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Selected Hydrologic and Geochemical Issues In Site Characterization for Nuclear Waste Disposal: Flood Basalts at the Hanford Reservation

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**Chalon L. Carnahan, Joan M. Delany, Jane C. S. Long
Robert J. Silva, David J. Watkins, Arthur F. White,
and Charles R. Wilson**

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University of California
Berkeley, California 94720

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Division of Waste Management
Office of Nuclear Material Safety and Safeguards
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SELECTED HYDROLOGIC AND GEOCHEMICAL ISSUES IN SITE CHARACTERIZATION FOR NUCLEAR WASTE DISPOSAL: FLOOD BASALTS AT THE HANFORD RESERVATION

Chalon L. Carnahan, Joan M. Delany, Jane C.S. Long,
Robert J. Silva, David J. Watkins, Arthur F. White, and Charles R. Wilson

Earth Sciences Division
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

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ABSTRACT

Four issues are considered that must be addressed by a site characterization program designed to evaluate the suitability of the flood basalts of the Pasco Basin in central Washington as a site for the construction of a repository for the disposal of high-level nuclear waste. The four issues are (1) identification of hydrostratigraphic units within a sequence of flood basalts, (2) mechanisms and points of groundwater recharge and discharge, (3) solubility of radionuclides, and (4) phase transformation of fracture filling materials. Each issue is discussed in terms of its significance to waste isolation. Available approaches for resolving the issues are presented and their limitations identified. Where appropriate, research programs for overcoming these limitations are indicated.

TABLE OF CONTENTS

LIST OF FIGURES xi

LIST OF TABLES xiii

EXECUTIVE SUMMARY 1

1. INTRODUCTION 6

1.1 Background 6

1.2 Geology of the Pasco Basin 6

1.3 Reference Repository Location and Repository Horizon . . . 11

1.4 Selection of Site Characterization Issues 11

1.5 Arrangement and Content of Report 13

2. IDENTIFICATION OF HYDROSTRATIGRAPHIC UNITS WITHIN A SEQUENCE OF FLOOD BASALTS 14

2.1 Statement of Issue 14

2.2 Importance of Issue 14

2.3 Considerations in Defining Hydrostratigraphic Units . . . 15

2.3.1 Hydraulic Properties of Hydrostratigraphic Units . . 16

2.3.2 Effect of the Purpose of the Model on the Choice of Hydrostratigraphic Units 17

2.3.3 Continuum and Noncontinuum Treatment of Hydrostratigraphic Units 17

2.4 Methods of Identifying Hydrostratigraphic Units 20

2.4.1 Observations of Present Behavior 21

2.4.1.1 Groundwater head 22

2.4.1.2 Groundwater chemistry and age dating . . . 23

2.4.2 Rock and Water Hydraulic Property Measurements . . 23

2.4.3 Special Considerations for the Disturbed Zone . . . 24

2.5 Recommended Hydrologic Approaches for Resolving the Issue of Hydrostratigraphic Units 25

2.5.1 Stages of Field Investigation 25

2.5.2 The Role of Groundwater Models 25

2.5.3 Field Program Development Using Standard Technology . 26

2.5.4 Hydrologic Data Needs 27

2.5.4.1 Standard tests to obtain hydrologic data . 27

2.5.4.2 Limitations of standard tests for collection of hydrologic data 30

2.5.5 Hydrochemical Data Needs 31

2.5.5.1 Analyses to obtain hydrochemical data . . 32

2.5.5.2 Limitations to hydrochemical approaches . . 36

2.5.6 Considerations in Test Program Design 37

2.6 Refined Approaches for Resolving the Issue of Hydrostratigraphic Units 39

2.6.1 Hydrologic Tests used to Refine Selection of Hydrostratigraphic Units 40

2.6.1.1 Large-scale hydrologic data 40

2.6.1.2 In situ generation of constant gradient, parallel flow fields 48

2.6.1.3 Large-scale measurement of vertical hydraulic conductivity 52

2.6.1.4 General limitations to refined hydrologic tests 55

2.6.2 Hydrochemical Tests Used to Refine Selection of Hydrostratigraphic Units 55

2.7 Uncertainties Remaining in Resolution of the Issue . . . 56

2.8 Recommendations for Research 58

3. DETERMINATION OF AREAS AND MECHANISMS OF NATURAL GROUNDWATER RECHARGE AND DISCHARGE FOR THE HYDROSTRATIGRAPHIC UNITS WITHIN A SEQUENCE OF FLOOD BASALTS 60

3.1 Statement of Issue 60

3.2 Importance of Issue 60

3.3 Nature of Groundwater Movement in Flood Basalts 61

3.4 Methods of Identifying Areas and Mechanisms of Recharge and Discharge 62

3.4.1 Basic Data Needs 62

3.4.2 Methods of Data Analysis 64

3.5 Metholologies for Resolution of Issue 65

3.5.1 Standard Approaches and their Limitations 65

3.5.1.1 Water budget techniques 65

3.5.1.2 Numerical model techniques 72

3.5.1.3 Direct synthesis techniques 79

3.5.2 Alternative Approaches and their Limitations . . . 80

3.6 Recommended Approaches and their Limitations 80

3.7 Uncertainties Remaining in Resolution of the Issue 85

3.8 Recommendations for Research 85

4. SOLUBILITY OF RADIONUCLIDES 87

4.1 Statement of Issue 87

4.2 Importance of Issue 87

4.3 Site Characterization Methods 89

4.3.1 Characterization of Groundwater 89

4.3.1.1 Groundwater sampling 90

4.3.1.2 Analytical methods 93

4.3.1.2.1 Chemical analyses 93

4.3.1.2.2 Redox measurements 95

4.3.2 Determination of Solubility 97

4.3.2.1 Solubility measurement methods 99

4.3.2.1.1 Characterization of solid phase . 100

4.3.2.1.2 Separation of solid and solution phases 101

4.3.2.1.3 Analysis of the aqueous phase . . 101

5. PHASE TRANSFORMATION OF FRACTURE FILLING MATERIALS 103

5.1 Statement of Issue 103

5.2 Importance of Issue 103

5.3 Host Rock Geochemistry 105

5.3.1 Geologic Setting 105

5.3.2 Primary Mineralogy 105

5.3.3 Secondary Mineralogy 106

5.4 Hydrothermal Conditions 107

5.4.1 Pasco Basin Geothermal Gradients 108

5.4.2 Potential Repository Conditions 108

5.4.3 Groundwater-Basalt Interactions 108

5.5 Phase Transformations 109

5.5.1 Smectites 112

5.5.2 Zeolites 113

5.5.3 Silica Minerals 114

5.6 Site Characterization Methodologies 114

5.6.1 Host Rock Field Studies 115

5.6.2 Laboratory Experiments 116

5.6.3 Theoretical Modeling Techniques 117

5.7 Research Needs and Limitations 119

ACKNOWLEDGEMENTS 121

APPENDIX A. Geologic Heterogeneities in Flood Basalts 122

A.1 Heterogeneities Within Single Basalt Flows 122

A.2 Heterogeneities Within a Sequence of Basalt Flows 124

APPENDIX B. Technical Basis for Identifying Hydrostratigraphic Units in Heterogeneous Media 128

B.1 Kinematic Considerations for Hydrostratigraphic Units Defined on the Basis of Continuum Behavior 128

B.2 Identification of Hydrostratigraphic Units Defined on the Basis of Hydraulic Properties and Continuum Behavior . . . 131

B.2.1 Identification in the Far-Field 131

B.2.2 Identification in the Disturbed Zone 135

B.3 Identification of Hydrostratigraphic Units Defined on the Basis of Noncontinuum Behavior 136

B.4 Kinematic Considerations in Choosing Hydrostratigraphic Units for Transport Modeling 137

APPENDIX C. Identification of Hydrostratigraphic Units in Flood Basalts: An Illustrative Example 138

C.1 Groundwater Head 138

C.2 Groundwater Chemistry and Age Dating 140

C.3 Geologic and Stratigraphic Methods 142

C.3.1 Single-Layer Case: Entire Basalt Section 142

C.3.2 Multiple-Layer Case: Principal Basalt Formations 142

C.3.3 Multiple-Layer Case: Structural Components of Individual Flows 144

C.4 Hydrogeologic Methods 144

C.4.1 Hydraulic Conductivity Basis for Unit Identification 144

C.4.2 Storage Coefficient, Effective Porosity, and Diffusion Basis for Unit Identification . . . 145

C.5 Geophysical Methods 147

C.6 Synthesis of Available Information 147

APPENDIX D. Mechanisms of Recharge and Discharge in Flood Basalts: An Illustration from the Pasco Basin . . . 150

D.1 Lateral Transfer Mechanisms 150

D.2 Vertical Transfer Mechanisms 153

D.3 Groundwater Extraction Mechanisms 153

D.4 Synthesis of Alternatives 154

REFERENCES 155

LIST OF FIGURES

Figure 1.1. Location of the Pasco Basin. 7

Figure 1.2. Northern Pasco Basin and Hanford Reservation 8

Figure 1.3. Simplified sections through the Pasco Basin 9

Figure 1.4. Pasco Basin stratigraphic nomenclature 10

Figure 1.5. Interpretation of stratigraphic units in the central Pasco Basin 12

Figure 2.1. Schematic definition of a representative elementary volume (REV) as applied to a flood basalt sequence . . . 19

Figure 2.2. Trilinear plots of major inorganic constitutents of groundwater from upper Wanapum Basalt, showing progressive hydrochemical change related to increasing distance from recharge area. 33

Figure 2.3. Generalized groundwater flow direction within the Mabton Interbed, based on oxygen-18/oxygen-16 ratios. 35

Figure 2.4. Schematic drawing of macropermeability experiment at Stripa Test Station, Sweden. 42

Figure 2.5. Distance-drawdown plot for steady radial flow into underground drift in macropermeability experiment. Numbers used as data points indicate borehole in which measurement was made 44

Figure 2.6. Change in average hydraulic conductivity as a function of test volume for the Stripa granite 45

Figure 2.7. Schematic representation of large-scale underground test facility in basalt 46

Figure 2.8. Banks of wells for parallel flow measurement 50

Figure 2.9. Underground arrangement of boreholes for measurement of vertical permeability. 54

Figure 3.1. Example of groundwater recharge and discharge in the Swale Creek Valley area, Washington 63

Figure 3.2. Typical components of a water budget. 68

Figure 3.3. Schematic drawing of U.S. Geological Survey stream gauging network for the Pasco Basin 70

Figure 3.4. Example of the subdivision of a study area into an array of blocks for the purpose of numerical modeling. . 73

Figure 3.5. Plan view of three-dimensional finite element mesh of the Pasco Basin used to produce the results shown in Figure 3.6 76

Figure 3.6. Contours of computed hydraulic heads for the Mabton Interbed at the top of the Wanapum Basalt for a model calibration run 77

Figure 4.1. Approximate time to remove contamination due to fluid losses during drilling 92

Figure 5.1. Local equilibrium mass transport as modeled by the EQ3/EQ6 Mass Transfer Simulation Code 118

Figure A.1. Schematic diagram showing structure of a basalt flow . . 123

Figure A.2. Fence diagram of the Umtanum flow in the Pasco Basin . . 126

Figure B.1. Example of the kinematic effect, showing parallel flow lines under a uniform gradient (Case A) and converging flow lines under a nonuniform hydraulic gradient (Case B). 129

Figure B.2. Example of hydrostratigraphic units identified for the purpose of numerical modeling in the vicinity of a repository in a sequence of flood basalts 130

Figure B.3. The relationship between REV's, scale of fractures (or other heterogeneities), and scale of isopotentials for two different constant scales of continuum flow analysis. 132

Figure B.4. Example of inconsistent relationship between the REV and the gradient field 134

Figure C.1. Variations of hydraulic head with depth. Case A: boreholes DC-1 and DC-2; Case B: DC-1/DC-2, DC-6 and DC-8. . 139

Figure C.2. Comparison of directions of groundwater movements within the Mabton Interbed as inferred by hydraulic head (Case A) and total dissolved solids (Case B) 141

Figure C.3. Generalized basalt stratigraphy within the Pasco Basin . 143

Figure C.4. Observed range of hydraulic conductivity across columnar zones within the Grande Ronde Basalt 146

Figure D.1. Map of the Pasco Basin and vicinity, showing neighboring groundwater basins 151

LIST OF TABLES

Table 5.1. Summary of Repository Equilibrium Conditions. 110

Table 5.2. Summary of Groundwater Compositions. 111

Table A.1. Nominal Hydrologic Properties of Umtanum Flow in the Pasco Basin 125

Table C.1. Example of Preliminary Regional Hydrostratigraphic Units for Studies of Groundwater Flux Within the Pasco Basin. 149

EXECUTIVE SUMMARY

This report considers four issues that must be addressed by a site characterization program designed to evaluate the suitability of the flood basalts of the Pasco Basin in central Washington as a site for the construction of a repository for the disposal of high-level nuclear waste. The four issues are (1) identification of hydrostratigraphic units within a sequence of flood basalts; (2) mechanisms and points of groundwater recharge and discharge; (3) solubility of radionuclides; and (4) phase transformation of fracture filling materials. A summary of the principal results of the studies of each of the issues is presented below.

IDENTIFICATION OF HYDROSTRATIGRAPHIC UNITS WITHIN A SEQUENCE OF FLOOD BASALTS

Hydrostratigraphic units (HSU's) are bodies of rock that function as distinct hydrologic systems for the problem being studied. HSU's serve to simplify a geologically complex study area by representing it as a smaller number of units that are more tractable for analysis by conceptual or numerical methods. Hydrostratigraphic units have traditionally been identified to facilitate a conceptual understanding of groundwater flow systems, and the units have been defined primarily on the basis of contrasts in the hydraulic properties of the different bodies of rock. Thus HSU's have been defined, for example, on the basis of a relatively higher or lower permeability as compared with the permeability of the neighboring strata. For the purposes of numerical modeling, however, the HSU's must also meet the specific criteria of the models.

In identifying HSU's to facilitate numerical modeling of a groundwater system, it is useful to supplement the criterion of contrasts in hydraulic properties between units with the criterion of similarity in hydraulic properties within units. This is because in preparing numerical models it is convenient to identify bodies of rock that can be assigned the same or similar hydraulic properties throughout. Because of this additional criterion, the identification of HSU's for modeling is closely linked with the purpose for which the HSU is defined and with the magnitude of the hydraulic properties that govern the characteristics being studied. Units defined for a study of groundwater flux, for example, must exhibit similar average conductivity and specific storage properties throughout their lateral and vertical extent when measured on a scale appropriate to the problem being studied. Further, numerical models for regional groundwater movement are generally based on the assumptions that each separately identified elemental volume (1) behaves as a continuum, (2) is a statistically representative sample of the average properties of the HSU, and (3) is small enough that internal hydraulic gradients are essentially uniform. To be appropriate for numerical modeling, the HSU's must also be capable of subdivision into elemental volumes that satisfy these three assumptions. Emphasis in this paper is placed upon the identification of HSU's for the purpose of numerical modeling.

The first assumption in numerical modeling--that of continuum behavior--asserts that the rock behaves as a homogeneous, anisotropic porous medium on the scale of the smallest elemental volume being studied. Flood basalt is in reality a heterogeneous mass of fractured rock that must be shown to behave as a porous medium on the scale of the elemental volumes used in modeling. Thus the appropriate HSU is one that may be subdivided into elemental volumes that exhibit continuum behavior on the correct scale.

The second assumption--that of statistical representation--asserts that the elemental volumes being studied contain a large enough sample of heterogeneities to be statistically representative of the rock mass as a whole. For example, permeability is controlled by the size, shape, and degree of interconnection of the void spaces in the rock. To be statistically representative, the elemental volume must contain a sufficiently large sample of these void spaces so that the permeability of one such volume will be similar to the permeability of any other such volume within the HSU. The smallest elemental volume that meets the criteria of statistical representation is called the representative elementary volume (REV).

The third assumption asserts that the elemental volumes must be scaled relative to the groundwater flow patterns such that the average hydraulic gradient within the element is uniform. Uniformity is necessary to assure that the heterogeneities within the elements are stressed in a predictable manner. If this criterion is not met, continuum behavior cannot be assured.

Field data on hydraulic head, hydrochemistry, geologic structure, and hydraulic properties of the rock will be required to identify appropriate HSU's in the Pasco Basin. These data must be collected throughout the three-dimensional volume of rock to be characterized. Resolution of this issue will be accomplished through the selective application of both standard and innovative field techniques. The results will be periodically checked through the field validation of numerical models based upon the HSU's identified.

DETERMINATION OF AREAS AND MECHANISMS OF NATURAL GROUNDWATER RECHARGE AND DISCHARGE FOR THE HYDROSTRATIGRAPHIC UNITS WITHIN A SEQUENCE OF FLOOD BASALTS

Radionuclides that escape the engineered barriers and leave the disturbed zone of a repository will enter the regional groundwater system. The moving groundwater will then transport the nuclides from the recharge areas to the discharge areas. The travel time to the accessible environment will depend upon the length of the flow path and the hydrologic and geochemical conditions encountered along that flow path. Knowledge of the recharge and discharge areas, and of the groundwater flow patterns between these areas, is an important element in assessing the safety of a proposed waste repository.

Three fundamental conventional approaches are expected to be adequate for resolution of this issue: (1) water budget techniques, (2) numerical model techniques, and (3) direct observational methods.

The first two involve the use of analytical models. The water budget technique is relatively simple, but yields only approximate results. It is best used in reconnaissance-level studies during the early phases of the exploration program. Numerical model techniques are the most sophisticated and potentially the most accurate methods available for resolving this issue. They are capable of providing detailed, quantitative information on groundwater movement throughout the study area and are thus ideal for identifying areas and mechanisms of recharge and discharge. The third approach--direct observational methods--provides important qualitative information. These three approaches are complementary, and together are expected to be adequate for resolving the issue.

The recommended field exploration program consists of conventional techniques that should be capable of identifying, in a qualitative sense, the areas and mechanisms of recharge and discharge. Quantitative resolution of this issue in terms of accurate estimates of groundwater flux will require additional research into the field verification of the usual assumptions of continuum behavior that are made in regional groundwater models.

SOLUBILITY OF RADIONUCLIDES

Radionuclides released from a waste form will enter the local groundwater system, where they will react with chemical components of groundwater, and possibly the host rock, to form insoluble compounds and solution species that can provide significant controls on solution concentrations and migration rates of the radionuclides. Knowledge of the processes controlling residence times of radionuclides in the aqueous and solid phases is required for prediction of rates of migration of radionuclides from an underground storage facility to the accessible environment.

Prediction of possible stable solid phases and solution species will depend on two critical kinds of information. These are (1) complete characterization of the chemical composition and oxidation-reduction behavior of the groundwater, and (2) knowledge of the nature and solubility of radionuclide compounds likely to form under groundwater conditions at the repository site.

Characterization of groundwater involves two categories of methodology: sampling and chemical analysis. In general, existing methodologies are adequate for nearly complete characterization, provided certain precautions are observed.

The inability to obtain uncontaminated, representative samples from a repository site places a significant limitation on the reliability of

geochemical analysis of groundwater. Groundwater samples taken from vertical boreholes drilled from the ground surface are subject to contamination or other perturbations from three principal sources: (1) drilling fluids and other materials may be introduced during the drilling process, (2) groundwaters from different aquifers may be mixed by cross flow in a borehole, and (3) exchange of dissolved gases may be caused by changes of pressure and temperature during and immediately after the sampling process. Sampling methods exist that can minimize or avoid these sources of error.

On the other hand, samples obtained from boreholes extending horizontally from a test facility at depth and analyzed in situ are likely to be more representative of groundwaters near the repository, and less subject to contamination, than samples obtained from vertical boreholes originating at the ground surface.

Existing analytical methods are, in general, adequate for characterization of groundwaters. The use of two or more different analytical methods is advised for the determination of certain elements present at low concentrations.

The determination of oxidation-reduction potential (Eh) is the only analytical procedure subject to significant uncertainty. In natural groundwaters, potentiometric measurement of Eh is not always reliable. In some cases, it is possible to obtain reasonably close approximations of Eh by using the results of other chemical analyses. If these methods fail, it will be necessary to determine oxidation states of radionuclides by direct chemical measurement. Further research is needed for development of more reliable methods of Eh measurement.

Two methods are available, in principle, for determination of solubilities of solid phases containing radionuclides. The solubility can be calculated by use of thermochemical data (e.g., heat of solution, free energy of formation) for the solid of interest and the aqueous species in equilibrium with it. Alternatively, the solubility can be measured directly.

To calculate a solubility, the identities of the solid phase and associated aqueous complexes must be known. In natural systems, solid phases likely to contain radionuclides are expected to be complex. In general, thermochemical data are not available for these phases because of experimental difficulties in making the necessary measurements.

Although direct measurement of solubilities can produce useful results, this method does not provide fundamental thermochemical data needed for extrapolation to future conditions, which might be beyond the range of the parameter values studied.

