}U, ^{237}Np, ^{239}Pu, ^{243}Am, ^{244}Cm • Si

TABLE 3.8. Leaching Studies for Doped and High-Level NFS Glasses and Spent Fuel

A. Actinide Doped Glasses (IAEA Leach Procedure)^(a)

	<u>Isotopes Doped</u>	<u>Solutions</u>	<u>Replicates</u>	<u>Experiments</u>
1.	$^{233}\text{U} + ^{243}\text{Am}$	5	3	15
2.	$^{239}\text{Pu} + ^{237}\text{Np}$	5	3	15
3.	^{244}Cm	5	3	15
4.	^{99}Tc	5	3	
				<hr/> 60

B. Actinide Doped Glasses (anoxic IAEA test)

1.	$^{299}\text{U} + ^{237}\text{Np}$	3	3	9
2.	^{99}Tc	3	3	<hr/> 9
				18

C. Actinide Doped Glasses (Static Leach Procedure)

1.	$^{239}\text{Pu} + ^{237}\text{Np}$	Salt	$3^{(b)}$	18
2.	$^{239}\text{Pu} + ^{237}\text{Np}$	Bicarbonate	$3^{(b)}$	<hr/> 18
				36

D. Full Level Glass (NFS or AGNS Composition, IAEA Procedure)

NFS or AGNS	5	3	15
Devitrified	5	3	<hr/> 15
			30

E. Spent Fuel (IAEA Procedure)^(a)

5	3	15
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(a) Started in FY1977

(b) Each is sampled 6 times: after 1 week, 1 month, 3 months, 6 months, 1 year, and 5 years

for spent fuel leaching studies. A representative sample of these spent fuel pellets has been crushed, dissolved and a sample is being analyzed for α , β and γ emitters.

Fifteen batches of this spent fuel were weighed out, photographed, rinsed with acetone, and placed in the same leaching containers as with the doped glass leach experiments. The geometric surface areas were approximately 30 cm² for the spent fuel batches. IAEA leach tests were initiated on these spent fuel fragments, using the solutions described in Table 3.4.

3.2 RADIONUCLIDE GEOCHEMICAL INTERACTION DATA

3.2.1 Evaluation of Sorption Measurement Methods

A number of methods can be used to measure the sorption of radionuclides by geologic media. Past experience has shown that the experimental results are sometimes dependent on the method used. Work was initiated in FY77 to compare the results of the various methods with the ultimate goal of choosing the best methods, determining their ranges of applicability, and developing standardized measurement procedures. The methods were evaluated using a range of geologic materials, nuclide-spiked ground waters, and experimental conditions. The methods studied in FY77 included:

1. batch, static, shaking or jar
2. low pressure, flow-through column
3. axial filtration
4. channel chromatography.

Preparations were also made to study the high-pressure, intact-core, flow-through column method. The details of these studies are presented in PNL-SA-6957, "Waste Isolation Safety Assessment Program, Task 4 Contractor Information Meeting Proceedings."⁽¹⁾

3.2.1.1 Method Descriptions

In the batch method a solution of known radionuclide concentration is placed in a container with geologic medium of known weight and/or surface

area. The liquid phase is sampled until its radionuclide concentration, macro constituents, and pH are constant with time. The phases are then separated and counted. From this information the distribution of radionuclide between the two phases is calculated (K_d or K_a). This information can then be used together with knowledge about the bulk density, porosity, and fracture characteristics of the geologic medium in its in-situ state to estimate the retardation factor, K , for ground-water transport of that radionuclide (the quantity needed for the assessment model calculations) using either of the two equations below:

$$K = 1 + \frac{K_d}{\rho_b} \quad (\text{for unconsolidated media}) \quad (1)$$

where:

$$K_d = \text{distribution coefficient} = \left[\frac{\text{activity of nuclide in sorbed state}}{\text{mass of medium}} \div \frac{\text{activity of nuclide in dissolved state}}{\text{volume of solution}} \right]$$

$$= \text{bulk density of medium} = \frac{\text{mass of medium}}{\text{volume of medium}}$$

$$= \text{void fraction} = \left[\frac{\text{volume of pore space}}{\text{volume of medium}} \right]$$

$$K = 1 + K_a R_f \quad (\text{for fractured media}) \quad (2)$$

where:

$$K_a = \text{distribution coefficient} = \left[\frac{\text{activity of nuclide in sorbed state}}{\text{surface area}} \div \frac{\text{activity of nuclide in dissolved state}}{\text{volume of solution}} \right]$$

$$R_f = \text{surface to volume ratio of fracture system} = \left[\frac{\text{surface area of fracture}}{\text{volume of fracture}} \right]$$

Advantages of the batch method include experimental simplicity; low cost; short duration experiments; ability to perform many experiments simultaneously; ability to use crushed rock, chunks, shards, or rock tablets; ability to calculate K_d or K_a ; ability to monitor pH, Eh, and K_d time dependence; and reversibility. Disadvantages include inability to address multiple oxidation states and species; difficulty in solid-liquid phase separation; unrealistically high (sometimes) solution to solids ratios; disregard for hydrodynamic or flow effects; and alteration of the geologic material of interest by crushing and grinding.

In the low pressure column method a column of known length is loaded with the geologic medium of known density and porosity, and ground water is pumped through the column at constant velocity. After steady-state is reached either a pulse or continuous injection of radionuclide solution is injected into the flowing ground water. The experiment continues until the radionuclide discharges from the column. From the length of the column, the velocity of the water and the time for discharge of the radionuclide, the retardation factor (K) can be calculated using Equation 3 or 4.

Assuming saturated flow and ideal chromatographic curves are obtained, then

For a pulse input:

$$\begin{aligned} K &= \text{number of pore volumes needed to reach peak nuclide concentration in effluent} \\ &= \frac{\text{volume to reach peak effluent concentration}}{\text{volume of column pore space}} \end{aligned} \quad (3)$$

For a continuous input:

$$\begin{aligned} K &= \text{number of pore volumes needed to reach 50\% breakthrough} \\ &= \frac{\text{volume to reach 50\% breakthrough}}{\text{volume of column pore space}} \end{aligned} \quad (4)$$

The 50% breakthrough occurs when

$$\frac{\text{concentration in effluent}}{\text{concentration in influent}} = 0.50$$

The distribution coefficient is then back-calculated using either Equation 1 or Equation 2.

The low pressure, flow-through column method permits the nuclide migration rates to be measured directly for porous materials without significant sample alteration. Reversibility, multiple oxidation states or species, and physical transport of colloids and fine particulates can be studied under realistic solution to solids ratios. Porous and fracture flow experiments are possible. Disadvantages include long duration experiments, inability to create practical flow rates in rock materials with low permeability, experimental phenomena such as channeling, greater difficulty in control of Eh and pH, and data reduction difficulties for non-ideal discharge curves.

The axial filtration method uses a rotating cylindrical filter which is enclosed in a coaxially-mounted pressure vessel as shown in Figure 3.5. Solution flows into the outer chamber, through the filter into the cylindrical space within the filter, and finally out through a tube mounted on the axis of rotation. The rotation of the filter (typically at several thousand rpm) keeps the geologic material uniformly distributed in the outer chamber. A slurry of the crushed geologic material is first placed in the outer (reaction) chamber and the system brought to steady state. The radionuclide solution is then introduced into the system as a step change in the inflow concentration and the radionuclide concentration in the outflow is recorded with time. The distribution coefficient is determined by recording the activity C and the effluent volume V with time and plotting the data using Equation 5.

$$\ln[1 - (C/C_0)] = -V/(V_f + m K_d) \quad (5)$$

where:

C = activity of the effluent

C_0 = influent activity

V = accumulated volume of the effluent

V_f = volume contained within outer chamber of filter

m = the weight of the adsorbent

K_d = the distribution coefficient.

The distribution coefficient is determined from the slope of the curve.

FIGURE 3.5. Schematic Diagram of Axial Filtration Apparatus

The principal advantages of this method are the ease and rapidity with which distribution coefficient determinations may be made and the capability to determine the reversibility and kinetics of the sorption. Variable oxidation state or multiple species can be identified. Eh, pH can also be monitored and controlled. Disadvantages include the necessity of using unconsolidated geologic media, the cost of the equipment, and potential interpretation problems on unsymmetric data peaks.

As the strength of sorption decreases, data reduction using the axial filtration method becomes difficult and prone to error because C rapidly approaches C_0 making the equation difficult to solve. Thus, there is a practical limit to the utilization of axial filtration methods for weakly sorbed nuclides.

In the channel chromatography method, crushed geologic material is slurried with water until moderately fluid and then applied to chemical chromatography plates by using a conventional spreader. Strips of blotter paper are used as wicks for transporting the radionuclide solution to the geologic media in the channels. The radionuclide is introduced into the column chromatograph either through the feed solution or by spotting the radionuclide directly onto the geologic media. The velocities of movement of both the eluting water and the nuclide are recorded. The retardation factor is calculated by Equation 6:

$$K = \frac{V_w}{V_n} \quad (6)$$

where:

V_w = water velocity

V_n = nuclide velocity

The distribution coefficient is then back-calculated by Equation 1. Advantages of channel chromatography include the ability to compare rapidly the migration rate of nuclides through many geologic media, the ability to study several wetting and drying cycles nondestructively, and

the ability to study multiple-oxidation states of species. Disadvantages include the need to use crushed materials, lack of control of flow rates, and the complexity in data reduction techniques. As the strength of the sorption increases, the nuclide moves so slowly that the velocity cannot be accurately measured. From the work to date it appears that the method is not useful when the K_d is greater than about 15.

The high-pressure, intact core, flow-through column method forces the radionuclide solution through unaltered rock core at elevated pressures. Except for the experimental difficulties posed by working at elevated pressures, the high-pressure and low-pressure column methods are quite similar. Work in FY77 focused on constructing a prototype apparatus. A schematic diagram is shown in Figure 3.6. The apparatus is designed for longitudinal driving pressures of 500 psi and radial confining pressures up to 6000 psi. The rock samples may be either 13 or 26 mm in diameter and 26 mm in length and are covered along the sides by cast plastic jackets to prevent radial leakage from the core. The jackets also seal the samples to the end fittings and prevent leakage of the confining pressure fluid. Brass and stainless steel have been specified for the prototype sample holder because they have mechanical properties which are adequate for the initial tests and are more quickly and cheaply fabricated than high pressure steel. The injection valve and supply line are made of Teflon to minimize extraneous sorption effects. The 6000 psi pressure limit corresponds to the lithostatic pressure imposed by 5700 ft of a geologic medium with a density of 2.4 g/cm^3 , and thus is adequate to simulate reasonable repository depths.

3.2.1.2 Comparison of Sorption Measurements by Different Methods

During FY77 the sorption of cesium was compared for the batch and low-pressure column methods, and the sorption of copper was compared for the batch and axial filtration methods. Both studies used sodium chloride brine solutions and montmorillonite clays. The results are shown in Table 3.9.

FIGURE 3.6. Schematic Diagram of High-Pressure Intact Core Flow-Through Column Apparatus

TABLE 3.9. Comparison of K_d by the Batch, Low-Pressure Column, and Axial Filtration Methods

<u>K_d Cs vs NaCl Brine Concentration</u>				
Brine Molarity	4	2	1	0.5
Batch K_d	2.0	5.0	10	20
Column K_d	2	5.8	13	20

<u>K_d Cu vs NaCl Brine Concentration</u>				
Brine Molarity	4.1	2	1.1	0.6
Batch K_d	14	16	16	12
Axial Filter K_d			11	

The sorption of strontium, nickel, and sodium was compared for the batch and channel chromatography methods using 0.1 N calcium nitrate solutions and a Muscatine silt loam. The results are shown in Table 3.10.

TABLE 3.10. Comparison of K_d by the Batch and Soil Channel Chromatography Methods

	<u>Soil Channel</u>	<u>Batch</u>
Sr-85	3.0	2.1
Na-22	0.23	4.3
Ni-63	15	27

The agreement for cesium, copper, and strontium is very good, for nickel qualitatively acceptable, and for sodium poor.

These preliminary results suggest that method independent distribution coefficients can be obtained in some situations. More comparisons must be performed on important radionuclides before final conclusions can be made. Work was also performed in FY77 to measure the sorption of plutonium, americium, neptunium, and cesium by the batch and low-pressure column methods. However, it was difficult to interpret the

results because small fractions of all four nuclides appeared to move down the column at higher velocities than the bulk of the nuclides. The cause of this behavior is being investigated.

3.2.1.3 Effects of Important Experimental Parameters on Sorption

Studies to determine the effects of such experimental parameters as time, temperature, particle size (surface area), solution pH, sodium chloride concentration, and direction of measurement (sorption or desorption) were started in FY77. Although the data obtained to date are too sparse to make final conclusions, some general observations can be made.

Batch measurements of Pu and Am sorption on small tablets of some rocks showed that equilibrium was reached very rapidly but similar experiments with other rocks showed that over 25 days were required to reach equilibrium. Other experiments using crushed minerals showed that the sorption of Np, Am, Tc, Sr, Cs, and I from solution showed only small time dependency when observed between 3 and 47 days of contact with geologic media. Still other studies showed that Sr, Cs and Sb reached equilibrium within 3 days when contacted with crushed alluvium but that Co and Nb needed at least 14 days.

Temperature differences (between 20°C and 70°C) appear to affect the sorption of Sr, Co, and Sb but not Cs. The sodium chloride concentration has a large effect on the sorption of Sr, a small effect on Cs, a still smaller effect on Np, and little or no effect on Tc and Cu. Also, a number of experiments showed that the sorption process was not totally reversible under some conditions but completely reversible under others.

A difficulty in the interpretation of FY77 work in this area was randomness in the choice of geologic materials and ground waters by the subcontractors. In FY78 standard (and well characterized) samples of a number of rocks and recipes for synthetic ground waters will be distributed so that experiments can be performed by all subcontractors on the same materials.

3.2.2 Generic Sorption Data Bank

As previously discussed in Section 2.2.1.1, there are a number of models available for predicting the transport of radionuclides through geologic media. However, there have been very little sorption data available for deep geologic materials which could be used to define the sorption parameters in these models.⁽²⁾ This situation resulted in the repeated use of one set of partly estimated sorption parameters by many workers in the field.⁽³⁻⁵⁾ Thus, work was initiated in FY77 to provide a data bank of sorption values for a large number of geologic materials and nuclides. In order to make these data interpretable a standard format for collection was developed. This format is presented in Table 3.11. As shown detailed characterizations of the geologic materials and ground waters as well as the details of the sorption experiment methodology are necessary to provide data of maximum usefulness. The data obtained in FY77 are listed in Appendix D. Sorption measurements were made for Tc, I, Sr, Cs, Np, Am, Pu, Eu, Co, Ce, Sb, U, Nb, and Ru. The geologic materials included: limestone, dolomite, marble, sandstone, siltstone, shale, tuff, soapstone, anhydrite, galena, chalcopryrite, greenstone, granite, gneiss, basalt, rock salt, montmorillonite, illite, kaolinite, vermiculite, quartz, apatite, argillite, albite, anorthite, microcline, biotite, hornblende, enstatite, pyroxene, chalk and bentonite.

3.2.3 Analysis of Generic Sorption Data

Using information from the data bank about the geologic material properties, ground water properties, and experimental conditions, it should be possible to develop empirical relationships between the measured sorption values and the independent experimental variables. Such relationships can then be used to predict sorption behavior in situations which are similar to (but not the same as) the situations investigated.

3.2.3.1 Statistical Analyses

Two statistical methods, linear regression and adaptive learning networks, were investigated in FY77 in order to evaluate methods of developing empirical equations to predict sorption. The details of these

studies are present in PNL-SA-6957.⁽¹⁾ The investigations showed that it was feasible to model K_d empirically as a function of geologic media and ground water characteristics. A number of the parameters in Table 3.11 were shown to be statistically significant variables with respect to sorption. Adaptive learning networks performed better than linear regression in correlating the limited number of data sets attempted in FY77. This suggests that nonlinear interactions were present between the geologic media and groundwater properties. However, the same interactions were not present for all nuclides.

The statistical analyses in FY77 used sorption measurement data for four nuclides (Tc, Sr, Cs, and Np), taken at three time intervals after the start of the experiments (3, 10 and 29 days), eight minerals (illite, kaolinite, montmorillonite, quartzite, albite, anorthite, and microcline), and four groundwaters (salt brine with 5130 meq/l NaCl, high sodium with 30 meq/l NaCl, high calcium with 30 meq/l, and high bicarbonate with 30 meq/l). Eight independent variables were measured for each geologic media-groundwater combination: cation-exchange capacity (CEC), surface area (SA), sodium content (Na), calcium content (Ca), chloride content (Cl), bicarbonate content (HCO_3), pH and Eh. With the addition of the time variable (t), nine experimental parameters were measured for each nuclide-media-groundwater system. Table 3.12 contains the results of the preliminary linear regression correlations on both time-independent and time-dependent bases. The results of the adaptive learning network correlations are presented in Reference 1.

3.2.3.2 Comparative Analyses

Although the generic data base is not complete, several preliminary comparisons can be made. Table 3.13 compares the strontium, cesium, americium and plutonium sorption data for basalt with two plagioclase feldspars. Basalt contains labradorite, an intermediate composition plagioclase feldspar. The K_d for strontium appears to be sensitive to pH or HCO_3 concentration perhaps due to greater sorption by carbonate

TABLE 3.11. Information Requirements for Generic Data Bank

Independent Variables				Methodology
Geologic Material Properties		Ground-Water Properties	Nuclide Properties	
Mineralogy	Amount	pH	(a) Tracer Concentration	(a) Method Details
Primary Minerals	%	Eh	(b) Tracer Valence	(b) Soil to Solution Ratio
Secondary Minerals	%	Major Cations	State Distribution	
CaCO ₃	%	Major Anions	(c) Contact Time	(c) Misc.
Hydrous Oxides	%	Soluble Organic Composition	(d) Direction (adsorption or desorption)	
Organic Content	%	Soluble SiO ₂		
Cation-Exchange-Capacity		Soluble Minor Species		
Anion-Exchange-Capacity		Temperature		
Surface Area				
Hydrologic Properties				
Hydraulic Conductivity				
Permeability				
Porosity				
Water Velocity				
Percentage Saturation				
Fissure Surface Area to Volume Ratio				

TABLE 3.12. Preliminary Empirical Sorption Correlations Using Linear Regression

Time Independent

$$K_{dTc} = 2.1 - 0.80 (CEC) - 0.31 (SA) - 0.86 (Ca) + 1.2 (Cl) - 0.61 (HCO_3) - 1.3 (pH) - 1.57 (Eh)$$

$$\ln(K_{dSr}) = 4.2 + 0.49 (CEC) + 0.07 (SA) - 1.4 (Ca) - 1.4 (Cl) + 0.40 (HCO_3) + 1.1 (pH) + 0.60 (Eh)$$

$$\ln(K_{dCs}) = 7.0 + 3.6 (CEC) - 2.7 (SA) - 3.8 (Na) - 4.4 (pH) - 4.0 (Eh)$$

$$\ln(K_{dNp}) = 3.7 - 0.40 (CEC) + 0.50 (SA) + 0.88 (Na) - 0.43 (Ca) - 0.80 (HCO_3) + 1.8 (pH) + 0.64 (Eh)$$

Time Dependent

$$K_{dTc} = 0.90 - 0.52 (CEC) - 0.22 (SA) - 0.20 (Ca) + 0.67 (Cl) - 0.50 (HCO_3) - 0.41 (pH) - 0.93 (Eh) - 0.09 (t)$$

$$\ln(K_{dSr}) = 4.3 + 0.60 (CEC) - 0.04 (SA) - 1.4 (Ca) - 1.8 (Cl) + 0.28 (HCO_3) + 0.43 (pH) - 0.12 (Eh) - 0.24 (t)$$

$$\ln(K_{dCs}) = 6.9 + 1.7 (CEC) - 0.86 (SA) - 1.7 (Na) + 0.63 (HCO_3) - 0.90 (pH) + 0.13 (Eh) + 0.32 (t)$$

$$\ln(K_{dNp}) = 3.5 + 0.38 (SA) - 0.40 (Ca) + 0.34 (Cl) - 0.63 (HCO_3) + 1.1 (pH) + 0.12 (Eh) + 0.22 (t)$$

where:

CEC = cation exchange capacity (milliequivalents/100 g)

SA = surface area (m²/g)

Ca, Na,

Cl, HCO₃ = ionic concentration (meq/l)

Eh = electromotive potential (millivolts)

t = time

TABLE 3.13. Preliminary Distribution Coefficients for Strontium, Cesium, Americium and Plutonium with Basalt and Plagioclase Feldspars Similar to those Present in Basalt

	<u>Experiment</u>	<u>Ground Water</u>	<u>pH</u>	<u>K_d_{Sr}</u>	<u>K_d_{Cs}</u>	<u>K_d_{Am}</u>	<u>K_d_{Pu}</u>
Columbia River Basalt	Tablets	Rock Equilibrated	-	-	-	250	150
	16-20 mesh		-	-	-	83	88
	30-40 mesh		-	-	-	130	120
	50-70 mesh		-	-	-	180	130
Umtanum Basalt	Crushed	0.003N NaHCO ₃	8.6	-	300	-	-
			7.9	150	-	-	-
			8.8	-	-	230	20
Albite	Crushed	0.03N NaHCO ₃	9.4	550	530	-	-
			-	-	-	5400	-
		0.3N CaCl ₂	7.7	4	820	170	-
Anorthite	Crushed	0.3N NaHCO ₃	9.4	460	610	-	-
			-	-	-	3800	-
		0.3N CaCl ₂	7.7	3	770	180	-

precipitation. The K_d for cesium does not appear to be as sensitive as strontium to solution pH. The americium data of the three groups compares well, but the plutonium data for the rock equilibrated groundwater is about five times larger than that for bicarbonate groundwater. The equilibrium water composition of the data for the rock equilibrated experiments was not measured, but it probably contains significantly less HCO_3^- ion (which is capable of forming soluble complexes). Thus, the lower K_d Pu found for bicarbonate ground water could reflect soluble carbonate complexation. Plutonium tracer concentration and/or speciation distribution could also be affecting the results. The pure mineral data for strontium suggest a strong effect of calcium concentration on strontium sorption.

Table 3.14 shows cesium sorption data for montmorillonite with a salt brine groundwater as a function of cesium concentration. The sorption was greater at the lower Cs concentration. This result may support the conclusion that a few selective sorption sites can cause a large K_d for some nuclides present at very low concentrations (such as those expected in many waste repository release scenarios).

TABLE 3.14. Preliminary Distribution Coefficients for Cesium with Montmorillonite

<u>Material</u>	<u>Experiment</u>	<u>Ground Water</u>	<u>Cesium Concentration</u>	<u>K_dCs</u>
Montmorillonite	Crushed	4N NaCl	10^{-3} M	3-10
		0.6N NaCl	10^{-3} M	11-35
	Crushed	5N NaCl	10^{-11} M	33
		0.03N NaCl	10^{-11} M	1000

Sorption data for plutonium and americium were obtained for both tablets and crushed material. These data are shown in Table 3.15. In seven out of nine experiments the sorption was greater for the crushed material than for the tablets suggesting that sorption increases as

TABLE 3.15. Preliminary Distribution Coefficients for Plutonium and Americium with Tablets and Crushed Material

<u>Material</u>		<u>K_dPu</u>	<u>K_dAm</u>
Limestone	Tablet	62 ± 76	59 ± 87
	Crushed	290	2200
Basalt	Tablet	150 ± 71	250 ± 97
	Crushed	88 to 130	83 to 180
Tuff	Tablet	24 ± 21	140 ± 98
	Crushed	11	23
Low Temperature Metamorphic	Tablet	81 ± 57	0.9 ± 1.5
	Crushed		2600
Marble	Tablet	100 ± 68	180 ± 34
	Crushed	720	3100
Soapstone	Tablet	20 ± 10	65 ± 41
	Crushed		>47000
Dolomite (NTS)	Tablet	17 ± 16	62 ± 77
	Crushed		3500
Chalcopyrite	Tablet	11 ± 12	0.5 ± 0.2
	Crushed		14
Galena	Tablet	3.9	0.1
	Crushed	930	23

surface area increases. The tablet data had large error bands which suggests that this experimental design has low potential for reproducibility.

The sorption of Cs, Pu, Am, and Np by chalk, shale, tuff, sandstone, and limestone was measured using the low pressure column method. The break-through curves and nuclide distributions in the rock columns did not appear to have the Gaussian shape expected for equilibrium sorption of a

single species of each nuclide. In all experiments a small fraction of each nuclide appeared to move more rapidly than the majority of the material. This phenomenon may be attributed to: multiple speciation (i.e., the presence of more than one chemical species of each nuclide), channeling (the presence of a low resistance flow pathway which permits some of the nuclide to move through the column without contacting the solid phase enough to maintain the sorption equilibrium condition), rate controlled sorption (the condition which results when the groundwater moves through the column too fast or the sorption process is too slow to maintain equilibrium between the dissolved and sorbed phases), and colloidal transport (the physical movement of nuclide as small particles rather than as individual ions). More work is necessary to resolve these unexpected (certainly for cesium) and difficult to interpret results.

3.2.4 Validation Studies

An important consideration concerning sorption data is the relationship between the results of short-term laboratory experiments and long-term in-situ behavior. Among the methods of quantifying this relationship are thermodynamic studies of nuclide-groundwater-geologic media systems and the observed nuclide behavior at natural and man-initiated migration situations (Oklo, Nevada Test Site, uranium ore deposits, existing radioactive waste disposal sites, and large-scale in-situ tests). Work in FY77 focused on the thermodynamic studies although a small amount of support was provided to enhance migration studies under way at the Nevada Test Site.

Plots of nuclide activity in solution versus pH and Eh were constructed for antimony, cerium, cesium, cobalt, europium, promethium, radium, ruthenium, strontium, thorium, uranium, zirconium, plutonium, neptunium, americium, and curium. These data are being incorporated into a computer program to facilitate rapid calculation of nuclide activities for any groundwater composition. After long time periods the concentration of nuclide species in various ground-water-geologic media

systems should approach that predicted by the thermodynamic calculations. Thus, the thermodynamic results can be used to predict the maximum solution concentrations possible for geologic environments of interest to radioactive waste disposal. The details of these studies are presented in PNL-2651, "Solid Phases and Solution Species of Different Elements in Geologic Environments"⁽⁶⁾ and PNL-SA-6957.⁽¹⁾

3.2.5 Sorption Mechanism Studies

A more complete understanding of the controlling sorption mechanisms for important nuclides in geologic environments relevant to waste isolation will increase our ability to predict radionuclide behavior at one site from data taken at another site. This in turn can result in time and cost savings during subsequent site-specific investigations. During FY77 studies were initiated on the effects of solution ionic strength on nuclide sorption, microstructural configuration of sorption sites on specific geologic materials, controlled pH-Eh sorption experiments for Pu and the solubility of plutonium compounds. The preliminary results of this work are presented in PNL-SA-6957.⁽¹⁾

4.0 WORKSHOPS

Four workshops were held during FY77 for the purpose of communicating WISAP results and obtaining peer review from the technical community. The workshops also served to improve the short- and long-term plans for WISAP.