PHASE TRANSFORMATION OF FRACTURE FILLING MATERIALS

Phase transformation of materials filling fractures in the host rock could result in either an increase or a decrease in the rate of release of radionuclides from a nuclear waste repository. Because flow of groundwater in the Hanford basalts occurs principally within fractures, changes in the permeability of materials in the fractures would directly affect the rate of flow. In addition, changes in the sorptive properties of fracture filling materials would directly affect the rate of movement of radionuclides relative to the groundwater flow rate.

Site characterization procedures designed to resolve this issue must include not only identification of existing conditions of fracture fillings, but also assessment of the kinds and magnitudes of changes caused in fracture fillings by repository-induced hydrothermal processes.

Existing primary and secondary mineral assemblages in the Umtanum basalt flow have been extensively characterized. The sorptive capacity of the basalt has been attributed to secondary mineralization in fractures and voids, specifically smectite clay and the zeolite clinoptilolite.

Although no experiments have been performed to investigate the stability of secondary mineral assemblages, the thermal alteration of clay minerals has been recognized from field data. In particular, the transformation of smectite to mixed-layer illite-montmorillonite results in layer contraction, causing an increase of pore space, reduction of ion-exchange capacity, and decrease of swelling capacity. However, there is a lack of experimental data regarding the stability of smectite in the range 100°C to 300°C. Further investigations in this temperature range are needed. Similarly, there is a need for hydrothermal experimental data on the stability of clinoptilolite at elevated temperatures.

Prediction of the potential consequences of phase transformation of secondary minerals will depend on assessment of potential hydrothermal conditions near the repository and their effects on subsequent phase transformations. Because little is known about the response of natural mineral assemblages to changes in thermal conditions, resolution of the issue must rely almost entirely on future research and the development of new methodologies for site characterization. Existing methodologies are limited to collection of site-specific data from field experiments and boreholes; at best, they can provide a preliminary data base that could serve as a starting point for further research.

Recent attempts to theoretically model the generation of secondary phase assemblages in the Pasco Basin basalts have had little success. Limitations of existing theoretical models are their inability to simulate the extensive compositional variations, metastability, and nonequilibrium (both steady-state and time-dependent) processes that appear to exist in low-temperature geochemical systems. This theoretical lack is compounded by the absence of data on these effects and processes. Extension of theoretical concepts to the modeling stage will be critically dependent on acquisition of experimental data for use in model verification and in data bases for predictive modeling.

1. INTRODUCTION

1.1 BACKGROUND

The United States Department of Energy (DOE) has the responsibility to identify sites and construct repositories for the geologic disposal of high-level nuclear waste. These facilities will be licensed by the United States Nuclear Regulatory Commission (NRC) under the rules and procedures defined in the Code of Federal Regulations (10 CFR Part 60). As part of a program designed to identify and select candidate sites for construction of waste repositories, the DOE is evaluating areas within DOE-owned reservations to determine which, if any, might exhibit desirable characteristics. This effort has led to the selection of the Hanford Reservation in eastern Washington for further characterization studies (Shipler and Evans, 1980). The Hanford Reservation lies within the Pasco Basin near the center of the Columbia River flood basalt physiographic province, which spans parts of Washington, Oregon, and Idaho (see Figures 1.1 and 1.2).

If the DOE elects to submit an application for construction of a repository at the Hanford Reservation, a Site Characterization Report will be submitted to the NRC prior to the application for a license. The Site Characterization Report will include a description of the candidate site based on the available data and a description of site characterization activities proposed to address the ability of the site to host a safe repository for radioactive waste. The NRC will review the Site Characterization Report and may make specific objections or recommendations regarding the proposed program. This report considers four site characterization issues that are expected to be included among those that will have to be addressed in a site characterization program for a proposed waste repository at the Hanford Reservation.

1.2 GEOLOGY OF THE PASCO BASIN

Geologic data for the Columbia Plateau and the Pasco Basin have been compiled by Myers and Price (1979). The Pasco Basin is one of several structural and topographic basins within the western Columbia Plateau. It is a semiarid, sparsely vegetated steppe that occupies about 5200 km^2. The basin is underlain by three major rock units: (1) pre-Columbia River Basalt Group rocks, (2) the Columbia River Basalt Group, which includes the Ellensburg Formation, and (3) late Cenozoic sediments including the Ringold Formation, the Palouse Soil, and the Hanford Formation. A simplified section through the Pasco Basin is shown in Figure 1.3, and the stratigraphic nomenclature is given in Figure 1.4. The bed rock is overlain by 0 to 220 m of fluvial, lacustrine, and glaciofluvial sediments of Pliocene and Pleistocene age. The late Cenozoic sedimentary rocks and the Columbia River Basalt Group rocks, which are at least 1460 m thick, crop out throughout the Pasco Basin. The pre-Columbia River Basalt Group rocks do not crop out within the basin.

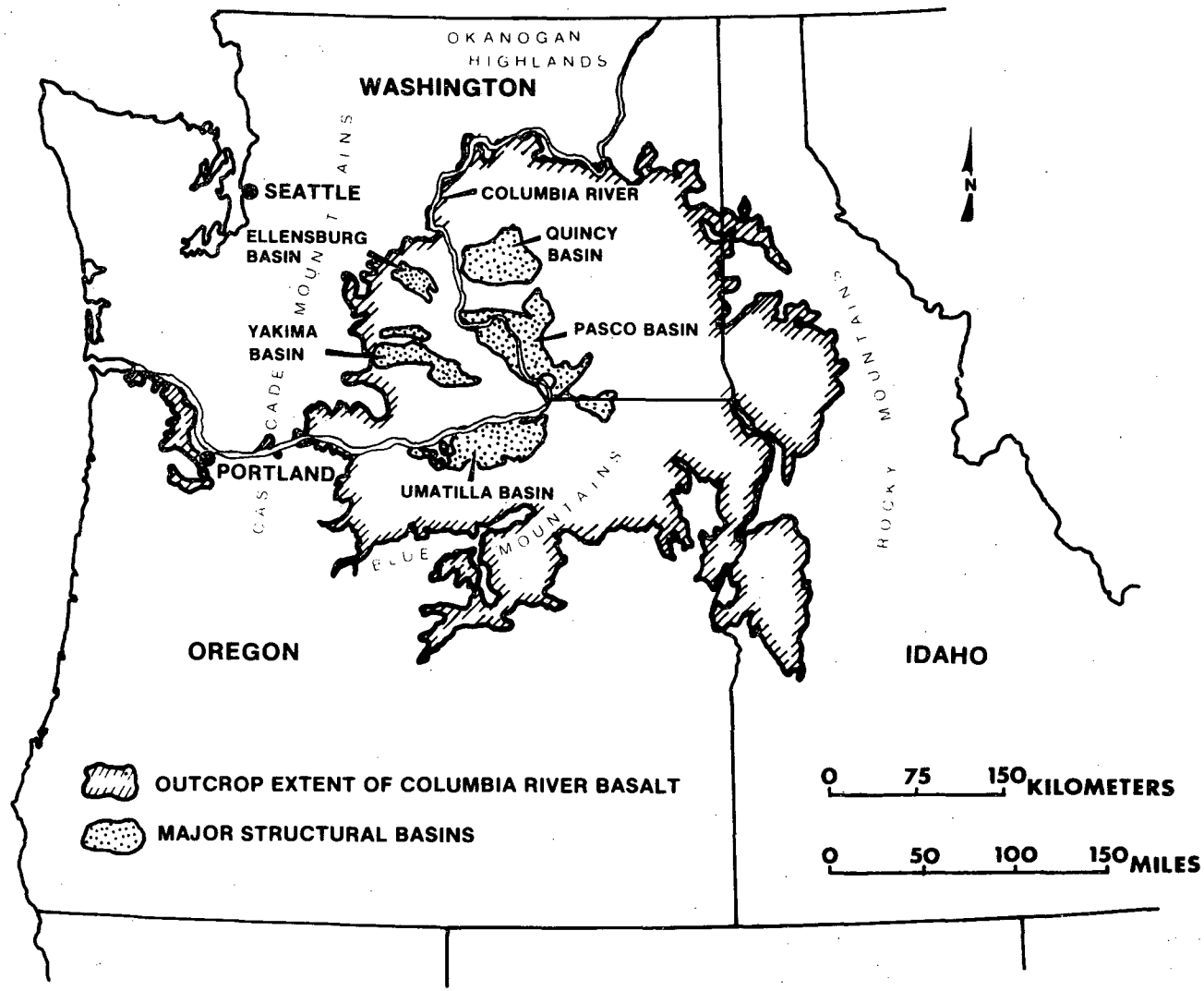


Figure 1.1. Location of the Pasco Basin (from Apps et al., 1979, Figure I-1).
[XBL 792-8312]

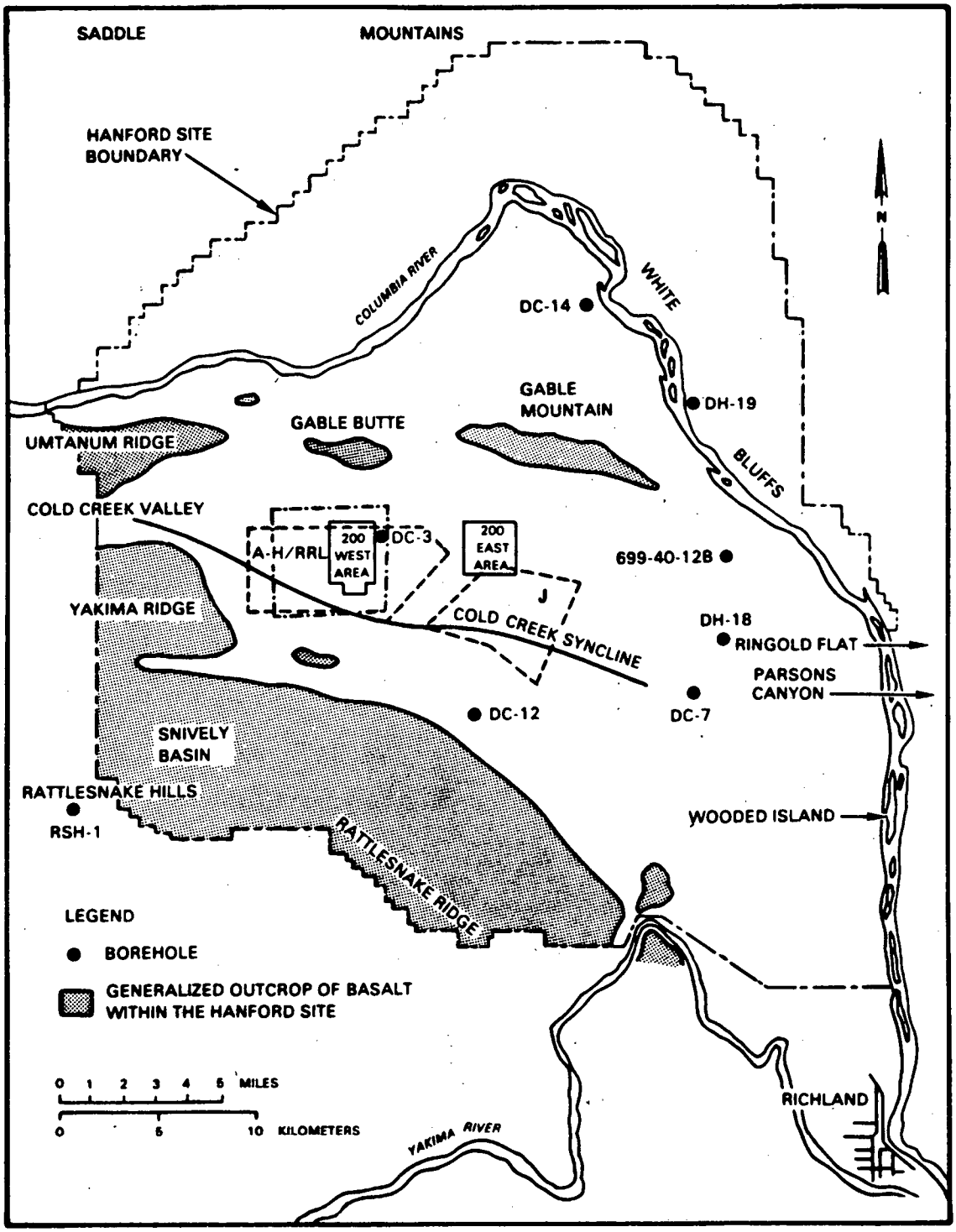


Figure 1.2. Northern Pasco Basin and Hanford Reservation (from Deju, 1981, Figure 3). [XBL 826-10481]

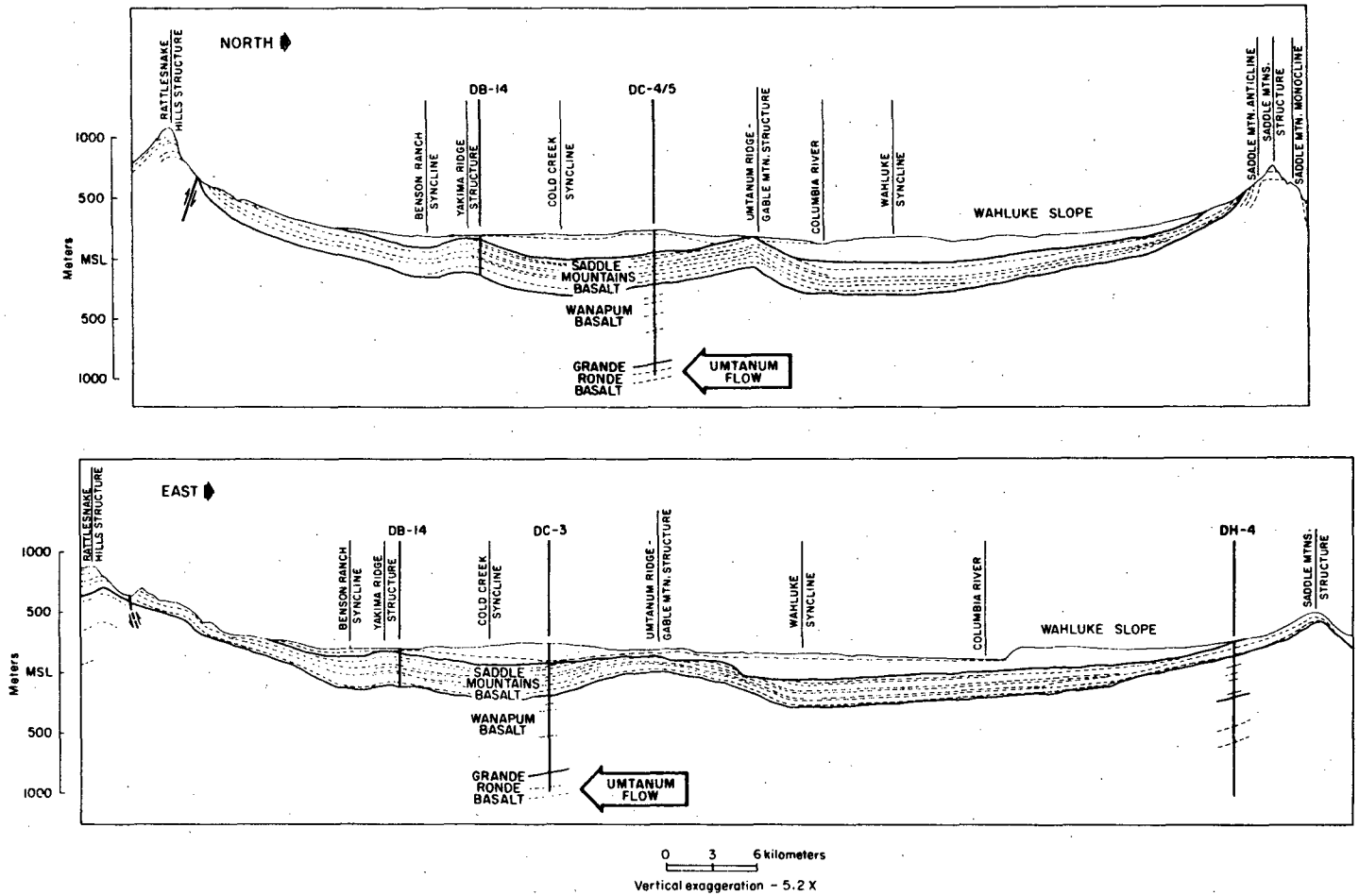


Figure 1.3. Simplified sections through the Pasco Basin. [XBL 818-3381]

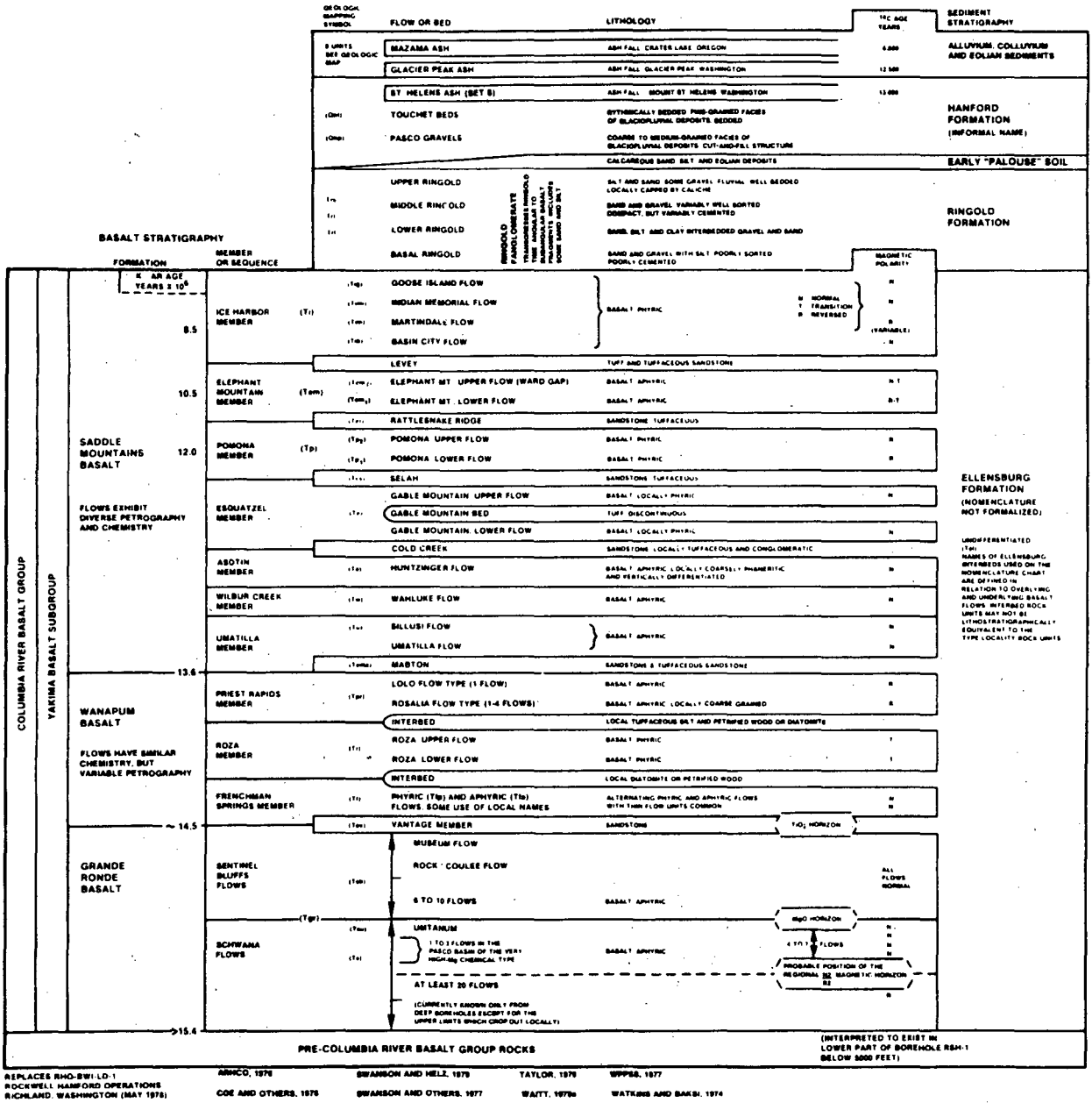


Figure 1.4. Pasco Basin stratigraphic nomenclature (from Myers et al., 1979, Table III-1). [XBL 826-10482]

Volcanoclastic sediment layers are interbedded between the basalt flows in the upper part of the bedrock section. Throughout the section, many of the basalt flows appear to extend laterally as single rock-stratigraphic units across the Pasco Basin and beyond, whereas other units are less extensive and pinch out within the basin. A few flows in the upper part of the section were emplaced as valley fills and are of restricted lateral extent.

1.3 REFERENCE REPOSITORY LOCATION AND REPOSITORY HORIZON

As part of the Basalt Waste Isolation Project (BWIP), studies have been conducted at the Hanford Reservation to define suitable candidate sites for construction of a waste repository (Woodward-Clyde Consultants, 1979; Rockwell Hanford Operations, 1980a). This work has progressed through a series of steps leading to the selection of a preferred site located within the Cold Creek Syncline area of the Pasco Basin. This preferred site, designated the "reference repository location," or site A-H, is shown in Figure 1.2. Site J in the same figure has been designated the "first alternate" (Deju, 1980b). The Umtanum flow unit, at an appropriate depth of 1130 m below the surface, has been selected as the reference storage horizon (Rockwell Hanford Operations, 1980b). The Umtanum unit is a member of the Schwana Sequence of the Grande Ronde Basalt (see Figure 1.5). For the purposes of this report, it is assumed that a site characterization program would be directed to evaluation of site A-H or a similar site in the Cold Creek Syncline area and that the repository would be constructed in the Umtanum flow. However, this use of the reference site and horizon is intended only to illustrate issues and site characterization methodologies. Unless otherwise noted, material presented in this report may be considered generally applicable to other candidate sites and horizons of the Pasco Basin.

1.4 SELECTION OF SITE CHARACTERIZATION ISSUES

The term "issues" has been used to include all characteristics of a site that may affect its ability to host a geologic repository (Nuclear Regulatory Commission, 1981). In this report, "site characterization" is used as it is defined in 10 CFR Part 60, Section 60.2(p). Thus the term refers to a program of laboratory and field studies undertaken to develop the information needed to determine the suitability of a site for a geologic repository. The information required includes establishing the site's existing conditions and determining the properties of the host rock. These properties must be known in order to predict the site's response to the changed conditions that will result from the repository construction and operation.

This report is restricted to four selected site characterization issues in the disciplinary areas of hydrogeology and geochemistry that are expected to be of importance in evaluating the suitability of a repository site within the Hanford Reservation. These issues are: (1) the identification of hydrostratigraphic units (HSU's), (2) the identification of areas of

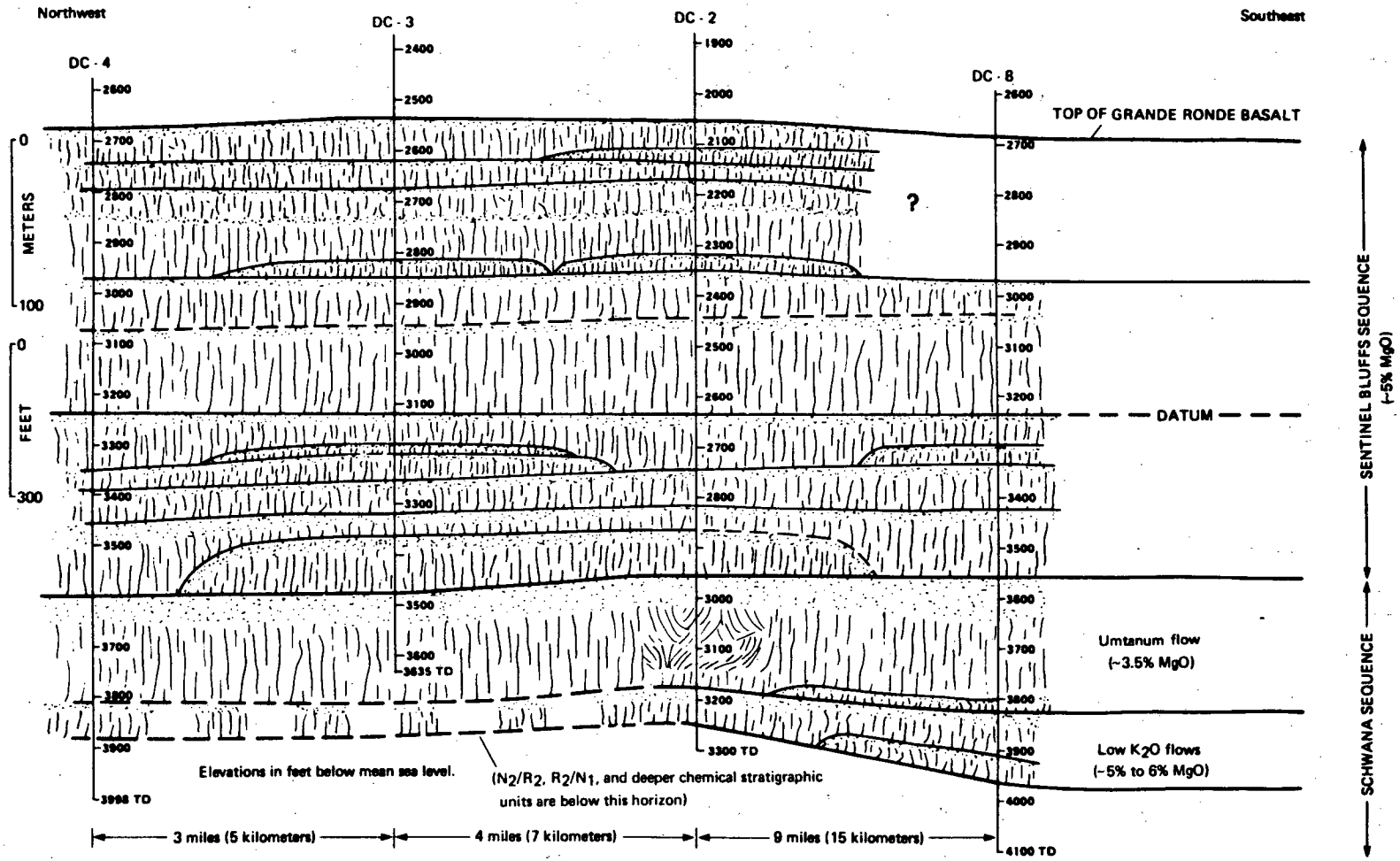


Figure 1.5. Interpretation of stratigraphic units in the central Pasco Basin (from Rockwell Hanford Operations, 1979, Figure 3).

[XBL 826-10483]

groundwater recharge and discharge to the deep hydrologic strata, (3) the solubility and precipitation of radionuclides, and (4) the phase transformation of fracture filling materials. This selection of issues was based on a review of the currently available data regarding the geology of the Hanford Reservation and the requirements of 10 CFR Part 60. The specific issues were selected by the NRC from short lists of major issues developed by Lawrence Berkeley Laboratory (LBL) and the NRC. The issues selected do not necessarily reflect those that will be of greatest technical importance in a site characterization program for a waste repository in the Pasco Basin. Some, however, are significant issues for which currently available data are limited and whose resolution is expected to be of concern in reaching a determination as to the suitability of the site for disposal of nuclear waste and in evaluating aspects of repository design.

1.5 ARRANGEMENT AND CONTENT OF REPORT

Four major sections follow this introduction. The issue of identifying HSU's is treated in Section 2. The identification of mechanisms and areas of groundwater recharge and discharge is addressed in Section 3. Site characterization techniques associated with prediction of radionuclide solubility are discussed in Section 4, and site characterization methodologies related to phase transformation of fracture filling materials are presented in Section 5.

In each section recommended site characterization methodologies that may be used to obtain the necessary data required for resolution of the issue are described. Descriptions of the methodologies include a presentation of the general procedures to be used, conceptual designs of testing methods, and general measurement techniques and instrumentation needs. Detailed descriptions of specific instrumentation systems, standards of practice, and other details that depend upon design controlled configurations or are dictated by findings developed during the progress of the site characterization program are not included.

During the preparation this report a review was made of the current literature to obtain data on specific conditions in the Pasco Basin; thus the recommended site characterization procedures are those considered most relevant to this site. The site characterization methodologies described are limited to those pertinent to the disciplinary areas of hydrology and geochemistry. Where appropriate, references are provided to methods and techniques from other disciplinary areas. The limitations of each site characterization procedure are noted, and recommendations are made for research and technology development that may be required to improve existing methods or reduce uncertainties in the resolution of an issue.

2. IDENTIFICATION OF HYDROSTRATIGRAPHIC UNITS WITHIN A SEQUENCE OF FLOOD BASALTS

2.1 STATEMENT OF ISSUE

An understanding of groundwater movement within the Pasco Basin will require separation of the complex sequence of flood basalts and interbeds into hydrostratigraphic units (HSU's). This is accomplished by identifying bodies of rock that function as distinct hydrologic systems for the problem being studied (Maxey, 1964). The identification of such units will depend primarily upon observation of their behavior, the physical properties of the rock, and the scale and nature of the particular groundwater flow system to be studied.

2.2 IMPORTANCE OF ISSUE

Hydrostratigraphic units form the basis of both conceptual and numerical groundwater flow models. These models are the primary tools that hydrologists use to predict groundwater flux and velocity. In a groundwater model, the HSU is generally a subdomain of the model that behaves as a continuum and has similar hydraulic properties throughout. If the actual HSU does not behave as a continuum or does not have similar properties, then such a model would be in error. Appropriate definition of HSU's is critical to accurate groundwater modeling. Correct identification of HSU's will be vital to the performance assessment of a site for nuclear waste disposal.

Hydrostratigraphic units selected for resolving a specific problem necessarily represent a compromise between conflicting demands for accuracy and simplicity. Accuracy requires knowledge of the details of the hydrogeologic system. However, economic and practical limitations require that the system be simplified. Therefore, the degree of detail used in the model must be commensurate with the available data. It makes little sense to produce a detailed model that calls for significant amounts of data that cannot be made available. The most appropriate selection of HSU's is the one that best balances these conflicting demands.

The primary consideration in identifying HSU's is that such identification be strongly coupled with the specific problem to be studied. Secondarily, it must be recognized that different HSU's may be required to study different types of hydrologic behavior. Both of these considerations are discussed later in this section. A general discussion of basic concepts governing the definition of HSU's follows in Section 2.4. Recommended approaches to the resolution of the issue are presented in Sections 2.5 and 2.6, and uncertainties that are expected to remain after the HSU's are identified are discussed in Section 2.7. Recommendations for further research are given in Section 2.8. Detailed technical discussions and an illustrative example are presented in Appendices. Appendix A presents a

review of the types of heterogeneities that are common in Columbia River basalts. Appendix B gives the scientific basis for identification of HSU's. Appendix C gives examples of HSU's that may be tentatively identified from available data on the Pasco Basin.

In summary, the importance of appropriately identifying HSU's is that these units form the basis for an understanding of the hydrology of the site. The need for a careful and thorough understanding of this issue is reflected in several sections of 10 CFR part 60:

1. Section 60.21(c) requires that the Safety Analysis Report contain an analysis of the hydrologic aspects of the site that bear significantly on its suitability for disposal of radioactive waste.

2. Section 60.31(a) indicates that the Commission must determine whether the DOE has adequately described the hydrologic characteristics of the proposed site prior to construction authorization.

3. Sections 60.111(b) and 60.112(c) require that the ability of the geologic setting to contain nuclear waste must be adequately demonstrated; this necessitates an accurate groundwater model.

4. Section 60.122 specifies those hydrologic conditions at the site that may be considered favorable in their effects on the ability of the site to meet performance objectives.

5. Section 60.123 specifies those hydrologic conditions that would have potentially adverse effects on the ability of the site to meet performance objectives.

2.3 CONSIDERATIONS IN DEFINING HYDROSTRATIGRAPHIC UNITS

A hydrostratigraphic unit was defined earlier as a body of rock that functions as a distinct hydrologic system for the problem being studied. For example, an aquifer that has a relatively higher permeability than the neighboring aquitards could qualify as an HSU because of its specific function in the hydrologic system of transmitting water. Hydrostratigraphic units differ from hydrogeologic units in that the HSU need not be constrained to conform to lithologic units. The concept of the HSU was originally introduced by Maxey (1964).

Traditionally, HSU's have been identified as bodies of rock with hydraulic properties that contrast in a uniform way with the properties of the surrounding rock. For example, an HSU defined on the basis of its relatively higher permeability as compared with the neighboring strata should maintain this permeability contrast throughout its lateral extent

even though the actual magnitudes of the permeabilities may systematically vary. However, if the unit is being defined to subdivide the rock mass for the purpose of numerical modeling, additional criteria will be required. In addition to a contrast in hydraulic properties between units, there must be a similarity of hydraulic properties within units. Moreover, the units must be amenable to subdivision into elemental volumes that satisfy the requirements of (1) continuum behavior, (2) statistically representative samples, and (3) uniform hydraulic gradients. The identification of HSU's for the purpose of numerical modeling will be emphasized in this report, and each of these requirements will be explained below.

2.3.1 Hydraulic Properties of Hydrostratigraphic Units

The hydraulic properties of a medium are the physical properties that govern the flow of fluids within the medium. The primary hydraulic properties that govern transient groundwater flux are hydraulic conductivity and specific storage. If transport phenomena are to be studied, additional properties are required, such as effective porosity, dispersivity, diffusion coefficient, and distribution coefficient. If other phenomena such as heat transfer are to be coupled, still more physical properties are required, such as thermal conductivity, heat capacity, and thermal expansion coefficients. Most of these properties are discussed by Freeze and Cherry (1979), and an example application is given by King et al. (1981).

Whichever set of physical properties is required for a particular problem, the principles used in identifying HSU's are the same. The complex geologic structure must be simplified in order to develop either qualitative or quantitative models of the properties being studied. In order to simplify the discussion of HSU's, definition of these units will be illustrated primarily with reference to the material properties governing groundwater mass flux and velocity.

Hydrostratigraphic units determined with respect to flux are not necessarily the same as units determined with respect to, say, velocity or chemical sorption. The flux field and the velocity field, for instance, depend on different geometric characterisitics of the medium. Therefore, there is a possibility that the HSU associated with flux may be different from the unit for velocity.

Identification of HSU's for groundwater models will require a demonstration that the pertinent hydraulic properties are statistically similar over the extent of the proposed unit. That is, there must exist test volumes on a scale smaller than the volume of the unit itself for which repeated measurements of a given hydraulic property will belong to the same statistical distribution. This criterion is routinely assumed in constructing numerical models because of its value in estimating hydraulic properties at unmeasured locations. Despite its widespread

use, the assumption of statistical similarity is rarely substantiated by direct field measurement because of economic constraints.

2.3.2 Effect of the Purpose of the Model on the Choice of Hydrostratigraphic Units

For analysis of a site such as the Pasco Basin, it would be advisable to prepare a series of nested groundwater flow models. These models would be of increasing detail and decreasing areal coverage. The first would be a regional model. It would be the most coarsely defined and cover the greatest area. The next would be a basin model covering the Pasco Basin. The last would be a repository, or "control zone," model. The control zone includes the rock around the repository and extends to the boundaries of the "accessible environment" as defined by the EPA. Each model would provide the boundary conditions and overall framework for the next more detailed model. The specific implications of this scheme on data collection will be discussed in Section 2.5.

In general, the data input for each model must be appropriate to the scale and detail of the particular model. Thus, on a regional scale, many basalt flows may be grouped together over a large volume as a single HSU whose average properties are internally similar but distinguishable from the average properties of the groups of flows above and below it. For the basin model, this same rock might be subdivided into individual basalt flows or structural components of flows. For example, the entablature of the Umtanum flow could be treated as a separate HSU apart from the surrounding basalts. On the control zone scale, it may be desirable to treat as a separate HSU every entablature and interflow zone in the Grande Ronde in the vicinity of the reference repository horizon. Further, it is conceivable that the detail around the repository itself could be analyzed on a scale as small as that of single fractures. On this scale, each separately identified fracture would be an HSU. Thus identification of HSU's, even at the same location in the basin, will depend on the purpose and scale of the groundwater model analysis being considered.

2.3.3 Continuum and Noncontinuum Treatment of Hydrostratigraphic Units

The type of analysis used, porous continuum or noncontinuum, will determine which hydraulic properties are measured. Treating the HSU as a continuum is the logical first choice, because the data requirements of existing techniques for treating HSU's as noncontinuous, discrete fractures are essentially impossible to satisfy except perhaps in the immediate vicinity of the repository. Because of this difficulty, emphasis in this discussion will be on the identification of HSU's from the standpoint of a continuum. A discussion of the continuum and noncontinuum approaches is presented by Kanehiro et al. (1981, p. 187).

Intrinsically heterogeneous fractured rock can behave like a homogeneous porous medium under certain conditions. Techniques for determining

when these conditions exist are being developed. An approach recently developed by Long et al. (1981) is based upon the representative elementary volume (REV) concept. The concept of the REV has developed as an attempt to define the minimum volume of a particular geologic medium that will exhibit homogeneous behavior with respect to groundwater flux (Hubbert, 1956, p. 227). A volume is considered representative when small increases in the test volume have no significant effect on the averaged value of the material property being measured. In the case of a basalt flow, the average hydraulic conductivity of a volume element would be representative of the average hydraulic conductivity of, say, the entablature of the flow when further enlargement of the test volume at a given location in the entablature results in no further significant change in the measured average hydraulic conductivity. A discussion of geologic nomenclature as applied to typical basalt flows is presented in Appendix A.

The principle of the REV is shown schematically in Figure 2.1. On the scale of the single fracture, measured parameters are likely to be highly variable. On the slightly larger scale of a principal component of an individual basalt flow, such as the entablature, it may be possible to identify an REV. As the scale of observation increases to include combinations of entablatures and flow tops, some variation in measured parameters may be anticipated until enough flows are included to obtain a sufficiently large sample of heterogeneities that the effects of the individual units are averaged and the volume can again be considered representative. From this discussion and Figure 2.1, it is evident that REV's can exist on more than one scale within the same rock.

In order to have an accurate continuum analysis, the REV must be at least as small as the HSU and must also be of a size appropriate to the kinematic effects of the groundwater flow patterns. The reason for this is illustrated briefly below and in detail in Appendix B. Consider the identification of HSU's for a small-scale, detailed model. As increasing detail is required, smaller and smaller HSU's must be defined, because finer contrasts in hydraulic properties and finer changes in the gradient field become significant as we look at the problem in detail. Each HSU must be made up of at least one REV that behaves as a continuum in order to have an accurate continuum analysis as described by Hubbert (1956). However, the heterogeneities in the rock may be such that it does not behave as a continuum on a scale at least as small as that of the HSU. This would be the case for the rock shown in Figure 2.1 if the HSU desired is much smaller than v_1. If the basalt does not behave as a continuum on the appropriate scale, the errors associated with a continuum analysis can be quite large.

The appropriate scale for analysis is determined primarily by the kinematic effects of the groundwater flow patterns being studied. In order to be mathematically modeled as a continuum, the basalt must be divisible into discrete elements at least as large as the REV, within which the hydraulic gradient is generally uniform. If the gradient is not generally

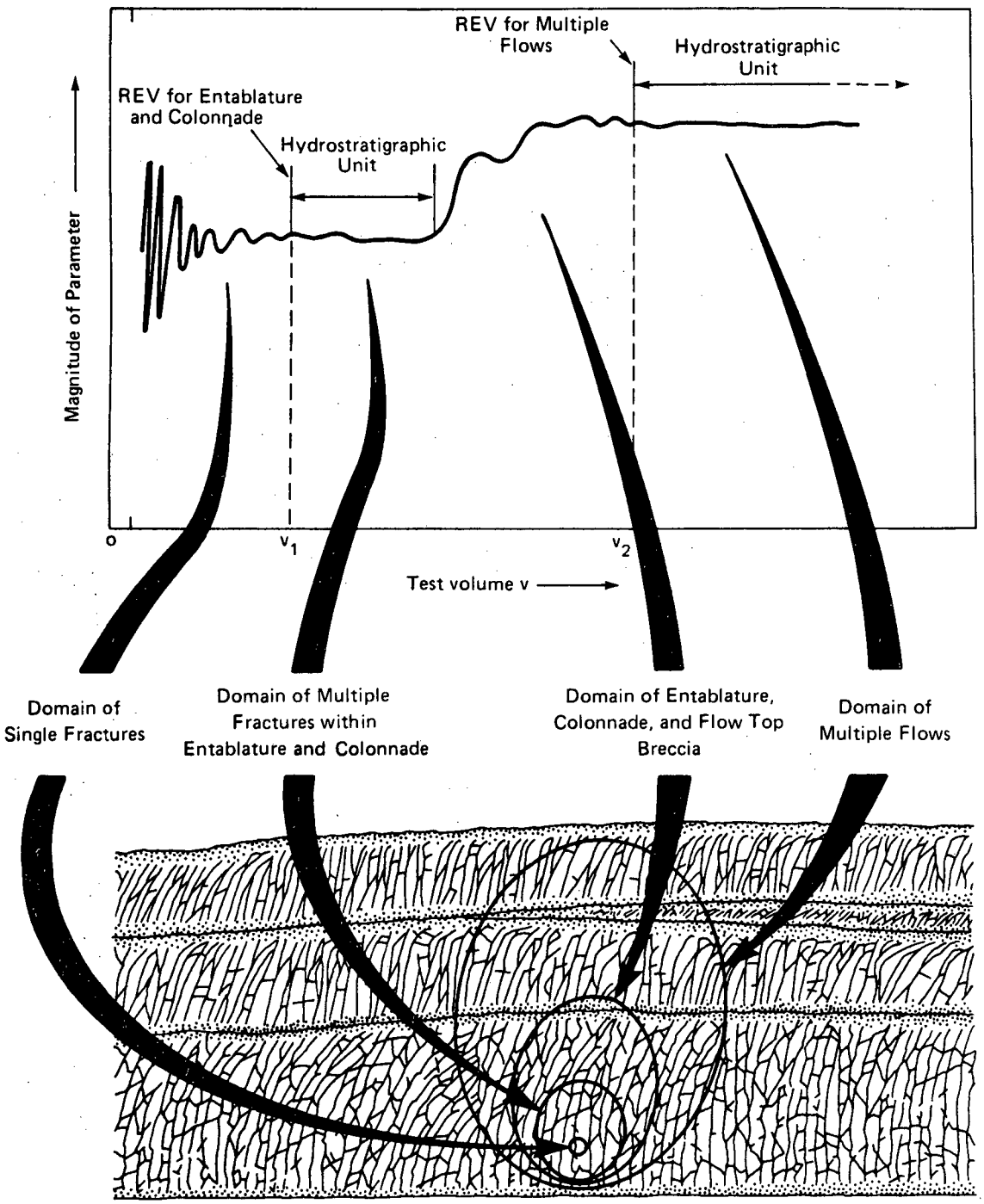


Figure 2.1. Schematic definition of a representative elementary volume (REV) as applied to a flood basalt sequence (adapted from Hubbert, 1956). [XBL 8110-12138]

uniform within each element and the elements are near the size of the REV, continuum behavior of the elements cannot be assured. Additional discussion of the kinematic requirements for uniform gradients is presented in Appendix B.