4.1 SAFETY ASSESSMENT METHODS WORKSHOP

The first WISAP workshop was held at the Pacific Northwest Laboratory (PNL), Richland, Washington, on February 23-24, 1977. Representatives were present from PNL; Electric Power Research Institute; Energy Research Group, Inc.; Office of Waste Isolation; Science Applications, Inc.; United Nuclear Industries; U.S. Geological Survey; and the University of Washington. The objective of the workshop was to review potentially applicable safety assessment methods and the proposed WISAP release scenario analysis concept.

There was considerable discussion concerning the strengths and weaknesses of the various methods that could be potentially applied to assess the long-term safety performance of geologic isolation repositories. Although a consensus was not reached, there was significant support for the use of a Monte Carlo method. It was believed that the use of biasing techniques would make it possible to obtain the proper statistics for very low probability events. Peripheral discussion focused on the interface of WISAP with related programs under way elsewhere, nuclear waste isolation objectives, and public perceptions of the geologic isolation of nuclear waste materials.

4.2 HYDROLOGIC AND CONTAMINANT TRANSPORT METHODS WORKSHOP

A workshop on hydrologic and contaminant transport modeling was held July 25-26, 1977, at the Battelle Seattle Research Center, Seattle, Washington. Organizations represented included: Battelle Columbus Laboratories; PNL; Boeing Computer Services, Inc.; George Maddox & Associates; Intera Corporation; Lawrence Berkeley Laboratory; Lawrence Livermore Laboratory; Princeton University; Rockwell Hanford Operations; Rocky Mountain Arsenal; Sandia Laboratories; U.S. Geological Survey;

University of Illinois; University of New Mexico; and University of Waterloo. The objectives of the workshop were to: 1) discuss the basic assumptions and requirements for the geosphere transport portion of the WISAP release consequence analysis system, 2) obtain critiques of the proposed model systems from other experts in the field, and 3) obtain ideas for making models more useful to the long-term safety assessment problem.

Objective 1 was achieved by reviewing a list of assumptions and requirements which had been previously prepared by PNL. There was general agreement on the content of the statements but significant disagreement about statement wording. A number of suggestions for improving statement clarity were made.

Objective 2 was achieved by reviewing a categorization of hydrologic and contaminant transport models that had been previously prepared by PNL. This categorization had four levels of model complexity. The point was made that increasing model complexity in the absence of supporting data does not produce a more accurate prediction of nuclide transport behavior. Furthermore, there is no point in developing models whose parameters cannot be set in a rational way for the long-term safety assessment problem. Some members of the group felt that two levels of modeling sophistication were sufficient. The first level would employ simple models and would be used for scoping, sensitivity, and uncertainty analyses for the multitude of the possible release scenarios. The second level would be used for in-depth study of important scenarios and for technical backup in licensing hearings.

Objective 3 was accomplished only to a limited extent. The only specific suggestion was that the format arrangement of the data and information be such that it is easily used in the selected transport and dose models. It was generally agreed that sensitivity studies are necessary and that the models and codes should be validated and verified (to the extent possible) and fully documented in publicly available reports.

The details of this workshop will be presented in PNL-2707, "Workshop on Transport Modeling for the Safety Assessment Program on Nuclear Waste Isolation."

4.3 GEOLOGIC ANALYSIS WORKSHOP

A workshop on the geologic data requirements for analysis of potentially disruptive phenomena for geologic isolation repositories was held July 27-28, 1977, at Battelle Seattle Research Center, Seattle, Washington. Organizations represented included PNL; Energy Research Group, Inc.; Lamont Geological Observatory; Lawrence Livermore Laboratory; Los Alamos Scientific Laboratory; Louisiana State University; Office of Waste Isolation; Ohio State University; Planetary Science Institute; Sandia Laboratories; Stanford University; TERA Corporation; U.S. Geological Survey; University of Illinois; and Western Washington State University.

The objectives of this workshop were to: 1) assess and generate input for the use of "subjective probabilities" as a technique for obtaining geologic information from earth scientists, 2) develop or improve submodels of the various geologic processes for use in the WISAP release scenario analysis method, 3) determine quantitative bounds on disruptive process rates and disruptive event frequencies, and 4) exchange information about analysis methods and data from similar NRC-supported programs at Sandia and Lawrence Livermore Laboratories.

The objectives were achieved only in a qualitative sense at the workshop itself. However, objectives 1, 2, and 3 were partially achieved in a quantitative sense in reports submitted by the earth science consultants after the meeting. The workshop also served to introduce the waste isolation safety assessment problem to the team of consultants as a prelude to more in-depth technical activities in FY78. The details of this workshop will be presented in PNL-SA-7197, "WISAP Workshop on Potentially Disruptive Phenomena for Nuclear Waste Repositories."

4.4 GEOCHEMICAL INTERACTION DATA WORKSHOP

The fourth WISAP workshop was held September 20-23, 1977, at Battelle Seattle Research Center, Seattle, Washington, to review FY77 progress in obtaining radionuclide geochemical interaction data. Organizations represented included: Adaptronics, Inc.; Argonne National Laboratory; Atomic Energy of Canada, Ltd.; PNL; Bechtel Corporation; Brookhaven National Laboratory; Georgia Institute of Technology; Lawrence Berkeley Laboratory; Lawrence Livermore Laboratory; Los Alamos Scientific Laboratory; Louisiana State University; Nuclear Assessments, Inc.; NUS Corporation; Oak Ridge National Laboratory; Office of Waste Isolation; Pennsylvania State University; Rockwell Hanford Operations; Sandia Laboratories; U.S. Geological Survey; University of California at Davis; University of Waterloo; University of Wisconsin; and Yale University.

The major objective of this workshop was to obtain peer review of the technical results from this part of WISAP during FY77. Among the conclusions reached at the workshop were the following:

1. The selection of particular sorption measurement methods and the specification of experimental procedures are premature at the present time.
2. A "standard" sample program is needed to cross-verify the techniques of all subcontractors.
3. The development of a generic sorption data bank is needed.
4. Some subcontractors need to improve their characterization of geologic materials and ground waters used in their experiments.
5. The range of study in this area needs to be narrowed in order to speed up the delivery of usable output for the overall program.

The details of this workshop are reported in PNL-SA-6957, "Waste Isolation Safety Assessment Program Task 4 Contractor Information Meeting Proceedings" (see Reference 1, Section 3.2).

5. REFERENCES

SECTION 2.1 - RELEASE SCENARIO ANALYSIS

1. K. J. Schneider and A. M. Platt (eds.), High-Level Waste Management Alternatives. BNWL-1900, Pacific Northwest Laboratory, Richland, WA, 1974.
2. S. F. Logan (chairman), Workshop on Geologic Data Requirements for Radioactive Waste Management Assessment Models. Y/OWI/SUB-76/81726, Office of Waste Isolation, Oak Ridge, TN, 1976.
3. National Academy of Sciences, Disposal of Radioactive Wastes on Land. Publication 519, Washington, DC, 1957.
4. A. Mazur, "Disputes Between Experts," Minerva. 11, 1973.
5. G. Benveniste, The Politics of Expertise. Glenessary Press, Berkeley, CA, 1972.
6. L. King and P. H. Melanson, "Knowledge and Politics," Public Policy. 20, 1972.
7. N. C. Dalkey and O. Helmer, "An Experimental Application of the Delphi Method to the Use of Experts," Management Science. 9 (3), 1963.
8. T. J. Gordon and O. Helmer, Report on a Long-Range Forecasting Study. Rand Paper P-2982, Rand Corporation, Santa Monica, CA, 1964.
9. O. Helmer, Social Technology. Basic Books, New York, NY, 1966.
10. Lord Rayleigh, "On the Instability of Jets," Proc. London Math. Soc. 10 (4), 1878.
11. C. C. Lin, The Theory of Hydrodynamic Stability. Cambridge University Press, Cambridge, England, 1955.
12. D. K. Cheng, Analysis of Linear System. Addison-Wesley Publishing Co., New York, NY, 1959.
13. Y. Rocard, Dynamic Instability: Automobiles, Aircraft, and Suspension Bridges. Frederick Ungar Company, 1957.
14. D. L. Hetrick, Dynamics of Nuclear Reactors. University of Chicago Press, Chicago, IL, 1971.

15. H. C. Burkholder, J. A. Stottlemire and J. R. Raymond, "Safety Assessment and Geosphere Transport Methodology for the Geologic Isolation of Nuclear Waste Materials," Risk Analysis and Geologic Modeling in Relation to the Disposal of Radioactive Wastes into Geologic Formations. OECD Nuclear Energy Agency, Paris, France, 1977.
16. Nuclear Regulatory Commission, Reactor Safety Study. WASH-1400, Washington, DC, 1975.
17. J. B. Fussell, E. B. Henry and N. H. Marshall, MOCUS - Computer Program to Obtain Minimal Sets from Fault Trees. ANCR-1156, 1974.
18. W. J. Van Slyke and D. E. Griffing, ALLCUTS - A Fast, Comprehensive Fault Tree Analysis Code. ARH-ST-112, Atlantic Richfield Hanford Company, Richland, WA, 1975.
19. W. E. Vesely and R. E. Narum, PREPP and KITT: Computer Codes for the Automatic Evaluation of a Fault Tree. IN-1349, 1970.
20. G. R. Burdick, N. H. Marshall and J. R. Wilson, COMCAN - A Computer Program for Common Cause Analysis. ANCR-1314, 1976.
21. D. P. Wagnen, C. L. Cate and J. B. Fussell, "Common Cause Failure Analysis Methodology for Complex Systems," Nuclear Systems Reliability and Safety. Society for Industrial and Applied Mathematics, 1977.
22. T. H. Smith et al., A Risk Based Fault Tree Analysis Method for Identification, Preliminary Evaluation, and Screening of Potential Accidental Release Sequences in Nuclear Fuel Cycle Operations. BNWL-1959, Pacific Northwest Laboratory, Richland, WA, 1976.
23. P. J. Pelto and W. L. Purcell, MFAULT: A Computer Program for Analyzing Fault Trees. BNWL-2145, Battelle, Pacific Northwest Laboratories, Richland, WA, 1977.
24. W. Hammer, Handbook of System and Product Safety. Prentice-Hall, Englewood Cliffs, NJ, 1972.
25. H. E. Lambert and G. Yakigarolu, "Fault Trees for Diagnosis of System Fault Conditions," Nuclear Science and Engineering. 62, 1977.
26. D. F. Hassl, "Advanced Concepts in Fault Tree Analysis," Proceedings of System Safety. University of Washington and The Boeing Company, Seattle, WA, 1965.

27. G. R. Burdick and J. B. Fussell, "On the Adaptation of Cause-Consequence Analysis to U.S. Nuclear Power Systems Reliability and Risk Assessment," A Collection of Methods for Reliability and Engineering. ANCR-1273, 1976.
28. J. L. Carter, ACORN: A Computer Program for Plotting Fault Trees. BNWL-2144, Pacific Northwest Laboratory, Richland, WA, 1977.
29. G. D. Seybold, RAFT: A Computer Program for Fault Tree Risk Calculations. BNWL-2146, Pacific Northwest Laboratory, Richland, WA, 1977.
30. S. E. Logan and M. C. Berbano, "Geologic Modeling in Risk Assessment Methodology for Radioactive Waste Management," Risk Analysis and Geologic Modeling in Relation to the Disposal of Radioactive Wastes into Geological Formations. OECD Nuclear Energy Agency, Paris, France, 1977.
31. R. Proske, "Previous Results of Risk Analysis of Repositories for Radioactive Wastes in Geologic Salt Formation in the Federal Republic of Germany," Risk Analysis and Geologic Modeling in Relation to the Disposal of Radioactive Wastes into Geologic Formations. OECD Nuclear Energy Agency, Paris, France, 1977.
32. G. Bertozzi, M. D'Alessandro, F. Girardi and M. Vanossi, "Evaluation of the Safety of Storing Radioactive Wastes in Geological Formation: A Preliminary Application of the Fault Tree Analysis to Salt Formations," Risk Analysis and Geologic Modeling in Relation to the Disposal of Radioactive Wastes into Geological Formations. OECD Nuclear Energy Agency, Paris, France, 1977.
33. J. S. Hammond, "Better Decisions with Preference Theory," Harvard Business Review. 1967.
34. P. D. Newendorp, "Use of Decision Trees Can Help Simplify Complex Problems," The Oil and Gas Journal. 1976.
35. IBM, General Purpose Systems Simulator II Reference Manual. International Business Machines Corporation, New York, NY.
36. H. M. Markowitz, Bernard Hausner and W. H. Karr, SIMSCRIPT: A Simulation Programming Language. RM-3310, The Rand Corporation, Santa Monica, CA, 1962.
37. P. J. Kiviat, GASP - A General Activity Simulation Program. 17-019(2), Applied Research Laboratory, United States Steel Corporation, Monroeville, PA, 1963.

38. Systems Development Corporation, SIMPAC User's Manual. TM 602/00/00, Santa Monica, CA, 1962.
39. A. L. Pugh, DYNAMO User's Manual. The MIT Press, Cambridge, MA, 1963.
40. C. C. Holt, R. W. Shirey, D. V. Steward, J. L. Midler and A. Stroud, Program SIMULATE, A User's and Programmer's Manual. Social Systems Research Institute, University of Wisconsin, Madison, WI, 1964.
41. J. M. Hammersley and D. C. Handscomb, Monte Carlo Methods. Wiley & Sons, Inc., New York, NY, 1964.
42. E. Parzen, Stochastic Processes. Holden-Day, New York, NY, 1972.

SECTION 2.2 - RELEASE CONSEQUENCE ANALYSIS

1. Holcomb Research Institute, International Assessment of Groundwater Modeling as an Aid to Water Resource Management. Butler University, 1978.
2. D. L. Streng, E. C. Watson, and J. G. Droppo, Review of Computational Models and Computer Codes for Environmental Dose Assessment of Radioactive Release. BNWL-B-454, Pacific Northwest Laboratory, Richland, WA, 1976.
3. F. O. Hoffman, C. W. Miller, D. L. Shaeffer, and C. T. Garten, Jr., "Computer Codes for the Assessment of Radionuclides Released to the Environment," Nuclear Safety. 18:343, 1977.
4. D. H. Lester, G. Jansen, and H. C. Burkholder, "The Migration of Radionuclide Chains Through an Adsorbing Medium," AICHE Symposium Series No. 152, Adsorption and Ion Exchange. 71:202, 1975.
5. R. W. Nelson, Evaluating the Environmental Consequences of Groundwater Contamination. BCSR-6/UC-11, BCS Richland, Inc., Richland, WA, 1976.
6. C. Van der Akker, "Performance of a Recharge and Recovery System in an Aquifer with Uniform Flow," Hydrologic Sciences Bulletin. 21:3, 1976.
7. J. Danielson, D. K. Sunada, and D. B. McWhorter, Management of Streamaquifer Systems Through Use of Analytical Models. American Geophysical Union Conference, 1974.

8. S. W. Ahlstrom and H. P. Foote, Multicomponent Mass Transport-Discrete Parcel Random Walk Model Theory and Numerical Implementation. BNWL-2127, Pacific Northwest Laboratory, Richland, WA, 1977.
9. R. L. Cooley, Finite Element Solutions for the Equations of Groundwater Flow. Hydrology and Water Resources Pub. No. 18, Desert Research Institute, Las Vegas, NV, 1974.
10. K. L. Kipp, A. E. Reisenauer, C. R. Cole, and C. A. Bryan, Variable Thickness Transient Groundwater Flow Model Theory and Numerical Implementation. BNWL-1703, Pacific Northwest Laboratory, Richland, WA, 1972 (updated 1976).
11. D. W. Chorley, A Finite Element Model for Analysis of Multiaquifer Systems. M. Sc. Thesis, University of Waterloo, Canada, 1976.
12. J. D. Bredehoeft and G. F. Pinder, "Mass Transport in Flowing Groundwater," Water Resources Research. 9(1):194-210, 1973.
13. C. L. Lin, "Digital Simulation of the Boussinesq Equation for a Water Table Aquifer," Water Resources Research. 8(3):691-698, 1972.
14. S. K. Gupta, K. K. Tanji, and J. N. Luthin, A Three-Dimensional Finite Element Ground Water Model. University of California, Davis, CA, 1975.
15. J. F. Fletcher and W. L. Dotson, Compilers, HERMES: A Digital Computer Code for Estimating Regional Radiological Effects from the Nuclear Power Industry. HEDL-TME-71-168, Hanford Engineering Development Laboratory, Richland, WA, 1971.
16. J. K. Soldat, N. M. Robinson, and D. A. Baker, Models and Computer Codes for Evaluating Environmental Radiation Doses. BNWL-1754, Pacific Northwest Laboratory, Richland, WA, 1974.
17. D. K. Truby and S. V. Kaye, The EXREM III Computer Code for Estimating External Radiation Doses to Populations from Environmental Releases. ORNL-TM-4322, Oak Ridge National Laboratory, Oak Ridge, TN, 1973.
18. L. Bramati et al., "VADOSCA: A Simple Code for the Evaluation of Population Exposure Due to Radioactive Discharges," Proceedings of the Third International Congress of the International Radiation Protection Association. Washington, DC, September 9-14, 1973, CONF-730907-P2, pp. 1072-1077, 1973.

19. J. R. Watts, "Modeling of Radiation Doses from Chronic Aqueous Releases," presented at Health Physics Society Annual Meeting, San Francisco, June 27-July 2, 1976, CONF-760652-1, Savannah River Laboratory, 1976.
20. D. A. Baker, G. R. Hoenes, and J. K. Soldat, FOOD: an Interactive Code to Calculate Internal Radiation Doses from Contaminated Food Products. BNWL-SA-5523, Pacific Northwest Laboratory, Richland, WA, 1976.
21. R. S. Booth and S. V. Kaye, A Preliminary Systems Analysis Model of Radioactivity Transfer to Man from Deposition in Terrestrial Environment. ORNL-TM-3135, Oak Ridge National Laboratory, Oak Ridge, TN, 1971.
22. R. S. Booth, "System Analysis Model for Calculating Radionuclide Transport Between Receiving Waters and Bottom Sediments," Environmental Toxicity of Aquatic Radionuclides: Models and Mechanisms, Proceedings of the 8th International Conference on Environmental Toxicity, June 2-4, 1975, University of Rochester, Rochester, NY, pp. 133-164, Ann Arbor Science; also ORNL-TM-4751, Oak Ridge National Laboratory, Oak Ridge, TN, 1975.
23. Oak Ridge National Laboratory, RSIC Computer Code Collection: ACRA-II-Kernal Integration Code Estimation of Radiation Doses Caused by a Hypothetical Reactor Accident. CCC-213, Oak Ridge, TN, 1974.
24. J. M. Otter and P. A. Conners, Description of the COMRADIX-III Code. TI-001-130-053, Atomics International, 1975.
25. L. L. Bonzon and J. B. Rivard, Computational Method for Calculation of Radiological Dose Resulting from Hypothetical Fission Product Release. SC-RR-70-338, Sandia Laboratories, Albuquerque, NM, 1970.
26. D. L. Streng, M. M. Hendrickson, and E. C. Watson, RACER: A Computer Program for Calculating Potential External Dose from Airborne Fission Products Following Postulated Reactor Accidents. BNWL-B-69, Pacific Northwest Laboratory, Richland, WA, 1971.
27. D. R. Wenzel, "A Computer Code to Calculate Doses Resulting from Release of Radionuclides to the Atmosphere," Health Physics. 27:641 (Abstr), 1974.
28. D. L. Streng, E. C. Watson, and J. R. Houston, SUBDOS: A Computer Program for Calculating External Doses from Accidental Atmospheric Releases of Radionuclides. BNWL-B-351, Pacific Northwest Laboratory, Richland, WA, 1975.

29. J. R. Houston, D. L. Strenge, and E. C. Watson, DACRIN: A Computer Program for calculating Organ Dose from Acute or chronic Radionuclide Inhalation. BNWL-B-389, Pacific Northwest Laboratory, Richland, WA, 1974.
30. G. G. Killough, P. S. Rohwer, and W. D. Turner, INREM: A FORTRAN Code Which Implements ICRP 2 Models of Internal Radiation Dose to Man. ORNL-5003, Oak Ridge National Laboratory, Oak Ridge, TN, 1975.
31. R. E. Moore, AIRDOS: A computer Code for Estimating Population and Individual Doses Resulting from Atmospheric Releases of Radionuclides from Nuclear Facilities. ORNL-TM-4687, Oak Ridge National Laboratory, Oak Ridge, 1975.
32. J. A. Martin, Jr., J. C. B. Nelson, and P. A. Cuny, AIREM Program Manual: A Computer Code for Calculating Doses, Population Doses, and Ground Depositions Due to Atmospheric Emissions of Radionuclides. EPA-520/1-74-004, Office of Radiation Programs, U.S. Environmental Protection Agency, 1974.
33. D. L. Strenge and E. C. Watson, KRONIC: A Computer Program for Calculating Annual Average External Doses from Chronic Atmospheric Releases of Radionuclides. BNWL-B-264, Pacific Northwest Laboratory, Richland, WA, 1973.
34. R. Fukai and C. N. Murray, "Adsorption and Desorption of Plutonium and Americium in Fresh Water-Sediment and Seawater-Sediment Systems," IAEA-163, Activities of the International Laboratory of Marine Radioactivity 1974 Report, 96 (1974).
35. C. R. Frink, "Fixation of ^{137}Cs by Soil Clays," NYO-2955-25, 1971.
36. H. C. Claiborne and F. Gera, Potential Containment Failure Mechanisms and Their Consequences at a Radioactive Waste Repository in Bedded Salt in New Mexico. ORNL-TM-4639, Oak Ridge National Laboratory, Oak Ridge, TN, 1974.
37. H. C. Burkholder, M. O. Cloninger, D. A. Baker, and G. Jansen, "Incentives for Partitioning High-Level Waste," Nuclear Technology. 31:202, 1976.
38. D. S. Jenkinson and J. H. Rayner, "The Turnover of Soil Organic Matter in Some of the Rothamsted Classical Experiments," Soil Science. 123:298, 1977.
39. The Effects on Populations of the Exposure to Low Levels of Ionizing Radiation. National Academy of Science, National Research Council Advisory Committee on Biological Effects of Ionizing Radiation, Washington, DC, (1972).

40. Environmental Radiation Dose Commitment: An Application to the Nuclear Power Industry, EPA-520/4-73-002, U.S. Environmental Protection Agency, (1974).
41. B. K. Trimble and J. H. Doughty, "The Amount Hereditary Disease in Human Populations," American Human Genetics, 38, 199 (1974).
42. H. B. Newcombe, "Mutation and the Amount of Human Ill Health," Radiation Research: Biomedical, Chemical, and Physical Perspectives, Academic Press, New York, NY, 937 (1975).

SECTION 3.1 - WASTE FORM RELEASE RATE DATA

1. D. E. Larsen and W. F. Bonner, editors, High Level Waste Vitrification by Spray Calculation/In-Can Melting. BNWL-2092, Pacific Northwest Laboratory, Richland, WA, 1976.
2. J. E. Mendel, Annual Report on the Characteristics of High Level Waste Glasses. BNWL-2252, Pacific Northwest Laboratory, Richland, WA, 1977.

SECTION 3.2 - RADIONUCLIDE GEOCHEMICAL INTERACTION DATA

1. R. J. Serne, Waste Isolation Safety Assessment Program. Task 4 Contractor Information Meeting Proceedings, September 20-23, 1977. PNL-SA-6957, Pacific Northwest Laboratory, Richland, WA.
2. H. C. Burkholder, "Methods and Data for Predicting Nuclide Migration in Geologic Media," Proceedings of the International Symposium on the Management of Waste from the LWR Fuel Cycle. U.S. Energy Research and Development Administration, Washington, DC, 1976.
3. K. J. Schneider and A. M. Platt, editors, High-Level Waste Management Alternatives. BNWL-1900, Pacific Northwest Laboratory, Richland, WA, 1974.
4. H. C. Burkholder, M. O. Cloninger, D. A. Baker, and G. Jansen, "Incentives for Partitioning High-Level Waste," Nuclear Technology. 31:202, 1976.
5. S. E. Logan and M. C. Berbano, "Geologic Modeling in Risk Assessment Methodology for Radioactive Waste Management," Risk Analysis and Geologic Modeling in Relation to the Disposal of Radioactive Wastes into Geologic Formations. OECD Nuclear Energy Agency, Paris, France, 1977.
6. Dhanpat Rai and R. J. Serne, Solid Phases and Solution Species of Different Elements in Geologic Environments. PNL-2651, Pacific Northwest Laboratory, Richland, WA, 1978.

APPENDICES

APPENDIX A
DETAILS OF REPOSITORY SIMULATION MODEL DEVELOPMENT

J. A. Stottlemire

Pilot Program Example Logic

Flow Diagram for Preliminary Repository Simulation Model

APPENDIX B
DESCRIPTIONS OF POTENTIALLY APPLICABLE MODELS
FOR RELEASE CONSEQUENCE ANALYSIS

R. W. Nelson

APPENDIX B

DESCRIPTIONS OF POTENTIALLY APPLICABLE MODELS FOR RELEASE CONSEQUENCE ANALYSIS

This section contains descriptions of hydrologic, contaminant transport, water-dose and air dose models which are potentially useful in analyzing the consequences of releases from geologic isolation repositories. The descriptions are presented in the order in which they are referenced in Tables 2.4 and 2.5.

B.1 HYDROLOGIC AND CONAMINANT TRANSPORT MODELS

Name of Model - GETOUT

Description - Predict the long-term migration of radionuclides through the geosphere from nuclear waste disposal sites. The model interfaces directly with the water-dose models, ARRRG and FOOD, and together they are used to predict the dose consequences to man from radionuclide releases.

The model analyzes the transport of radionuclides by flowing ground water following a leach incident at an underground nuclear waste disposal site. This model assumes that at some arbitrary time after the waste is deposited, the contents of the site are dissolved at a specified constant rate by ground water. The ground water flows at constant velocity through a homogeneous one-dimensional column of the geologic medium and discharges to a surface water body. The dissolved radionuclides are assumed to be in sorption equilibrium at all points in the geologic medium. Radioactive decay (including chain decay of the actinides) is modeled both at the disposal site and during migration through the geologic medium. Trace concentrations of the dissolved nuclides are assumed, and as a result the adsorption equilibrium constants are independent of concentration. A constant axial dispersion coefficient is also assumed. This model is applicable to particulate and fractured media provided the necessary input data are obtained properly and can be applied to heterogeneous media if a weighted averaging technique is properly applied to the relevant input parameters.

Solution Method - The equations describing the one-dimensional nuclide transport of radionuclide decay chains are solved (by the Laplace transform technique) for both impulse and decaying band releases.

Applications - Consequence estimations for radionuclide releases from geologic isolation.

Name of Modeler - G. Jansen and H. C. Burkholder
Pacific Northwest Laboratory
P. O. Box 999
Richland, WA 99352

Name of Model - PATHS

Description - The original purpose of the model was to provide an easily used two-dimensional analysis tool to determine the movement of water transported contaminants accidentally released from a waste storage facility.

The model was purposely designed to provide a balance between modeling sophistication and the limited data usually available for initial evaluations of subsurface contamination problems. Accordingly, the basis of the code is an idealized two-dimensional analytical solution for the ground-water potential distribution. From the potential distributions the pathline differential equations are written and then numerically solved by the code to give the paths of the fluid particles and their advance with time toward the outflow boundary.

After finishing the original version of the code, it became apparent that the combination of moderately short running times to get results, the moderate field data requirements, and the ease of running the code, made it useful in a wider variety of situations. In fact, its main strength lies in providing initial "first cut" evaluations inexpensively and quickly.

Solution Methods - Flow Potential--The usual potential energy or head problem was solved analytically using the classical potential theory for a doublet superimposed on a uniform flow. The entire strength of the doublet is dissipated at a finite outer radial distance and the doublet strength is expressed in terms of a time dependent head at the cylindrical doublet wall. Also, point sources or sinks (i.e., vertical line sources) are superimposed to represent the transient completely penetrating wells.

Flow Kinematics--The analytical expression for the potential was differentiated, substituted into Darcy's Law and the uniform porosity incorporated to yield the two pore velocity component equations which are the pathline characteristics differential equations. These two equations are solved numerically using a fourth order Runge Kutta solution scheme, modified slightly to enable stopping at prescribed distances around a well or at a remote river type boundary.

Applications - Developed in original form (without wells) as an initial model for movement from deep underground caverns.

- Initial Model of Accidental Release from a Fuels Reprocessing Facility in South Carolina.
- Initial Evaluation of Accidental Failure of Earthen Sewage Holding Ponds, Kennewick, Washington.
- Initial Evaluation of Seepage from a Copper Tailings Reservoir.
- Used during short course in "Groundwater Engineering Short Source," sponsored by Agricultural Research Service, Chickasha, Oklahoma.
- Example evaluation for State of Idaho Department of Water Administration.
- Evaluation of a numerical generation scheme for pathlines for ARHCO in cooperation with PNL for the U.S. Energy Research and Development Administration.
- Evaluation of potential hazard from subsurface reactor accidental releases for Sandia Laboratories, Albuquerque, New Mexico.

Date of Completion - May of 1974 (present version)

Name of Modeler - R. William Nelson
BCS Richland, Inc.
Richland, Washington 99352

Name of the Model - FLOP - 1

Description - Calculation of pathlines or streamlines in a confined, homogeneous aquifer without storage, and the residence times of a number of water particles. (Very similar to FRONT-N except no storage term is involved in the analytical well solutions used in this model.)

Solution Method - The analytical closed form expression for a uniform flow in an infinite horizontal permeable slab containing pumping or injection wells is used in the velocity component equations. These two simultaneous differential equations are solved using the Runge-Kutta Method to obtain the pathlines and flow time for fluid particles.

Applications - Classroom instruction and several field problems.

Date of Completion - 1974

Name of Modeler - C. van den Akker
Municipal Waterworks of Amsterdam
Condensatorweg 54
Amsterdam-Sloterdijk

Name of the Model - FLOP - 2

Description - Calculation of pathlines in a semi-confined, homogeneous aquifer without storage, and the residence times of a number of water particles in the aquifer. (Very similar to FLOP - except that the aquifer is semi-confined.)

Solution Method - The analytical closed form expression for a uniform flow in an infinite horizontal permeable slab containing pumping or injection wells is used in the velocity component equations. These two simultaneous differential equations are solved using the Runge-Kutta Method to obtain the pathlines and flow time for fluid particles.

Applications - Classroom instruction and several field problems.

Date of Completion - 1975

Name of Modeler - C. van den Akker
Municipal Waterworks of Amsterdam
Condensatorweg 54
Amsterdam-Sloterdijk

Name of the Model - FRONT-N

Description - Calculation of pathlines in a confined, homogeneous aquifer with storage and the residence times of a number of water particles. The flow is two-dimensional in the horizontal plane. In the aquifer is a lateral uniform ground-water flow. A number of sources and/or sinks are possible (fully penetrating) representing wells.

Solution Method - The analytical closed form expression for a uniform flow in an infinite horizontal permeable slab containing pumping or injection wells is used in the velocity component equations. These two simultaneous differential equations are solved using the Runge-Kutta Method to obtain the pathlines and flow time for fluid particles.

Applications - Classroom instruction and several field problems

Date of Completion - 1975

Name of Modeler - C. van den Akker
Municipal Waterworks of Amsterdam
Condensatorweg 54
Amsterdam-Sloterdijk

Name of Model - RCPIGW

Description - Compute potentiometric heads in a two-dimensional aquifer using the Error Function, Well Function and the exponential integral function. Specifically the model describes a saturated, homogeneous, isotropic aquifer, and homogeneous, incompressible fluid. Model includes arrays to define areally a) recharge, b) discharge. Boundary condition options include specified head and impermeable boundaries.

Solution Method - The model solves analytic expressions for the flow equations.

Applications - Water allocation problems in Colorado

Date of Completion - October, 1972 (refinements will continue).

Name of Modeler - David B. McWhorter
Dept. Agric. Engr.
Colorado State Univ.
Fort Collins, CO 80523

Daniel K. Sunada
Dept. Civil Engr.
Colorado State Univ.
Fort Collins, CO 80523

W. W. Burt
State Engineer's Office
Denver, CO 80203

A. Prakash
Chicago, IL

Name of the Model - Hydrologic Contaminant Transport Model (HCTM)

Description - Solution of heads (pressures) and contaminant transport with dispersion in a three-dimensional heterogeneous aquifer.

1. Fluid flow utilizes continuity and Darcy's Law.
2. Single solute or contaminant transport includes
 - (a) hydrodynamic dispersion;
 - (b) convection;
 - (c) adsorption-desorption.
3. Solution provides concentration and pressure (head) in each grid block as a function of time.

Solution Method - Finite difference approximations to both the water and solute material balance equations. The water flow equation may be solved by a Line Successive Overrelaxation (LSOR) technique with optimum parameter selection or a direct matrix inversion method. The contaminant transport equation may be solved by either of the above plus a method of characteristics (point tracking) method.

Applications

<u>Client</u>	<u>Application Type and Site</u>
(Confidential)	Transport and Diffusion of Groundwater Contaminants Downstream from Surface Mining, Utah
Atlantic Richfield Hanford Company	Investigation of Three-Dimensional Effects in Tritium Transport at Hanford Reservation, Washington
(Confidential)	Interaction Between Industrial Aquifer Withdrawals for Water Flooding and City Use, Alberta
(Confidential)	Design of Well Field for In Situ Leaching Project, Arizona
(Confidential)	Mine Dewatering Needs, Wisconsin

The above applications illustrate the range of problems for which the model has been used. The use of the model for ARHCO above is the only one available in open literature.

Date of Completion - 1975 (most recent version)

Name of Modeler - INTERA Environmental Consultants Inc.
1201 Dairy Ashford, Suite 200
Houston, TX 77079

Name of the Model - TRIGAT - HS 1, or XYZ - HS 5

Description - Prediction of piezometric heads in three-dimensional underground unsteady flow in confined aquifers or unconfined aquifers.

Specifically:

- In each point of the model, the flow is three-dimensional.
- Possible connection of the aquifer with surface water (rivers, lakes, oceans).
- Each cell of the model can be assigned a value of specific yield or storage coefficient.
- All the cells are not necessarily of the same size.
- Boundary conditions can be of different types:
 - steady or unsteady piezometric head (input or output),
 - steady or unsteady flow rate (input or output),
 - rate of flow $Q = \delta (P - P_0)$, i.e. the rate flow is a linear function of piezometric head,
 - impermeable boundary,
 - drain condition,
 - in unconfined aquifers, the free surface can move from one layer to the other,
 - in unconfined aquifers the change of water table level gives automatically a change of the Kh value in the concerned cells,
 - it is possible to change the value of the storage coefficient when a confined layer becomes unconfined or vice versa.

Solution Method

- finite difference implicit discretization
- linear equation solved by Gauss-Seidel method with over-relaxation.

Applications

- Direction Departementale de l'Equipement des Alpes-Maritimes
Head and leakage rate prediction in the alluvial aquifer of the river near a projected dam.

- Société d' Aménagement de la Vallée de l'Authion
Head prediction and study of exchange flow between la Loire river, l'Authion river, and a multilayered aquifer system in connection with an irrigation and drainage problem.
- Entente Départementale pour l'Aménagement d'Origny-Ste-Benoite
Prediction of leakage rate by the chalk aquifer near projected dam of Origny-Ste-Benoite (North-East of Paris).
- Régie Autonome des Transports Parisiens (R.A.T.P.)
 - a) Prediction of piezometric heads increases around the projected underground railway station of "Chatelet" for the new line R.E.R. related to the possibility of high level in Seine river.
 - b) Same study for the projected station of "Gare de Lyon".
- World health Organization
Study of Maestrichian aquifer in the area of Pout and Sebikotane (Sénégal)
- Ministère de l'Eau et de l'Electricité d'Iran - Bureau d'études MAHAB; Water management in Varamin plain (Iran)

Date of Completion - 1968

Name of Modelers - P. Prudhomme, J. L. Henry, F. Biesel
Geohydraulique
10, rue Eugène Renault
94700 MAISONS-ALFORT

Name of the Model - none

Description - Prediction of transient or steady-state hydraulic head distribution in confined, semiconfined, or unconfined aquifer. Specifically, the aquifer may be given an areal (plan view) description or may be cross-sectional. Aquifer parameters may be distributed or zoned and the system may be anisotropic with the principal components aligned with the global coordinate axes. If the areal description is used, leakage from confining beds (or river bottoms, etc.) is vertical and storage in the confining beds is neglected. The Dupuit-Forchheimer assumptions and delayed (or no delayed) yield concept are used for the water-table case in plan view.

Solution Method - The basic discretization method is the subdomain finite element method with the time domain discretized by a weighted average technique. The matrix equation is solved by the strongly implicit procedure; the iterative alternating direction implicit procedure; or line successive over-relaxation, with or without single line correction. Each method is incorporated into a separate computer program.

Applications - The program is on line at Dames and Moore and is used routinely by them. It is also distributed by the University of Colorado Computing Center. It has been used at the Desert Research Institute for the following projects:

- Management of ground-water in Ash Meadows, Nevada (R. L. Bateman)
- Analysis of the effects of waste-water discharge on the shallow ground-water flow system, Las Vegas Valley, Nevada (J. A. Westphal)
- Hydrogeologic effects of a gravel-pit operation in Reno, Nevada (R. L. Cooley)
- Ground-water and river-water interchange, Winnemucca reach of Humboldt River, Nevada (R. L. Cooley and J. A. Westphal) (program modified to interface with river-stage predictive model)

- Effects of energy losses in a pumping well on draw down around well (R. L. Cooley and A. Cunningham) (program modified to interface with model for flow in the well bore)
- Other as yet incomplete projects at the Desert Research Institute

Date of Completion - January 1974

Name of Modeler - R. L. Cooley
U.S.G.S.
Water Resources Division
Box 25046, Stop 413
Denver, CO 80225

Name of the Model - VTT

Description - Forecasting the piezometric head in a multiaquifer ground-water system. Specifically it is a Multiaquifer-Two-Dimensional Boussinesq Model with provisions for interaquifer transfer between aquifers and transfer to a water body through a semipervious layer. The system can handle heterogenous isotropic parameters and confined as well as unconfined aquifers. Water is treated as incompressible. The model can handle a variety of boundary conditions and boundary configurations.

Solution Method -

Steady-State Solution: When a steady-state is requested, the model utilizes a finite-difference formulation involving Newton's Method and a disk based direct Gaussian elimination procedure. This allows a converged solution of the nonlinear unconfined problem to be computed in four-five iterations. When the system is confined or the starting point is far from the steady-state, another faster version is available which uses direct disk based on Cholesky decomposition. This method is approximately two times faster but for a nonlinear-unconfined problem, 10-12 iterations are sometimes required.

Transient Model: When the Transient Model is requested, a finite difference SLOR (Successive Line Over Relaxation) is used. For reasonable sized time steps, only seven-ten iterations per time step are required.

Applications - Moxee-Ahtanum Valley for Washington State Department of Ecology. A multiaquifer irrigation problem using pumped ground water.

Eastern third of Long Island for Brookhaven National Laboratory. Travel times and direction of waste in ground water determined.

Southport Region of Brunswick County, North Carolina for Nuclear Regulatory Commission, the investigation of brackish water infiltrations from sea level power plant canal.

Southern Tier Central 208 Study Area, N.Y. Model being used to investigate water recharge and discharge characteristics of the aquifer. Aid in defining nonpoint pollution problems and as a water resource evaluation for:

Hanford Reservation - Model forecasts ground-water levels under different operating conditions and provides series of transient potential distributions from which pathlines and travel times can be determined.

Clark County, Washington - The model is used as a resource development and management tool for testing future land use scenarios.

Date of Completion - August 1975 (current version, but under continual revision)

Name of Modeler - C. R. Cole and A. E. Reisenauer
Pacific Northwest Laboratory
Water and Land Resources Department
Richland, Washington 99352

Name of the Model - Multiaquifer model

Description - Determination of piezometric heads and/or watertable in multiaquifer system. Specifically:

- Aquifers are represented in 2-D in the horizontal plane. Non-homogeneous and anisotropic aquifers. Principal directions of anisotropy can vary.
- Flow in aquitards is represented by 1-D (vertical) continuity equation
- Watertable aquifer at top, impermeable boundary at bottom
- Dirichlet or Neuman boundaries on any layer
- Recharge flux on top
- Any number of pumping or recharge wells can be put into any of the aquifers
- Dupuit approximation for watertable aquifer
- Flow of water in aquitards - represented by 1-D vertical transient continuity equation (valid at all values of time).
- Leakage flux at aquifer - aquitard interfaces is determined by differentiating the aquitard heads and applying Darcy's Law.

Solution Method - Galerkin Finite Element formulation of transient continuity equation for both aquifers and aquitards.

Iterative solution. Cycle starts with calculation of aquifer heads, then aquitard heads, then leakage fluxes. These are substituted back into aquifer equation, and cycle is repeated.

Cholesky solver for solution of equations.

Applications - None listed

Date of Completion - June 1976

Name of Modeler - E. O. Frind (with D. W. Chorley)
Dept. of Earth Sciences
University of Waterloo
Waterloo, Ontario, Canada

Name of the Model - MOC

Description - Compute potentiometric heads and solute transport in flowing water. Specifically:

- Flow of water according to Darcy's Law and continuity equation.
- Solute transport by convection and hydrodynamic dispersion.
- Dispersion coefficient treated as second-order tensor.
- Transient or steady-state flow.
- Can readily incorporate simple chemical reactions (radioactive decay or adsorption).

Solution Methods - The model solves a finite difference form of the flow equation using an iterative ADI procedure. The solute-transport equation is solved using the method of characteristics.

Application - Pinder and Cooper (1970)--Transient position of interface between fresh water and salt water; cross-sectional model; flow is density dependent.

Bredehoeft and Pinder (1973)--Movement of salt water in confined limestone aquifer; vertical leakage through confining bed; area in Georgia.

Konikow and Bredehoeft (1974)--Salinity increases in alluvial stream-aquifer system were related to irrigation practice; coupled streamflow routing model; applied to management problems; area in Colorado.

Robertson (1974)--Movement of industrial and low-level radioactive liquid wastes in inter-bedded basalt flows and unconsolidated sediments; effects of radioactive decay and adsorption included in model; area in Idaho.

Robertson (1974)--Contamination of shallow alluvial aquifer by seepage from sewage-treatment ponds; area in California.

Konikow (1976)--High chloride industrial wastes seeped out of unlined disposal ponds and spread through underlying alluvial aquifer; area in Colorado.

Date of Completion - November 1976

Name of Modeler - L. F. Konikow
U.S.G.S.
Box 25046, Mail Stop 413
Denver Federal Center
Denver, CO 80225

J. D. Bredehoeft
U.S.G.S.
National Center
Mail Stop 413
Reston, VA 22092

Name of the Model - Boussinesq Equation for Water Table Aquifer

Description - Simulation of the Boussinesq Equation for a Two-Dimensional Water Table Aquifer. Specifically:

- the aquifer is given by a 2-D discrete representation in the horizontal plane.
- the aquifer boundary is irregular and mixed
- the aquifer is superposed by a meandering stream
- aquifer parameters are assigned to each nodal point and can be slightly anisotropic and nonhomogeneous
- transient ground-water flow through a water table aquifer is described by the Boussinesq equation which assumes the Dupuit-Forchheimer assumptions are valid,
- the principal conductivity components are colinear with the coordinate systems x and y ,
- the water is released from storage mainly by gravity drainage with an instantaneous decline in head,
- the stream bed is semi-confined and the leakage obeys Darcy's law,
- the flow from the unsaturated zone is negligible,
- the change in fluid density over time is negligible,
- the replenishment to the aquifer system occurs through gravity drainage and stream bed leakage.

Solution Method - The model simulates the transient ground-water flow through a two-dimensional water table aquifer, described by the Boussinesq equation, using the alternating direction implicit method.

- the Boussinesq equation is approximated by a two-dimensional finite difference equation of linearized form, employing the noniterative alternating direction implicit method. The linearized finite difference equation is written for two half time steps, and is done for each node along either a row or column

- The resulting simultaneous equations are solved by the Thomas algorithm
- The calculation is carried on successional row by row for the first half time step and a similar calculation is carried on column by column for the second half time step.
- the results of the second half time step are the approximations to the transient solution of the problem under discussion

Applications - The model was initially developed to simulate the two-dimensional nonsteady Boussinesq Equation for an outwash aquifer located at Elmsvale, Musquodoboit River Valley, Nova Scotia, Canada. It is one of two groundwater models developed during this study. Specifically, this model attempts to answer the following questions:

1. Usefulness of the noniterative alternating direction implicit method in simulating the Boussinesq Equation.
2. What are the differences if an outwash aquifer is treated separately under confined and unconfined conditions.
3. Can the aquifer be discretized by an irregular mesh matrix for simulation purpose.

Date of Completion - May 1970

Name of Modeler - Dr. Chang L. Lin
N.S. Department of the Environment
P.O. Box 2107, Halifax, Nova Scotia
Canada

Name of the Model - MTMVMC

Description - Prediction of piezometric heads in a multilayered aquifer.
Specifically:

- Each aquifer layer is given a 2-D discrete representation in the horizontal plane.
- Leakage between two layers is assumed to be vertical.
- The aquifer can be phreatic or confined.
- Replenishment of the first layer can be natural, either through rainfall or from lakes, rivers, etc...
- Replenishment of the lower layers occurs through leakage from the overlying or underlying horizons.
- Outlets for the various layers can be springs, lakes, rivers, wells, artificial drains, evaporation, etc...
- Boundary conditions are discretized along the sides of the meshes by prescribed heads or fluxes.
- Flow of water according to Darcy's law and the continuity equation.
- Dupuit approximation and variation of the transmissibility with the saturated thickness of the aquifer.
- Permeability varies according to the X and Y coordinates and is constant in each mesh representing an average value of the different permeabilities encountered along the vertical.

Solution Method - Integration of the flow equation in a porous medium is done by the method of finite differences. In a steady-state, the system of linear equations is solved by an over-relaxation method with an optimized relaxation factor. In a transient state, implicit or explicit methods can be used.

Applications -

- hydroagricultural development of TRIPOLITANIA (LIBYA)
- hydroagricultural development of the NEKOR Plain (MOROCCO)
- hydroagricultural development of the LOWER EUPHRATES VALLEY (SYRIA)
- hydroagricultural development of SIRTE-ZEMZEM (LIBYA).

Date of Completion - August 1976

Name of Modeler - A. Carriere
Hydraulic Engineer
GERSAR
B.P. 4001
3001 - Nimes, FRANCE

Name of the Model - ISOQUAD2

Description - To simulate transient two-dimensional areal ground-water flow in confined and unconfined aquifers. Specifically:

- Distributed parameter model
- Boundaries of arbitrary geometry, including curved surfaces
 - Sources and sinks. Distributed or point
 - Leakage is taken care of internally.
 - Confined or unconfined
 - Homogeneous compressible fluid

Solution Method - The model solves the ground-water flow equations using a Galerkin-finite element scheme and a band algorithm matrix solver.

Applications - Approximately 100 individuals have and are applying the code.

Date of Completion - January 1974

Name of Modelers - George Pinder, Princeton University
Emil Frind, Waterloo University

Name of the Model - NEWSAM

Description - Prediction of piezometric heads and salt transport in a multi-layered aquifer. Specifically:

1. Flow of water according to Darcy's law and the continuity equation in each layer (aquifer and semi-pervious).
2. Dupoit approximation in the layers (horizontal flow), and variation of the transmissivities with the saturated thickness of the phreatic aquifer.
3. Principal direction of anisotropy of permeability assumed constant and parallel to the x and y coordinates.
4. For semi-pervious layers, flow is given by Darcy's law in steady state; in transient state, flow is approximated by a few terms of the development of the complete analytical solution.
5. Transport of salt with the water with only the convective term (neglecting dispersion) and assuming instantaneous mixing in each mesh of the flux over one time step.
6. Adsorption of salt by the immobile phase can be represented assuming an instantaneous linear and reversible adsorption isotherm (relation between concentration in the mobile and immobile phases).

Solution Method - Integrated finite differences yield, in steady state, a set of linear equations which is solved by a point successive over-relaxation method (PSOR) with an optimised relaxation factor. In transient state, two methods are available: implicit (solved by PSOR) and integrated polynomial approximation. Leakage in semi-pervious layers is given by an analytical expression convoluted with the previous drawdowns in each overlying and underlying meshes. These convolution integrals are approximated by a few terms of their development, making it unnecessary to store in the core the values of drawdown for previous time-steps. For salt transport, a fully implicit backward differences scheme is solved by PSOR.

Application - Empresa Nacional ADARO, Spain

- Head prediction and well planning, coastal aquifers of Camao de Nijar, America, Southern Spain (2 layers).
- Head prediction and well planning, secondary and tertiary aquifers of the Bassin Aquitain, Southern France (7 layers).

Direction des Etudes de Milieu et de la Recherche Hydraulique, Algeria:

- Head prediction, salt concentration prediction and well pattern optimization (with program PLIN) in the Quad R'hir, Northern Sahara (3 layers).
- Head prediction in the Mascara plain, Northern Algeria (2 layers).

Direction des Ressources en Eau et en Sol, Ministère de l'Agriculture, Tunisia:

- Head prediction, salt concentration prediction, well field design, and recharge prediction along ephemeral streams after building of a dam in the Kairouan plain, Tunisia (2 layers).
- Head prediction in five coastal aquifers in Northern Tunisia (Mornag, Manouba, Raf-Raf, Oued Guenich, Cap Bon Oriental).

Bureau de Recherches Géologiques et Minières, France:

- Head and flux prediction in the aquifers under "Les Halles" inside Paris (2 layers).
- Head prediction in the alluvial aquifer of the Seine river, near Rouen (2 layers).

Agence de Bassin Seine-Normandie, France:

- Head prediction and well design in the Orne basin, in Normandy (3 layers).

University de Louvain-la-Neuve, Louvain, Belgium:

- Head prediction in the Bruxellian aquifers at Louvain (Belgium) (2 layers).

Aluminum Pechiney, France:

- Head and flux prediction in the aquifer underneath the bauxite mine of Mazauges (Var), Southern France (1 layer).

University of Aachen, Germany:

- Study of the alluvial valley of the Rhine near the wasserwerk Wolfsbachtal (1 layer).

Société des Eaux de Marseille, France:

- Head prediction in the alluvial valley of the Huveaune (1 layer).

Date of Completion - June 1976

Name of Modeler - E. LEDOUX

Centre d'Informatique Géologique
Ecole des Mines de Paris
35, rue Saint-Honoré
77305 - Fontainebleau, France - Tel: (1) 422.48.21

Former version of the model, named SAMMIT (1973) developed by A. DREYFUS, J. P. DELHOMME, P. ARMISEN, M. BESBES, same address.

Name of the Model - DAVIS/FE3D

Description - Prediction of transient piezometric heads and salt transport in large natural multiaquifer basins. The layers of various geologic materials encountered are described by 3-D mixed order finite elements. Each material can be nonisotropic. The aquifers are confined. Sources or sinks associated with the given elements are considered. Boundary conditions discretized along the outer boundary include prescribed head or flux. For salt transport, the boundary conditions are prescribed by concentration or flux of solute. The fluid phase is considered as compressible through the storage coefficient of the confined aquifers. Variation of density and viscosity with salt concentration is considered.

Solution Methods - Galerkin finite element method is used for solution. Backward difference scheme is used for transient cases. To reduce the core storage and computation time, the intermediate results which are needed repeatedly for obtaining solutions for each time step or for iterations with different material properties are stored on disk or tape.

For solution of large sparse system of equations, use of partially compressed matrix is developed by storing only nonzero coefficients and their column identifications.

Applications - Applied initially in California also to Long Island, New York and in a Consulting Engineering Firm application more recently.

Date of Completion - November 1975

Name of Modeler - S. K. Gupta (with K. K. Tanji & J. N. Luthin)
Land, Air and Water Resources
Water Science and Engineering Section
University of California
Davis, CA 95616

Name of Model - Deep Well Disposal Model (DWDM)

Description - Solves pressure as well as temperature and contaminant transport and dispersion in a three-dimensional heterogeneous aquifer.

Specifically:

1. Allows description of three-dimensional heterogeneous aquifer.
2. Source-sink terms allow handling a well field or connection with surface water.
3. Single solute transport and diffusion at concentration sufficiently high to affect fluid density and viscosity.
4. Energy equation is solved to provide temperature distribution.
5. A recently added option would allow N trace constituents, such as a decay chain, to be solved with the above equations.

Solution Methods - Finite difference approximations to water, solute and energy balance equations. Each of the above equations are solved simultaneously and can be solved by a Line Successive Over-relaxation (LSOR) technique with optimum parameter selection or a direct matrix inversion method.

Applications - Developed by INTERA for the U.S.G.S. who has applied the model. Sandia Laboratories also is using the program.

Date of Completion - 1975

Name of Modeler - INTERA Environmental Consultants, Inc.
INTERCOMP Resource Development and Engineering Inc.
1201 Dairy Ashford, Suite 200
Houston, TX 77079

Name of Model - VCHFLD

Description - Describe the movement of from two to six chemical species in a porous medium by solving the coupled transport equation using Galerkin methods. When needed for resolution, a separate locally refined grid can be employed for each dependent variable.

Primary design of the program is for two-dimensional simulation, either areally or as a two-dimensional cross section. Local grid refinement may be employed in these two principle dimensions. A limited capability is provided for a third dimension when necessary. This dimension should be chosen as the one in which the minimum changes occur and the least resolution is required. The reservoir is confined and all boundaries are no flow. Injection and production is from point (line) sources and sinks. The carrier fluid (water) convects up to five different chemical species. Chemical species may sorb and desorb on the reservoir rock according to user specified sorption isotherms, with possible complex interactions between the species.

Solution Method - Spatial discretization in the two principle dimensions is achieved using Galerkin methods with a bilinear basis (Chapeau functions). In the accumulation and transmissibility terms, coefficients which are functions of the dependent variables are dated explicitly. Time discretization is at the user's option either (a) backward differencing or (b) Crank-Nicholson. The resulting linear equations are solved by Gaussian Elimination or, for large problems when storage is critical, by SOR.

Applications - Not reported.