In standard practice the appropriate size of an element is assumed, without the benefit of field measurements, to verify the assumption of continuum behavior or even to show that a representative volume exists on any scale. All continuum models inherently assume that the volumes they are dealing with are representative volumes, and therefore assume that the representative elementary volume is smaller than the smallest volume treated. Thus essentially every approach to groundwater modeling is an "REV approach," though this may not be explicitly recognized. Many successful models have been developed without directly demonstrating either the size or presence of an REV. Such models have been verified by standard head matching techniques that provide an indirect indication that the assumptions of representative continuum behavior are acceptable. This type of approach may or may not be successful with fractured basalts. The extent to which the REV's must actually be verified by field measurements cannot be specified a priori. The number of such measurements required will depend on the validity of the groundwater models developed from standard field tests. This will be explained more fully in Section 2.6.

If a particular mass of basalt does not behave as a continuum, its hydraulic properties may be expected to vary significantly with small changes in test volume. It may be necessary to identify such HSU's on the basis of contrasts in hydrologic function with neighboring units, without regard to questions of statistical similarity of hydraulic properties within the unit. The mathematical treatment of HSU's that do not exhibit continuum behavior, but must be considered in regional flow analysis, is a difficult technical question that largely goes beyond the issue of unit identification addressed here. A stochastic approach is the only feasible analytic technique, but such an approach would be a topic for research.

2.4 METHODS OF IDENTIFYING HYDROSTRATIGRAPHIC UNITS

Two basic methods are available for HSU identification: those involving observations of present behavior and those involving physical property measurements. Direct observation of the present behavior of the groundwater can serve to identify rock volumes that function as distinct hydrologic systems. Such rock volumes are by definition HSU's, but HSU's identified in this manner may not be applicable to the hydrologic system when it is perturbed. For example, an HSU identified in this manner may be correct for regional, unperturbed flow but not for analysis of flow in the control zone. An alternative approach is to measure directly the physical properties of the rock and water that control the hydrologic functions of interest in site characterization. Thus, for the functions of flux and velocity, for example, one would want to measure hydraulic conductivity,

specific storage, and effective porosity. Variations in hydrologic functions among the various bodies of rock could be inferred from such measurements, which would then serve as the basis for identifying HSU's. The fundamentals of these two approaches are described below. Appendix C gives an example of the use of these methods by identifying potential HSU's on the basis of data currently available from the Pasco Basin.

2.4.1 Observations of Present Behavior

Observations of present behavior include all tests that measure the present, in situ, ambient conditions in order to identify the hydrologic systems present within the rock. An example of such a test would be the use of linear hydraulic gradients across a sequence of strata as an indication that these strata, as a unit, are behaving as a distinct and relatively uniform hydrologic function with regard to groundwater flux.

The advantage of such "behavioral" tests is that they can be truly long-term and large-scale indicators, because they rely upon long-term natural perturbations. The disadvantage of behavioral tests is that they provide only qualitative information regarding those systems established in response to the particular perturbations that now exist at the site. For example, a uniform hydraulic gradient across several strata may be evidence that the strata are behaving as a single HSU in response to the natural field gradient, but this provides no information regarding the response of the unit to a gradient in another direction. The perturbations induced by repository excavation and operation and by some hypothetical breach scenarios must be superimposed upon the natural perturbations. System response to these types of activities would not be the same as the existing natural system behavior. Interpretations of the hydrologic system drawn from natural behavioral tests are therefore not necessarily applicable to HSU's within the disturbed zone of the repository. These types of tests are best suited for studying field conditions that will remain unaffected by significant repository-induced perturbations.

Listed below with brief descriptions are examples of classes of measurements based on present behavior.

1. Groundwater head and hydraulic gradient measurements. A uniform or regularly changing groundwater head or hydraulic gradient can be an indication that the strata are behaving as single hydrologic units in response to that gradient.

2. Groundwater chemistry and geochemical gradient measurements. Uniform or regularly changing geochemical characteristics of groundwater are indications that the strata are behaving as single hydrologic units with regard to ion migration under existing hydraulic and geochemical gradients.

3. Groundwater age dating. Uniform or regularly changing groundwater ages are indications that the strata are behaving as single hydrologic units with regard to groundwater movement under existing hydraulic and geochemical gradients.

2.4.1.1 Groundwater head

Measurement of groundwater head provides an indication of the hydraulic response of the rock to the existing boundary conditions. Any conclusions derived from this technique may be applicable only to the hydrologic systems established by these boundary conditions and may not be valid for flow patterns established by other boundary conditions. Groundwater head is expected to be most useful in indicating HSU's for the far-field, where the perturbations introduced by the repository are not expected to be significant. Erroneous inferences can be drawn from groundwater head data if significant pressure transients exist. This method is best suited for flow regimes that are essentially in steady state.

As can be seen from the foregoing discussion and from Appendix B, HSU's appropriate for modeling essentially steady-state, natural conditions would be indicated by uniform hydraulic gradients that result in linear variations in hydraulic head with distance. If the average gradient through structural units of significantly different permeabilities is uniform, the hydrologic system is behaving as if it were homogeneous. This implies that the conditions for an REV may be satisfied on the scale of observation of the uniform gradient and for the natural steady conditions and direction of groundwater movement observed. Groundwater head measurements thus can be useful in identifying HSU's in the far-field, where natural conditions are not expected to be perturbed by the repository.

2.4.1.2 Groundwater chemistry and age dating

Groundwater chemistry and age dating serve as indicators of HSU's in much the same way as hydraulic head. Both techniques are measurements of the behavioral response of the groundwater to natural conditions and thus are primarily applicable to far-field analyses.

The chemical constituents of groundwater at a particular location within the rock mass are a function of the initial chemistry of the water at the recharge point, the environmental conditions along the subsurface flow path, and the travel time from the point of recharge. Environmental conditions would include the ambient temperature, the water pressure, the chemical constituents of the rock, the chemical constituents of the fracture coatings along the flow path, and the antecedent groundwater chemistry.

Hydrostratigraphic units would tend to be indicated by either uniform or regularly changing hydrochemical conditions, which are signs of hydrologic similarity. Rapidly changing hydrochemical conditions, on the other hand,

might be an indication of major hydrologic changes. Information gained from age dating is useful in the same sense, and if the data are reliable, age dates can provide good indications of groundwater velocities. The degree of confidence placed in hydrochemical methods should be commensurate with the reliability of the data. It is necessary to support conclusions based on hydrochemical data with stratigraphic and hydrologic data.

2.4.2 Rock and Water Hydraulic Property Measurements

Groundwater moves in a network of interconnected void spaces consisting of fractures and pores within the basalt flows and interbeds. Resistance to groundwater movement results from the physical geometry of this network of flow conduits, the compressibility of the basalt, and the specific weight, viscosity, and compressibility of the water. Those hydraulic properties related to the physical properties of the basalt are the most important for field measurement, particularly properties related to the highly variable geometry of the flow conduits. The physical properties of the water are not highly variable under normal environmental conditions and are consequently less difficult to characterize in the field.

Hydraulic property measurements include all direct and indirect analytical methods that are independent of existing ambient conditions. That is, these methods rely either on direct measurement of a physical parameter, such as counting the frequency of natural open fractures in a drill core, or on indirect measurements of response to an induced perturbation of the natural system, such as a borehole injection test. Many hydraulic properties are measured by recording the response to an artifically induced perturbation that is stronger than any similar natural perturbation that would be expected to occur at the site. An example of this would be the creation of a strong vertical hydraulic gradient within the proposed repository horizon to measure vertical hydraulic conductivity if no strong natural vertical hydraulic gradient exists under natural conditions.

Examples of classes of physical property measurements are given below along with brief descriptions:

1. Geologic and stratigraphic measurements. These include all information obtained by direct observation on the stratigraphy and structure of the geologic units and on the geometry of the fracture systems, faults, and folds.

2. Hydrological measurements. These include all field and laboratory tests involving measurement of the response of the geologic system to induced hydrologic perturbations. This category includes all permeability and tracer tests that rely upon induced hydraulic gradients.

3. Geophysical measurements. These include all surface and borehole tests that utilize electromagnetic, seismic, sonic, radiological, and other means to obtain indirect information on the physical properties of the rock mass.

4. Associated rock property measurements. These include all field and laboratory tests that measure rock properties through other than hydrologic perturbations. They include rock compressibility, fracture stiffness, thermal conductivity, and geochemical properties.

The first three of these classes of measurements--the geologic and stratigraphic, the hydrogeologic, and the geophysical measurements--are the most important in the identification of HSU's. They are the most directly concerned with defining statistical similarity within candidate rock bodies because they provide measurements of the properties that most closely control groundwater movement.

The fourth class--the rock property tests measurement--generally yields data needed to predict rock response to repository-induced perturbations within the disturbed zone. Some of these perturbations may locally alter the hydraulic properties of the rock in a manner that may, in some cases, be significant. It must be decided on a case-by-case basis whether these changes are sufficient to constitute local redefinition of the HSU. Because the rock property measurements are in general not fundamental to the identification of HSU's for flux or transport, they will not be considered further here.

2.4.3 Special Considerations for the Disturbed Zone

The foregoing discussion has been primarily directed toward considerations of HSU identification for the regional and especially the basin model where existing hydraulic head and hydrochemical information can be used as aids in identification. In the disturbed zone of the repository, the flow patterns are expected to be considerably altered as a result of repository construction and waste emplacement. Thus the value of existing hydraulic head and geochemical data will not be as great as in the far-field. The effect of this consideration will be to retain the same basic approach to identifying HSU's as for the far-field, but the role of material property measurements will be emphasized and the role of existing "behavioral" data de-emphasized. The creation of gradient fields by repository excavation and waste emplacement will have to be anticipated if HSU's are to be identified on a scale that is kinematically appropriate for continuum behavior. The development of a test facility at depth within the repository horizon would help to identify the types of gradient fields to expect. Examples of the types of tests that might be performed in such a facility are given in Section 2.6. Similar considerations will apply to the identification of HSU's appropriate for studying the various breach scenarios.

2.5 RECOMMENDED HYDROLOGIC APPROACHES FOR RESOLVING THE ISSUE OF HYDROSTRATIGRAPHIC UNITS

A field exploration program directed toward the identification of HSU's in flood basalts is discussed here in general terms. The approach is iterative, and specific decisions as to which tests to perform at which locations must be made after a thorough review of all field data available at each step in the process. The field techniques are dictated by the need to characterize the behavior of various volumes of rock on scales appropriate for the required fluid flow analysis. The approach recommended here assumes that the analysis will be based upon continuum mechanics whenever feasible; thus emphasis is placed on identifying conditions for continuum behavior with regard to groundwater flow. The approach relies upon the use of standard site characterization techniques and the continuing refinement of numerical models to verify the accuracy of the field data and appropriateness of the HSU's. Refined field techniques are also provided, and should be used as needed to increase the accuracy of the groundwater model. The standard site characterization techniques are described in this section, and the refined techniques are described in Section 2.6.

2.5.1 Stages of Field Investigation

As previously discussed, it is recommended that analysis proceed in stages. The first stage should be a regional analysis, the second a basin analysis, and the third a "control zone" analysis as defined by EPA standards. These three stages of analysis pertain to increasingly smaller volumes. As part of each analysis, a numerical model will be developed of the study area. An iterative procedure will be implemented for each stage, wherein the models will be continuously refined by newly acquired data and used to guide the acquisition of additional data. Although it is expected that stages would be initiated successively, there is no reason why overlap of stages should not occur. Indeed, it would be desirable to choose potential repository locations well in advance so that excessive drilling could be avoided in those areas.

The basic principles of data collection specific to each of the three stages are presented in the following paragraphs. Primary emphasis will be placed on hydrologic and hydrochemical approaches. Geologic and geophysical approaches, though important to the identification of the physical properties of the rock mass, do not provide direct hydrologic information, and detailed review of these approaches is outside the scope of this report.

2.5.2 The Role of Groundwater Models

For the purpose of repository siting on the Hanford Reservation, the regional model, perhaps of the entire Columbia Plateau, will help determine the boundary conditions for the smaller model of the Pasco Basin itself. The boundary conditions acting on the Pasco Basin are important in identification of HSU's for modeling because they determine the kinematic conditions in the basin.

The regional model should include enough of the Columbia River Plateau to determine where water enters and leaves the Pasco Basin. Thus the Pasco Basin should be entirely included within the regional model and should not share common boundaries. It would not be inappropriate to use the whole Columbia River Plateau, but a smaller area would also suffice. In any case, the boundaries for this regional model should be chosen mainly for convenience. Some logical choices might be major rivers, surface water divides that reflect groundwater divides, areas for which considerable well data are available, or outcrops thought to be recharge or discharge zones. Head data should be used only from the most permeable zones, where the majority of the water flow is concentrated and data are the most accurate.

For the most part, the regional model will be based on existing data because of its large areal extent. Well drilling and testing will be limited. Identification of HSU's for this model will mainly use the behavioral techniques described in Section 2.4.

The basin model will be smaller and more detailed than the regional model. More effort will be put into actively obtaining data for the basin model. Both behavioral and direct hydraulic property testing techniques are expected to be used. An active well drilling and testing program will be required.

The control zone model will be smaller and more detailed than the basin model. It will differ from the previous two models in that the flow systems that must be predicted will include perturbations of the existing flow system. Therefore, greater emphasis will be placed on hydraulic property testing.

2.5.3 Field Program Development Using Standard Technology

The conventional approach to identifying HSU's in the field for the purpose of numerical modeling is to assume that an REV exists on a scale kinematically appropriate for the analysis at hand. In many cases, it is also assumed that the field measurements of hydraulic parameters are representative of average rock properties on this same scale, without making an effort to assure that the appropriate volume of rock has been perturbed by the test. Hydrostratigraphic units are identified primarily on the basis of expected or measured functional contrasts with adjacent units, and are assigned hydraulic properties on the basis of very little information.

The conventional approach has been successful largely because the demands for accuracy have historically not been stringent. Estimation of many hydraulic properties to within an order of magnitude of the actual field value is often considered "good." The cost of refined approaches is generally high, and the assumptions made have proved to be acceptable for many studies, particularly predictions of groundwater flux in porous media. The use of this approach in flood basalts may or may not be successful.

The conventional approach has been preferred for characterization of flood basalts because the high degree of fracturing commonly found in the entablatures, and particularly in the flow-top breccias, provides some confidence that the conventional approach will be acceptable. Further, the conventional approach has been used with some success in similar rock types elsewhere on the Columbia Plateau--e.g., at Idaho National Engineering Laboratory (Barraclough and Jensen, 1976).

As discussed earlier, verification of the numerical model is expected to provide the most realistic indication of the appropriateness of the HSU's and the hydraulic properties obtained with conventional techniques. If an acceptable model cannot be developed using these techniques, refinements will be required. The most obvious refinement--which, in fact, should be implemented from the outset of the program--is to assure that the volumes perturbed by the conventional tests are on a scale appropriate to the magnitude of the heterogeneities. For instance, if a sequence of basalt flows is to be considered as a single HSU, then the hydraulic properties should be measured in such a way that their values are averaged over the whole sequence. In the refined techniques discussed in Section 2.6, procedures for making large-scale tests are presented for measuring the size of the REV and for considering kinematic effects.

2.5.4 Hydrologic Data Needs

Groundwater flux depends upon the material properties of hydraulic conductivity and storage coefficient. If only steady flow is considered, then only hydraulic conductivity is required. Effective porosity is required in addition to the other two properties if groundwater velocity is to be made a part of the definition of HSU's.

2.5.4.1 Standard tests to obtain hydrologic data

Hydraulic head and the parameters of hydraulic conductivity and storage coefficient required to evaluate groundwater flux are routinely measured in the field using techniques that are described in a number of publications. Field tests for these parameters have been described specifically for application to flood basalts by Long and Wilson (1978). The application of borehole tests to low-permeability rock has been reviewed by Wilson et al. (1979). Other general tests providing measurements of permeability and storage coefficient have been reviewed by Ferris et al. (1962), Zeigler (1976), Earlougher (1977), and Raghavan (1978).

Selected papers are also available for specific types of tests. The standard tests, their specific limitations, and key references are listed below. General limitations to these tests are discussed in the following subsection.

1. Slug test. Measures isotropic horizontal hydraulic conductivity accurately and storage coefficient approximately by monitoring the perturbation caused by falling head in a vertical pipe under

the influence of gravity. The principle limitations for low-permeability basalts are long test times and small test volume. Key reference: Cooper et al. (1967).

2. Pulse test. Measures isotropic horizontal hydraulic conductivity accurately and storage coefficient approximately by monitoring the perturbation caused by rapid injection of water into an isolated cavity. Principle limitation in basalts is small test volume. Key reference: Bredehoeft and Papadopulos (1980).

3. Injection test. Measures isotropic horizontal hydraulic conductivity accurately by monitoring the perturbation caused by injection of water under constant head or flow rate. Measures storage coefficient accurately with observation wells. Principle limitation is requirement for clean water supply. Key reference: Doe and Remer (1981).

4. Pump test. Measures isotropic horizontal hydraulic conductivity accurately by monitoring the perturbation caused by withdrawal of water under constant flow rate or head. Measures storage coefficient accurately with observation wells. Principle limitation is pumping from significant depth in small diameter boreholes as required at Hanford. Key reference: Stallman (1971).

5. Leaky aquifer tests. Measures vertical hydraulic conductivity in aquitards with observation wells by monitoring the perturbation caused by either pumping or injection methods. Principle limitation is requirement for high-permeability contrast between aquifer and aquitard, and may be only a point measurement. Also has limitations of pump or injection tests. Long test times and low sensitivity for low-permeability rock. Key references: Hantush (1956) and Neuman and Witherspoon (1972).

6. Tracer tests. Permits computation of effective porosity if hydraulic conductivity is known by measuring the linear velocity of groundwater from the travel time and linear travel distance of a tracer. Dispersion can be determined from the concentration of tracer as a function of arrival time. Requires multiple wells. Is only standard hydrologic test available for effective porosity and dispersion. Principal limitations are long test times for low-permeability media or large test volumes and uncertainty about representativeness of results. Nonsorbing tracers should be used. Key reference: Freeze and Cherry (1979).

7. Interference tests. Measures anisotropic horizontal permeability and detects orientation of flow barriers by monitoring the perturbations caused by either pumping or injection methods. Limitations same as those of pump or injection test. Key references: Ramey (1975 and 1981).

8. Numerical model calibration. Estimates regional average horizontal or vertical hydraulic conductivity by monitoring the perturbations caused by natural phenomena or large-scale pumping or injection tests. Many observation wells required over large area. Principle limitations are large data requirements, large time requirements, low precision, and need for appropriate perturbations. Key reference: Neuzil and Bredehoeft (1981).

9. Hydraulic head. Measures natural in situ groundwater head. A portion of a borehole is isolated hydraulically from the balance of the borehole and allowed to come to equilibrium with natural pressure of the rock mass. Principle limitations are difficulty of isolation and long test times in low-permeability basalts. Key reference: Veneruso and McConnell (1981).

Test selection will depend upon the conditions at the site and the types of measurement required. The greatest variety of test methods is for hydraulic conductivity. Pumping tests are the most desirable because they are well known, can be run for very long times, and have the widest range of available analytical solutions. Injection tests are good alternatives, particularly for applications to low-permeability rock, where water supply demands are not excessive and the control of injection pressure will permit more rapid testing. Pulse or slug tests may also be appropriate for lower-permeability zones if large test volumes are not required. Interference and leaky aquifer tests should be conducted in multiple borehole clusters to obtain information on vertical permeability, flow barriers, and horizontal anisotropy. Multiple well pumping tests are particularly good for large-scale measurements of higher-permeability zones. Tracer tests should be considered in the design of every multiple well test to obtain measurements of effective porosity and dispersion.

Hydraulic head should be measured in specific basalt horizons in a hydraulically isolated part of the well. Isolation can be achieved either by temporary packers or a permanent seal, but in either case isolation from the hydraulic effects of the well bore must be complete. Good head measurements may take a considerable amount of time, particularly in low-permeability media, because the water pressure in the rock must recover from perturbations caused by exposure to the open well. The effectiveness of packer seals may be demonstrated by a four packer system that creates three isolated zones. The seals of the two center packers, which straddle the test zone, can be checked by changing water pressure in the outer zones and monitoring the test zone for a response.

Numerical model calibration is an acceptable technique for estimating regional average hydraulic conductivity values when field measurements are sparse or of questionable accuracy. This is particularly true for vertical conductivity, which is difficult to measure accurately on a regional basis with surface borehole tests.

2.5.4.2 Limitations of standard tests for collection of hydrologic data

In addition to the specific limitations described above, standard hydrologic tests have several important general limitations. These fall into three categories: (1) the size of the test, (2) the manner of measurement, and (3) the properties that are measured.

Size of Test. Most tests are conducted in such a way that they perturb a relatively small volume of rock compared to the volumes that may be required to identify statistical homogeneity for some of the larger HSU's. Thus, although small-scale tests will be adequate to evaluate HSU's on the order of tens of cubic meters, they may not be adequate to evaluate larger units. Methodologies are needed for field tests to identify hydraulic properties at a given location on a series of scales, which can range into very large volumes, or for integrating the results of a large number of smaller-scale tests.

Several of the standard tests described above are easily adaptable to long-term, large-scale testing. The pump test is particularly well suited for this, as previously mentioned, and has been used effectively for this purpose on many occasions. Multiple well pumping or injection tests are recommended as the best of the standard tests for long-term, large-scale testing.

Manner of Measurement. Most tests are conducted from boreholes that induce a radial perturbation. The resulting patterns of flow into the borehole are therefore not occurring in response to a uniform, linear hydraulic gradient, and the average hydraulic properties that are measured are biased by the properties of the rock nearest the borehole. Methodologies are needed for in situ tests that measure unbiased average hydraulic properties over the volume of the rock.

This limitation may be partially overcome by standard multiple well tests, which can provide an indication of variations in hydraulic properties with distance and direction. If such variations are determined to be minor, the borehole test results will probably provide sufficient indication of continuum behavior of the basalts. If the variations are not minor, then a refined testing technique that produces a uniform, linear hydraulic gradient may be required to verify continuum behavior. Such tests are discussed in Section 2.6.

Properties Measured. Tests for measuring the properties controlling the vertical movement of groundwater are not well developed. The leaky aquifer test is the only standard technique for directly measuring vertical hydraulic conductivity from surface boreholes. Depending on the nature of the heterogeneities and the duration of the test, only a point measurement may be obtained, which may not accurately predict large-scale behavior. Numerical model calibration provides an indirect method of estimating vertical (or horizontal) conductivity on a regional scale. Considerable head data and a perturbation that generates moderate vertical groundwater movement must be available for reliable results.

Tests for measuring effective porosity and dispersion in heterogeneous, fractured rock are also not well developed. Standard tracer techniques are based on porous media flow assumptions, thus it must be known a priori that the volume tested behaves as a continuum. Methods for testing the assumption of continuum behavior with respect to these properties are required, as well as methods for integrating the results of large numbers of small-scale tests to approximate large-scale behavior.

2.5.5 Hydrochemical Data Needs

In general, any type of hydrochemical data that can be interpreted to indicate the nature of groundwater flow patterns may be suitable to assist in the identification of HSU's. Hydrochemical data may be used in two basic ways: (1) to identify hydrochemical contrasts and (2) to identify ongoing hydrochemical processes.

Analysis of data for hydrochemical contrasts involves using the relative proportions of specific cations and anions present in the water as indicators of hydrochemical similarity. Abrupt changes in these proportions in water samples taken at different locations will indicate hydrochemical contrasts, which may coincide with hydrostratigraphic boundaries. An example of a hydrochemical contrast would be a change from water rich in sodium bicarbonate to water rich in sodium chloride over a relatively short distance. The apparent ability of the geohydrologic system to maintain such an abrupt contrast over a long period of time may result from the presence of a physical restriction to groundwater movement that has prevented mixing. Other, nonstructural causes for such hydrochemical contrasts are also possible, and should be considered in interpreting groundwater movement in terms of hydrochemical data alone. An example of a nonstructural cause for a hydrochemical contrast that could lead to a misinterpretation of data is given in Section 2.5.5.2.

The second method of data analysis involves the use of progressive hydrochemical change to indicate the direction and possibly the velocity of groundwater movement. The chemical constituents and isotopic content of groundwater are normally expected to change with time, with variations in environmental conditions such as water temperature, and with variations in the chemical constituents of the rock. An example of this method is the use of radioactive tracers to indicate groundwater age. Another example is measurement of the concentration of total dissolved solids (TDS) in the water at various locations. The TDS concentration can, under favorable conditions, progressively increase with groundwater residence time. Such an increase may indicate the direction of groundwater movement. An example of the use of TDS content to indicate the direction of groundwater movement within the Mabton Interbed in the Pasco Basin is shown in Figure C.2. Regular flow patterns with no abrupt changes in direction or velocity are indications of continuous HSU's.

The number of specific hydrochemical constituents, chemical reactions, and isotopic decay patterns that can be profitably studied for input to the identification of HSU's is very large. Data analysis for hydrochemical contrast relies upon the detection of variations in the natural chemical constituents of the groundwater. The specific constituents or hydrochemical processes that may be studied will depend upon the chemistry of the basalt, the initial chemical composition of the water, and the environmental conditions encountered along the groundwater flow path. Because these factors cannot all be anticipated in advance, the specific techniques that will prove successful cannot be known until a regional baseline study which is broad both in terms of chemical species and areal extent can be completed.

Application of hydrochemical data to identification of HSU's requires a well-grounded understanding of the basic principles of interpreting field data, such that maximum advantage can be taken from whatever actual field conditions are encountered. A number of analytical techniques have, however, been applied with some success to flood basalts and will be used as examples in the following discussions of alternative approaches to the problem of data interpretation.

2.5.5.1 Analyses to obtain hydrochemical data

Comparison of the relative proportions of specific anions and cations of various waters in terms of their concentrations expressed in equivalents per liter has been shown to be an effective approach in basalt. This method is capable of indicating sharp contrasts in chemical character; moreover, data plotted in a trilinear fashion can also indicate progressive chemical reactions. The method is well suited for the study of ion-exchange processes, but also provides information on other types of reactions, such as precipitation. A discussion of the principle graphic techniques for data analysis is presented by Freeze and Cherry (1979, p. 247). Examples of the application of these techniques to Pasco Basin flood basalts is presented by Gephart et al. (1979, Figures III-45 and III-49). Figure II-45 from Gephart et al. (1979), showing a trilinear diagram, is reproduced as an example in Figure 2.2 of this report.

The major inorganic constituents of groundwater normally considered in hydrochemical studies are silica, calcium, magnesium, sodium, potassium, chloride, sulfate, carbonate, and bicarbonate. In addition, a multitude of minor or trace constituents, as well as characteristic properties (such as pH), also exist, which can be used to differentiate groundwater types and flow patterns. Examples are tritium, whose presence in significant quantity may indicate relatively young groundwater (Apps et al., 1979, p. III-7), and nitrates, which can indicate recharge by irrigation water (Gephart et al., 1979, Figure III-43).

Data indicating progressive hydrochemical change are generally derived from studies of major and minor inorganic constituents and elemental isotopes. The relative concentrations of certain inorganic constituents is sometimes

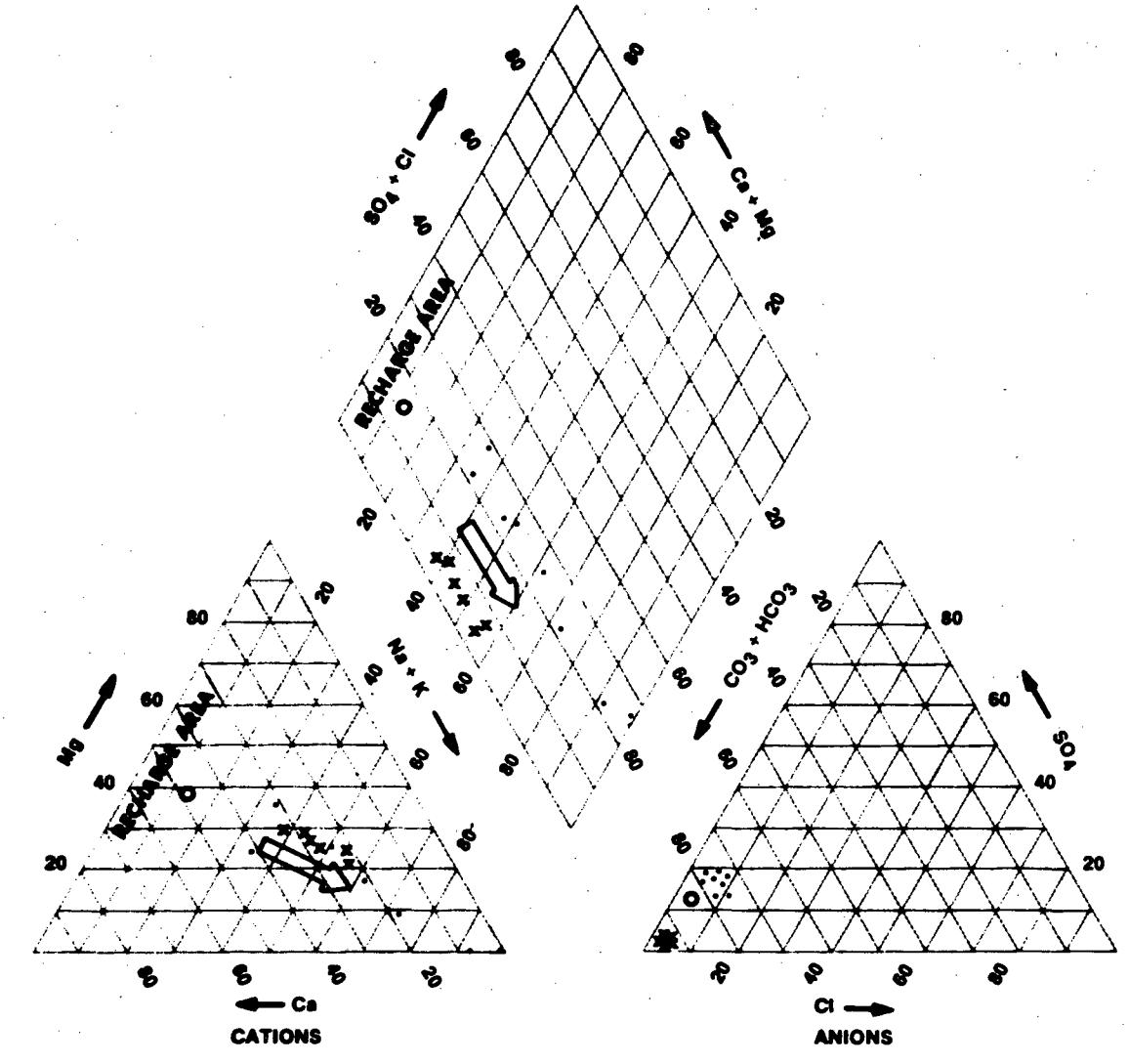


Figure 2.2. Trilinear plots of major inorganic constituents of groundwater from upper Wanapum Basalt, showing progressive hydrochemical change related to increasing distance from recharge area (from Gephart et al., 1979, Figure III-45). [XBL 826-10495]

seen to change progressively along a flow path as the groundwater reacts chemically with the rock. These trends can also be affected by such processes as bacterial action, and are subject to other environmental conditions such as changes in temperature. Progressive change can also be seen in areas of groundwater mixing. An example of a progressive change in groundwater in the upper Wanapum Basalt was prepared by Gephart et al. (1979, Figure III-45) and appears in this report as Figure 2.2. This example shows a progressive shift from calcium carbonate enrichment to sodium carbonate enrichment as the groundwater moves away from the area of recharge.

Both stable and radioactive isotopes can be studied from the standpoint of progressive hydrochemical change to indicate direction of groundwater movement. Some isotopes can be used to determine groundwater age. A summary of the principles behind the various isotopic measurements is presented by Apps et al. (1979, p. III-6).

One isotope technique that has been successfully applied to the Pasco Basin basalts is use of the oxygen-18/oxygen-16 ratio to identify the direction of groundwater movement. This stable isotope technique relies upon isotopic exchange between water and host rock, which causes a progressive decrease in the oxygen-18/oxygen-16 ratio with residence time. Application of this technique to the Mabton Interbed in the Pasco Basin yielded groundwater flow patterns similar to those obtained from hydraulic head and total dissolved solids data (Gephart et al., 1979, Figure III-44). These results are shown in Figure 2.3 and may be compared with results based on hydraulic head and total dissolved solids data shown in Figure C.2.

The oxygen-18/oxygen-16 ratio technique is summarized along with other stable isotope techniques by Faure (1977) and by Fritz and Fontes (1980). Other stable isotope techniques that may be applicable to flood basalts are the carbon-13/carbon-12 ratio, the deuterium/hydrogen ratio, and the sulfur-34/sulfur-32 ratio.

Additional methods involve use of radioactive isotopes such as tritium, carbon-14, and the uranium-234/uranium-238 equilibrium relationship. Tritium is generated in the atmosphere by cosmic ray bombardment and by thermonuclear explosions. Its half-life of 12.3 years permits age dating of water up to 25 years old by conventional methods. Carbon-14 is also produced in the atmosphere through cosmic ray bombardment. With a half-life of about 5730 years, it is capable of yielding age determinations up to 40,000 years before present by conventional methods. Uranium-234 is sometimes found to be strongly out of equilibrium with its parent, uranium-238. The subsequent reapproach to equilibrium conditions can be used to date the water, provided enough is known about the in situ environment and the conditions that caused the initial disequilibrium. Uranium-234 has a half-life of 2.44×10^5 years, and groundwaters as old as 5×10^5 years might feasibly be dated, although many questions on the behavior of uranium isotopes in groundwater remain to

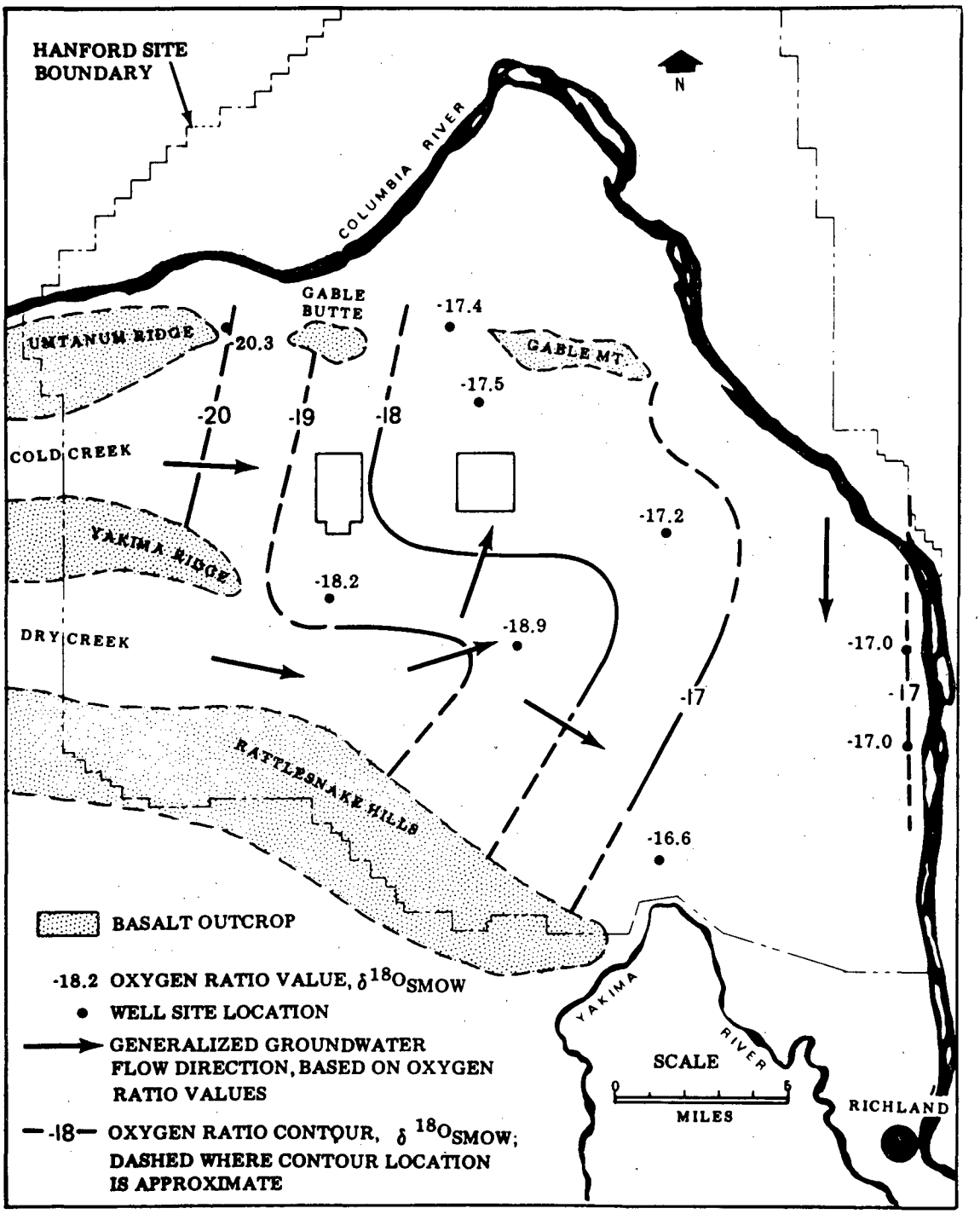


Figure 2.3. Generalized groundwater flow direction within the Mabton Interbed; based on oxygen-18/oxygen-16 ratios (from Gephart et al., 1979, Figure III-44).
[XBL 826-10496]

be answered. Further discussion of these techniques is supplied by Apps et al. (1979, p. III-7). Because radioactive isotopes can provide age data as well as information on progressive hydrochemical change, they can be used to determine the velocity as well as the general pattern of groundwater movement.

2.5.5.2 Limitations to hydrochemical approaches

Limitations to both conventional and unconventional approaches are similar and will be discussed together in this section. Several limitations are of fundamental importance.

First, all hydrochemical data are, from a hydrologic standpoint, essentially measurements of system response to long-term, natural groundwater movement. Thus inferences based on these data can be interpreted only in terms of HSU's appropriate for the natural, regional flow system and may not be adequate for identification of HSU's appropriate to repository-induced flow conditions, particularly within the disturbed zone.

Second, hydrochemical data are only indirectly indicative of hydrologic behavior and may, in some circumstances, be misleading. For example, a sharp hydrochemical contrast may be the result of a geochemical barrier (such as a zone with strongly reducing characteristics) rather than a hydrologic barrier. Thus, although nuclide migration may be strongly affected, groundwater flux may be unaffected. A hydrologic basis should be identified to substantiate any significant conclusions regarding HSU's derived from hydrochemical data.

Third, hydrochemical techniques, and particularly those involving progressive chemical changes with distance or time, rely strongly in their interpretation upon assumptions of basalt chemistry and environmental conditions that may be difficult to verify. For example, successful application of the uranium-234/uranium-238 disequilibrium technique requires detailed information on the location and environmental conditions at the initiation of disequilibrium as well as during the subsequent reapproach to equilibrium. This point has been succinctly made by Apps et al. (1979, p. III-9): "These . . . conditions can vary for each site and create uncertainties with this and most other dating methods since the "clock" radionuclide is not isolated in a completely closed system during the decay, but is subject to continuous interactions with its environment, some of which could disturb the clear interpretation of the decay data."

Fourth, hydrochemical data are commonly rendered unreliable by contamination during field sampling, resulting from such diverse causes as drill bit wear against the rock, drilling fluid invasion, and interaquifer mixing through an open well. A discussion of field sampling problems and precautions is presented by Apps et al. (1979, p. III-9).