Date of Completion - March 1977

Name of Modeler - INTERCOMP Resource Development and Engineering, Inc.
1201 Dairy Ashford, Suite 200
Houston, TX 77079

Name of the Model - MMT

Description - Prediction of the movement of radionuclides and other contaminants in ground water and in the vadose zone.

The saturated or partially saturated flow vectors are defined at the center of each rectangle circumscribed by four nodes. Boundary types which are also defined at the center of the rectangles are either reflecting or flow boundaries. At inflow boundaries the concentration of the incoming fluid can be a continuous function of time at each node. Concentrations entering an aquifer from above are assumed to impact a specific size circular or trapezoidal area of the aquifer and mass is added to all coincident rectangles (cells). Specifically the processes involved are:

1. Mass transport of components of phases - chemical, physical and radioactive species (advection, hydrodynamic dispersion).
2. Reactions - chemical, radioactive (instant equilibria constraint).
3. Processes at Interfaces - adsorption, ion exchange, precipitation and dissolution (instant equilibria constraint).

Solution Methods - The model solves the problem of transport of multicomponent species in ground water using a technique referred to as the Discrete-Parcel-Random-Walk (DPRW) approach. This is a Lagrangian, particle-of-mass based approach that simulates dispersion using a random walk analogy. The soil-waste reaction submodel has a rapid equilibrium assumption as its basis, and the resulting system of non-linear equations is solved using a simultaneous Newton-Raphson algorithm.

Applications - Although the program is generic, to date it has only been applied to various portions of the Hanford Reservation in Southeast Washington State on behalf of DOE. It has been used for a variety of problems concerned with predicting the movement of radiocontaminants in the Hanford subsurface.

Date of Completion - July 1976

Name of Modelers - S. W. Ahlstrom, H. P. Foote, R. J. Serne
Pacific Northwest Laboratory
Water and Land Resources Department
Richland, WA 99352

B.2. WATER-DOSE AND AIR-DOSE MODELS

Name of Program - ACRA II

Description - ACRA II (Stallman and Kam, 1973; Binford, 1968) was developed for estimation of external and inhalation doses from atmospheric releases of radioactive material during hypothetical nuclear reactor accidents.

The radioactive material is assumed to be uniformly mixed within the reactor containment system and released to the atmosphere at a uniform rate. Filtration upon release may be included. Dispersion of the material leaving the stack is described as three-dimensional normal distribution with symmetric horizontal distribution ($\sigma_x = \sigma_y$). Reflections off the ground plane and off an inversion layer are described by the virtual cloud image technique. The effective release height is calculated by the method of Holland, "Meteorology and Atomic Energy" (1955).

The inhalation dose is a function of the air concentration at the exposure point while the external dose depends on the distribution of material throughout the plume. The external gamma dose rate is calculated as the volume integral of the contributions from all photons for each nuclide as a function of time. The total dose is then calculated as the time integral of the dose rate. The amount of each nuclide is calculated as a function of time after the accident and transit time to the exposure point according to a linear decay sequence.

The volume integral is calculated as a function of gamma energy and cloud dimensions only and is, therefore, independent of time after the accident. The dimensions of the cloud are specified as a function of distance from the release point to the exposure point.

Special Notes -

- Numerical instabilities in the radioactive decay calculation are avoided by using a technique similar to that developed by H. H. Van Tuyl (1964).
- Radionuclide decay is handled as a linear sequence without branching. Branching may be included by splitting the decay sequence into a number of independent linear chains through manipulation of input.

- The program does not depend on any particular internal dosimetry model. Dose conversion factors are supplied as input to convert to rem from μCi uptake. Breathing rate is also supplied.
- All nuclide and dosimetric data are supplied via data cards.
- The authors of ACRA II have given considerable attention to the external gamma dose space integration. The mathematical treatment is thorough and numerical approximations are employed where appropriate.
- Gamma ray buildup is modeled by the following expression:

$$B = 1 + C\mu r \exp(D\mu r)$$

where C and D are functions of gamma energy and μr represents the mean free path length traveled by photons. This expression is valid in the energy range $0.5 \text{ MeV} \leq E \leq 5 \text{ MeV}$.

Programming Considerations - ACRA II is written in FORTRAN IV for an IBM Computer.

Name of Program - AIRDOS

Description - AIRDOS (Moore, 1975) estimates population and individual doses resulting from the continuous atmospheric release of radionuclides from a nuclear facility. This program was prepared for use at Oak Ridge National Laboratory (ORNL) in the United States Plowshare Gas Program (Moore and Barton, 1972, 1973) in the ORNL Cumulative Exposure Index (CUEX) Project (Kaye, 1973) and has been used in preparation of environmental impact statements.

Five pathways to man are considered: 1) inhalation, 2) submersion in air, 3) exposure to contaminated ground surfaces, 4) ingestion of food, and 5) immersion in water. Dose and dose commitment are estimated for each pathway and the following eleven reference organs: whole body,^(a) GI tract, bone, thyroid, lungs, muscle, kidneys, liver, spleen, testes, and ovaries.

The environmental model in AIRDOS consists of a 20 x 20 square grid (variable size) with the nuclear facility located at the center. Human population, numbers of beef and dairy cattle, and whether an area is predominately used for production of vegetable crops or is a water area specified for each of the 400 grids. Air concentrations are modeled as a bivariate Gaussian plume with dispersion parameters determined by Pasquill stability categories A-F and a seventh stability G. Plume rise may be calculated by equations of Briggs (1968), Rupp (1948) or by input. All doses are calculated as proportional to the ground level concentration. Joint frequency of occurrence meteorological data is used for population and long-term individual dose calculations.

AIRDOS estimates radionuclide intake via ingestion using the terrestrial model TERMOD of Booth, Kaye and Rohwer (1971). Intakes result from eating beef and vegetable crops and drinking milk.

Special Notes -

- AIRDOS allows for continuous simultaneous releases from as many as six plant stack or roof vents (all at the same site).

(a) Whole body and total body are used interchangeably throughout this appendix.

- The external gamma dose calculation uses the semi-infinite cloud model.
- Dose from daughter buildup within the plume is not estimated.
- The program requires dose conversion factors as input.
- The external dose to each organ (equivalent to whole body dose) is added to the 50 year internal dose commitment for each organ resulting from inhalation and ingestion.
- Dose reduction factors are applied to account for cattle pasturing practices in the area and time elapsed between production of vegetable crops, milk and beef and consumption by humans.
- Average annual air concentration and depositions are calculated for each of 16 compass directions. The resulting concentrations are averaged over each of the 16 sections and converted to a square grid specification.

Programming Considerations - AIRDOS is written in FORTRAN IV for an IBM Computer.

Name of Program - AIREM

Description - The AIREM code (Martin, 1974) was developed as part of the Office of Radiation Program's Comprehensive Dose Computational System (CDCS) for analysis of emissions and effluents from nuclear fuel cycle facilities. The program may be used to estimate air concentration, ground deposition (both wet and dry) and doses from external gamma radiation and from inhalation. The dispersion calculation, based on the sector-averaged Gaussian diffusion model, produces results as a function of direction and distance for each nuclide. Contributions from the first daughter are included. The release is assumed to be at a constant rate over a specified release period. In-plant holdup time and decontamination factors may be supplied as input. Inhalation doses are calculated using conversion factors for each organ (four per run) and nuclide (twenty per run). For the external gamma dose, a table of dose integrals is to be supplied relating dose to release height, cloud size and gamma energy. A modified version of EGAD (Cooper, 1972) is given in the AIREM report (Martin, 1974) for calculation of the dose integrals.

Special Notes -

- The code requires dose conversion factors as input for each radionuclide, organ and population group. A table of dose conversion factors is also required for the finite cloud gamma dose calculation.
- Meteorological data are supplied as the frequency (percent of time) that the wind blows in a sector under a given stability class. An average wind speed must be supplied for each direction and stability combination. This procedure carries less information than supplying frequency data as a function of direction, stability and wind speed class.
- Air concentrations and wet and dry ground deposition are calculated and printed for each nuclide as a function of distance and direction, with effects of decay in transit included.
- The contribution to external body exposure from nuclides in adjacent sectors is included in the dose integrals calculated by EGAD. This is accomplished by integrating in the lateral direction over all distances

contributing significantly to dose without respect to sector boundaries.
Inherent in this procedure is the assumption that the wind blows uniformly in all sectors adjacent to the given sector.

Programming Considerations - AIREM is written in FORTRAN IV for an IBM 370 system.

Name of Programs - ARRRG/FOOD/GRONK

Description - This set of computer codes was developed at Battelle-Northwest (BNW) for calculation of annual radiation doses and long-term dose commitments to the total body and selected organs of individuals and population groups, from both internal and external sources of radiation. The computer codes were developed to evaluate radiological impact in the USAEC's Environmental Statements for commercial power reactors and are usable for any nuclear facility releasing radioactive materials to the environment. They were derived from mathematical models and codes developed for the "Year 2000 Study" HERMES computer program.

ARRRG (Soldat, 1974) calculates annual individual and population doses resulting from radionuclides released with liquid effluents. Presently nine exposure pathways may be selected by the operator: consumption of fish, crustacea, mollusc, algae and drinking water; and direct external radiation from shoreline, water immersion (swimming) and surface water (boating). Doses are calculated for skin (external only), total body, GI-LLI, thyroid and bone. Individual contributions to dose by nuclide and by pathway are output.

FOOD (Denham, 1973) calculates annual individual doses from the consumption of garden foods and animal products contaminated from air deposition or water (sprinkler irrigated). Presently 14 food types may be selected.

GRONK (Soldat, 1974) calculates annual dose resulting from radionuclides released with gaseous effluents. Skin and total body dose to an individual and total body dose to the population are calculated for a standard matrix of points made up by 16 sectors and up to 10 annular rings out to 50 miles from release point. Options permit calculation of dose at other specified distances. An optional calculation for thyroid dose from radioiodine via inhalation, milk and leafy vegetables may be made.

Special Notes -

- Currently ARRRG is operational with the capability of calculating doses for 6 organs and ~200 radionuclides.
- The user inputs the following variables to ARRRG from an interactive terminal: the name of the facility under investigation; decay between

release and point of exposure (holdup), usages, and mixing ratios by pathway; reactor coolant flow, shoreline width factor and reconcentration factor parameters.

- Data files are used to minimize input for each run.
- Terminal input for FOOD includes: facility name, holdups, usages, irrigation rates, air concentration, crop yields and growing periods for 14 food types (for animal products the parameters refer to animal's feed); coolant flow and mixing ration, and reconcentration factor parameters in the case of liquid release.
- FOOD is operational with 136 nuclides.
- Terminal input to GRONK includes: facility name, a string of code letters signifying what σ_z model to use (Pasquill or Hanford) and the various options selected and up to 10 ranges, if ranges other than the internally set standard ranges are required. Other inputs are required depending on the options selected, such as release height for elevated release, plume rise constant for plume rise consideration, building height for wake effect correction and sensor level for translating meteorological data from actual height of wind sensor to height selected for dose estimate. For the thyroid dose calculation, the child and adult vegetable consumptions, the cow grazing period and the leafy vegetable consumption period are entered for the milk and leafy vegetable pathways.
- GRONK is operational with 136 radionuclides available; however, only 52 may be used at any one time because of core allocation limitations.

Programming Considerations - These codes are all written in the Computer Sciences Corporation's version of BASIC denoted by CSTS for interactive use from a remote terminal. This system operates on a UNIVAC 1108 computer. The interactive mode enhances the flexibility of varying data parameters and shortens the turnaround time required to obtain results.

Name of Program - COMRADEX

Description - The COMRADEX code (Spangler, 1967; Willis, 1968) was developed to calculate radiation doses from postulated accidental release of radio-nuclides from nuclear reactors.

The code considers up to four levels of containment with independent time varying leak rates. Filtration, particle coagulation and fallout, and special cleanup systems are also included in the containment model. Material reaching the atmosphere is dispersed according to the bivariate Gaussian model with dispersion parameters (σ_y and σ_z) defined by the Pasquill curves A-F (Pasquill, 1962; Hilsmeier and Gifford, 1962). Plume rise is considered by specifying an effective height of release.

Doses calculated by COMRADEX include direct dose from contained activity, external cloud gamma dose, and internal dose from inhalation of contaminated air. The external cloud gamma dose is calculated by a space integration over the active volume of the plume (finite cloud approach). The inhalation dose may be for as many as 14 organs of interest by specifying appropriate dose conversion factors.

Special Notes -

- The initial inventory is specified as disintegrations per second for each nuclide.
- Shielding between various containment shells is accounted for by an attenuation factor in calculating the direct dose from contained material. Air attenuation for this calculation is done for one photon energy.
- Volume sources are modeled by a virtual source technique.
- For the finite cloud integration, σ_y and σ_z are held constant about the exposure point.
- The space integration is performed by dividing the Y-Z plane into small rectangles and evaluating the dose kernel at the center of each rectangle.
- The finite cloud integration is performed for only one photon energy.

Programming Considerations - COMRADEX is written in FORTRAN IV for an IBM 360.

Name of Program - DACRIN

Description - DACRIN (Houston, 1974; Streng, 1975), developed at BNW, calculates the effective radiation dose to the human respiratory tract and other organs from the inhalation of radioactive aerosols. The program follows the basic precepts of the ICRP Task Group on Lung Dynamics (1959, 1966, 1972) and a simple exponential model for retention by an organ of interest. As an adjunct to the organ dose model, mathematical models describing atmospheric dispersion have been included for the purpose of evaluating doses resulting from either accidental or chronic atmospheric releases of radionuclides.

The program calculates the effective radiation dose to any of 18 organs and tissues from inhalation of any one or combination of radionuclides considered by the ICRP. A maximum of 10 organs may be selected for any one case (run). In addition, up to five multiple intake intervals and 10 time intervals measured from the last intake may be selected for each case. Organ doses from inhalation can be calculated by specifying either the quantity of a radionuclide inhaled or the quantity released to the atmosphere. In the latter case, the duration of release, the release height, wind speed, atmospheric dispersion parameters and downwind distance at which the dose is to be calculated must also be specified. As many as 10 distances may be specified for each case.

Special Notes -

- Radioactive decay during transit is calculated for decay chains with branching to and from isomeric states.
- Two data libraries are used by DACRIN; data for 242 nuclides are included. A radionuclide data library contains half-lives and branching ratios while an organ data library contains data of ICRP Publication 2 (1959): biological half-life, effective energy and transfer fractions.
- Doses to each portion of the G.I. tract may be summed and reported as G.I. tissue dose.

Programming Considerations - DACRIN is written in FORTRAN IV for a CDC CYBER computer and requires 144k (octal) words of core to execute.

Name of Program - EGAD

Description - EGAD (Cooper, 1972) calculates external gamma dose integrals as a function of release height, inversion lid height, gamma energy and vertical dispersion parameter σ_z . The material is assumed to be normally distributed in the vertical direction about the release height and uniformly distributed in the crosswind direction. Sector boundaries are not considered in the model.

The results of EGAD may be used as input to chronic release computer codes. The code AIREM uses output from EGAD.

Special Notes -

- Because EGAD ignores sector boundaries, the resulting dose integrals are high for distances close to the release point (narrow sector width). However, use of the dose integrals in this case is one method for accounting for contributions from material in adjacent sectors. The method assumes a uniform directional frequency for nearby sectors.

Programming Considerations - EGAD is written in FORTRAN IV. The program is quite short and can be made to run on most computers without difficulty.

Name of Program - EMERALD

Description - EMERALD (Brunot, 1971) was designed for calculation of releases and exposures resulting from normal and abnormal operation of a large pressurized water reactor. The code models each component or volume within the plant by a separate subroutine. Activity is transferred from subroutine to subroutine in the code as it would be from place to place within the plant. The amount of material released to the atmosphere is calculated for a series of time periods.

The activity released during each time period is used to calculate thyroid dose and total body dose from beta and gamma radiation. The semi-infinite cloud approach is used for the external gamma dose. Corresponding doses are calculated for persons inside the containment building. The population doses in man-rem may also be calculated from input of population and atmospheric dilution data for each sector.

Special Notes -

- The code contains a library of data for 25 nuclides of interest in licensing calculations.
- The code assumes no downwind decay and no depletion of the cloud due to rain-out, fallout, or plate-out of any kind.
- Thyroid dose is calculated using dose conversion factors.

Programming Considerations - EMERALD was written in FORTRAN IV for operation on an IBM computer.

Name of Program - EXREM III

Description - EXREM III is the third in a series of computer programs (Trubey and Kaye, 1973; Turner, 1968; Turner, 1969) developed at Oak Ridge National Laboratory for estimating external radiation exposure from submersion in contaminated water and air and from exposure to contaminated surfaces. The initial program EXREM was improved to include contributions from daughter products (EXREM III). The codes were developed for estimating radiation dose rates and doses from construction of a sea-level canal with nuclear explosive. As such, the codes calculate doses for accidental releases rather than chronic releases.

The air concentration is defined via input by specifying "location correction factors" as a function of distance, nuclide and exposure mode (beta, gamma position or electron). The submersion doses are estimated as semi-infinite cloud calculations proportional to the air concentration at the exposure point.

Special Notes -

- The code includes contributions from gamma rays, x-rays, positron, electron and beta radiations.
- Radioactive decay is calculated in a detailed manner with branching to and from isomeric states included.
- A nuclear data base is available with the code which includes data for 189 nuclides.

Programming Considerations - The code is written in FORTRAN for an IBM computer.

Name of Program - FISSP/CLOUD

Description - The linked computer programs FISSP and CLOUD (Bonzon, 1970) perform a reactor excursion analysis involving: 1) the fission product inventory immediately preceding the release, 2) the release from the containment structure to the atmosphere, 3) the transport of the released fission products to the exposure point, and 4) the resulting external and internal dose. FISSP performs the fission product inventory and release calculation while CLOUD performs the fission product transport and dose calculation.

CLOUD models transport by a three-dimensional Gaussian dispersion equation with Sutton's dispersion parameter representation. The time integrated air concentration is calculated numerically for use in determining external dose and inhalation dose. The external dose from gamma radiation is calculated using the semi-infinite cloud assumption. Contributions to external dose from both beta and gamma radiations are included. The dose to organs from inhaled material is calculated using MPC values. The doses calculated are the 50-year dose commitments from uptake over a specified uptake period.

Special Notes -

- A puff release to the atmosphere of the inventory at the end of the operating history is assumed. Fractional releases may be assigned to the nuclide groups-noble gases, halogens, high temperature volatiles and the remainder.
- One neutron energy group is allowed.
- FISSP performs a double precision calculation.
- CLOUD applies a factor of 0.64 to the external beta dose to account for perturbation of the average energy of the beta field by preferential absorption of the high energy particles.
- Inhalation doses for nuclides not listed in ICRP Publications 2 (1959) or 6 (1964) are calculated using "artificial" MPC values.

Programming Considerations - This code is written in FORTRAN IV for a CDC 6600 and requires 60k (octal) to run.

Name of Program - INREM

Description - INREM (Turner, 1968; Killough, 1975) is a computer code to estimate dose commitments to organs from continuous inhalation or ingestion of radionuclides. Organ parameters may be specified as a function of age (of exposed individual), and the uptake may be a function of time after start of release. Dose calculations are based on recommendations in ICRP Publication 2 (1959).

The nuclide source term is specified as an intake rate ($\mu\text{Ci/day}$) as a function of time. Therefore, meteorological dispersion data are not considered by the code but may be factored into the nuclide source term or applied to the results.

Special Notes -

- The G.I. tract dose calculation is based on MPC input values.
- Although the code was specifically written to estimate doses to individuals from construction of a sea-level canal, it may be useful in other studies involving releases of radioactive material to the atmosphere.

Programming Considerations - INREM is written in FORTRAN for an IBM computer and has been converted for use on a CDC CYBER at BNW.

Name of Program - KRONIC

Description - KRONIC (Streng and Watson, 1973), developed at BNW, calculates annual external total body tissue dose from chronic release of radionuclides to the atmosphere. The external total body tissue dose is calculated as a function of the 1) radionuclides present, 2) climatology for the site, 3) time dependence of fission product concentrations, 4) photon and beta particles emitted from nuclides, and 5) physical properties describing interaction of photons and beta particles with air and tissue.

Atmospheric dispersion effects are estimated using data on joint frequency of occurrence of wind speed, wind direction and stability for a particular site. Each sector is considered to be a plume for which the center line ground-level dose is calculated for specified downwind distances. The result of the calculation is a table of annual dose rates as a function of direction and distance from the release point.

Both photons and beta particles contribute to the external total body dose. The beta dose contribution is calculated using a semi-infinite cloud model. The gamma dose calculation is performed by space integration over the plume volume. The gamma dose can be calculated at any specified tissue depth.

Special Notes -

- KRONIC uses extensive data bases to minimize input requirements.
- Radioactive chain decay with branching is calculated for chains with up to seven members.
- Multiple releases may be specified with results summed.

Programming Considerations - KRONIC is written in FORTRAN IV for a CDC CYBER computer.

Name of Program - LONGTM

Description - LONGTM, operational but only partially documented (Streng, 1973), calculates the normalized air concentration at ground level as a function of wind speed, direction, atmospheric stability, release height and distance from point of release. The bivariate normal mathematical model is the basis for this program. The program is capable of accepting 1) almost any set of values describing horizontal and vertical dispersion coefficients including those attributable to Sutton (1953) and Pasquill (1962), and 2) the Hanford Model parameters (Fuquay, 1964) for stable atmospheres.

Special Notes -

- LONGTM performs a normalized dispersion calculation only and does not use data for specific nuclides.
- Terrain elevation effects are considered as a function of distance and direction.

Programming Considerations - LONGTM is written in FORTRAN IV for a CDC CYBER. The program is short and could easily be converted for use on other computers.

Name of Program - RACER

Description - RACER (Streng, 1971), developed at BNW, calculates tissue dose in rads at a downwind location, delivered over a specified time, from gamma radiation emitted by a cloud of airborne radionuclides the distribution of which is described by a bivariate normal equation. The location can be any point downwind of the release on or off the centerline of the cloud at ground level. No restrictions have been placed on release height. The penetrating dose; i.e., dose at five centimeters, and the dose to organs of interest resulting from inhalation have not been incorporated in this computer code.

The program includes a fission product inventory calculation using the computer code RIBD (Gumprecht, 1968, 1969) as a subroutine. The fission product inventory, with additional activation products specified, is released to the atmosphere through a three barrier containment system with depletion and filtration in each barrier.

Special Notes -

- Nuclide decay is considered during production, release and transport using a chain decay scheme with branching to and from isomeric states.
- The dose is calculated as the space-time intergral of air concentration.
- A data base is used to minimize input requirements.
- The space-time integration causes long typical running times.

Programming Considerations - RACER is written in FORTRAN IV for a UNIVAC 1108 computer.

Name of Program - RADOS

Description - RADOS (Cooper, 1968) was developed to evaluate external gamma dose from a finite cloud of radioactive material. A bivariate Gaussian distribution is assumed with dispersion parameters described by Sutton's equation or by input. The dose calculation is performed for a source of specific energy emission rate with one daughter. The source is supplied as total energy per second release in one energy group.

The simplifying assumptions used to minimize computation time are:

- The material release is instantaneous and results in a radioactive cloud of unit thickness in the X or downwind direction.
- There is no change in the size and shape of the cloud during passage over the effective range of the receptor.
- The gamma buildup factors can be expressed analytically with sufficient accuracy.

These assumptions limit the applicability of RADOS as follows: the material release must occur over a relatively short time; the receptor distance must be more than 600 m downwind from the release point; and the gamma energies must be in the specified range (0.5 to 2.0 MeV).

Special Notes -

- Dispersion parameters for the bivariate normal dispersion equation can be specified in either Sutton's form or as the general Gaussian dispersion form.
- An analytic expression is used to evaluate the dose from a line source (downwind direction) which is integrated numerically in the lateral and vertical directions using Gaussian quadrature techniques.
- Buildup is calculated by the expression

$$B = 1 + \mu a + \frac{(\mu a)^2}{7E^{2.4}}$$

- The calculation is limited to gamma energies of from 0.5 to 2 MeV.
- For release under inversion conditions with a lid, the distribution of material is assumed to be uniform in the vertical direction.
- The source is specified as MeV/sec in a particular energy group. Specific nuclides are not considered.
- Contributions from one daughter may be included.

Programming Considerations - RADOS is written in FORTRAN for an IBM 360 computer.

Name of Program - RSAC-2

Description - The Radiological Safety Analysis Computer Code (RSAC) (Coates and Horton, 1966; Richardson, 1968; Wenzel, 1974) is used to calculate the radiological consequences from accidental release of radionuclides to the atmosphere. RSAC-2 can be used to calculate 1) fission product inventory source terms, 2) lung doses using either the ICRP Task Group on Lung Dynamics Lung Model (TGLM) (ICRP, 1966) or the initial ICRP Lung Model (ILM) (ICRP 2, 1959), 3) gastrointestinal tract doses using either the model of Dolphin and Eve (1966) or the ICRP Publication 2 (1959) model, 4) dose to various internal organs using the ILM, 5) ground deposition gamma doses, and 6) cloud gamma doses using either a "finite" or "semi-infinite" cloud model. Cloud concentration is determined by the bivariate normal distribution model.

Special Notes -

- Containment features are modeled as a ten term exponential function.
- Straight chain decay is considered. Branching is simulated by dividing the chain branches into two or more straight chains.
- Special attention is given to the finite cloud integration using Gaussian quadrature techniques applied to a variable interval.
- Buildup is modeled as a third-order polynomial.

Programming Considerations - RSAC-2 is written in FORTRAN IV for an IBM computer and requires ~125 (decimal) core.

Name of Program - RUBY

Description - RUBY (Kniazewycz, 1974) is a modified version of the EMERALD (Brunot, 1971) code and was designed to be used for calculations associated with the operation of the Shearan Harris Nuclear Power Plant. The program was developed to approximate most PWR plants.

The code models a reactor system using an analog simulation procedure with each component or control volume in the plant represented by a subroutine which keeps track of production, transfer, decay and removal of radioactivity in the volume. The activity released to the atmosphere is used to calculate individual and population doses at various distances and sectors for individual nuclides and sums of nuclides.

Special Notes -

- The code contains a library of physical data for the 55 nuclides of most interest in licensing calculations.
- Nuclides can be separated into four classes: iodines, noble gases, soluble particulates and insoluble particulates.
- "The program contains very little new scientific or engineering material, data, models, or assumptions, and many of the models are identical to those used by the Regulatory Staff of the Atomic Energy Commission."

Programming Considerations - The code is written in FORTRAN IV for an IBM 370 computer and requires 384K of storage for execution.

Name of Program - SUBDOSA

Description - SUBDOSA, (Streng, 1975), developed at BNW, calculates external gamma and beta doses to an individual from accidental release of radionuclides to the atmosphere. Both gamma and beta doses may be calculated as a function of depth in tissue. Combinations of gamma and beta doses may be summed and reported as skin, eye or genetic dose. Doses are calculated for up to six periods of release with separate nuclide inventories and dispersion considered for each period. Nuclide decay is considered during release and/or transit using a chain decay scheme with branching to account for transitions to and from isomeric states.

Special Note -

- An extensive data base is used to minimize input requirements.
- SUBDOSA includes a program to calculate the effective beta energy as a function of tissue depth for radiations from 494 radionuclides.
- The external gamma dose is calculated using the finite cloud approach.