2.5.6 Considerations in Test Program Design

The amount of data that would be required to identify HSU's sufficient to characterize a nuclear waste disposal site is not easily specified. For the Pasco Basin, Long and Wilson (1978) have shown that data collected from some 12 to 15 wells may be sufficient for development of a preliminary basin model that would serve to indicate the principal patterns of groundwater movement and show where additional data are needed.

If the basin is believed to be essentially in a state of equilibrium, it would be desirable to measure hydraulic heads during drilling. This will permit more rapid head measurement because perturbations caused by the well will be small. The head profile can be examined for indications of zones of constant average gradient. These data can be used as early indications of possible HSU's.

The indications provided by head measurements should be verified by direct measurement of hydraulic properties pertinent to the problem. For radionuclide transport, the principal hydraulic properties are hydraulic conductivity, specific storage, effective porosity, and dispersion. Of these, specific storage has the least importance in regional flow. Although reasonable estimates of horizontal hydraulic conductivity can be made from one well, the remaining parameters require multiple well tests.

Site characterization will most likely be conducted in stages, beginning with more general, regional scoping studies and narrowing in time to highly detailed studies of a well-defined control zone for a specific candidate repository location. During the regional scoping studies of the early stages of site characterization, hydraulic conductivity will be the most important parameter to measure because of its significance in governing regional flow patterns and because of its high variability. Single wells are sufficient for these measurements because in flood basalts and other stratified systems, the large-scale average horizontal hydraulic conductivities are significantly greater than average regional vertical conductivities, and under natural flow conditions the greatest length of flow path is generally in the horizontal direction. Multiple well tests to permit measurement of vertical hydraulic conductivity are expensive and will have to be used selectively at this stage of site characterization. Multiple well tests should be emphasized in areas of suspected significant vertical groundwater flow. Vertical permeability is particularly important to predictions of contaminant migration if flow paths to the accessible environment cross basalt flows. Measurements of specific storage, effective porosity, and dispersion should also be made wherever multiple wells are available.

Horizontal hydraulic conductivity should be measured in each of the reconnaissance wells in order to determine a continuous profile and an overall average. The conductivity profile would be developed from the results of a continuous series of tests conducted in packed-off intervals

of the well, with the aim of testing the entire depth of the well. The purpose of this approach is to assure that no important water-bearing aquifer or tight aquitard is overlooked, so that all significant HSU's can be identified. The packer spacing for these tests can vary at different depths, depending upon the sizes of the HSU's indicated by the head measurements or required for future modeling. The type of test selected will depend upon rock conditions, test duration, and other considerations as discussed in Section 2.5.4. Hydrochemical data should also be taken at this stage.

Data on vertical hydraulic conductivity, specific storage, effective porosity, and diffusion will be taken from the multiple well sites. The amount of available data for these parameters is expected to be less than that for horizontal hydraulic conductivity because of the greater cost in acquiring these data. The locations for these tests should be carefully selected to provide representative samples for flow tops, interbeds, and entablatures, with emphasis on the strata in the vicinity of potential repository horizons.

Preliminary indications of HSU's will be provided by contrasts in the collected data. Head and hydrochemical data provide indirect measurements, and should be used as guides. Primary emphasis should be placed on measured hydraulic properties. The choice of HSU's and their average properties can be put into the model and checked for accuracy by model verification techniques. It should be noted that these techniques, though generally appropriate for flux, are not appropriate for verifying predictions of velocity or dispersion. The best verification of transport characteristics is obtained by inference from hydrochemical data or by direct, large-scale tracer testing. If refinements in the initial choices of HSU's are needed, they can be based either on additional data collected at different locations by the same standard techniques (to improve areal coverage) or they can be based on refined testing techniques like those described in Section 2.6 (to improve measurement reliability).

The initial studies described above are intended primarily to gain an understanding of flow patterns on the scale of the basin. The results of these studies are expected to aid in the selection of a reference repository location within the basin and to provide boundary conditions for the control zone. The final series of tests will be conducted to characterize the control zone and to focus upon specific questions that may remain concerning the behavior of the basin. The procedures are expected to be similar to those described above, except that the level of detail and the demands for accuracy are expected to be considerably greater. Specialized tests for clarifying the hydrologic significance of specific geologic features will probably be required to complete the basin-wide studies, but a series of refined tests will be required to obtain complete information on hydraulic properties in the control zone.

Nearly every test to characterize the control zone should be a multiple hole test, and far greater emphasis should be placed on vertical conductivity, specific storage, effective porosity, and diffusion than in the basin-wide

studies. Particular emphasis should be placed on determining hydraulic properties within and in the vicinity of the reference repository horizon as well as on identifying any geologic structures or aquifers that may establish the limits of the control zone. There is also expected to be heavier reliance on the refined testing techniques discussed in Section 2.6, particularly with regard to underground tests in and near the reference repository horizon. Hydrostratigraphic units would continue to be defined principally on the basis of contrasts in hydraulic properties, but with increased reference to questions of continuum behavior, statistically representative samples, and kinematic effects. Tests to characterize the control zone must be planned to minimize borehole penetration, which may impair site integrity. Alternative strategies could include statistical inference, which may be gained from data collected on the periphery of the zone, or long-term interference tests, which may also be conducted from the periphery of the zone.

2.6 REFINED APPROACHES FOR RESOLVING THE ISSUE OF HYDROSTRATIGRAPHIC UNITS

From Appendix B it can be seen from theory that it is important to know both the gradient field and the hydraulic properties on many scales in order to identify appropriate HSU's and properly assign hydraulic properties. For any subdomain of the flow region that is to be identified as an HSU, the refined approaches, if needed, should be selected to provide answers for the following questions.

1. Is there an appropriate REV for the subdomain?

2. If there is an appropriate REV, are the values of the hydraulic properties (e.g., hydraulic conductivity) statistically similar for the REV volumes throughout the subdomain?

3. If there is no appropriate REV, how can the HSU be characterized for numerical modeling?

The first step in answering these questions is to examine the nature of any weaknesses in the preliminary conceptual model of the site. Topography, stratigraphy, and available data on hydraulic head distribution, the hydraulic properties of the basalt, and the chemical constituents of groundwater would already have been used to approximate the gross regional flow system in three dimensions. One of the first steps in refinement should be to assure that sufficient hydraulic head data are available to adequately define the flow system. Additional measurements should be made at important, unmeasured locations, as dictated by the preliminary flow model. The new data should check the existing hypotheses on flow patterns and provide direction for further measurements.

Once the flow patterns are adequately determined, it may be desirable to verify the size of the REV in certain critical locations by field measurements. This can be approached in either of two ways. A series of

small-scale tests can be run and the results integrated to find the size of the REV. Alternatively, tests of increasing size can be run in order to obtain a direct plot like that shown in Figure 2.1.

In porous media, the kinds of data that are useful from small-scale tests are measurements of the average hydraulic properties of equal size volumes of rock. In fractured media, useful small-scale test data include information on distributions of fracture orientations, fracture apertures, fracture size, and fracture density. Orientation distributions can be obtained from borehole logs. Fracture aperture and size are currently difficult to measure in situ, but can possibly be estimated in well tests if single fractures can be isolated by packers. Fracture density can be estimated from core data if the fracture size distribution is known (Baecher and Einstein, 1977). Integration of such data and determination of the size of the REV might be done using a method like that proposed by Long et al. (1981).

Alternatively, permeability tests can be performed on many scales at the same site. The smaller-scale tests could be standard well tests, whereas the larger-scale ones would be less conventional tests, which are described below. These large-scale tests would also serve to confirm the integration of small-scale tests at the same site. Thus some large-scale testing may be desirable even if a decision is made to rely primarily upon the results of small-scale tests. For both small- and large-scale tests, it will be important to recognize that media which do not exhibit continuum behavior in radial flow may still exhibit such behavior in parallel flow. Thus a further refinement of testing techniques is to utilize parallel flow fields in hydraulic property measurement. Because these refined tests are generally more expensive than the standard tests, it is practical to emphasize measurements only in the directions that flow is expected to occur in the field. Thus vertical permeability must be well quantified in areas where vertical flow is expected to be significant. Refined tests for vertical permeability are also described below.

2.6.1 Hydrologic Tests Used to Refine Selection of Hydrostratigraphic Units

Refined hydrologic tests will be required to overcome the limitations to the standard approaches. These are discussed below for each major type of limitation. Emphasis in this discussion is given to those methods not well described in the published literature. The specific limitations of each method are also discussed in this section.

2.6.1.1 Large-scale hydrologic data

Large-scale average hydraulic properties are required for identifying the large-scale HSU's appropriate for regional groundwater modeling, as discussed in Appendix B. Large-scale hydrologic data can, in theory, be

obtained either directly from large-scale field tests in which the properties of large volumes of rock are averaged, or indirectly by integrating the results of a large number of smaller-scale tests. Field tests aimed at increasing our understanding of these two approaches have recently been completed and are in the process of analysis (Gale and Witherspoon, 1978). The first approach, that of obtaining large-scale data directly from large-scale field tests, has been attempted by several investigators and is discussed in detail below. The second approach, that of integrating the results of a large number of small-scale tests to approximate large-scale behavior, is not well resolved and will require further research and comparison with the results of large-scale tests, particularly for application to fractured basalt.

The capability to perform large-scale hydrologic tests must be available if the average hydraulic properties of large HSU's are to be determined. Large-scale tests can be considered to fall into two categories: (1) those that measure natural conditions of responses to natural perturbations and (2) those that measure responses to induced perturbations.

Natural conditions or phenomena that can be measured to estimate large-scale hydraulic properties include hydraulic head, earth tides or earthquake-induced pressure waves, geothermal gradients, and anomalous pressures in geopressured regions. Examples of the application of these techniques are provided by Nesterov and Ushatinskii (1971), Anderson and Whitcomb (1973), Ohtake (1974), Anderson et al. (1977), Kanehiro (1979), Norton and Taylor (1979), and Neuzil and Bredehoeft (1981). Each of these methods has the disadvantages of the general behavioral methods discussed in Section 2.4.1. In particular, they are often limited to the measurement of responses to natural perturbations occurring in a particular direction, and thus may not provide good information on all the directional components of a particular hydraulic property. Their principal attribute is that they are truly large-scale tests and can provide information on some types of large-scale properties. Hydrochemical tests are also behavioral tests but will be discussed separately.

Perhaps of greatest interest in identifying HSU's are the large-scale hydrologic tests that measure responses to artificially induced perturbations. The boundary conditions and orientation of the perturbation can be known in advance and directed in such a way that the physical properties of greatest interest can be measured. The macropermeability experiment conducted at the Stripa Test Station in Sweden is an example of such a test.

The macropermeability experiment was designed to measure the average permeability of approximately 200,000 m^3 of low-permeability, fractured rock. The experiment was designed to measure the in situ averaged properties of the rock mass. The general experimental design philosophy has been described by Witherspoon et al. (1979). Flow of water into an enclosed portion of an underground drift was measured as the net moisture pickup in the ventilation system, and hydraulic gradients driving this seepage were measured from boreholes in the rock surrounding the drift. A schematic drawing of the experiment is shown in Figure 2.4.

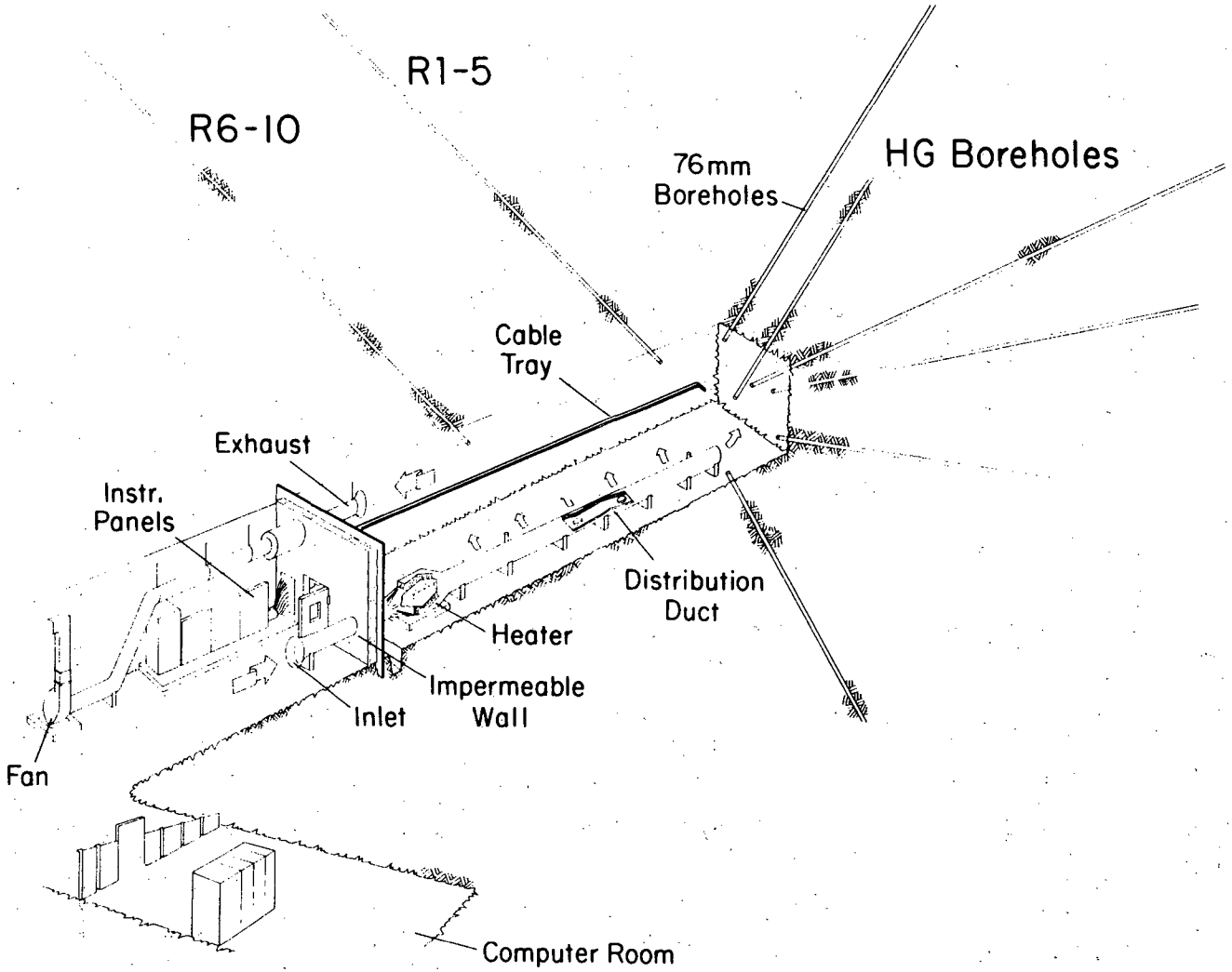


Figure 2.4. Schematic drawing of macropermeability experiment at Stripa Test Station, Sweden. [XBL 819-11583]

Some of the results of the macropermeability experiment are shown in Figure 2.5, which is a semilog distance-drawdown plot of hydraulic head as a function of radial distance from the axis of the drift. The scatter of points is primarily an indication of the heterogeneity of the rock, but is due partly to a superposed field gradient. Weighted average values are shown as small open circles.

If the rock mass had behaved, on the average, as a porous medium, and if steady-state conditions had prevailed, then the weighted average hydraulic heads in Figure 2.5 should plot as a straight line. The solid line drawn through the weighted average points was fitted by regression techniques and has a correlation coefficient of 0.98, indicating very close approximation to a straight line. Thus, in this experiment, the rock mass, on the average, did indeed exhibit continuum behavior on the scale of measurement of the experiment.

The averaged effects of increasing test volume can also be seen from Figure 2.6. Average hydraulic conductivity is proportional to the slope of the straight line between any of the weighted average data points. An evaluation of the change in average hydraulic conductivity as a function of test volume can be made by first computing conductivity from the slope of the first two points, then from the average slope of the first three points, and so on. By doing this for the data in Figure 2.5, but ignoring the data between the drift wall and the first point, which may have been affected by drift excavation, we obtain the results shown in Figure 2.6. These data tend to indicate that oscillations are still occurring on the largest scale of measurement but that they are small in magnitude for hydraulic conductivity measurements, being within $\pm$ 10% of the mean value. Similar tests could be conducted at other locations within the rock mass to determine the range of possible outcomes on this scale of measurement.

A limitation of large-scale underground testing is that most field experience has been acquired in low-permeability, fractured, massive granite. Some changes in test design may be required to adapt the macropermeability test concept to a stratified series of flood basalts and to conduct the test at a potential repository site. Such modifications are shown schematically in Figure 2.7.

With regard to seepage rate, the ventilation technique used at Stripa proved to be very successful. Provided that the range of moisture flow rates in basalt would be similar to those observed at Stripa, modification could be limited to conditioning the incoming air supply to provide a more stable humidity and temperature within the enclosed room.

Modifications to the pressure monitoring system may also be desirable. First, it may be necessary to avoid long radial boreholes, particularly in a vertical direction, as they could impair the capability of a relatively thin entablature to contain waste if the site were eventually used as a

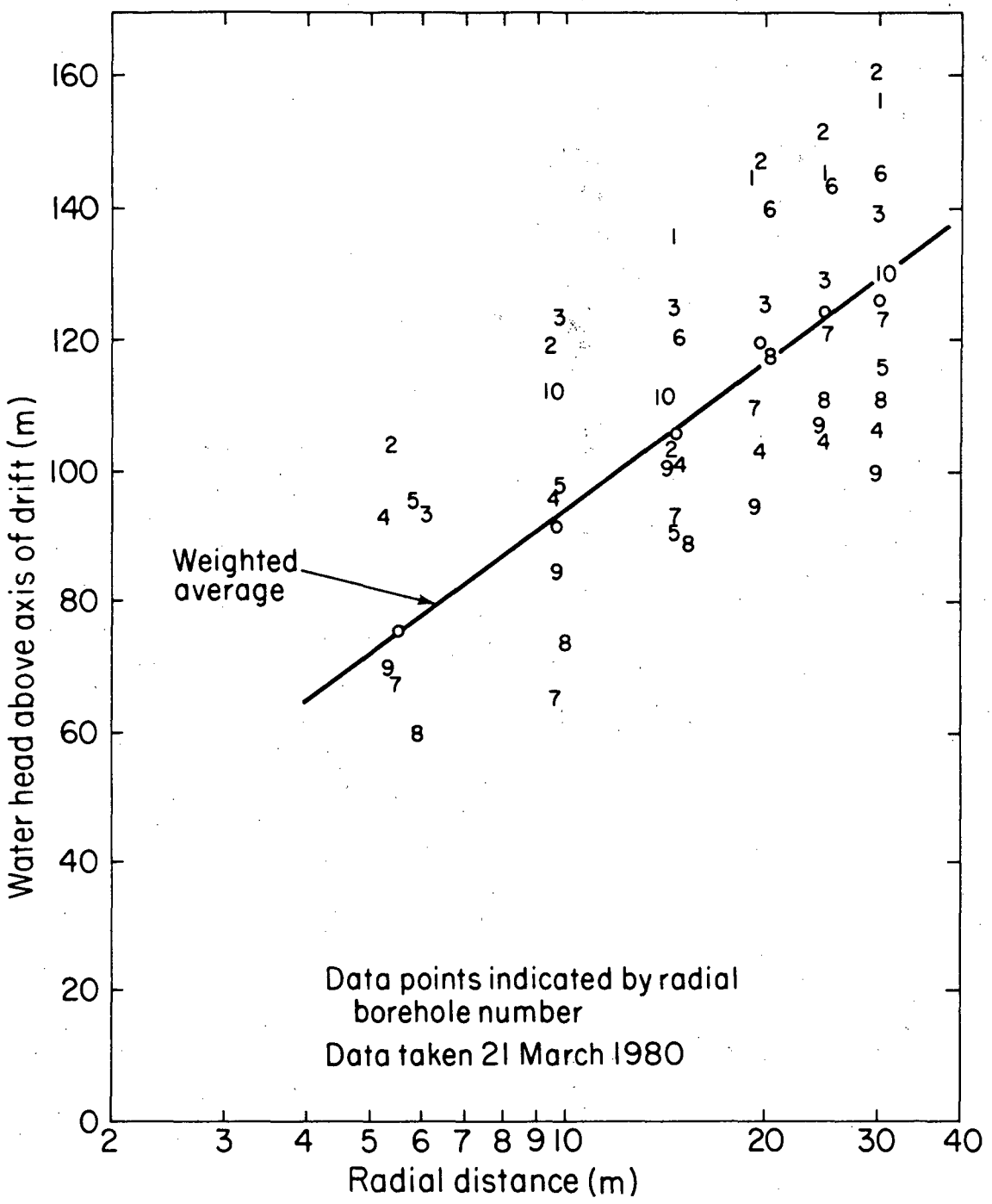


Figure 2.5. Distance-drawdown plot for steady radial flow into underground drift in macropermeability experiment. Numbers used as data points indicate borehole in which measurement was made. [XBL 8110-11691]