Programming Considerations - SUBDOSA is written in FORTRAN IV for a CDC CYBER.

Name of Program - SUBPOPA

Description - SUBPOPA, developed and in use at BNW but not yet documented, calculates the population dose resulting from accidental releases of radio-nuclides to the atmosphere. Population doses are calculated by assuming that the cloud travel and dispersal to any point surrounding the release are represented by the joint frequency distribution of wind vector and atmospheric stability. A sector average concentration and a 1-hr release are assumed.

Special Notes -

- Radioactive chain decay with branching is calculated for chains with up to seven members.
- Contributions to external dose from both beta and gamma radiations are calculated.
- Dose is calculated as a function of depth in tissue.
- Extensive data bases are used to minimize input requirements.
- Up to five release inventories may be specified with results from each release summed.
- A finite cloud approach is used for the external gamma dose calculation.

Programming Considerations - SUBPOPA is written in FORTRAN IV for a CDC CYBER computer and requires 143k (octal) words of core to execute.

Name of Program - (USNRDL CODE)

Description - This program (Wong, 1967) was developed to calculate organ doses from uptake via inhalation, ingestion and injection. The code also computes the effective energy absorbed by each organ. The dose is calculated for various periods of intake and internal exposure. The code uses methods of ICRP Publication 2 (1959) for the effective absorbed energy calculation.

Special Notes -

- Straight chain decay is included. Branching is accounted for by dividing the chain into two or more chains.
- ICRP (1959) models are used to calculate effective absorbed energies with options of other models where the ICRP (1959) model gives low results.
- Intake time is assumed to be generally less than 12 hours for accidental releases.
- Atmospheric dispersion is not calculated. Input is supplied as $\mu\text{Ci}/\text{m}^3$ for inhalation calculations.
- When the transfer fraction from inhalation to organ is not given, the code uses the fraction to total body weighted by the ratio of organ mass to total body mass.

Programming Considerations - The code is written in FORTRAN for an unspecified computer.

Name of Program - YIELDS

Description - The code (Chester, 1974) calculates the fission product activity as a function of time for a specified refuel schedule. Activity may be reported as 1) curies, 2) an energy-activity product, or 3) an energy-activity product integrated over time.

Additional calculations can be made to give MeV-Ci, lifetime dose in rem to an organ of specified mass, gamma ray dose rate 1 m above a plane, or an energy-Ci product where the average energy for disintegration for fission product nuclides is an input parameter. The internal doses are calculated for either an instantaneous or constant uptake.

Special Notes -

- Radioactive decay with branching to and from isomeric states is calculated. Simplifications are made in decay schemes where appropriate.
- Doses may be calculated for a multisection biological system with exponential clearance.
- The average beta energy is calculated from the endpoint energy and atomic number of the daughter by integrating the Fermi equation with coulomb correction.
- Decay chain data are read in from cards as a library.
- Atmospheric dispersion does not appear to be included.

Programming Considerations - YIELDS is written in FORTRAN for an IBM computer.

REFERENCES

F. T. Binford, J. Barish, and F. B. K. Kam. Estimation of Radiation Doses Following a Reactor Accident. ORNL-4086, Union Carbide Corporation, Oak Ridge National Laboratory, Oak Ridge, TN, 1968.

L. L. Bonzon, and J. B. Rivard. Computational Method for Calculation of Radiological Dose Resulting from Hypothetical Fission Product Release. SC-RR-70-338, Sandia Laboratories, Albuquerque, NM, 1970.

R. S. Booth, S. V. Kaye, and P. S. Rohwer. "A Systems Analysis Methodology for Predicting Dose to Man from a Radioactively Contaminated Terrestrial Environment." Proceedings of the Third National Symposium on Radioecology, May 10-12, 1971, Oak Ridge, TN, D. J. Nelson, Ed, CONF-710501, pp. 877-893, 1971.

G. A. Briggs. Plume Rise, AEC Critical Review Series. TID-25075, U. S. Atomic Energy Commission, Washington, DC, 1968.

W. K. Brunot, EMERALD - A Program for the Calculation of Activity Releases and Potential Doses from a Pressurized Water Reactor Plant. Pacific Gas and Electric Company, San Francisco, CA, 1971.

R. O. Chester, Biological Dose and Radiological Activity from Nuclear Reactor or Nuclear Weapon Fission Products. Oak Ridge, TN, 1974.

R. L. Coates, and N. R. Harton, Rnac - a Radiological Safety Analysis Computer Program. IDO-17151, Phillips Petroleum Company, National Reactor Testing Station, Idaho Falls, ID, 1966.

R. E. Cooper, RADOS - A Code to Estimate Gamma Dose from a Cloud of Radioactive Gases. DP-1098 (Rev. 1), E. I. duPont de Nemours & Co., Savannah River Laboratory, Aiken, SC, 1968.

R. E. Cooper, EGAD - A Computer Program to Compute Dose Integrals from External from External Gamma Emitters. DP-1304, E. I. duPont de Nemours & Co., Savannah River Laboratory, Aiken, SC, 1972.

D. H. Denham, D. A. Baker, J. K. Soldat, and J. P. Corley, Radiological Evaluations for Advanced Waste Management Studies. BNWL - 1764, Battelle, Pacific Northwest Laboratories, Richland, WA, 1973.

G. W. Dolphin, and I. S. Eve, "Dosimetry of the Gastrointestinal Tract." Health Physics, Vol. 12, pp 163-172, 1966.

R. O. Gumprecht, Mathematical Basis of Computer Code RIBD. DUN-4136, Douglas United Nuclear, Inc., Richland, WA, 1968.

R. O. Gumprecht, Computer Code RIBD. DUN-SA-69, Douglas United Nuclear, Inc., Richland, WA, 1969.

W. F. Hilsmeier, and F. A. Gifford Jr., Graphs for Estimating Atmospheric Dispersion. ORO-545, 1962.

J. R. Houston, D. L. Streng, and E. C. Watson, DACRIN - A Computer Program for Calculating Organ Dose from Acute or Chronic Radionuclide Inhalation. BNWL-B-389, Battelle Pacific Northwest Laboratories, Richland, WA, 1974. (Reissued 1975).

International Commission on Radiological Protection, ICRP Publication 2, Pergamon Press, Oxford, 1959.

International Commission on Radiological Protection, ICRP Publication 6, Pergamon Press, Oxford, 1964.

International Commission on Radiological Protection, Task Group of Committee II, "Task Group on Lung Dynamics for Committee II of the ICRP." Health Physics, Vol. 12, p. 173, 1966.

S. V. Kaye et al, "Environmental Hazards Studies." Environmental Sciences Division Annual Progress Report, September 30, 1973, ORNL-4935, p. 1, Union Carbide Corporation, Oak Ridge National Laboratory, Oak Ridge, TN, 1973.

G. G. Killough, P. S. Roher, and W. D. Turner, INREM - A FORTRAN Code Which Implements ICRP 2 Models of internal Radiation Dose to Man. ORNL-5003, Union Carbide Corporation, Oak Ridge National Laboratory, Oak Ridge, TN, 1975.

B. G. Kniazewycz, J. S. Boone, and G. L. Parks, RUBY - A Dynamic Radioactivity Model. Paper No. 120 presented at the 19th Annual Health Physics Society Meeting, Carolina Power & Light Company, P. O. Box 1551, Raleigh, NC, 1974.

J. A. Martin Jr., C. B. Nelson, and P. A. Cury, AIREM Program Manual: A Computer Code for Calculation Doses, Population Doses, and Ground Depositions Due to Atmospheric Emissions of Radionuclides. EPA-5201/-74-004, U. S. Environmental Protection Agency, Washington, DC, 1974.

Meteorology and Atomic Energy. AECU-3066, prepared by U. S. Weather Bureau for USAEC, p. 72, 1955.

R. E. Moore, AIRDOS - A Computer Code for Estimating Population and Individual Doses Resulting from Atmospheric Releases of Radionuclides from Nuclear Facilities. ORNL-TM-4687, Union Carbide Corporation, Oak Ridge National Laboratory, Oak Ridge, TN, 1975.

R. E. Moore, and C. J. Barton, Progress Report on Radiological Safety of Peaceful Uses of Nuclear Explosives: Preliminary Equations and Computer Techniques for Estimating and Controlling Tritium Doses from Nuclearly Stimulated Natural Gas ORNL-TM-3755, Union Carbide Corporation, Oak Ridge National Laboratory, Oak Ridge, TN, 1972.

R. E. Moore, and C. J. Barton, Dose Estimations for the Hypothetical Use of Nuclear Stimulated Natural Gas in the Cherokee Steam Electric Station, Denver, Colorado. ORNL-TM-4026, Union Carbide Corporation, Oak Ridge National Laboratory, Oak Ridge, TN, 1973.

F. Pasquill, Atmospheric Diffusion. D. Van Nostrand Co. LTD, 1962.

L. C. Richardson, User's Manual for the FORTRAN Version of RSAC. IDO-17261, Phillips Petroleum Company, National Reactor Testing Station, Idaho Falls, ID, 1968.

A. F. Rupp, S. E. Beall, L. P. Bornwasser and D. H. Johnson, Dilution of Stack Gases in Crosswinds. USAEC Report AECD-1811 (CE-1620), Clinto Laboratories, 1948.

J. K. Soldat, N. M. Robinson, and D. A. Baker, Models and Computer Codes for Evaluating Environmental Radiation Doses. BNWL-1754, Battelle, Pacific Northwest Laboratories, Richland, WA, 1974.

G. W. Spangler et al., Description of the COMRADEX Code, AI-67-TDR-108, McDonnell Douglas Corporation, Santa Monica, CA, 1967.

F. W. Stallman, and F. B. K. Kam, ACRA - Computer Program for the Estimation of Radiation Doses Caused by a Hypothetical Reactor Accident. ORNL-TM-4082, Union Carbide Corporation, Oak Ridge National Laboratory, Oak Ridge, TN, 1973.

D. L. Streng, DACRIN - A Computer Program for Calculating Organ Dose from Acute or Chronic Radionuclide Inhalation: Modification for Gastrointestinal Tract Dose. BNWL-B-389 SUPP, Battelle, Pacific Northwest Laboratories, Richland, WA, 1975.

D. L. Streng, M. M. Hendrickson, and E. C. Watson, RACER - A Computer Program for Calculating Potential External Doses from Airborne Fission Products Following Postulated Reactor Accidents. BNWL-B-69, Battelle, Pacific Northwest Laboratories, Richland, WA, 1971.

D. L. Streng, and E. C. Watson, KRONIC - A Computer Program for Calculating Annual Average External Doses from Chronic Atmospheric Releases of Radionuclides. BNWL-B-264, Battelle, Pacific Northwest Laboratories, Richland, WA, 1973.

D. L. Streng, E. C. Watson, and J. R. Houston, SUBDOS - A Computer Program for Calculating Individual External Doses from Accidental Atmospheric Radionuclides. BNWL-B-351, Battelle, Pacific Northwest Laboratories, Richland, WA, 1975.

O. G. Sutton, Micrometeorology. McGraw-Hill Book Company, NY, 1953.

D. K. Trubey, and S. V. Kaye, The EXREM III Computer Code for Estimating External Radiation Doses to Populations from Construction of a Sea-level Canal with Nuclear Explosives. CTC-8, Union Carbide Corporation, Oak Ridge, TN, 1969.

W. D. Turner, S. V. Kaye, and P. S. Rohwer, EXREM and INREM Computer Codes for Estimating Radiation Doses to Populations from Construction of a Sea-level Canal with Nuclear Explosives. K-1752, Union Carbide Corporation, Oak Ridge, TN, 1968.

H. H. Van Tuyl, ISOGEN - A Computer Program Code for Radioisotope Generation Calculations. HW-83785, General Electric Company, Richland, WA, 1964.

D. R. Wenzel, A Computer Code to Calculate Doses Resulting from Release of Radionuclides to the Atmosphere. Paper 119 presented at the 19th Annual Health Physics Society Meeting, Allied Chemical Corporation, Idaho Falls, ID 83401, 1974.

C. A. Willis, G. E. Spangler, and E. A. Rhoades, A New Technique for Reactor Siting Dose Calculations. Douglas Paper 10241, McDonnell Douglas Corporation, Santa Monica, CA, 1968.

P. Wong, A FORTRAN Program to Determine Absorbed Organ Dose Due to Inhalation of Radionuclides. USNRDL-TR-67-7, U. S. Naval Radiological Defense Laboratory, San Francisco, CA, 1967.

APPENDIX C

DETAILS OF GETOUT MODEL EXTENSION FOR IMPULSE RELEASE

H. C. Burkholder

APPENDIX C

DETAILS OF GETOUT MODEL EXTENSION FOR IMPULSE RELEASE

This appendix describes the derivation of the closed form mathematical expressions necessary to predict the transport through geologic media of a two-member decay chain, each member of which exists as two different but interacting chemical species. The background of this work was described in Section 2.2.3.1.

The linear partial differential equations which describe the material balances of the two nuclide, four species system (see Figure 2.4 in Section 2.2.3.1) over a differential volume of the geologic medium and a differential time are:

$$D \frac{\partial^2 C_{1,1}}{\partial z^2} - V \frac{\partial C_{1,1}}{\partial z} - K_{1,1} \frac{\partial C_{1,1}}{\partial t} - K_{1,1} \lambda_1 C_{1,1} - L_{1,1} \lambda_{1,1} C_{1,1} - M_{1,1} \lambda_{1,1}^m C_{1,1} = 0 \quad (1)$$

$$D \frac{\partial^2 C_{1,2}}{\partial z^2} - V \frac{\partial C_{1,2}}{\partial z} - K_{1,2} \frac{\partial C_{1,2}}{\partial t} - K_{1,2} \lambda_1 C_{1,2} - L_{1,2} \lambda_{1,2} C_{1,2} + L_{1,1} \lambda_{1,1} C_{1,1} - M_{1,2} \lambda_{1,2}^m C_{1,2} = 0 \quad (2)$$

$$D \frac{\partial^2 C_{2,1}}{\partial z^2} - V \frac{\partial C_{2,1}}{\partial z} - K_{2,1} \frac{\partial C_{2,1}}{\partial t} - K_{2,1} \lambda_2 C_{2,1} + K_{1,1} \lambda_1 C_{1,1} - L_{2,1} \lambda_{2,1} C_{2,1} - M_{2,1} \lambda_{2,1}^m C_{2,1} = 0 \quad (3)$$

$$D \frac{\partial^2 C_{2,2}}{\partial z^2} - V \frac{\partial C_{2,2}}{\partial z} - K_{2,2} \frac{\partial C_{2,2}}{\partial t} - K_{2,2} \lambda_2 C_{2,2} + K_{1,2} \lambda_1 C_{1,2} - L_{2,2} \lambda_{2,2} C_{2,2} + L_{2,1} \lambda_{2,1} C_{2,1} - M_{2,2} \lambda_{2,2}^m C_{2,2} = 0 \quad (4)$$

where:

$C_{i,j}$ = concentration of the "i"th nuclide and "j"th species
(g-atoms/m³)

z = distance (m)

t = time (yr)

D = dispersion coefficient (m²/yr)

V = the water velocity (m/yr)

λ_i = the radioactive decay rate coefficient (yr⁻¹)

$\lambda_{i,j}$ = the chemical reaction rate coefficient (yr⁻¹)

$\lambda_{i,j}^m$ = the irreversible mineralization rate coefficient (yr⁻¹).

The sorption retardation factor, $K_{i,j}$, is determined using either of the two equations shown below and on the following page:

$$K_{i,j} = 1 + \frac{Kd_{i,j} \rho}{\epsilon} \text{ (unconsolidated media)} \quad (5)$$

where:

$Kd_{i,j}$ = distribution coefficient

ρ = bulk density of medium

ϵ = void fraction

$$\left[\frac{\text{activity of nuclide in sorbed state}}{\text{mass of medium}} \right] \div \left[\frac{\text{activity of nuclide in dissolved state}}{\text{volume of pore space}} \right] \left[\frac{\text{mass of medium}}{\text{volume of medium}} \right] \left[\frac{\text{volume of pore space}}{\text{volume of medium}} \right]$$

$$K_{i,j} = 1 + K_{a,i,j} R_f \text{ (fractured media)} \quad (6)$$

where:

$K_{a_{i,j}}$ = distribution coefficient

R_f = surface to volume ration of fracture system

$$\left[\frac{\text{activity of nuclide in sorbed state}}{\text{surface area of fracture}} \right] \left[\frac{\text{activity of nuclide in dissolved state}}{\text{volume of fracture}} \right] \left[\frac{\text{surface area of fracture}}{\text{volume of fracture}} \right]$$

The factor $L_{i,j}$ equals $K_{i,j}$ if the chemical reaction occurs in both the dissolved and sorbed states, equals 1 if the reaction occurs in the dissolved state only, and equals $K_{d_{i,j}} \rho/\epsilon$ or $K_{a_{i,j}} R_f$ if the reaction occurs in the sorbed state only. The factor $L_{i,j}$ equals $K_{d_{i,j}} \rho/\epsilon$ or $K_{a_{i,j}} R_f$ depending upon whether the system is best described as porous or fractured. The factor $M_{i,j}$ equals $K_{d_{i,j}} \rho/\epsilon$ or $K_{a_{i,j}} R_f$.

The equations were nondimensionalized and solved simultaneously using the Laplace transform technique for both impulse and band releases. The impulse release assumes that the entire contents of the repository are instantaneously released to the water when intrusion occurs. The band release assumes that the repository contents are released at a constant rate until the repository becomes empty. Only the result for the impulse release is presented here. The appropriate boundary conditions are shown in Table C.1. The mathematical results for the impulse release are:

$$C_{1,1} = F_1(1,1) \quad (7)$$

$$\begin{aligned} C_{1,2} = & F_1(1,2) \\ & + F_2(1,1) F_3(1,1,1,2) F_6(1,1,1,2) \left[F_7^-(1,1,1,2) (F_8^-(1,1,1,2,1,2) \right. \\ & - F_8^-(1,1,1,2,1,1)) + F_7^+(1,1,1,2) (F_8^+(1,1,1,2,1,2) \\ & \left. - F_8^+(1,1,1,2,1,1)) \right] \end{aligned} \quad (8)$$

$$\begin{aligned}
C_{2,1} &= F_1(2,1) \\
&+ F_2(1,1) F_4(1,1,2,1) F_6(1,1,2,1) \left[F_7^-(1,1,2,1) (F_8^-(1,1,2,1,2,1) \right. \\
&- F_8^-(1,1,2,1,1,1)) + F_1^+(1,1,2,1) (F_8^+(1,1,2,1,2,1) \\
&- F_8^-(1,1,2,1,1,1)) \left. \right] \quad (9)
\end{aligned}$$

$$\begin{aligned}
C_{2,2} &= F_1(2,2) \\
&+ F_2(1,2) F_4(1,2,2,2) F_6(1,2,2,2) \left[F_9^-(1,2,2,2) (F_{10}^-(1,2,2,2,2,2) \right. \\
&- F_{10}^-(1,2,2,2,1,2)) + F_9^+(1,2,2,2) (F_{10}^+(1,2,2,2,2,2) \\
&- F_{10}^+(1,2,2,2,1,2)) \left. \right] + F_2(2,1) F_3(2,1,2,2) F_6(2,1,2,2) \\
&\left[F_7^-(2,1,2,2) (F_8^-(2,1,2,2,2,2) - F_8^-(2,1,2,2,2,1)) \right. \\
&+ F_7^+(2,1,2,2) (F_{10}^+(2,1,2,2,2,2) - F_{10}^+(2,1,2,2,2,1)) \\
&+ \frac{F_2(1,1) F_3(1,1,1,2) F_4(1,2,2,2)}{F_5(1,2,2,2) - F_5(1,1,1,2)} \left[F_6(1,1,1,2) \left[F_{11}^-(1,1,1,2,2,2) \right. \right. \\
&F_{12}^-(1,1,1,2,2,2) + F_{11}^+(1,1,1,2,2,2) F_{12}^+(1,1,1,2,2,2) \left. \right] \\
&- F_6(1,2,2,2) \left[F_{11}^-(1,2,2,2,2,2) F_{12}^-(1,2,2,2,2,2) \right. \\
&+ F_{11}^+(1,2,2,2,2,2) F_{12}^+(1,2,2,2,2,2) \left. \right] \left. \right] \\
&- \frac{F_2(1,1) F_3(1,1,1,2) F_4(1,2,2,2)}{F_5(1,2,2,2) - F_5(1,1,1,2)} \left[F_6(1,1,1,2) \left[F_{11}^-(1,1,1,2,1,2) \right. \right. \\
&F_{12}^-(1,1,1,2,1,2) \\
&+ F_{11}^+(1,1,1,2,1,2) F_{12}^+(1,1,1,2,1,2) \left. \right] - F_6(1,2,2,2) \\
&\left[F_{11}^-(1,2,2,2,1,2) F_{12}^-(1,2,2,2,1,2) + F_{11}^+(1,2,2,2,1,2) \right. \\
&F_{12}^+(1,2,2,2,1,2) \left. \right] \left. \right] \\
&+ \frac{F_2(1,1) F_3(1,1,2,1) F_4(2,1,2,2) F_6(1,1,2,1)}{(F_5(2,1,2,2) - F_5(1,1,2,1))} \\
&\left[F_{11}^-(1,1,2,1,2,2) F_{12}^-(1,1,2,1,2,2) \right. \\
&+ F_{11}^+(1,1,2,1,2,2) F_{12}^+(1,1,2,1,2,2) \left. \right] \quad (10)
\end{aligned}$$

where:

$$F_1(i, j) = N_{i, j}^0 \frac{v_n}{2Wl} \sqrt{\frac{K_{i, j}^p}{\pi \theta^3}} \exp \left[- \left(R_i + \frac{L_{i, j} R_{i, j}}{K_{i, j}} + \frac{M_{i, j} R_{i, j}^m}{K_{i, j}} \right) \theta - \frac{P \theta}{4K_{i, j}} \left(\frac{K_{i, j}^n}{\theta} - 1 \right)^2 \right]$$

$$F_2(i, j) = \frac{N_{i, j}^0 v}{2Wl}$$

$$F_3(i, j, k, 1) = \frac{L_{i, j} R_{i, j}}{K_{i, j} - K_{k, 1}}$$

$$F_4(i, j, k, 1) = \frac{K_{i, j} R_i}{K_{i, j} - K_{k, 1}}$$

$$F_5(i, j, k, 1) = \frac{K_{i, j} R_i - K_{k, 1} R_k + L_{i, j} R_{i, j} - L_{k, 1} R_{k, 1} + M_{i, j} R_{i, j}^m - M_{k, 1} R_{k, 1}^m}{K_{i, j} - K_{k, 1}}$$

$$F_6(i, j, k, 1) = \exp \left(- \frac{K_{i, j} R_i - K_{k, 1} R_k + L_{i, j} R_{i, j} - L_{k, 1} R_{k, 1} + M_{i, j} R_{i, j}^m - M_{k, 1} R_{k, 1}^m}{K_{i, j} - K_{k, 1}} \theta \right)$$

$$F_7(i, j, k, 1) = \exp \left[\frac{P_n}{2} \left(1 \pm \sqrt{1 + \frac{4(K_{i, j} L_{k, 1} R_{k, 1} - K_{k, 1} L_{i, j} R_{i, j} + K_{i, j} M_{k, 1} R_{k, 1}^m - K_{k, 1} M_{i, j} R_{i, j}^m)}{P(K_{i, j} - K_{k, 1})}} \right) \right]$$

$$F_8(i, j, k, 1, m, n) = \operatorname{erfc} \left[\frac{n}{2} \sqrt{\frac{K_{m, n}^p}{\theta}} + \sqrt{\frac{P}{4K_{m, n}} + \frac{K_{i, j} L_{k, 1} R_{k, 1} - K_{k, 1} L_{i, j} R_{i, j} + K_{i, j} M_{k, 1} R_{k, 1}^m - K_{k, 1} M_{i, j} R_{i, j}^m}{K_{m, n}(K_{i, j} - K_{k, 1})}} \theta \right]$$

$$F_9(i, j, k, 1) = \exp \left[\frac{P_n}{2} \left(1 \pm \sqrt{1 + \frac{4(K_{i, j} K_{k, 1} R_{k, 1} - K_{i, j} K_{k, 1} R_{i, j} + K_{i, j} L_{k, 1} R_{k, 1} - K_{k, 1} L_{i, j} R_{i, j} + K_{i, j} M_{k, 1} R_{k, 1}^m - K_{k, 1} M_{i, j} R_{i, j}^m)}{P(K_{i, j} - K_{k, 1})}} \right) \right]$$

$$F_{10}(i, j, k, 1, m, n) = \operatorname{erfc} \left[\frac{n}{2} \sqrt{\frac{K_{m, n}^p}{\theta}} + \sqrt{\frac{P}{4K_{m, n}} + \frac{K_{i, j} K_{k, 1} R_{k, 1} - K_{i, j} K_{k, 1} R_{i, j} + K_{i, j} L_{k, 1} R_{k, 1} - K_{k, 1} L_{i, j} R_{i, j} + K_{i, j} M_{k, 1} R_{k, 1}^m - K_{k, 1} M_{i, j} R_{i, j}^m}{K_{m, n}(K_{i, j} - K_{k, 1})}} \theta \right]$$

$$F_{11}(i, j, k, l, m, n) = \exp \left[\frac{p}{2} \left(1 + \sqrt{1 + \frac{4K_{m,n}^R R_m}{p} + \frac{4L_{m,n}^R R_{m,n}}{p} + \frac{4M_{m,n}^R R_{m,n}^m}{p} - \frac{4K_{m,n}}{p} \left(\frac{K_{i,j}^R i^{-K_{k,l}^R} + L_{i,j}^R i, j^{-L_{k,l}^R} + M_{i,j}^R i, j^{-M_{k,l}^R} + R_{k,l}^m}{K_{i,j}^{-K_{k,l}}} \right)} \right) \right]$$

$$F_{12}(i, j, k, l, m, n) = \operatorname{erfc} \left[\frac{\eta}{2} \sqrt{\frac{K_{m,n}^p}{\theta} + \sqrt{\frac{p}{4K_{m,n}} + R_m + \frac{L_{m,n}^R R_{m,n}}{K_{m,n}} + \frac{M_{m,n}^R R_{m,n}^m}{K_{m,n}} - \frac{K_{i,j}^R i^{-K_{k,l}^R} + L_{i,j}^R i, j^{-L_{k,l}^R} + M_{i,j}^R i, j^{-M_{k,l}^R} + R_{k,l}^m}{K_{i,j}^{-K_{k,l}}}} \right] \theta$$

$$p = \frac{VL}{D}$$

$$R_i = \frac{\lambda_i L}{V}$$

$$R_{i,j} = \frac{\lambda_{i,j} L}{V}$$

$$R_{i,j}^m = \frac{\lambda_{i,j}^m L}{V}$$

$$\eta = \frac{Z}{L}$$

$$\theta = \frac{tV}{L}$$

TABLE C.1 Boundary Conditions for Impulse Release

<u>Initial</u> <u>t=0, all z</u>	<u>Inlet</u> <u>t=0, z=0</u>	<u>Outlet</u> <u>t=0, z= L</u>
$C_{1,1} = 0$	$C_{1,1} = \frac{N_{1,1}^0}{W} (t)$	$C_{1,1} = \text{finite}$
$C_{1,2} = 0$	$C_{1,2} = \frac{N_{1,2}^0}{W} (t)$	$C_{1,2} = \text{finite}$
$C_{2,1} = 0$	$C_{2,1} = \frac{N_{2,1}^0}{W} (t)$	$C_{2,1} = \text{finite}$
$C_{2,2} = 0$	$C_{2,2} = \frac{N_{2,2}^0}{W} (t)$	$C_{2,2} = \text{finite}$

where:

(t) = the unit impulse function (y^{-1})

W = the volumetric flow rate of the water (m^3/yr)

$N_{i,j}^0$ = the nuclide inventory at the time of release (g-atoms).

APPENDIX D

SORPTION DATA BASE DETAILS

R. J. Serne

KEY TO SYMBOLS

<u>Geologic Material Properties</u>	<u>Groundwater Properties</u>	<u>Nuclide Properties</u>	<u>Kd ml/g</u>	<u>pH</u>	<u>Method</u>
Mineralogy (most abundant first others in decreasing abundance) CaCO ₃ = calcium carbonate OX = hydrous iron and manganese oxides OM = organic content CEC = cation exchange capacity AEC = anion exchange capacity SA = surface area	Eh = oxidation reduction potential	(a) Tracer concentration (b) Tracer valence (c) Shaking time (d) direction (adsorption or desorption)			a. Method details b. Soil to solution ratio c. Miscellaneous

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Illite		(a) $6 \times 10^{-11} \text{ M } ^{95}\text{mTc}$			a. Batch	Appendix 3.3.C
Poorly crystallized		(b) TcO_4^-	4.7 ± 0.5	6.3	(3 cold washes)	
Minor amount Kaolinite.	Eh 390 mv	(c) 29 days			(Blank corrected)	
$\text{CaCO}_3 = 0\%$					b. 0.5 g to 15 ml	
OX = ?	$\text{Na}^+ 5130 \text{ meq/l}$				c. Kd avg of 3 values	
OM = 0%	$\text{Cl}^- 5130 \text{ meq/l}$	(a) $2 \times 10^{-7} \text{ M } ^{237}\text{Np}$				
CEC = $13.8 \pm 0.8 \text{ meq/100 g}$		(b) NpO_2^+	42.0 ± 3.9	6.7		
AEC = ?	20-27°C	(c) 19 days				
SA = $165.4 \pm 3.3 \text{ m}^2/\text{g}$		(a) $3 \times 10^{-11} \text{ M } ^{137}\text{Cs}$				
		(b) Cs^+	564 ± 35	6.3		
		(c) 29 days				
		(a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$		6.3		
		(b) Sr^{2+}	1.2 ± 0.5			
		(c) 29 days				
		(a) $8 \times 10^{-12} \text{ M } ^{85}\text{Am}$				
		(b) Am^{3+}	2800 ± 3700	6.9		
		(c) 17 days				
		(a) $8 \times 10^{-5} \text{ M } ^{129}\text{I}$				
		(b) I^-	30 ± 33	6.9		
		(c) 17 days				
(Same)	Eh 490	(a) $6 \times 10^{-11} \text{ M } ^{95}\text{mTc}$			(Same)	(Same)
	$\text{Ca}^{2+} 30 \text{ meq/l}$	(b) TcO_4^-	0.5 ± 0.5	7.0		
	$\text{Cl}^- 30 \text{ meq/l}$	(c) 19 days				
		(a) $5 \times 10^{-7} \text{ M } ^{237}\text{Np}$				
		(b) NpO_2^+	14 ± 6	6.6		
	20-27°C	(c) 19 days				
		(a) $3 \times 10^{-11} \text{ M } ^{137}\text{Cs}$				
		(b) Cs^+	$4.4 \times 10^4 \pm 6.9 \times 10^4$	7.0		
		(c) 29 days				

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Illite (continued)		(a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$ (b) Sr^{2+} (c) 29 days	6.2 ± 1.5	7.0		
		(a) $4 \times 10^{-12} \text{ M } ^{241}\text{Am}$ (b) Am^{3+} (c) 17 days	330 ± 33	7.0		
		(a) $8 \times 10^{-5} \text{ M } ^{129}\text{I}$ (b) I^- (c) 17 days	1.7 ± 5.0	7.6		
(Same)	Eh 525 mv	(a) $6 \times 10^{-11} \text{ M } ^{95\text{m}}\text{Tc}$ (b) TcO_4^- (c) 29 days	10.3 ± 1.1	5.9	(Same)	(Same)
	$\text{Na}^+ 30 \text{ meq/l}$ $\text{Cl}^- 30 \text{ meq/l}$					
	20-27°C	(a) $5 \times 10^{-7} \text{ M } ^{237}\text{Np}$ (b) NpO_2^+ (c) 19 days	26.8 ± 1.0	5.7	(Same)	(Same)
		(a) $3 \times 10^{-11} \text{ M } ^{137}\text{Cs}$ (b) Cs^+ (c) 29 days	$13,000 \pm 6,000$	5.9		
		(a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$ (b) Sr^{2+} (c) 29 days	36.5 ± 1.0	5.9		
		(a) $8 \times 10^{-10} \text{ M } ^{241}\text{Am}$ (b) Am^{3+} (c) 17 days	920 ± 35	7.0		
		(a) $8 \times 10^{-5} \text{ M } ^{129}\text{I}$ (b) I^- (c) 17 days	1.3 ± 0.9	7.0		

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference	
Illite (continued)	Eh 405 mv	(a) $8 \times 10^{-12} \text{ M } ^{241}\text{Am}$	$6.3 \times 10^4 \pm 3.2 \times 10^4$	9.1	(Same)	(Same)	
		(b) Am^{3+}					
		(c) 17 days					
	Na^+ 30 meq/l						
	HCO_3^- 30 meq/l						
	20-27°C	(a) $6 \times 10^{-11} \text{ M } ^{95\text{m}}\text{Tc}$	-0.9 ± 0.4	8.7	a. Batch Constant Eh maintained with coulometer) b. 1 g to 30 ml c. Blank corrected	Appendix 3.3.D	
		(b) TcO_4^-					
		(c) 29 days					
		(a) $5 \times 10^{-7} \text{ M } ^{237}\text{Np}$	295 $\pm$ 25	8.9			
		(b) NpO_2^+					
		(c) 19 days					
		(a) $3 \times 10^{-11} \text{ M } ^{137}\text{Cs}$	$5.5 \times 10^4 \pm 8.2 \times 10^4$	8.7			
		(b) Cs^+					
		(c) 29 days					
		(a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$	298 $\pm$ 84	8.7			
		(b) Sr^{+2}					
		(c) 29 days					
		(a) $8 \times 10^{-5} \text{ M } ^{129}\text{I}$	-1.8 ± 2.1	9.1			
	(b) I^-						
	(c) 17 days						
Kaolinite	Eh 1140 mv	(a) $3 \times 10^{-7} \text{ M } ^{239}\text{Pu}$	55.9	4.0			
	Minor amount of mica.	(b) Pu^{+4}					
	CaCl_2 30 meq/l	(c) 2 days					
	$\text{CaCO}_3 = 0\%$						
	OM = 0%						
	CEC = 5.0 ± 0.9 meq/100 g	Eh 1340 mv	(a) $1.7 \times 10^{-6} \text{ M } ^{239}\text{Pu}$	-1.9	4.0		
	AEC = ?	CaCl_2 30 meq/l	(b) PuO_2^{2+}				
	SA = $30.7 \pm 0.5 \text{ m}^2/\text{g}$	20-27°C	(c) 14 days				
		Eh 1140 mv	(a) $2.1 \times 10^{-7} \text{ M } ^{239}\text{Pu}$	158	7.0		
	CaCl_2 30 meq/100 g	(b) PuO_2^{2+}					
	20-27°C	(c) 4 days					

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Kaolinite (continued)	Eh 440 mv	(a) $6 \times 10^{-11} \text{M } ^{95\text{m}}\text{Tc}$	0.4 ± 1.0	6.7	a. Batch (3 cold washes) (Blank corrected) b. 0.5 g in 15 ml c. Kd avg of 3 values	Appendix 3.3.C
		(b) TcO_4^-				
		(c) 29 days				
	Na^+ 5130 meq/l	(a) $2 \times 10^{-7} \text{M } ^{237}\text{Np}$	4.2 ± 1.8	6.1		
		(b) NpO_2^+				
		(c) 19 days				
	Cl^- 5130 meq/l	(a) $3 \times 10^{-11} \text{M } ^{137}\text{Cs}$	7.3 ± 0.8	6.7		
		(b) Cs^+				
		(c) 29 days				
	20-27°C	(a) $2 \times 10^{-11} \text{M } ^{85}\text{Sr}$	0.2 ± 1.0	6.7		
		(b) Sr^{2+}				
		(c) 29 days				
		(a) $1.6 \times 10^{-9} \text{M } ^{241}\text{Am}$	252 ± 17	6.9		
		(b) Am^{3+}				
		(c) 17 days				
		(a) $8 \times 10^{-5} \text{M } ^{129}\text{I}$	3.1 ± 2.0	6.9		
		(b) I^-				
		(c) 17 days				
(Same)	Eh 480 mv	(a) $6 \times 10^{-11} \text{M } ^{95\text{m}}\text{Tc}$	3.0 ± 5.3	5.7	(Same)	(Same)
		(b) TcO_4^-				
		(c) 29 days				
	Ca^{2+} 30 meq/l	(a) $5 \times 10^{-7} \text{M } ^{237}\text{Np}$	0.5 ± 1.9	6.5		
		(b) NpO_2^+				
		(c) 19 days				
	Cl^- 30 meq/l	(a) $3 \times 10^{-11} \text{M } ^{137}\text{Cs}$	$4.6 \times 10^4 \pm 6.7 \times 10^4$	5.7		
		(b) Cs^+				
		(c) 29 days				
	20-27°C					

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Kaolinite (continued)	(Same)	(a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$ (b) Sr^{2+} (c) 29 days (a) $4 \times 10^{-12} \text{ M } ^{241}\text{Am}$ (b) Am^{3+} (c) 17 days (a) $8 \times 10^{-5} \text{ M } ^{129}\text{I}$ (b) I^- (c) 17 days	0.6 ± 0.2 295 ± 141 -1.7 ± 1.5	5.7 6.9 6.9	(Same)	(Same)
(Same)	Eh 480 mv Na^+ 30 meq/l Cl^- 30 meq/l 20-27°C	(a) $6 \times 10^{-11} \text{ M } ^{95\text{m}}\text{Tc}$ (b) TcO_4^- (c) 29 days (a) $5 \times 10^{-7} \text{ M } ^{237}\text{Np}$ (b) NpO_4^+ (c) 19 days (a) $3 \times 10^{-11} \text{ M } ^{137}\text{Cs}$ (b) Cs^+ (c) 29 days (a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$ (b) Sr^{2+} (c) 29 days (a) $8 \times 10^{-10} \text{ M } ^{241}\text{Am}$ (b) Am^{3+} (c) 17 days (a) $8 \times 10^{-5} \text{ M } ^{129}\text{I}$ (b) I^- (c) 17 days	-0.4 ± 0.6 3.6 ± 2.0 909 ± 215 77 ± 3 1780 ± 520 5.4 ± 5.3	6.8 6.4 6.8 6.8 7.3	(Same)	(Same)

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Kaolinite (continued)	Eh 385 mv Na ⁺ 30 meq/l HCO ₃ ⁻ 30 meq/l 20-27°C	(a) $6 \times 10^{-11} \text{ M } ^{95\text{m}}\text{Tc}$			(Same)	(Same)
		(b) TcO_4^-	-0.2 ± 0.9	9.4		
		(c) 29 days				
		(a) $5 \times 10^{-7} \text{ M } ^{237}\text{Np}$				
		(b) NpO_4^+	122 ± 19	9.2		
		(c) 19 days				
		(a) $3 \times 10^{-11} \text{ M } ^{137}\text{Cs}$				
		(b) Cs^+	863 ± 37	9.4		
		(c) 29 days				
		(a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$				
		(b) Sr^{2+}	284 ± 107	9.2		
		(c) 29 days				
		(a) $1.6 \times 10^{-9} \text{ M } ^{241}\text{Am}$				
		(b) Am^{3+}	$4.2 \times 10^4 \pm 2.1 \times 10^4$	9.4		
Montmorillonite	Eh 410 mv No significant crystalline impurities OX = ? CaCO ₃ = 0% OM = 0% CEC = 87.4 ± 2.7 meq/100 g	(a) $8 \times 10^{-5} \text{ M } ^{129}\text{I}$			(Same)	(Same)
		(b) I^-	-1.0 ± 1.2	9.4		
		(c) 17 days				
		(a) $6 \times 10^{-11} \text{ M } ^{95\text{m}}\text{Tc}$				
		(b) TcO_4^-	0.2 ± 0.5	8.1		
		(c) 29 days				
		(a) $2 \times 10^{-7} \text{ M } ^{237}\text{Np}$				
		(b) NpO_4^+	80 ± 7	8.0		
		(c) 19 days				

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Montmorillonite (continued)						
AEC = ?						
SA = $722 \pm 7 \text{ m}^2/\text{g}$		(a) $3 \times 10^{-11} \text{ M } ^{137}\text{Cs}$ (b) Cs^+ (c) 29 days	33.2 ± 1.6	8.1		
		(a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$ (b) Sr^{2+} (c) 29 days	1.4 ± 0.6	8.1		
		(a) $8 \times 10^{-12} \text{ M } ^{241}\text{Am}$ (b) Am^{3+} (c) 17 days	382 ± 207	7.9		
		(a) $8 \times 10^{-5} \text{ M } ^{129}\text{I}$ (b) I^- (c) 17 days	4.8 ± 0.9	7.9		
(Same)	Eh 450 mv Ca^+ 30 meq/l Cl^- 30 meq/l 20-27°C	(a) $6 \times 10^{-11} \text{ M } ^{95m}\text{Tc}$ (b) TcO_4^- (c) 29 days	-0.6 ± 0.1	7.7	(Same)	(Same)
		(a) $5 \times 10^{-11} \text{ M } ^{237}\text{Np}$ (b) NpO_2^+ (c) 19 days	17.7 ± 2.3	7.8		
		(a) $3 \times 10^{-11} \text{ M } ^{137}\text{Cs}$ (b) Cs^+ (c) 29 days	218 ± 5	7.7		
		(a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$ (b) Sr^{2+} (c) 29 days	28 ± 1	7.7		
		(a) $4 \times 10^{-12} \text{ M } ^{241}\text{Am}$ (b) Am^{3+} (c) 17 days	230 ± 190	7.5		

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Montmorillonite (continued)	(Same)	(a) $8 \times 10^{-5} \text{M}$ ^{129}I (b) I^- (c) 17 days	0.3 ± 2.4	7.5	(Same)	(Same)
(Same)	Eh 400 mv Na^+ 30 meq/l Cl^- 30 meq/l 20-27°C	(a) $6 \times 10^{-11} \text{M}$ ^{95m}Tc (b) TcO_4^- (c) 29 days	-0.6 ± 0.4	8.7	(Same)	(Same)
		(a) $2 \times 10^{-7} \text{M}$ ^{237}Np (b) NpO_2^+ (c) 19 days	46 ± 5	8.5		
		(a) $3 \times 10^{-11} \text{M}$ ^{137}Cs (b) Cs^+ (c) 29 days	1020 ± 80	8.7		
		(a) $2 \times 10^{-11} \text{M}$ ^{85}Sr (b) Sr^{2+} (c) 29 days	1070 ± 90	8.7		
		(a) $8 \times 10^{-10} \text{M}$ ^{241}Am (b) Am^{3+} (c) 17 days	2190 ± 100	8.3		
		(a) $8 \times 10^{-5} \text{M}$ ^{129}I (b) I^- (c) 17 days	1.7 ± 1.7	8.3		
(Same)	Eh 390 mv Na^+ 30 meq/l HCO_3^- 30 meq/l 20-27°C	(a) $6 \times 10^{-11} \text{M}$ ^{95m}Tc (b) TcO_4^- (c) 29 days	-1.5 ± 0.3	9.3	(Same)	(Same)

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Montmorillonite (continued)	(Same)	(a) $5 \times 10^{-7} \text{ M } ^{237}\text{Np}$ (b) NpO_2^+ (c) 19 days	9.1 ± 1.3	9.2	(Same)	(Same)
		(a) $3 \times 10^{-11} \text{ M } ^{137}\text{Cs}$ (b) Cs^+ (c) 29 days	1560 ± 370	9.3		
		(a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$ (b) Sr^{2+} (c) 29 days	1353 ± 330	9.3		
		(a) $1.6 \times 10^{-9} \text{ M } ^{241}\text{Am}$ (b) Am^{3+} (c) 17 days	$11,150 \pm 1920$	9.3		
		(a) $8 \times 10^{-5} \text{ M } ^{129}\text{I}$ (b) I^- (c) 17 days	-2.2 ± 1.8	9.3		
(Same)	Eh 1140 mv CaCl_2 30 meq/l 20-27°C	(a) $1.7 \times 10^{-6} \text{ M } ^{239}\text{Pu}$ (b) PuO_2^{2+} (c) 7 days	23.7	4.0	a. Batch, Eh maintained with colometric cell (Blank corrected) b. 1.0 g to 30 ml	Appendix 3.3.D
Vermiculite No significant crystalline impurities $\text{CaCO}_3 = 0\%$ $\text{OM} = 0\%$ CEC = 77 ± 5 meq/100 g AEC = ? SA = $312 \pm 8 \text{ m}^2/\text{g}$	Eh 365 mv Na^+ 5130 meq/l Cl^- 5130 meq/l 20-27°C	(a) $6 \times 10^{-11} \text{ M } ^{95\text{m}}\text{Tc}$ (b) TcO_4^- (c) 29 days	0.6 ± 0.7	8.6	a. Batch (3 cold washes) (Blank corrected) b. 0.5 g in 15 ml c. Kd avg of 3 values	Appendix 3.3.C
		(a) $2 \times 10^{-7} \text{ M } ^{237}\text{Np}$ (b) NpO_2^+ (c) 19 days	61 ± 14	7.9		

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Vermiculite (continued)	(Same)	(a) $3 \times 10^{-11} \text{ M } ^{137}\text{Cs}$ (b) Cs^+ (c) 29 days (a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$ (b) Sr^{2+} (c) 29 days (a) $8 \times 10^{-12} \text{ M } ^{241}\text{Am}$ (b) Am^{3+} (c) 17 days (a) $8 \times 10^{-5} \text{ M } ^{129}\text{I}$ (b) I^- (c) 17 days	 93 $\pm$ 9 1.9 $\pm$ 1.1 203 $\pm$ 83 5.1 $\pm$ 1.0	 8.6 8.6 8.2 8.2	(Same)	(Same)
(Same)	Eh 430 mv Ca^{++} 30 meq/l Cl^- 30 meq/l 20-27°C	(a) $6 \times 10^{-11} \text{ M } ^{95m}\text{Tc}$ (b) TcO_4^- (c) 29 days (a) $5 \times 10^{-7} \text{ M } ^{237}\text{Np}$ (b) NpO_2^+ (c) 19 days (a) $3 \times 10^{-11} \text{ M } ^{137}\text{Cs}$ (b) Cs^+ (c) 29 days (a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$ (b) Sr^{2+} (c) 29 days (a) $4 \times 10^{-12} \text{ M } ^{241}\text{Am}$ (b) Am^{3+} (c) 17 days	 -0.8 $\pm$ 0.3 27.7 $\pm$ 0.6 8.0 7.8 24 $\pm$ 1 440 $\pm$ 290	 8.0 7.8 7.8 7.4	(Same)	(Same)

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Vermiculite (continued)	(Same)	(a) $8 \times 10^{-5} \text{ M } ^{129}\text{I}$ (b) I^- (c) 17 days	0.6 ± 0.8	7.4	(Same)	(Same)
(Same)	Eh 360 mv Na^+ 30 meq/l Cl^- 30 meq/l 20-27°C	(a) $6 \times 10^{-11} \text{ M } ^{95\text{m}}\text{Tc}$ (b) TcO_4^- (c) 29 days (a) $5 \times 10^{-7} \text{ M } ^{237}\text{Np}$ (b) NpO_2^+ (c) 19 days (a) $3 \times 10^{-11} \text{ M } ^{137}\text{Cs}$ (b) Cs^+ (c) 29 days (a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$ (b) Sr^{2+} (c) 29 days (a) $8 \times 10^{-10} \text{ M } ^{241}\text{Am}$ (b) Am^{3+} (c) 17 days (a) $8 \times 10^{-5} \text{ M } ^{129}\text{I}$ (b) I^- (c) 17 days	0.4 ± 1.0 33 ± 6 $5.9 \times 10^4 \pm 7.1 \times 10^4$ 760 ± 18 2310 ± 10 1.2 ± 4.1	8.2 8.3 8.2 8.2 8.0 8.0	(Same)	(Same)
(Same)	Eh 385 mv Na^+ 30 meq/l HCO_3^- 30 meq/l 20-27°C	(a) $6 \times 10^{-11} \text{ M } ^{95\text{m}}\text{Tc}$ (b) TcO_4^- (c) 29 days (a) $5 \times 10^{-7} \text{ M } ^{237}\text{Np}$ (b) NpO_2^+ (c) 19 days	0.0 ± 0.2 16.9 ± 4.3	9.4 9.2	(Same)	(Same)

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Vermiculite (continued)	(Same)	(a) $3 \times 10^{-11} \text{ M } ^{137}\text{Cs}$ (b) Cs^+ (c) 29 days (a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$ (b) Sr^{2+} (c) 29 days (a) $1.6 \times 10^{-9} \text{ M } ^{241}\text{Am}$ (b) Am^{3+} (c) 17 days (a) $8 \times 10^{-5} \text{ M } ^{129}\text{I}$ (b) I^- (c) 17 days	$2.0 \times 10^4 \pm 1.5 \times 10^4$ 1040 ± 100 6650 ± 290 -1.3 ± 1.1	9.4 9.2 9.3 9.3	(Same)	(Same)
Quartz Reasonably pure $\text{CaCO}_3 = 0\%$ $\text{OM} = 0\%$ $\text{CEC} = 0.15 \pm 0.07 \text{ meq/100 g}$ $\text{AEC} = ?$ $\text{SA} = 2.8 \pm 0.2 \text{ m}^2/\text{g}$	Eh 420 mv $\text{Na}^+ 5130 \text{ meq/l}$ $\text{Cl}^- 5130 \text{ meq/l}$ 20-27°C	(a) $6 \times 10^{-11} \text{ M } ^{95m}\text{Tc}$ (b) TcO_4^- (c) 29 days (a) $2 \times 10^{-7} \text{ M } ^{237}\text{Np}$ (b) NpO_2^+ (c) 19 days (a) $3 \times 10^{-11} \text{ M } ^{137}\text{Cs}$ (b) Cs^+ (c) 29 days (a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$ (b) Sr^{2+} (c) 29 days (a) $8 \times 10^{-12} \text{ M } ^{241}\text{Am}$ (b) Am^{3+} (c) 17 days	1.6 ± 0.9 -0.1 ± 0.7 2.2 ± 0.8 1.1 ± 0.4 2.3 ± 5.1	6.9 6.5 6.9 6.9	(Same) a. Batch (3 cold washes) (Blank corrected) b. 0.5 g in 15 ml c. Kd avg of 3 values	(Same)

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Quartz (continued)	(Same)	(a) $8 \times 10^{-5} \text{ M } ^{129}\text{I}$ (b) I^- (c) 17 days	3.0 · 2.0	7.1	(Same)	(Same)
(Same)	Eh 450 mv Ca^{2+} 30 meq/l Cl^- 30 meq/l 20-27°C	(a) $6 \times 10^{-11} \text{ M } ^{95\text{m}}\text{Tc}$ (b) TcO_4^- (c) 29 days (a) $5 \times 10^{-7} \text{ M } ^{237}\text{Np}$ (b) NpO_2^+ (c) 19 days (a) $3 \times 10^{-11} \text{ M } ^{137}\text{Cs}$ (b) Cs^+ (a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$ (b) Sr^{2+} (c) 29 days (a) $4 \times 10^{-12} \text{ M } ^{241}\text{Am}$ (b) Am^{3+} (c) 17 days (a) $8 \times 10^{-5} \text{ M } ^{129}\text{I}$ (b) I^- (c) 17 days	0.7 · 1.0 3.6 · 2.3 34 · 14 -0.1 · 1.1 7.3 · 5.9 -1.8 · 1.9	7.0 6.8 7.0 7.0 6.9 6.9	(Same)	(Same)
(Same)	Eh 450 mv Na^+ 30 meq/l Cl^- 30 meq/l 20-27°C	(a) $6 \times 10^{-11} \text{ M } ^{95\text{m}}\text{Tc}$ (b) TcO_4^- (c) 29 days (a) $5 \times 10^{-7} \text{ M } ^{237}\text{Np}$ (b) NpO_2^+ (c) 19 days	1.4 · 1.5 4.1 · 1.0	7.1 7.0	(Same)	(Same)

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Quartz (continued)	(Same)	(a) $3 \times 10^{-11} \text{ M } ^{137}\text{Cs}$ (b) Cs^+ (c) 29 days	58 · 8	7.1	(Same)	(Same)
		(a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$ (b) Sr^{2+} (c) 29 days	8.8 · 1.6	7.1		
		(a) $8 \times 10^{-10} \text{ M } ^{241}\text{Am}$ (b) Am^{3+} (c) 17 days	43 · 13	7.4		
		(a) $8 \times 10^{-5} \text{ M } ^{129}\text{I}$ (b) I^- (c) 17 days	2.8 · 1.2	7.4		
(Same)	Eh 380 mv	(a) $6 \times 10^{-11} \text{ M } ^{95\text{m}}\text{Tc}$ (b) TcO_4^- (c) 29 days	-0.4 · 0.3	9.4	(Same)	(Same)
	Na^+ 30 meq/l HCO_3^- 30 meq/l	(a) $5 \times 10^{-7} \text{ M } ^{237}\text{Np}$ (b) NpO_2^+ (c) 19 days	6.6 · 4.3	9.4		
	20-27°C	(a) $3 \times 10^{-11} \text{ M } ^{137}\text{Cs}$ (b) Cs^+ (c) 29 days	37 · 5	9.4		
		(a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$ (b) Sr^{2+} (c) 29 days	348 · 70	9.4		
		(a) $1.6 \times 10^{-9} \text{ M } ^{241}\text{Am}$ (b) Am^{3+} (c) 17 days	131 · 41	9.4		