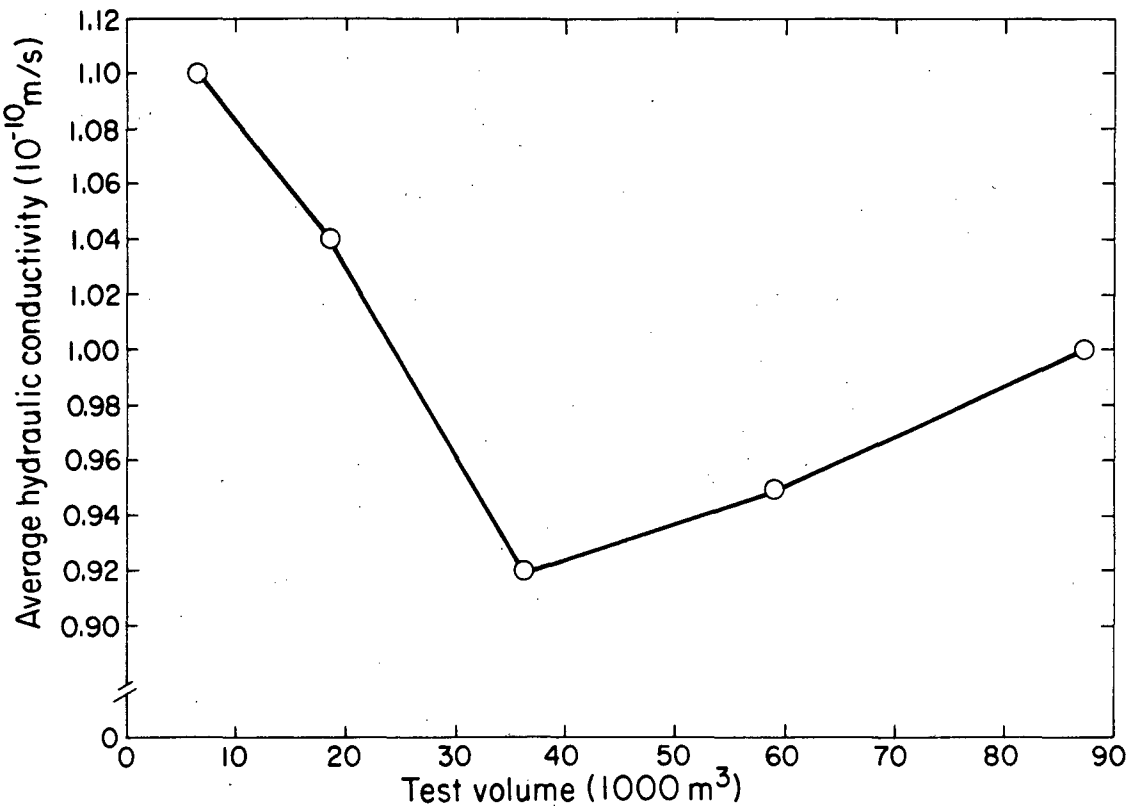


Figure 2.6. Change in average hydraulic conductivity as a function of test volume for the Stripa granite.

[XBL 8110-12139]

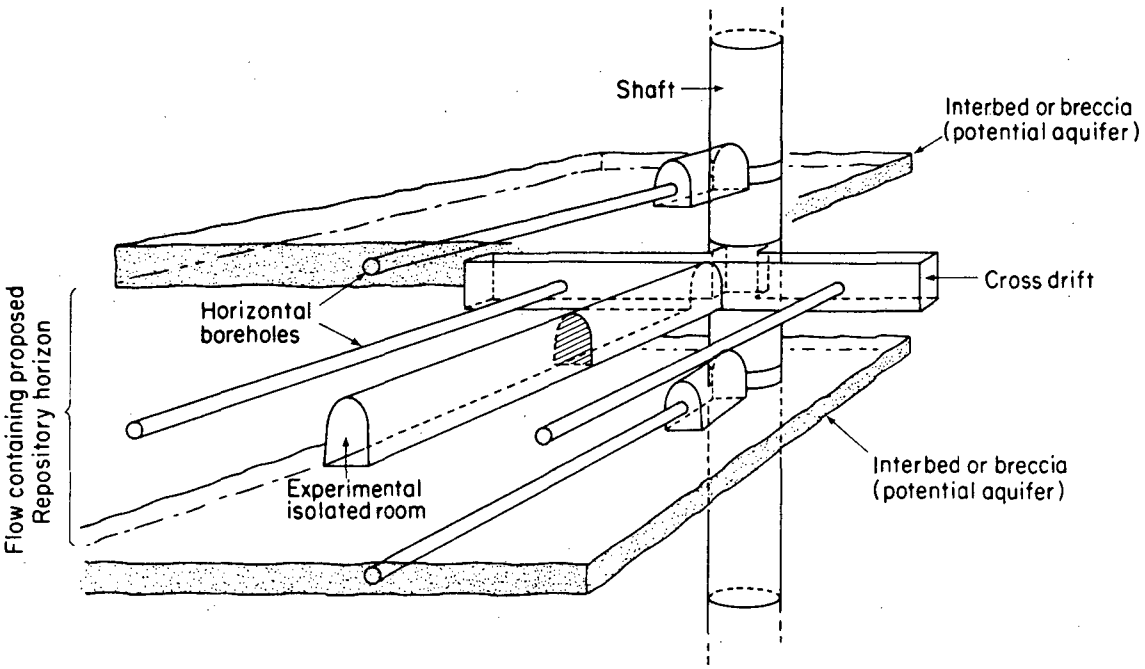


Figure 2.7. Schematic representation of large-scale underground test facility in basalt. [XBL 826-2288]

repository. Instead, horizontal boreholes could be drilled parallel to the axis of the drift; these boreholes could be within the dense host rock as well as within the overlying and underlying interflows. They would have the advantage of measuring pressure along equipotential lines rather than along flow lines (as in radial holes), and would therefore be less likely to alter in situ flow paths. The test design should retain, however, the ability to measure pressure at varying radial distances from the drift, so that the effects of increasing test volume can be determined.

An additional conceptual modification that may be desirable for macropermeability tests in flood basalt would be the artificial control of boundary conditions. This is expected to be somewhat simpler in basalt than in unbedded media because advantage can be taken of the higher permeability flow-top zones. The objective would be to maintain a fixed pressure along a boundary through control of pressure in a screen of parallel, closely spaced boreholes. This approach has been successfully used in granite in Sweden, where the boreholes were placed 1 m apart (Lindblom, 1979). The spacing of such boreholes in basalt would depend upon the permeability of the medium, and could be increased in a more permeable flow top. If the permeability of the flow top is significantly greater than that of the entablature, artificial head stabilization may not be required. Additional discussion of possible design features for large-scale underground tests is presented in a subsequent subsection on vertical permeability. Final design and dimensioning of the drift and boreholes will depend upon the physical properties of the site.

The primary advantage of underground macro tests like that described above is the ability to generate high gradients and directly measure average responses on a large scale in the vertical direction. Large-scale tests can be conducted from surface boreholes (e.g., see Miller et al., 1978, p. 89), but the results are largely limited to the measurement of properties in the horizontal direction, normal to the axis of the well. An exception is the measurement of vertical hydraulic conductivity by leaky aquifer methods (see Section 2.5.4.1), but these results are not guaranteed to provide large-scale averages. Large-scale tests in inclined wells are difficult to interpret for vertical conductivity and are best suited to massive media, which do not contain preferred directions for groundwater movement. In flood basalt, groundwater moving in response to perturbations from an inclined well will primarily follow paths of higher permeability, which are generally horizontal and parallel with the bedding, and the results might be expected to be similar to those from vertical wells. Underground testing resolves a primary limitation of testing from surface boreholes by permitting direct, large-scale measurement of hydrologic behavior in a vertical direction. Because of this, underground testing will be an essential part of repository site characterization.

The conceptual design for a macro test as described above is well suited for the identification of HSU's within the disturbed zone of the repository, because the flow patterns established by such a test configuration will be similar to those established by the repository tunnels.

For analysis of HSU's in the far-field, however, this design is limited because of the high cost of the test and because the convergent flow paths that are generated are not expected to occur in the far-field. The design of tests to resolve the limitation of convergent flow paths for far-field analysis is discussed in the following section of this report.

The high cost of underground experiments is primarily due to the cost of shaft sinking and preparing the underground support systems, such as the lift, ventilation, and electrical and water supplies. It should also be noted that these primary facilities are required for other purposes as well as the hydrologic testing. Once these primary facilities are installed, the incremental costs of performing large-scale tests from horizontal boreholes or drifts will probably be about the same as drilling and testing two or three deep surface boreholes. Although the cost of underground testing is expected to be large, the information to be gained on the parameters controlling vertical groundwater movement, particularly from the repository horizon, may be critical to the success of the site characterization program. Because of the high costs involved, the decision to use macro tests should be made only after the need for such a test has been clearly established by a thorough review and sensitivity analysis involving all available data.

2.6.1.2 In situ generation of constant gradient, parallel flow fields

The measurement of hydraulic properties in flow fields with a constant gradient provides the most powerful test for continuum behavior of a fundamentally heterogeneous rock. A constant average gradient throughout the flow field ensures that the properties of each part of the volume tested make an unbiased contribution to the measured data.

Hydraulic properties are, in general, determined from measurement of the flux or velocity occurring in response to an applied gradient, or vice versa. In the standard well test, a convergent flow pattern is produced in which the gradient decreases logarithmically with radial distance from the well. The emphasis of the measurement also falls off logarithmically with radial distance. For instance, if the permeability near the well is lower than the average permeability of the rock, flow into (or out of) the well will be decreased. In this case, an erroneously lower value of average permeability will be calculated from the well test results. Suppose a volume of rock has been identified that is a good statistical sample of the heterogeneities and is therefore a representative volume. Suppose further that this representative volume experiences approximately linear flow conditions in the regional flow system. Then in the regional flow system, the heterogeneities in the representative volume are all influencing the flux through the volume with equal emphasis. However, a radial flow well test would be unlikely to determine the correct average value of permeability for this volume, since its results will be logarithmically biased toward

the properties of the materials nearest the well. Additional discussion on the importance of parallel flow fields in testing a heterogeneous medium is presented in Appendix B.

Radial flow well tests can produce appropriate average measurements of hydraulic properties if the heterogeneities are small in relation to the length or diameter of the well. Larger diameter wells or longer test intervals are therefore more likely to provide accurate average values as long as the volume tested does not exceed the size of the HSU. An indication of the heterogeneity of the medium can be provided by multiple well tests, where the variation of hydraulic properties can be seen as a function of test volume. If continuum behavior is indicated by a well test, then that continuum behavior is probably valid. If, however, continuum behavior is not indicated by a well test, it may still be possible that continuum behavior exists but was not demonstrated because of the bias inherent in radial flow tests. The parallel flow test is the most powerful test for continuum behavior, and its results are conclusive. The radial flow test is less powerful, and its results may be inconclusive. Thus the parallel flow test provides a refined alternative to radial flow tests, to be used at critical locations within the flow field to resolve uncertainty concerning continuum behavior and the correct average hydraulic properties to use in modeling.

The question, then, is how can the "correct" average values of hydraulic properties be measured in the field? The volume over which these properties must be measured will govern the selection of HSU's suitable for regional modeling, and the values of these properties are those that will correctly predict hydrologic behavior in the regional flow system.

It is not easy to generate parallel flow conditions in the field. In the absence of any natural local boundaries, constant head boundaries must be created. This can be accomplished using the configuration for a parallel flow test, shown in Figure 2.8. Two parallel banks of wells, A and B, are drilled on either side of the region of measurement. These banks of wells can be drilled from the surface, as was done by Sauty (1978). They can also be drilled from an underground opening, as was done by Lindblom (1979). The wells need not be vertical.

Care must be taken to account for water entering bank A and flowing away from bank B, and vice versa. With vertical wells, for instance, it can be assumed that (1) the component of flow that comes from one bank of wells but does not go to (or come from) the other bank of wells is proportional to the difference between the head in the well and the head in the formation, and that (2)

$$\frac{h + \Delta h - h_o}{h - h_o} = n \ ,$$

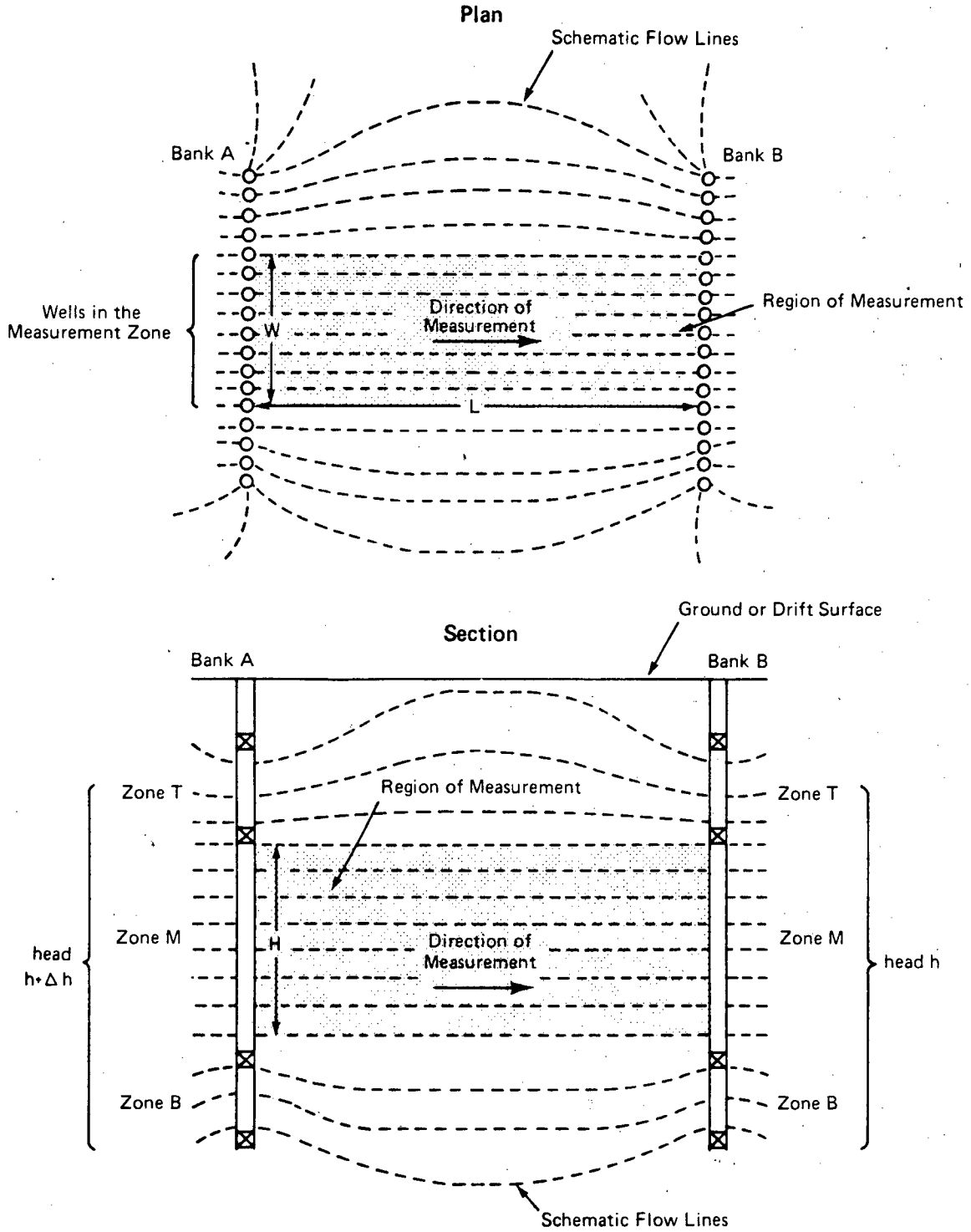


Figure 2.8. Banks of wells for parallel flow measurement.
[XBL 8111-4812]

where $h + \Delta h$ is the head in the A (injection) wells, h is the head in the B (withdrawal) wells, h_o is the ambient head, and n is an integer. Given these assumptions, the average hydraulic conductivity of the rock between the banks of wells can be shown to be

$$K = Q_{AB} \frac{L}{\Delta h H W} ,$$

where Q_{AB} is the flow from the A wells to the B wells, and L, H, and W are geometric parameters defined in Figure 2.8.

As in any large-scale test, consideration must be given to the size of the volume of rock that should be tested. This is probably best done through consideration of the results of small-scale tests. For instance, the small-scale tests could be performed in the first few boreholes drilled for the large-scale test. Small-scale tests should give information about the fracture geometry. An analysis of the fracture data, such as that used by Long et al. (1981), can then be used to decide on the appropriate scale for the test. The scale of the test and initial estimates of the hydraulic properties will in turn determine the length and spacing of the wells.

The orientation of the test wells is another problem. Hydraulic conductivity and dispersion both have directional properties. For the test configuration shown in Figure 2.8, the measurement direction is perpendicular to the planes formed by the wells. If the rock is strongly anisotropic, the direction of measurement can change the results by several orders of magnitude. In order to define an entire three-dimensional conductivity or dispersion tensor, a minimum of six measurements must be made in different directions if nothing is known about the system, or three measurements if the orientations of the principal axes are known. The extensive drilling requirements of the parallel flow test make it impractical for defining the entire tensor. Given the choice of a single direction of measurement for use in a regional flow model, the measurement should be made in the direction of the natural gradient. The properties measured will then be those that actually control flow under natural conditions.

Other test configurations for generating parallel flow are also possible. In flood basalts, the high-permeability horizons may act as constant head boundaries relative to the overlying or underlying strata. In this case, parallel flow can be established by drilling only one bank of wells parallel to the permeable formation from an underground facility. This technique would be applicable to the large-scale measurement of average vertical permeability of a low-permeability entablature above or below a highly conductive zone. The leaky aquifer method, a standard test described earlier, will also measure vertical permeability under similar circumstances with fewer boreholes, but does not provide a large-scale average value.

These methods of generating parallel flow fields are brute force by nature. They measure the parameters involved in the most direct possible way and thus have few technical limitations. Perhaps the most important technical limitation is the difficulty in obtaining an accurate estimate of the volume of water that moves opposite to the direction of measurement and thus is not involved in the test. This volume can be estimated, however, by approximations of the type presented above. The principal limitations in conducting this type of test will be economic rather than technical. They are very expensive, and may cost the equivalent of drilling and testing 20 or more single boreholes of equal depth. They can also be very time consuming, as it will be necessary, in general, to achieve steady-state conditions. The extensive drilling requirements will also cause great disturbance to the site. Despite the drawbacks, this type of test has already been used in at least two field studies, as indicated by the references given above. It is evident that the need for accurate, refined measurement can, in some circumstances, justify the cost of this type of test. But because of the high cost, it must be recognized that the use of this type of test will have to be strictly limited to measuring critical parameters where site disturbance has already occurred or will be tolerated. As with the previously discussed macro tests, the decision to use this large-scale test should be made only after the need has been clearly established.

2.6.1.3 Large-scale measurement of vertical hydraulic conductivity

In order to measure large-scale values, a method must be developed to directly induce a vertical hydraulic gradient over a large volume of rock and measure the resulting flux and velocity. In principle, every pressure perturbation creates a three-dimensional flow field that must include a vertical component, and measurement of the resulting three-dimensional pressure field should provide sufficient information (along with the flux used to generate the perturbation and the geometry of the problem) to compute the directional properties. In practice, however, only a few test geometries have been shown to be useful. These fall into two categories. The first method is the leaky aquifer test described in Section 2.5.4.1. This is a standard test performed from vertical boreholes, but may not provide a large-scale measurement. The second method consists in inducing a vertical gradient and measuring the resulting flux (or vice versa). This test, if properly designed, will provide a large-scale measurement.

The need for accurate large-scale measurements of vertical hydraulic conductivity has been mentioned earlier but will be stressed again because of its importance. The ultimate purpose of site characterization is to demonstrate the ability of the geologic media at the site to isolate radioactive waste. Waste deposited within the low-permeability entablature of a thick basalt flow will move initially in a vertical direction, perhaps only as far as the first permeable interflow zone, or perhaps farther depending on the relative hydraulic conductivities of the zones and the existing hydraulic gradient. This initial vertical movement cannot be predicted unless the vertical conductivities of these basalt strata are known over a large volume of rock.

In order to measure large-scale vertical conductivity, a vertical component of flow must be generated. This can be done by two methods. The first has been presented in the previous discussion of parallel flow. Two banks of horizontal wells can be drilled and the vertical conductivity of the rock between them can be measured. The banks of wells would be drilled from two drifts underground, each drift having the same orientation and one lying directly above the other. A schematic representation of this test configuration is shown in Figure 2.9. This method and its limitations have been discussed previously.