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Quartz (continued)	(Same)	(a) $8 \times 10^{-5} \text{ M } ^{129}\text{I}$ (b) I^- (c) 17 days	-1.6 - 1.4	9.4	(Same)	(Same)
Albite					(Same)	(Same)
Reasonably pure.	Eh 395 mv	(a) $6 \times 10^{-11} \text{ M } ^{95m}\text{Tc}$ (b) TcO_4^- (c) 29 days	18.0 - 3.3	7.4		
$\text{CaCO}_3 = 0\%$	$\text{Na}^+ 5130 \text{ meq/l}$					
OM = 0%	$\text{Cl}^- 5130 \text{ meq/l}$					
CEC = $1.5 \pm 0.3 \text{ meq/100 g}$		(a) $2 \times 10^{-7} \text{ M } ^{237}\text{Np}$ (b) NpO_2^+ (c) 19 days	39 - 4	7.0		
AEC = ?	20-27°C	(a) $3 \times 10^{-11} \text{ M } ^{137}\text{Cs}$ (b) Cs^+ (c) 29 days	20.4 - 2.2	7.4		
SA = $8.4 - 3.7 \text{ m}^2/\text{g}$		(a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$ (b) Sr^{2+} (c) 29 days	5.2 - 1.0	7.4		
		(a) $8 \times 10^{-12} \text{ M } ^{241}\text{Am}$ (b) Am^{3+} (c) 17 days	503 - 240	6.9		
		(a) $8 \times 10^{-5} \text{ M } ^{129}\text{I}$ (b) I^- (c) 17 days	3.7 - 1.8	6.9		
(Same)	Eh 430 mv	(a) $6 \times 10^{-11} \text{ M } ^{95m}\text{Tc}$ (b) TcO_4^- (c) 29 days	2.8 - 1.3	7.7	(Same)	(Same)
	$\text{Ca}^{2+} 30 \text{ meq/l}$					
	$\text{Cl}^- 30 \text{ meq/l}$					
	20-27°C	(a) $5 \times 10^{-7} \text{ M } ^{237}\text{Np}$ (b) NpO_2^+ (c) 19 days	7.0 - 2.5	7.7		

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Albite (continued)	(Same)	(a) $3 \times 10^{-11} \text{ M } ^{137}\text{Cs}$ (b) Cs^+ (c) 29 days	820 $\pm$ 120	7.7	(Same)	(Same)
		(a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$ (b) Sr^{2+} (c) 29 days	4.1 $\pm$ 0.4	7.7		
		(a) $4 \times 10^{-12} \text{ M } ^{241}\text{Am}$ (b) Am^{3+} (c) 17 days	173 $\pm$ 55	7.4		
		(a) $8 \times 10^{-5} \text{ M } ^{129}\text{I}$ (b) I^- (c) 17 days	11.8 $\pm$ 8.7	7.4		
(Same)	Eh 435 mv Na^+ 30 meq/l Cl^- 30 meq/l 20-27°C	(a) $6 \times 10^{-11} \text{ M } ^{95\text{m}}\text{Tc}$ (b) TcO_4^- (c) 29 days	0.7 $\pm$ 0.5	8.0	(Same)	(Same)
		(a) $5 \times 10^{-7} \text{ M } ^{237}\text{Np}$ (b) NpO_2^+ (c) 19 days	9.8 $\pm$ 2.1	7.9		
		(a) $3 \times 10^{-11} \text{ M } ^{137}\text{Cs}$ (b) Cs^+ (c) 29 days	519 $\pm$ 11	8.0		
		(a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$ (b) Sr^{2+} (c) 29 days	105 $\pm$ 2	8.0		
		(a) $8 \times 10^{-10} \text{ M } ^{241}\text{Am}$ (b) Am^{3+} (c) 17 days	1100 $\pm$ 960	7.7		

[illegible]

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Anorthite (continued)	(Same)	(a) $3 \times 10^{-11} \text{ M } ^{137}\text{Cs}$ (b) Cs^+ (c) 29 days (a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$ (b) Sr^{2+} (c) 29 days (a) $8 \times 10^{-12} \text{ M } ^{241}\text{Am}$ (b) Am^{3+} (c) 17 days (a) $8 \times 10^{-5} \text{ M } ^{129}\text{I}$ (b) I^- (c) 17 days	22.4 ± 1.2 5.0 ± 1.3 240 ± 58 3.6 ± 1.6	8.0 8.0 7.7 7.7	(Same)	(Same)
(Same)	Eh 390 mv Ca^{2+} 30 meq/l Cl^- 30 meq/l 20-27°C	(a) $6 \times 10^{-11} \text{ M } ^{95\text{m}}\text{Tc}$ (b) TcO_4^- (c) 29 days (a) $5 \times 10^{-7} \text{ M } ^{237}\text{Np}$ (b) NpO_2^+ (c) 19 days (a) $3 \times 10^{-11} \text{ M } ^{137}\text{Cs}$ (b) Cs^+ (c) 29 days (a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$ (b) Sr^{2+} (c) 29 days (a) $4 \times 10^{-12} \text{ M } ^{241}\text{Am}$ (b) Am^{3+} (c) 17 days (a) $8 \times 10^{-5} \text{ M } ^{129}\text{I}$ (b) I^- (c) 17 days	0.5 ± 0.7 6.4 ± 2.4 774 ± 48 3.0 ± 0.3 175 ± 120 0.8 ± 5.0	7.7 7.7 7.7 7.7 7.5	(Same)	(Same)

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Anorthite (continued)	Eh 420 mv	(a) $6 \times 10^{-11} \text{ M } ^{95}\text{Tc}$			(Same)	(Same)
		(b) TcO_4^-	1.8 ± 1.0	8.4		
		(c) 29 days				
	Na^+ 30 meq/l Cl^- 30 meq/l	(a) $5 \times 10^{-7} \text{ M } ^{237}\text{Np}$			8.4	
		(b) NpO_2^+	13.4 ± 2.4	8.4		
		(c) 19 days				
	20-27°C	(a) $3 \times 10^{-11} \text{ M } ^{137}\text{Cs}$			8.4	
		(b) Cs^+	440 ± 35	8.4		
		(c) 29 days				
		(a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$			8.4	
		(b) Sr^{2+}	51 ± 4	8.4		
		(c) 29 days				
		(a) $8 \times 10^{-10} \text{ M } ^{241}\text{Am}$			8.1	
		(b) Am^{3+}	304 ± 101	8.1		
		(c) 17 days				
		(a) $8 \times 10^{-5} \text{ M } ^{129}\text{I}$			8.1	
		(b) I^-	0.6 ± 0.7	8.1		
		(c) 17 days				
(Same)	Eh 395 mv	(a) $6 \times 10^{-11} \text{ M } ^{95}\text{Tc}$			(Same)	(Same)
		(b) TcO_4^-	0.0 ± 0.1	9.3		
		(c) 29 days				
	Na^+ 30 meq/l HCO_3^- 30 meq/l	(a) $5 \times 10^{-7} \text{ M } ^{237}\text{Np}$			9.3	
		(b) NpO_2^+	15.7 ± 4.5	9.3		
		(c) 19 days				
	20-27°C	(a) $3 \times 10^{-11} \text{ M } ^{137}\text{Cs}$			9.3	
		(b) Cs^+	608 ± 36	9.3		
		(c) 29 days				

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Anorthite (continued)	(Same)	(a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$ (b) Sr^{2+} (c) 29 days	459 $\pm$ 58	9.3	(Same)	(Same)
		(a) $1.6 \times 10^{-9} \text{ M } ^{241}\text{Am}$ (b) Am^{3+} (c) 17 days	3750 $\pm$ 1990	9.4		
		(a) $8 \times 10^{-5} \text{ M } ^{129}\text{I}$ (b) I^- (c) 17 days	0.8 $\pm$ 3.6	9.4		
Microcline	Eh 425 mv	(a) $6 \times 10^{-11} \text{ M } ^{95\text{m}}\text{Tc}$ (b) TcO_4^- (c) 29 days	15.5 $\pm$ 4.0	7.2	(Same)	(Same)
Reasonably pure.	Na^+ 5130 meq/l					
CaCO_3 = 0%	Cl^- 5130 meq/l					
OM = 0%	20-27°C					
CEC = 1.2 ± 0.2 meq/100 g		(a) $2 \times 10^{-7} \text{ M } ^{237}\text{Np}$ (b) NpO_2^+ (c) 19 days	43 $\pm$ 19	6.6		
AEC = ?		(a) $3 \times 10^{-11} \text{ M } ^{137}\text{Cs}$ (b) Cs^+ (c) 29 days	7.5 $\pm$ 1.8	7.2		
SA = $5.1 \pm 1.0 \text{ m}^2/\text{g}$		(a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$ (b) Sr^{2+} (c) 29 days	4.1 $\pm$ 1.1	7.2		
		(a) $8 \times 10^{-12} \text{ M } ^{241}\text{Am}$ (b) Am^{3+} (c) 17 days	640 $\pm$ 480	6.9		
		(a) $8 \times 10^{-5} \text{ M } ^{129}\text{I}$ (b) I^- (c) 17 days	7.0 $\pm$ 6.1	6.9		

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Microcline (continued)	(Same)	(a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$ (b) Sr^{2+} (c) 29 days	159 $\pm$ 7	7.8	(Same)	(Same)
		(a) $8 \times 10^{-10} \text{ M } ^{241}\text{Am}$ (b) Am^{3+} (c) 17 days	1450 $\pm$ 610	7.6		
		(a) $8 \times 10^{-5} \text{ M } ^{129}\text{I}$ (b) I^- (c) 17 days	2.9 $\pm$ 1.3	7.6		
(Same)	Eh 385 mv	(a) $6 \times 10^{-11} \text{ M } ^{95\text{m}}\text{Tc}$ (b) TcO_4^- (c) 29 days	0.6 $\pm$ 0.1	9.4	(Same)	(Same)
	Na^+ 30 meq/l HCO_3^- 30 meq/l	(a) $5 \times 10^{-7} \text{ M } ^{237}\text{Np}$ (b) NpO_2^+ (c) 19 days	8.0 $\pm$ 1.6	9.3		
	20-27°C	(a) $3 \times 10^{-11} \text{ M } ^{137}\text{Cs}$ (b) Cs^+ (c) 29 days	343 $\pm$ 21	9.4		
		(a) $2 \times 10^{-11} \text{ M } ^{85}\text{Sr}$ (b) Sr^{2+} (c) 29 days	461 $\pm$ 26	9.4		
		(a) $1.6 \times 10^{-9} \text{ M } ^{241}\text{Am}$ (b) Am^{3+} (c) 17 days	971 $\pm$ 95	9.4		
		(a) $8 \times 10^{-5} \text{ M } ^{129}\text{I}$ (b) I^- (c) 17 days	-1.6 $\pm$ 0.2	9.4		

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Microcline (continued)	Eh 450 mv Ca ²⁺ 30 meq/l Cl ⁻ 30 meq/l 20-27°C	(a) 6×10^{-11} M ^{95m} Tc	0.1 ± 0.4	7.6	(Same)	(Same)
		(b) TcO ₄ ⁻				
		(c) 29 days				
		(a) 5×10^{-7} M ²³⁷ Np	10.1 ± 2.5	7.6		
		(b) NpO ₂ ⁺				
		(c) 19 days				
		(a) 3×10^{-11} M ¹³⁷ Cs	222 ± 76	7.6		
		(b) Cs ⁺				
		(c) 29 days				
		(a) 2×10^{-11} M ⁸⁵ Sr	3.6 ± 0.9	7.6		
		(b) Sr ²⁺				
		(c) 29 days				
		(a) 4×10^{-12} M ²⁴¹ Am	173 ± 34	7.4	a. Batch (3 cold washes) (Blank corrected) b. 0.5 g in 15 ml c. Kd avg of 3 values	
		(b) Am ³⁺				
		(c) 17 days				
		(a) 8×10^{-5} M ¹²⁹ I	0.7 ± 3.5	7.4		
		(b) I ⁻				
		(c) 17 days				
(Same)	Eh 435 mv Na ⁺ 30 meq/l Cl ⁻ 30 meq/l 20-27°C	(a) 6×10^{-11} M ^{95m} Tc	5.8 ± 1.2	7.8	(Same)	(Same)
		(b) TcO ₄ ⁻				
		(c) 29 days				
		(a) 5×10^{-7} M ²³⁷ Np	68 ± 51	7.9		
		(b) NpO ₂ ⁺				
		(c) 19 days				
		(a) 3×10^{-11} M ¹³⁷ Cs	391 ± 18	7.8		
		(b) Cs ⁺				
		(c) 29 days				

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Magnetite	(Same)	(a) 750 $\mu\text{Ci}/\ell$ ^{90}Sr	$K_{d_{\text{Sr}}}$ 5.46 $\pm$ 0.45	7.92	(Same)	(Same)
Biotite		(b) Sr^+				
Titanite		(c) 2 days				
Apatite						
CaCO_3 zero or low		(a) 70 $\mu\text{Ci}/\ell$ ^{106}Ru	$K_{d_{\text{Ru}}}$ 210 $\pm$ 15	7.97		
OX = ?		(b) Ru^{+3}				
OM = ?		(c) 2 days				
CEC = ?						
AEC = ?		(a) 6.5 $\mu\text{Ci}/\ell$ ^{241}Am	$K_{d_{\text{Am}}}$ 60,436 $\pm$ 28,875	8.16		
SA = 0.9 m^2/g (B.E.T.)		(b) Am^{+3}				
		(c) 2 days				
		(a) 730 $\mu\text{Ci}/\ell$ Pu	$K_{d_{\text{Pu}}}$ 5,398 $\pm$ 1,123	8.15		
		(b) ?				
		(c) 2 days				
Argillite (Eleana, Nevada Test Site, VE17e 2200') crushed		(a) 52 $\mu\text{Ci}/\ell$ ^{137}Cs	$K_{d_{\text{Cs}}}$ 986 $\pm$ 114	8.69	(Same)	(Same)
Minerals identified	Eh = Oxidizing	(b) Cs^+				
Quartz	$\text{Na}^+ = 1.61 \text{ meq}/\ell$	(c) 2 days				
Clay (Chlorite)	$\text{Ca}^{+2} = 2.24 \text{ meq}/\ell$					
Orthoclase	$\text{Mg}^{+2} = 1.80 \text{ meq}/\ell$					
Calcite	$\text{HCO}_3^- = 1.61 \text{ meq}/\ell$					
TiO_2	$\text{CO}_3^{+2} = 4.04 \text{ meq}/\ell$					
CaCO_3 present	Room Temperature					
OX = ?						
OM = ?		(a) 750 $\mu\text{Ci}/\ell$ ^{90}Sr	$K_{d_{\text{Sr}}}$ 191 $\pm$ 44	8.74		
CEC = ?		(b) Sr^{+2}				
AEC = ?		(c) 2 days				
SA = 5.4 m^2/g (B.E.T.)						

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
(Same)	(Same)	(a) 70 $\mu\text{Ci}/\ell$ ^{106}Ru (b) Ru^{+3} (c) 2 days	$K_{d_{\text{Ru}}} 1,991 \pm 375$	8.62	(Same)	(Same)
		(a) 6.5 $\mu\text{Ci}/\ell$ ^{241}Am (b) Am^{+3} (c) 2 days	$K_{d_{\text{Am}}} 2,637 \pm 1,345$	8.72		
		(a) 730 $\mu\text{Ci}/\ell$ Pu (b) ? (c) 2 days	$K_{d_{\text{Pu}}} 318 \pm 49$	8.69		
Rocksalt (Carlsbad, New Mexico ERDA Drill Hole #9 2621')	pH = 7.41 Eh = oxidizing $\text{Na}^{+} = 5000 \text{ meq}/\ell$ $\text{Ca}^{+2} = 44.9 \text{ meq}/\ell$ $\text{K}^{+} = 0.47 \text{ meq}/\ell$	(a) 52 $\mu\text{Ci}/\ell$ $^{137}\text{Cs} + 0.1 \text{ mN}$ (b) Cs^{+} (c) 2 days	$K_{d_{\text{Cs}}} 0.07 \pm 0.09$	7.41	(Same)	(Same)
>99% Soluble Salt						
Minerals						
Decreasing Content						
Halite	$\text{Mg}^{+2} = 0.84 \text{ meq}/\ell$					
Gypsum	$\text{Fe}^{+3} = 0.11 \text{ meq}/\ell$					
Epsomite	$\text{Sr}^{+2} = 0.34 \text{ meq}/\ell$					
Clay	$\text{Rb}^{+} = 0.01 \text{ meq}/\ell$					
$\text{CaCO}_3 = \text{low}$	$\text{Cs}^{+} = 0.01 \text{ meq}/\ell$					
OX = ?	$\text{Cl}^{-} = 4957 \text{ meq}/\ell$					
OM = ?	$\text{SO}_4^{-2} = 84.5 \text{ meq}/\ell$					
CEC = ?	$\text{HCO}_3^{-} = 0.2 \text{ meq}/\ell$					
AEC = ?	$\text{Br}^{-} = 5.05 \text{ meq}/\ell$					

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
SA = ?	I ⁻ = 0.8 meq/l BO ₃ ⁻ = 0.08 meq/l Room temperature	(a) 750 μ Ci/l ⁹⁰ Sr + .34 mM (b) Sr ⁺² (c) 2 days (a) 70 μ Ci/l ¹⁰⁶ Ru (b) Ru ⁺³ (c) 2 days (a) 6.5 μ Ci/l ²⁴¹ Am (b) Am ⁺³ (c) 2 days (a) 730 μ Ci/l Pu (b) ? (c) 2 days	Kd _{Sr} 0.13 $\pm$ 0.15 Kd _{Ru} 3.55 $\pm$ 0.30 Kd _{Am} 2,265 $\pm$ 285 Kd _{Pu} 1,228 $\pm$ 627	7.39 7.49 7.37 7.34	(Same)	(Same)
Montmorillonite (University of Missouri and API)		(a) $\sim 10^{-3}$ M Cs (b) Cs ⁺ (c) ?	Kd _{Cs} at .6M Na ⁺ 20-65 at 1.1M Na ⁺ 11-35 at 2.1M Na ⁺ 7.5-20 at 4.1M Na ⁺ 3.5-10		a. Batch (no cold washes) (no blanks) b. Solution/Solid Ratio Variable	Appendix 3.3.I
CaCO ₃ = removed OX = ? OM = removed CEC = ? AEC = ? SA = ?	pH = 8 NaCl = 0.5 - 4.0M NaHCO ₃ = .1M Room temperature					
Montmorillonite (University of Missouri)	EH = air equilibrated NaCl 0.5 to 4.0M NaHCO ₃ .1M Room temperature	(a) $\sim 10^{-3}$ M Cs (b) Cs ⁺ (c) ?	Kd _{Cs} at 6M Na ⁺ 15 1.1M Na ⁺ 10 2.1M Na ⁺ 7.5 4.1M Na ⁺ 3.7	8.0	(Same)	(Same)
CaCO ₃ = removed OX = removed OM = removed CEC = ? AEC = ? SA = ? (Same)	EH = air equilibrated NaCl 0.5 to 4.0M Na Acetate 0.1M Room Temperature	(a) $\sim 10^{-3}$ M Cs (b) Cs (c) ?	Kd _{Cs} .6M Na ⁺ 13 1.1M Na ⁺ 9.5 2.1M Na ⁺ 7 4.1M Na ⁺ 4	5.0	(Same)	(Same)

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
(Same)	Air equilibrated NaCl 0.2 to 5.5M Room Temperature	(a) 5×10^{-4} M Sr (b) Sr^{+2} (c) 5 days	$K_{d\text{Sr}} = 111 \pm 4$ at Na = 0.2M $K_{d\text{Sr}} = 33 \pm 4$ at Na = 0.6M $K_{d\text{Sr}} = 8.7 \pm 0$ at Na = 2.1M $K_{d\text{Sr}} = 3.5 \pm 0$ at Na = 5.5M	7.6	Batch (cold b. 7.5 to 75 ml/g c. average of 2	(Same)
(Same)	Air equilibrated NaCl 0.1 to 4.6M Na acetate 0.1M Room Temperature	(a) 5×10^{-4} M Sr (b) Sr^{+2} (c) 5 day	$K_{d\text{Sr}} = 52.9 \pm 0$ at Na = 0.2M $K_{d\text{Sr}} = 29.4 \pm 1.3$ at Na = 0.6M $K_{d\text{Sr}} = 12.6 \pm 0.6$ at Na = 2.1M $K_{d\text{Sr}} = 1.3 \pm 0$ at Na = 4.7	5.0	(Same)	(Same)
(Same) Muscatine Silt Loam Soil Minerals - available	(a) 1.0 to .1 μCi spot Eh = air equilibrated	(b)	$K_{d\text{Sr}} = 3$ when eluting solution 100 meq/l Ca^{+2} $K_{d\text{Sr}} = >15$ when eluting solution 10 meq/l Ca^{+2}	?	Channel Chromatography V_{water} variable bulk density 1.21 g/cm ³ porosity 0.545	Appendix 3.3.J
CaCO_3 = available OX = ? OM = available CEC = available AEC = ?	Ca^{+2} 1 to 100 meq/l (initial) Cl^- 1 to 100 meq/l (initial) Room temperature	Sr^{+2} Ni^{+2} I^- TcO_4^-	$K_{d\text{Ni}} = >15$ when eluting			

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
SA = ?		(b) <1 day	100 meq/l Ca ⁺² Kd _{Ni} = >15 when eluting solution 10 meq/l Ca ⁺² Kd _I = 0 at all Ca eluting solution concentrations Kd _{Tc} = 0.1 when eluting solution 100 meq/l Ca ⁺² Kd _{Tc} = 0.1 when eluting solution 10 meq/l Ca ⁺² Kd _{Sr} = 0.28 (Ca) ^{-0.87}	?		
		(a) <10 ⁻⁶ M			a. Batch (soil Ca saturated no blanks)	(Same)
	Eh = air equilibrated Ca ⁺² = 10 ⁻¹ - 10 ⁻³ meq/l Cl ⁻ = 10 ⁻¹ - 10 ⁺³ meq/l Room temperature	(b) Sr ⁺² Ni ⁺² (c) 16-24 hours	Kd _{Ni} = 3.39 (Ca) ^{-0.90} where (Ca) is equilibrium concentration in meq/ml		b. 20 ml/g c. Spike added directly to slurry	
Fuquay Sand Soil		(a) .01 to .1 μ Ci spot	Kd _{Sr} = 0.5 when eluting solution 100 meq/l Ca ⁺²	?	Channel Chromatography	(Same)
Minerals = available CaCO ₃ = available	Eh = air equilibrated Ca ⁺² 10 to 100 meq/l (initial)	(b) Sr ⁺² Ni ⁽²⁾	Kd _{Sr} = 1.5 when eluting solution 10 meq/l Ca ⁺²		v _{water} variable	
OX = ? OM = available	Cl ⁻ 10 to 100 meq/l (initial) Room temperature	I ⁻ TcO ₄	Kd _{Ni} = 0.8 when eluting solution 100 meq/l Ca ⁺²		bulk density = 1.38 g/cm ³ porosity = 0.479	
CEC = Capacity available AEC = ?		(c) <1 day	Kd _{Ni} = 54 when eluting solution 10 meq/l Ca ⁺²			

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
SA = ?		$Kd_I = 0.02$ when eluting solution 100 meq/l Ca^{+2} $Kd_I = 0.0$ when eluting solution 10 meq/l Ca^{+2} $Kd_{TC} = .11$ when eluting solution 100 meq/l Ca^{+2} $Kd_{TC} = 0.02$ when eluting solution 10 meq/l Ca^{+2}				
Limestone (Salem Formation) tablets N(1x1x.25 cm)	Eh = air equilibrated water equilibrated with crushed limestone Room Temperature	(a) $8 \times 10^{-13} M$ $^{237}Pu + ^{239}Pu$ $5.8 \times 10^{-9} M$ ^{241}Am (b) Pu^{+4} Am^{+3} (c) ~500 hours	$Kd_{Pu} 62 \pm 76 t_{reaction}$ 74 ± 10^9 hours $Kd_{Am} 59 \pm 87 t_{reaction}$ 78 ± 70 hours	8.3	a. Batch (0 cold wash) (blank corrected) b. 4 to 6 ml/l g	Appendix 3.3.B
Granite (Winnsboro N.C.) Chicago Field Museum # Li-6152 tablets ~ (1x1x.25 cm)	Eh = air equilibrated water equilibrated with crushed granite Room temperature	(a) $8 \times 10^{-13} M$ $^{237}Pu + ^{239}Pu$ $5.8 \times 10^{-9} M$ ^{241}Am (b) Pu^{+4} Am^{+3} (c) ~500 hours	$Kd_{Pu} 37 \pm 6 t_{reaction}$ 45 ± 18 hours $Kd_{Am} 10 \pm 7 t_{reaction}$ 155 ± 7 hours	?	a. Batch (0 cold wash) (blank corrected) b. 2 to 3 ml/l g	
Basalt (Columbia River) tablets (.7x.7x.2 cm)	Eh = air equilibrated water equilibrated with crushed basalt Room Temperature	(a) $8 \times 10^{-13} M$ $^{237}Pu + ^{239}Pu$ $5.8 \times 10^{-9} M$ ^{241}Am (b) Pu^{+4} Am^{+3} (c) ~500 hours	$Kd_{Pu} 148 \pm 71 t_{reaction}$ 78 ± 20 hours $Kd_{Am} 245 \pm 97 t_{reaction}$ 167 ± 115 hours	7.4	a. Batch (cold wash) (blank corrected) b. 20 to 30 ml/g	
Tuff (Paint Brush Formation) Nevada Test Site Tunnel Bed N-10 tablets (.8x.9x.3 cm)	Eh = air equilibrated water equilibrated with crushed tuff Room temperature	(a) $8 \times 10^{-13} M$ $^{237}Pu + ^{239}Pu$ $5.8 \times 10^{-9} M$ ^{241}Am (b) Pu^{+4} Am^{+3} (c) ~500 hours	$Kd_{Pu} 24 \pm 21 t_{reaction}$ 240 ± 85 hours $Kd_{Am} 144 \pm 198 t_{reaction}$ 5 ± 0 hour	6.4	a. Batch (0 cold wash) (blank corrected) b. 7 to 10 ml/g	

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Low Temperature Metamorphic (Greenstone?)		(a) $8 \times 10^{-13} \text{ M } ^{237}\text{Pu} + ^{239}\text{Pu}$	$K_{d_{\text{Pu}}} 81 \pm 57 \text{ t}_{\text{reaction}}$ $550 \pm 87 \text{ hours}$	?	a. Batch (0 cold wash)	
Chicago Field Museum #Li-7509 tablets (.7x.8x.1 cm)	water equilibrated with crushed rock	$5.8 \times 10^{-9} \text{ M } ^{241}\text{Am}$ Am^{+3}	$K_{d_{\text{Am}}} 0.9 \pm 1.5 \text{ no reaction}$		(blank corrected) b. 15 to 20 ml/g	
tablets (.7x.8x.1 cm)	crushed rock Room temperature	(b) Pu^{+4} Am^{+3}				
		(c) 500 hours				
Dolomite - Salado, New Mexico Formation (Magenta - WIPP Site)	Eh = air equilibrated	(a) $8 \times 10^{-13} \text{ M } ^{237}\text{Pu} + ^{239}\text{Pu}$	$K_{d_{\text{Pu}}} 17 \pm 21 \text{ t}_{\text{reaction}}$ $21 \pm 25 \text{ hours}$	8.2	a. Batch (0 cold wash)	(Same)
tablets (.8x1.2x.25 cm)	water equilibrated with crushed Magenta	$5.8 \times 10^{-9} \text{ M } ^{241}\text{Am}$ Pu^{+4} Am^{+3}	$K_{d_{\text{Am}}} 20 \pm 24 \text{ t}_{\text{reaction}}$ $380 \pm 325 \text{ hours}$		(blank corrected) b. 4 to 6 ml/g	
	Room temperature	(c) ~500 hours				
Marble - Georgia White		(a) $8 \times 10^{-13} \text{ M } ^{237}\text{Pu} + ^{239}\text{Pu}$	$K_{d_{\text{Pu}}} 103 \pm 68 \text{ t}_{\text{reaction}}$ $6 \pm 2 \text{ hours}$	8.3	a. Batch (0 cold wash)	
Chicago Field Museum #Li ? tablets (.7x1.1x.25 cm)	Eh = air equilibrated water equilibrated with crushed marble Room temperature	(b) Pu^{+4} Am^{+3}	$K_{d_{\text{Am}}} 181 \pm 34 \text{ t}_{\text{reaction}}$ $5 \pm 0 \text{ hours}$		(blank corrected) b. 4 to 6 ml/g	
		(c) ~500 hours				
Oolitic Limestone		(a) $8 \times 10^{-13} \text{ M } ^{237}\text{Pu} + ^{239}\text{Pu}$	$K_{d_{\text{Pu}}} 487 \pm 254 \text{ t}_{\text{reaction}}$ $5 \pm 0 \text{ hours}$	8.3	a. Batch (0 cold wash)	
Bedford, Indiana	Eh = air equilibrated	(b) Pu^{+4} Am^{+3}	$K_{d_{\text{Am}}} 542 \pm 139 \text{ t}_{\text{reaction}}$ $< 5 \text{ hours}$		(blank corrected) b. 8 to 12 ml/g	
Chicago Field Museum #Li-2624 tablets (.7x1.2x.3 cm)	water equilibrated with crushed limestone Room Temperature	(c) ~500 hours				
		(a) $8 \times 10^{-13} \text{ M } ^{237}\text{Pu} + ^{239}\text{Pu}$	$K_{d_{\text{Pu}}} 11.5 \pm 7.4 \text{ t}_{\text{reaction}}$ $50 \pm 3 \text{ hours}$	8.0	a. Batch (0 cold wash)	
Sandstone		(b) Pu^{+4} Am^{+3}	$K_{d_{\text{Am}}} 10.3 \pm 2.2 \text{ t}_{\text{reaction}}$ $18 \pm 6 \text{ hours}$		(blank corrected) b. 5 to 8 ml/g	
Ohio Barrier Sandstone	Eh = air equilibrated	(c) ~500 hours				
Chicago Field Museum #Li ? tablets (.9x1.1x.2 cm)	water equilibrated with crushed sandstone Room temperature					

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Soapstone Chicago Field Museum #Li-3545 tablets (.7x.8x.2 cm)	Eh = air equilibrated water equilibrated with crushed soapstone Room temperature	(a) $8 \times 10^{-13} \text{ M } ^{237}\text{Pu} + ^{239}\text{Pu}$ $5.8 \times 10^{-9} \text{ M } ^{241}\text{Am}$ (b) Pu^{+4} Am^{+3} (c) ~500 hours	$\text{Kd}_{\text{Pu}} 19.8 \pm 10.2 \text{ t}_{\text{reaction}}$ $17 \pm 3 \text{ hours}$ $\text{Kd}_{\text{Am}} 65 \pm 41 \text{ t}_{\text{reaction}}$ $17 \pm 8 \text{ hours}$	8.2	a. Batch (0 cold wash) (blank corrected) b. 7 to 10 ml/g	(Same)
Dolomite (Salado Formation) Culebra WIPP Sample tablets (.8x.8x.2 cm)	Eh = air equilibrated water equilibrated with crushed Culebra Room temperature	(a) $8 \times 10^{-13} \text{ M } ^{237}\text{Pu} + ^{239}\text{Pu}$ $5.8 \times 10^{-9} \text{ M } ^{241}\text{Am}$ (b) Pu^{+4} Am^{+3} (c) ~500 hours	$\text{Kd}_{\text{Pu}} 18.3 \pm 2.1 \text{ t}_{\text{reaction}}$ $< 5 \text{ hours}$ $\text{Kd}_{\text{Am}} 67 \pm 15 \text{ t}_{\text{reaction}}$ $< 5 \text{ hours}$	8.2	a. Batch (0 cold washes) (blank corrected) b. 7 to 10 ml/g	
Gneiss Chicago Field Museum #Li-3896 tablets (.6x1.0x.2 cm)	Eh = air equilibrated water equilibrated with crushed Gneiss Room temperature	(a) $8 \times 10^{-13} \text{ M } ^{237}\text{Pu} + ^{239}\text{Pu}$ $5.8 \times 10^{-9} \text{ M } ^{241}\text{Am}$ (b) Pu^{+4} Am^{+3} (c) ~500 hours	$\text{Kd}_{\text{Pu}} 14.3 \pm 3.8 \text{ t}_{\text{reaction}}$ $108 \pm 38 \text{ hours}$ $\text{Kd}_{\text{Am}} 10 \pm 7 \text{ t}_{\text{reaction}}$ $> 600 \text{ hours}$	8.1	a. Batch (0 cold washes) (blank corrected) b. 7 to 10 ml/g	
Dolomite (Nevada Test Site) Core 2850' Area 7, Hole 47 ae tablets (.7x1x.25 cm)	Eh = air equilibrated water equilibrated with crushed dolomite Room temperature	(a) $8 \times 10^{-13} \text{ M } ^{237}\text{Pu} + ^{239}\text{Pu}$ $5.8 \times 10^{-9} \text{ M } ^{241}\text{Am}$ (b) Pu^{+4} Am^{+3} (c) ~500 hours	$\text{Kd}_{\text{Pu}} 17 \pm 16 \text{ t}_{\text{reaction}}$ $< 5 \text{ hours}$ $\text{Kd}_{\text{Am}} 62 \pm 77 \text{ t}_{\text{reaction}}$ $< 5 \text{ hours}$	9.3	a. Batch (0 cold washes) (blank corrected) b. 5 to 8 ml/g	
Chalcopyrite (Fe,Cu sulfide) Chicago Field Museum #E-19201 tablets (.5x.7x.3 cm)	Eh = air equilibrated water equilibrated with crushed chalcopyrite Room temperature	(a) $8 \times 10^{-13} \text{ M } ^{237}\text{Pu} + ^{239}\text{Pu}$ $5.8 \times 10^{-9} \text{ M } ^{241}\text{Am}$ (b) Pu^{+4} Am^{+3} (c) ~500 hours	$\text{Kd}_{\text{Pu}} 11 \pm 12 \text{ t}_{\text{reaction}}$ $150 \pm 50 \text{ hours}$ $\text{Kd}_{\text{Am}} 0.5 \pm 0.2 \text{ no reaction}$	5.4	a. Batch (0 cold washes) (blank corrected) b. 5 to 8 ml/g	

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Galena		(a) $8 \times 10^{-13} \text{ M } ^{237}\text{Pu} + ^{239}\text{Pu}$	$\text{Kd}_{\text{Pu}} 3.9$		a. Batch	(Same)
Last Chance Mine, Idaho	Eh = air equilibrated	$5.8 \times 10^{-9} \text{ M } ^{241}\text{Am}$	$\text{Kd}_{\text{Am}} 0.1$		(0 cold washes)	
Chicago Field Museum #E-13415	water equilibrated with	(b) Pu^{+4}			(blank corrected)	
tablets (.7x5x.8 cm)	crushed Galena	Am^{+3}			b. 1.5 to 2 ml/g	
	Room temperature	~500 hours				
Basalt		(a) Pu ?	$\text{Kd}_{\text{Pu}} 88 \pm 27$	7.4	a. Batch	
Columbia River	Eh = air equilibrated		(16-20 mesh size)		(no washes)	
Crushed materials	water equilibrated with	Am ?	adsorption $\text{Kd}_{\text{Am}} 83 \pm 11$		(not corrected)	
	crushed Basalt	(b) Pu^{+4}	B.E.T. Surface Area		b. 4-30 ml/g	
	24°C	Am^{+3}	$= 8.7 \text{ m}^2/\text{g}$			
		(c) 488 hours	desorption $\text{Kd}_{\text{Am}} 176 \pm 643$			
			$\text{Kd}_{\text{Pu}} 117 \pm 38$			
			(30 to 40 mesh size)			
			adsorption $\text{Kd}_{\text{Am}} 134 \pm 23$			
			B.E.T. Surface Area			
			$= 7.3 \text{ m}^2/\text{g}$			
			desorption $\text{Kd}_{\text{Am}} 249 \pm 86$			
			$\text{Kd}_{\text{Pu}} 126 \pm 31$			
			(50-70 mesh size)			
			Adsorption $\text{Kd}_{\text{Am}} 176 \pm 56$			
			B.E.T. Surface Area			
			$= 7.7 \text{ m}^2/\text{g}$			
			desorption $\text{Kd}_{\text{Am}} 284 \pm 60$			
Anhydrite		(a) ?		8.3	a. Batch	
Crushed	Eh = air equilibrated	(b) Pu^{+4}	$\text{Kd}_{\text{Pu}} 748 \pm 100$ (16-20 mesh)		(no washes)	
	water equilibrated with		surface area B.E.T.		(not corrected)	
	crushed anhydrite		$10.1 \text{ m}^2/\text{g}$		b. 12 ml/g	
	24°C		$\text{Kd}_{\text{Pu}} 994 \pm 69$ (30-40 mesh)			
			Surface Area B.E.T.			
			$7.5 \text{ m}^2/\text{g}$			
		(c) 819 hours	$\text{Kd}_{\text{Pu}} 2200 \pm 914$			
			(50-70 mesh)			
			Surface Area B.E.T. $8.9 \text{ m}^2/\text{g}$			

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Apatite Crushed	Eh = air equilibrated water equilibrated with crushed apatite 50°C	(a) ? (b) Pu ⁺⁴ Am ⁺³ Np ⁺⁵ (c) 24 hours	Kd _{Pu} 713 60-100 mesh Kd _{Am} 9353 Kd _{Np} 1284	?	a. Batch (0 cold washes) (not blank corrected) b. 5 ml/g	ANL unpublished
Argillite Crushed	Eh = air equilibrated water equilibrated with crushed argillite 50°C	(a) = ? (b) Pu ⁺⁴ Am ⁺³ Np ⁺⁵ (c) 24 hours	Kd _{Pu} 9 60-100 mesh Kd _{Am} 15 Kd _{Pu} 27	8.7	a. Batch (0 cold washes) (not blank corrected) b. 3 ml/g	(Same)
BaCO ₃ Crushed	Eh = air equilibrated water equilibrated with crushed BaCO ₃ 24°C	(a) = ? (b) Pu ⁺⁴ (c) 819 hours	Kd _{Pu} 2496 ± 785 (16-20 mesh) <0.1 m ² /g B.E.T. Surface Area Kd _{Pu} 2721 ± 2196 (30-40 mesh) <0.1 m ² /g B.E.T. Surface Area Kd _{Pu} 3822 ± 2610 (50-70 mesh) <0.1 m ² /g B.E.T. Surface Area	?	a. Batch (0 cold washes) (no blank corrected) b. 7.5 ml/g	(Same)
Bornite Crushed	Eh = air equilibrated water equilibrated with crushed bornite 50 °C	(a) ? (b) Pu ⁴ Am ³ Np ⁺⁵ (c) 24 hours	Kd _{Pu} 2453 (60-100 mesh) Kd _{Am} 5816 Kd _{Np} 1096	?	a. Batch (0 cold washes) (not blank corrected) b. 5 ml/g	(Same)

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Chalcopyrite (Fe,Cu sulfide) Chicago Field Museum #E-19201 Crushed	Eh = air equilibrated water equilibrated with crushed chalcopyrite 50°C	(a) ? (b) Pu ⁺⁴ Am ⁺³ Np ⁺⁵ (c) 24 hours	Kd _{Pu} 75 (60-100 mesh) Kd _{Am} 14 Kd _{Np} 27	5.4	a. Batch (0 cold washes) (not blank corrected) b. 7 ml/g	(Same)
Chalk Crushed	Eh = air equilibrated water equilibrated with crushed chalk 24°C	(a) ? (b) Pu ⁺⁴ Am ⁺³ (c) 488 hours	Kd _{Pu} 187,127 ± 191,153 (16-20 mesh) Kd _{Am} 166,233 ± 173,207 13.8 m ² /g B.E.T. Surface Area Kd _{Pu} 179,651 ± 104,910 (30-40 mesh) Kd _{Am} 338,603 ± 196,918 13.9 m ² /g B.E.T. Surface Area Kd _{Pu} 173,310 ± 217,970 (50-70 mesh) Kd _{Am} 321,625 ± 218,393 12.7 m ² /g B.E.T. Surface Area Kd _{Am} 743,185 (60-100 mesh) Kd _{Np} 752	8.5	a. Batch (0 cold washes) (not blank corrected) b. 10-15 ml/g	(Same)
	Same 50°C	(c) 24 hours				
Dolomite (Nevada Test Site) Core 2850' Area 7 Hole 47 ae Crushed	Eh = air equilibrated water equilibrated with crushed dolomite 50°C	(a) ? (b) Am ³⁺ Np ⁵⁺ (c) 24 hours	Kd _{Am} 3474 (60-100 mesh) Kd _{Np} 395	9.3	a. Batch (0 cold washes) (not blank corrected) b. 10 ml/g	(Same)
Dolomite (Quantin Quarry)	Eh = air equilibrated water equilibrated with crushed dolomite 50°C	(a) ? (b) Am ³⁺ Np ⁵⁺ (c) 24 hours	Kd _{Am} 8921 (60-100 mesh) Kd _{Np} 649	8.2	a. Batch (0 cold washes) (not blank corrected) b. 4 ml/g	(Same)

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Fe ₂ O ₃ Reagent Grade	Eh = air equilibrated water equilibrated with Fe ₂ O ₃ 50°C	(a) ? (b) Pu ⁺⁴ Am ⁺³ Np ⁺⁵	Kd _{Pu} 621 Kd _{Am} >78,016 Kd _{Np} 284	?	a. Batch (no cold washes) (not blank corrected) b. 8.5-9.5 ml/g	(Same)
Galena Last Chance Mine, Idaho Chicago Field Museum #E-19201 Crushed	Eh = air equilibrated water equilibrated with crushed galena 50°C	(a) ? (b) Pu ⁺⁴ Am ⁺³ Np ⁺⁵	Kd _{Pu} 929 (60-100 mesh) Kd _{Am} 23 Kd _{Np} 23	6.1	a. Batch (no cold washes) (not blank corrected) b. 2.7 ml/g	(Same)
Granite (Nevada Test Site) Crushed	Eh = air equilibrated water equilibrated with crushed granite 50°C	(a) ? (b) Pu ⁺⁴ Am ⁺³ Np ⁺⁵	Kd _{Pu} 2051 (60-100 mesh) Kd _{Am} 21 Kd _{Np} 21	8.5	a. Batch (no cold washes) (no blank corrected) b. 6.6-7.4 ml/g	(Same)
Limestone (Salem Formation) Crushed	Eh = air equilibrated water equilibrated with crushed limestone 50°C	(a) ? (b) Pu ⁺⁴ Am ⁺³ Np ⁺⁵	Kd _{Pu} 293 (60-100 mesh) Kd _{Am} 2231 Kd _{Np} >7544	8.3	a. Batch (no cold washes) (not blank corrected) b. 4.8-5.0 ml/g	(Same)
Marble (Georgia White) Chicago Field Museum #Li ? crushed	Eh = air equilibrated water equilibrated with crushed marble 50°C	(a) ? (b) Pu ⁺⁴ Am ⁺³ Np ⁺⁵	Kd _{Pu} 720 (60-100 mesh) Kd _{Am} 3075 Kd _{Np} 592	8.3	a. Batch (no cold washes) (not blank corrected) b. 5.5-6.8 ml/g	(Same)
Low Temperature Metamorphic (Greenstone?) Chicago Field Museum #Li-7509 Crushed	Eh = air equilibrated water equilibrated with crushed rock 50°C	(a) ? (b) Am ⁺³ Np ⁺⁵	Kd _{Am} 2573 (60-100 mesh) Kd _{Np} 40	8.7	a. Batch (no cold washes) (not blank corrected) b. 10.8 ml/g	(Same)

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Soapstone		(a) ?		8.1	a. Batch	(Same)
Chicago Field Museum #Li-3545	Eh = air equilibrated	(b) Am ⁺³	Kd _{Am} >47,183		(no cold washes)	
Crushed	water equilibrated with crushed soapstone 50°C	Np ⁺⁵	(60-100 mesh) Kd _{Np} 91		(not blank corrected)	
Tuff (Paintbrush Formation)		(a) ?			b. 6.3 ml/g	
Nevada Test Site Tunnel Bed N-10	Eh = air equilibrated	(b) Pu ⁺⁴	Kd _{Pu} 11 (60-100 mesh)	6.4	a. Batch	(Same)
crushed	water equilibrated with crushed Tuff	Am ⁺³ Np ⁺⁵	Kd _{Am} 23 Kd _{Np} 8		(no cold washes) (not blank corrected)	
Alluvium (Nevada Test Site)	RNM-2S	(a) ?	Kd _{Sr} 252 ± 46	8.3-	a. Batch	Appendix 3.3.H
Hole U5e 256M	Ca ⁺² 0.9 meq/l	(b) Sr ⁺² , Cs ⁺ , Co ⁺² , Eu ⁺³ ,	Kd _{Cs} 3700 ± 150	8.7	(pre-equilibrated	
Glass (quartz)	Mg ⁺² 0.46 meq/l	Ce ⁺³ , Sb?, Nb ⁺⁵ , I mixed	Kd _{Co} 6600 ± 4400		blank corrected	
Plagioclase	K ⁺ 0.26 meq/l	(c) 2.8 days	Kd _{Eu} >5000		spikes equilibrated	
Alkali feldspar	Na ⁺ 2.87 meq/l	(d) adsorption	Kd _{Ce} >10,000		and filtered before	
Calcite	HCO ₃ ⁻ 2.79		Kd _{Sb} 11 ± 10		rock contact	
Clinopyroxene	Cl ⁻ 0.65		Kd _{Nb} 529		b. 20-40 ml/g	
Orthopyroxene	F ⁻ 0.03		Kd _I 16.6			
CaCO ₃ = present	SO ₄ ⁻² 0.85		Kd _{Sr} 272			
OX present	Eh 400-435 mV	(a) ?	Kd _{Cs} 8090			
CEC = 10-17 meq/100 g	Room Temperature 20°C	(b) Sr ⁺² , Cs ⁺ , Co ⁺² , Eu ⁺³ ,	Kd _{Co} 7880			
OM = ?		Ce ⁺³ , Sb?, Nb, I mixed	Kd _{Eu} >5270			
AEC = ?		(c) 11.6 day	Kd _{Ce} >720			
SA = 10-20 m ² /g (B.E.T.)		(d) adsorption	Kd _{Sb} 14 ± 17			
crushed to 100 to 400 mesh			Kd _{Nb} 1520			
			Kd _I 25			

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Alluvium (continued)	(Same)	(a) ? (b) Sr^{+2} , Cs^{+} , Co^{+2} , Eu^{+3} , Ce^{+3} , Sb^{2+} , UO_2^{+2} , 2Nb(V) (c) 23-28 days (d) adsorption	$\text{Kd}_{\text{Sr}} 236 \pm 43$ $\text{Kd}_{\text{Cs}} 7500 \pm 1350$ $\text{Kd}_{\text{Co}} 21,000 \pm 15,000$ $\text{Kd}_{\text{Eu}} >40,000$ $\text{Kd}_{\text{Ce}} >20,000$ $\text{Kd}_{\text{Sb}} 11 \pm 9$ $\text{Kd}_{\text{U}} 7.4$ $\text{Kd}_{\text{Nb}} 2800$ $\text{Kd}_{\text{I}} 23.7$	8.3- 8.7	(Same)	(Same)
(Same)	(Same)	(a) ? (b) Sr^{+2} , Cs^{+} , Cs^{+2} , Eu^{+3} , Ce^{+3} , $\text{Sb}^{?}$, UO_2^{+2} , I mixed (c) 39-42 days (d) adsorption-desorption	$\text{Kd}_{\text{Sr}} 186$ adsorption $\text{Kd}_{\text{Cs}} 182$ adsorption $\text{Kd}_{\text{Cs}} 10,400$ adsorption $\text{Kd}_{\text{Cs}} 10,600$ desorption $\text{Kd}_{\text{Co}} 13,400$ adsorption $\text{Kd}_{\text{Co}} 25,000$ desorption $\text{Kd}_{\text{Eu}} >640$ adsorption $\text{Kd}_{\text{Eu}} >2700$ desorption $\text{Kd}_{\text{Ce}} >1090$ adsorption $\text{Kd}_{\text{Ce}} >9100$ desorption $\text{Kd}_{\text{Sb}} 6.3$ adsorption $\text{Kd}_{\text{Sb}} 19.5$ desorption $\text{Kd}_{\text{U}} 5.8$ adsorption $\text{Kd}_{\text{U}} 8.9$ desorption $\text{Kd}_{\text{Nb}} 2720$ adsorption $\text{Kd}_{\text{Nb}} 5100$ desorption $\text{Kd}_{\text{I}} 24.7$ adsorption $\text{Kd}_{\text{I}} 640 \pm 310$ desorption		(Same)	(Same)
(Same)	(Same)	(a) ? (b) Sr^{+2} , Cs^{+} , Co^{+2} , Eu^{+3} , Ce^{+3} , $\text{Sb}^{?}$, Nb(V)	$\text{Kd}_{\text{Sr}} 171 \pm 8$ $\text{Kd}_{\text{Cs}} 6770 \pm 760$ $\text{Kd}_{\text{Co}} 29,800 \pm 11,200$		(Same)	(Same)

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
(Same)	(Same)	(c) 144 days	Kd _{Eu} >15,000		(Same)	(Same)
		(d) desorption	Kd _{Ce} >2000			
			Kd _{Sb} 61 ± 14			
			Kd _{Nb} 2635 ± 7 desorption			
	70°C	(a) ?	Kd _{Sr} 416			
		(b) Sr ⁺² , Cs ⁺ , Co ⁺² , Eu ⁺³ , Ce ⁺³ , Sb?	Kd _{Cs} 5840			
			Kd _{Co} 17,500			
		(c) 2.7 days	Kd _{Eu} 28,800			
		(d) adsorption	Kd _{Ce} >28,000			
			Kd _{Sb} 8.6			
		(a) ?	Kd _{Sr} 596 ± 47			
		(b) Sr ⁺² , Cs ⁺ , Co ⁺² , Eu ⁺³ , Ce ⁺³ , Sb?	Kd _{Cs} 6600 ± 800			
			Kd _{Co} 13,400 ± 5400			
		(c) 23.7 days	Kd _{Eu} >10,000			
		(d) adsorption	Kd _{Ce} >13,000			
			Kd _{Sb} 8 ± 5			
Bentonite	RNM-25	(a) ?	Kd _{Sr} 2000 ± 890	8.3-	a. Batch	(Same)
CaCO ₃ = ?	Ca ⁺² 0.9 meq/l	(b) Sr ⁺² , Cs ⁺ , Co ⁺² , Eu ⁺³ , Ce ⁺³ , Sb?, Nb(V), UO ₂ ⁺²	Kd _{Cs} 1680 ± 141	8.7	(pre-equilibrated & blank corrected	
OX = ?	Mg ⁺² 0.46 meq/l		Kd _{Co} 1120 ± 700		spikes equilibrated	
OM = ?	K ⁺ 0.26 meq/l	(c) 2.8 days	Kd _{Eu} >5000		and filtered before	
CEC = 56-72 meq/100 g	Na ⁺ 2.87 meq/l	(d) adsorption	Kd _{Ce} >400		rock contact	
AEC = ?			Kd _{Sb} 6.4 ± 0.8		b. 0.5-2.0 g to	
SA = 33.8 m ² /g (B.E.T.)			Kd _{Nb} 600 ± 500		20 ml	
90% less than 85 µm	Room Temperature 20°C	(a) ?	Kd _{Sr} 1000 ± 160			
		(b) Sr ⁺² , Cs ⁺ , Co ⁺² , Eu ⁺³ , Ce ⁺³ , Sb?, Nb(V)	Kd _{Cs} 1500 ± 100			
			Kd _{Co} 470 ± 54			
		(c) 11.6 days	Kd _{Eu} >1400			
		(d) adsorption	Kd _{Ce} >500			
			Kd _{Sb} 69 ± 2.3			
			Kd _{Nb} 510 ± 4			

Geologic Material Properties	Groundwater Properties	Nuclide Properties	Kd ml/g	pH	Method	Reference
Bentonite (continued)	(Same)	(a) ? (b) Sr^{+2} , Cs^{+} , Co^{+2} , Eu^{+3} , Ce^{+3} , Sb? , Nb , UO_2^{+2} (c) 27-35 days (d) adsorption	Kd_{Sr} 1575 $\pm$ 660 Kd_{Cs} 1780 $\pm$ 420 Kd_{Co} 725 $\pm$ 370 Kd_{Eu} 1450 Kd_{Ce} >500 Kd_{Sb} 6.0 $\pm$ 1.0 Kd_{Nb} 650 $\pm$ 270 Kd_{U} 77.8		(Same)	(Same)
(Same)	(Same)	(a) ? (b) Sr^{+2} , Cs^{+} , Co^{+2} , Eu^{+3} , Ce^{+3} , Sb? , Nb , UO_2^{+2} (c) 39-66 days (d) Both	Kd_{Sr} 1800 $\pm$ 950 adsorption Kd_{Cs} 1950 $\pm$ 35 adsorption Kd_{Co} 2170 $\pm$ 130 adsorption Kd_{Eu} >4500 adsorption Kd_{Ce} >600 adsorption Kd_{Sb} 5.7 $\pm$ 1.1 adsorption Kd_{Nb} 1100 $\pm$ 870 adsorption Kd_{U} 73.1 adsorption		(Same)	(Same)
(Same)	(Same)	(a) ? (b) Sr^{+2} , Cs^{+} , Co^{+2} , Eu^{+3} , Ce^{+3} , Sb? , Nb , UO_2^{+2} (c) 39-66 days (d) Both	Kd_{Sr} 2440 $\pm$ 100 desorption Kd_{Cs} 2110 $\pm$ 106 desorption Kd_{Co} 3200 $\pm$ 2300 desorption Kd_{Eu} >6000 desorption Kd_{Ce} >700 desorption Kd_{Sb} 41 $\pm$ 25 desorption Kd_{Nb} 2200 $\pm$ 1000 desorption Kd_{U} 271 desorption		(Same)	(Same)
(Same)	(Same)	(a) ? (b) Sr^{+2} , Cs^{+} , Co^{+2} , Eu^{+3} , Ce^{+3} , Sb? , Nb , UO_2^{+2} (c) 141-145 days (d) desorption	Kd_{Sr} 2645 $\pm$ 245 Kd_{Cs} 2047 $\pm$ 210 Kd_{Co} 5600 $\pm$ 3400 Kd_{Eu} >10,000 Kd_{Ce} >1500 Kd_{Sb} 32 $\pm$ 20 Kd_{Nb} 1450 $\pm$ 64		(Same)	(Same)

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