The second method is to measure the flow into a larger horizontal "well." In order to distinguish the vertical component of conductivity, it is necessary to measure the head distribution in vertical planes perpendicular to the axis of the well. Care must be taken to eliminate end effects by measuring inflow into and head surrounding the central part of the well only. This method would constitute a large-scale test similar to that shown in Figure 2.7, but specifically designed to measure vertical conductivity.

Suppose the initial conditions are those of constant head everywhere and the head distribution is measured sufficiently far from the well to avoid steep gradients and to include a good statistical sample of the heterogeneities. If the rock behaves as a homogeneous, anisotropic porous medium, the isopotentials in a vertical plane will be elliptical. In this case, the results can be analyzed with the methods of Hantush (1966) and Hantush and Thomas (1966), in which the shape of the isopotential ellipses is used to derive the two-dimensional conductivity tensor in the vertical plane. The vertical component of this tensor will give the vertical conductivity. If a pre-existing, known regional hydraulic gradient exists at the test site, its effect can be analytically removed from the test results and the Hantush and Thomas solution can still be used. If the initial head distribution is not known, vertical permeability cannot be determined with this test.

The measurement of head distribution around the well should be made from an array of wells drilled parallel to the "pumping" well. Figure 2.7 shows the general well configuration required; however, more horizontal boreholes than are shown would be necessary in order to define the elliptical isopotentials.

In some respects, it might seem better to use isolated zones in radial holes for monitoring head, as shown in Figure 2.4, than to use holes parallel to the axis of the well. However, radial holes do not provide a value of head averaged parallel to the pumping well. By using horizontal monitoring wells, the head measurements will automatically yield the correct average vertical permeability for the monitored length of the pumping well.

Horizontal monitoring wells do have a major limitation: the long sections of open borehole may create significant leakage paths and erroneously increase the measured permeability. The farther the monitoring holes

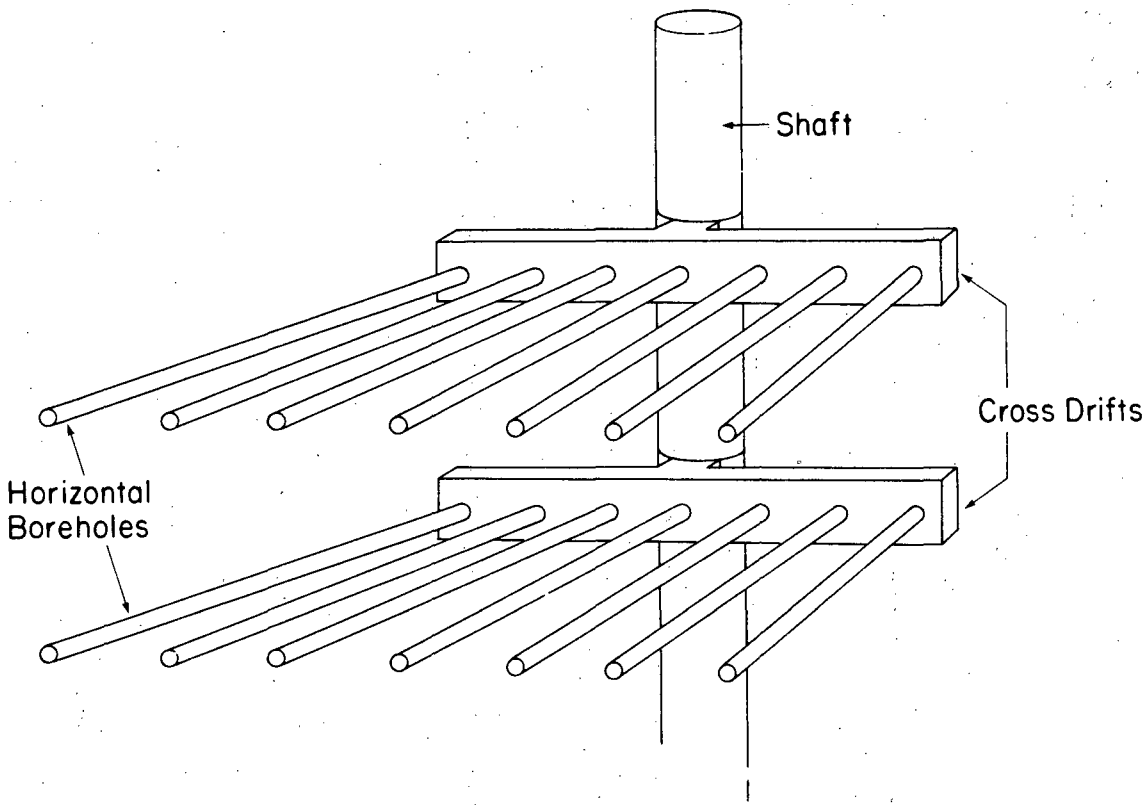


Figure 2.9. Underground arrangement of boreholes for measurement of vertical permeability. [XBL 8110-12140]

are from the pumping well, the less likely this is to be a problem. Packing off segments of the parallel holes would prevent leakage. The effect of this procedure on average pressure measurement, however, is not fully understood.

A further technical limitation of this method is the difficulty in defining the initial conditions. The head distribution in the test zone must be measured before the pumping well perturbs the system. Since the pumping well and monitoring holes must all be drilled from an underground opening, the initial head distribution might be quite complex and difficult to define accurately because of drainage into the drilling chambers. This can be minimized by locating the test facility far from pre-existing excavations.

Nontechnical limitations are similar to those discussed previously for underground testing and parallel flow measurement. Extensive and costly excavations and boreholes are necessary for this test, and the test can be quite time consuming. Because of the high costs involved, this test, as well as the other large-scale tests described in this report, should be used only after the need for such a test has been clearly established by a thorough review and sensitivity analysis involving all available data.

2.6.1.4 General limitations to refined hydrologic tests

The refined hydrologic tests discussed above have several limitations in common. The first limitation is cost. These tests are generally performed on a large scale, require more boreholes, more time to perform, and more underground access than the standard tests. This limitation will reduce the usefulness of these tests in regional analysis. The second limitation is that the refined tests are still generally in an early stage of development, and additional research is required to evaluate these techniques. A third limitation is that a methodology for analyzing data and applying field test results to a theoretically rigorous field identification of HSU's is still in the formative stages of development and has not yet been fully assessed for heterogeneous, fractured rock.

2.6.2 Hydrochemical Tests Used to Refine Selection of Hydrostratigraphic Units

Refined hydrochemical tests for identifying HSU's involve the use of chemical species, hydrochemical properties, or analytical techniques that are less well established. The general approach of looking for hydrochemical contrasts or progressive hydrochemical changes, however, remains the same. As with standard approaches, the refined approaches are numerous and highly specific to the hydrochemical conditions at the site.

The refined approaches showing greatest promise from the standpoint of resolution of the HSU issue in flood basalts are those dealing with radioactive isotopes that have the potential to indicate both the patterns and the rate of groundwater movement. Chlorine-36 may be useful for this purpose. It is relatively free of interference and is resistant to precipitation and adsorption. With a half-life of 3.08×10^5 years, it is potentially useful for measuring time periods of perhaps 2×10^6 years (Apps et al., 1979, p. III-8). However, measurement techniques have not been well developed and will require further study. Refinement of measurement techniques for the tritium and carbon-14 methods would increase their usefulness as well. Apps et al. (1979, p. III-7) report that increases in age dating capability from 25 years to 100 years may be feasible for tritium and that increases from 40,000 years to 100,000 years may be feasible for carbon-14.

An approach that is unconventional not necessarily in terms of technology but in terms of methodology is the simultaneous application of many hydrochemical techniques at a given site. This methodology has the obvious advantage of permitting comparison of results. Each technique yields a slightly different set of information about the site, and the inferences that can be drawn from comparing results adds significantly to our knowledge of the hydrochemistry of the site. The limitations of these refined procedures are the same as for the standard procedures.

2.7 UNCERTAINTIES REMAINING IN RESOLUTION OF THE ISSUE

The reason for identifying HSU's in flood basalts is to characterize the study area for the purpose of evaluating the isolation potential of this rock type for radioactive waste. Regional flow analysis has been done for many years on the basis of the continuum approach, and the errors involved in treating intrinsically heterogeneous fractured rock with continuum techniques basically developed for porous sediments have been generally accepted without rigorous analysis. Only recently have hydrologists realized the importance and complexity of the representative volume assumptions that are tacitly embedded in the continuum approach, and the need to verify these assumptions by field measurements.

It is currently uncertain whether the standard tests and assumptions described in Section 2.5 will be sufficient to adequately identify HSU's and assign hydraulic properties in flood basalts for the purpose of nuclear waste storage. As was previously mentioned, favorable experience with standard techniques in parts of the Columbia Plateau indicates that standard approaches may be successful, but existing evidence of a high degree of heterogeneity in the flood basalts of the Pasco Basin, as discussed in Appendix B, indicates the opposite. Because acceptable levels of uncertainty in nuclear waste disposal will be more stringent than for most other types of field problems, application of some refined tests will probably be necessary. These are particularly expected to include the large-scale underground measurement of hydraulic properties controlling vertical groundwater movement in and near the repository host horizon.

Field verification of representative volumes and continuum behavior, on the other hand, has not to our knowledge been applied to an actual problem in regional flow analysis in fractured rock. The ability to verify representative continuum behavior by direct field measurement has therefore not been demonstrated, and the success of such an effort cannot be assured. Criteria for continuum behavior have been developed, but just how well real rocks will meet these criteria remains unknown. Until further experience is gained in field tests, the use of these criteria is expected to be limited to resolving only the most crucial issues in site characterization. This is in fact happening at the WIPP site. A lawsuit by the State of New Mexico has resulted in a stipulated agreement by the DOE to re-evaluate by more refined techniques the conservativeness of initial assessments of the hydraulic properties of two fractured dolomite aquifers (U.S. District Court for New Mexico, 1981).

Uncertainties also remain in methods for determining large-scale average hydraulic properties in fractured media. These uncertainties involve the accuracy with which the results of small-scale borehole tests can be integrated to approximate the large-scale average behavior of the basalt strata, as well as techniques for verifying these approximations with large-scale tests. Uncertainties remain regarding the ability to measure appropriately averaged material properties on both small and large scales, for which the field generation of parallel flow lines is required. Uncertainties also remain in the ability to measure certain material properties, of which vertical hydraulic conductivity is most important in the context of identifying HSU's for studies of groundwater movement.

Another uncertainty concerns techniques for identifying the lateral extent of the HSU's. Field tests will be required within each major unit at a number of locations within the study area to confirm lateral continuity of the stratigraphic horizons and preservation of hydrologic function. For the purposes of modeling, these tests should also confirm statistical similarity in hydraulic properties. Assistance in dealing with this uncertainty will be provided by the iterative model verification process. This process can be expected to identify the type of additional data required, the location from which the data were obtained, and the sensitivity of the overall groundwater system to errors in that data.

Finally, uncertainty is also associated with the implications of identifying HSU's for developing numerical models of basalt when continuum behavior is not exhibited on an appropriate scale. Under these circumstances, statistical similarity of hydraulic properties would not be a strong criterion for identification of HSU's, because the hydraulic properties would be expected to be so highly variable that only very simple statistical parameters, such as mean and standard deviation, would be likely to be successful. Primary reliance would thus be upon interpretation of these parameters only as indicators of hydraulic

function. These statistical parameters will also provide relatively little guidance for the numerical treatment of these units in studies of groundwater flow. Practical techniques for treating units that do not exhibit continuum behavior are poorly developed, particularly in fractured rock, and little is known about the errors involved in such treatment.

2.8 RECOMMENDATIONS FOR RESEARCH

The most critical research needs are those associated with field identification of continuum behavior at scales appropriate for the hydrologic problems to be analyzed using the HSU's in flood basalts. Research is also needed in the identification of HSU's for basalts that do not exhibit continuum behavior. Proper unit identification is intrinsically linked with available methods of characterizing these units for studies of hydrologic behavior, thus uncertainties associated with the conceptual or numerical treatment of these units must also be considered in formulating a research program.

Research to help resolve the issue of HSU's in flood basalts is recommended in the following areas.

1. Identification of representative continuum behavior for intrinsically discontinuous geologic media: analytical and field methods are required for identifying representative volumes in both fractured and porous media, and to verify continuum behavior on the scale of the representative volume.

2. Integration of the results of small-scale tests to approximate large-scale behavior: small-scale tests are generally less costly and are more familiar than large-scale tests. Reliable techniques are required for approximating large-scale behavior from small-scale tests in flood basalts.

3. Techniques for large-scale tests to verify approximations based on small-scale tests: large-scale tests are the only realistic means of verifying techniques for the integration of small-scale tests. Techniques for performing large-scale tests in flood basalts are needed.

4. Techniques for field measurement of vertical permeability: methods for in situ measurement of vertical permeability, particularly on a large scale, are required for the proper identification and treatment of HSU's in flood basalts.

5. Techniques for field generation of parallel flow fields: field tests using constant gradient, parallel flow fields are the most powerful means of demonstrating continuum behavior, because test results are not biased toward the properties of any particular part of the medium. Techniques for performing such tests are needed at all scales.

6. Rapid borehole techniques for confirmation of the lateral extent of an HSU: simple, rapid tests that can be performed from small diameter boreholes are required to confirm the lateral extent of the HSU. These tests should be designed to eliminate the need for elaborate, multiscale testing to be performed at many locations within each HSU.

7. Techniques for evaluating the probable degree of statistical similarity of material properties at unmeasured locations within the study area: material properties pertinent to the identification of HSU's cannot be measured at every point within a study area, thus some uncertainty will exist regarding the appropriateness of unit identification at unmeasured locations. Techniques are required for estimating material properties at unmeasured locations and identifying the statistical similarity with material properties at known locations.

8. Techniques for conceptual and numerical treatment of HSU's that either do not meet or only approximately meet the continuum requirements: these must include methods for quantifying the uncertainty of the analysis.

9. Techniques for field measurement of dispersion: methods for in situ evaluation of dispersion are required, particularly for equivalent continuum values in fractured rock. A great deal of fundamental research is still required for application of both the dispersion and effective porosity concepts to fractured rock.

10. Improvements in hydrochemical age dating: age dating techniques are the most important hydrochemical tools for identification of HSU's because they provide information on both groundwater flow paths and velocities. In flood basalts, the chlorine-36 and carbon-14 methods appear promising, but research is needed on techniques for obtaining uncontaminated samples. In the case of chlorine-36, research is also needed on the interpretation of age from the chemical analysis.

3. DETERMINATION OF AREAS AND MECHANISMS OF NATURAL GROUNDWATER RECHARGE AND DISCHARGE FOR THE HYDROSTRATIGRAPHIC UNITS WITHIN A SEQUENCE OF FLOOD BASALTS

3.1 STATEMENT OF ISSUE

Radionuclides that migrate from the repository into the host rock will, upon leaving the disturbed zone, be subject to transport by the natural movement of groundwater away from the recharge areas and toward the discharge areas of the regional flow system. The ability of the site to isolate radionuclides will depend in part upon the areas and mechanisms of groundwater recharge and discharge for the HSU's containing flow paths that connect the repository with the accessible environment. The purpose of this section of the report is to identify technical approaches appropriate for the determination of areas and mechanisms of recharge and discharge for the existing natural groundwater system within a sequence of flood basalts.

3.2 IMPORTANCE OF ISSUE

Transport by moving groundwater is the most likely means of radionuclide escape from a mined repository. In the event that radionuclides should escape such a repository, they will enter the groundwater system and be transported toward an area of discharge. The specific flow paths to be followed by the waste will depend in part upon the size and hydrologic conditions of the disturbed zone and in part upon the hydrologic conditions at the areas of recharge and discharge for the regional groundwater system. The points at which radionuclides leave the disturbed zone will depend upon hydrologic conditions within that zone. Upon leaving that zone, they will enter the far-field, where natural in situ hydrologic conditions will predominate. If natural hydrologic conditions at the time of radionuclide escape are similar to present conditions, groundwater will transport the waste materials away from the present recharge areas and toward the present discharge areas. If travel time is sufficiently short and the sorptive capacity of the geologic medium is sufficiently low, migrating radionuclides could eventually reach the accessible environment.

Knowledge of the present areas of discharge to the biosphere is essential for determining the potential toxic hazard of radionuclide escape into the accessible environment. It will provide flow path information from which site characterization testing programs can be planned and radionuclide travel times and concentrations can be estimated. Further, the areas of discharge may be critical elements in defining the size of the control zone that must be evaluated in the site characterization process.

Knowledge of the present areas of recharge is also important to safe siting of a waste repository. In general, it is preferable to locate a repository closer to points of recharge than discharge in order to obtain a longer groundwater flow path. Longer flow paths will increase travel time

to the accessible environment and increase sorptive and dispersive effects. Hydraulic heads at the recharge and discharge areas generally determine the possible range of heads within the groundwater system. Knowledge of the principal areas of recharge will permit evaluation of potential changes in land and water use that could materially affect present hydraulic gradients. Finally, the locations of the principal recharge zones will also be critical elements in defining the size of the hydrologic system that must be characterized.

In summary, knowledge of the present areas and mechanisms of recharge and discharge for the host rock of a potential nuclear waste repository is essential to evaluating the ability of the site to successfully isolate nuclear waste. The need for resolution of this issue is reflected in several sections of 10 CFR part 60.

1. Section 60.11(a) requires that the Site Characterization Report include a description of the site to be characterized and sufficient information to demonstrate the adequacy of the candidate area to be studied.

2. Section 60.21(c) requires that the Safety Analysis Report contain an analysis of the hydrologic aspects of the site that bear significantly on its suitability for disposal of radioactive waste.

3. Section 60.31(a) requires that the DOE describe the hydrologic characteristics of the site in sufficient detail to permit the Commission to evaluate the safety of the site prior to construction authorization.

4. Sections 60.111(b) and 60.112(b) and (c) require that the ability of the geologic setting to contain nuclear waste must be adequately demonstrated.

5. Section 60.122 specifies those hydrologic conditions at the site that may be considered favorable in their effects on the ability of the site to meet performance objectives.

6. Section 60.123 specifies those hydrologic conditions that would have potentially adverse effects on the ability of the site to meet performance objectives.

3.3 NATURE OF GROUNDWATER MOVEMENT IN FLOOD BASALTS

Groundwater moves naturally in geologic media from areas of high groundwater head toward areas of low groundwater head. The paths taken by the water are generally those offering least resistance to movement. Groundwater will preferentially follow the more permeable beds unless they are disrupted by a crosscutting feature, such as a sharp fold, a fault, or a dike.

A simplified example of groundwater recharge and discharge is taken from Newcomb's work in the Dalles area of the Columbia Plateau. Figure 3.1 shows a simplified stratigraphic cross section of Swale Creek Valley. Primary recharge of the stratified basalts is thought to occur in the topographically high Columbia Hills Anticline to the southeast. From there, the groundwater is thought to move through essentially confined strata beneath Swale Creek Syncline, over a low, unnamed anticline northwest of Swale Creek Valley, and then into Little Klickitat River. The distance from the primary recharge area to the primary discharge area is about 22 km. According to Newcomb's conceptual model, minor mechanisms for recharge or discharge would include vertical movement of groundwater across confining beds and flow within any wells that penetrate the system. Flow directions across confining beds will depend upon local hydraulic gradients. These were expected by Newcomb to be generally upward beneath Swale Creek Valley and generally downward near the Little Klickitat River discharge area. Thus each of the deeper aquifers would tend to recharge its overlying aquifer within Swale Creek Valley and would tend to recharge its underlying aquifer near the discharge area.

Within the context of the Swale Creek example, each aquifer and each aquitard in the system can be considered to be a separate hydrostratigraphic unit (HSU). An HSU can be defined as a body of rock that functions as a distinct hydrologic system for the problem being studied. Hydrostratigraphic units identified for numerical modeling must behave as homogeneous bodies with respect to the parameters of interest and with respect to the groundwater flow patterns being studied. The identification of HSU's has been presented as a separate issue in this report and is discussed in Section 2. The identification of HSU's appropriate for describing regional groundwater flow will be essential to the proper delineation of flow paths and resolution of the recharge-discharge issue.

3.4 METHODS OF IDENTIFYING AREAS AND MECHANISMS OF RECHARGE AND DISCHARGE

3.4.1 Basic Data Needs

The basic data needs for identifying areas and mechanisms of groundwater recharge and discharge fall into two categories: (1) data on the physical properties of the geologic system, which would permit application of the theory of groundwater movement; and (2) data on the present patterns of groundwater movement.

The data required on the physical properties of the geologic system are essentially those that would be required to develop a regional model for groundwater flux. These data include

1. Bedrock geometry: the extent and thickness of beds; locations of faults, folds, major fractures, and other structural features.

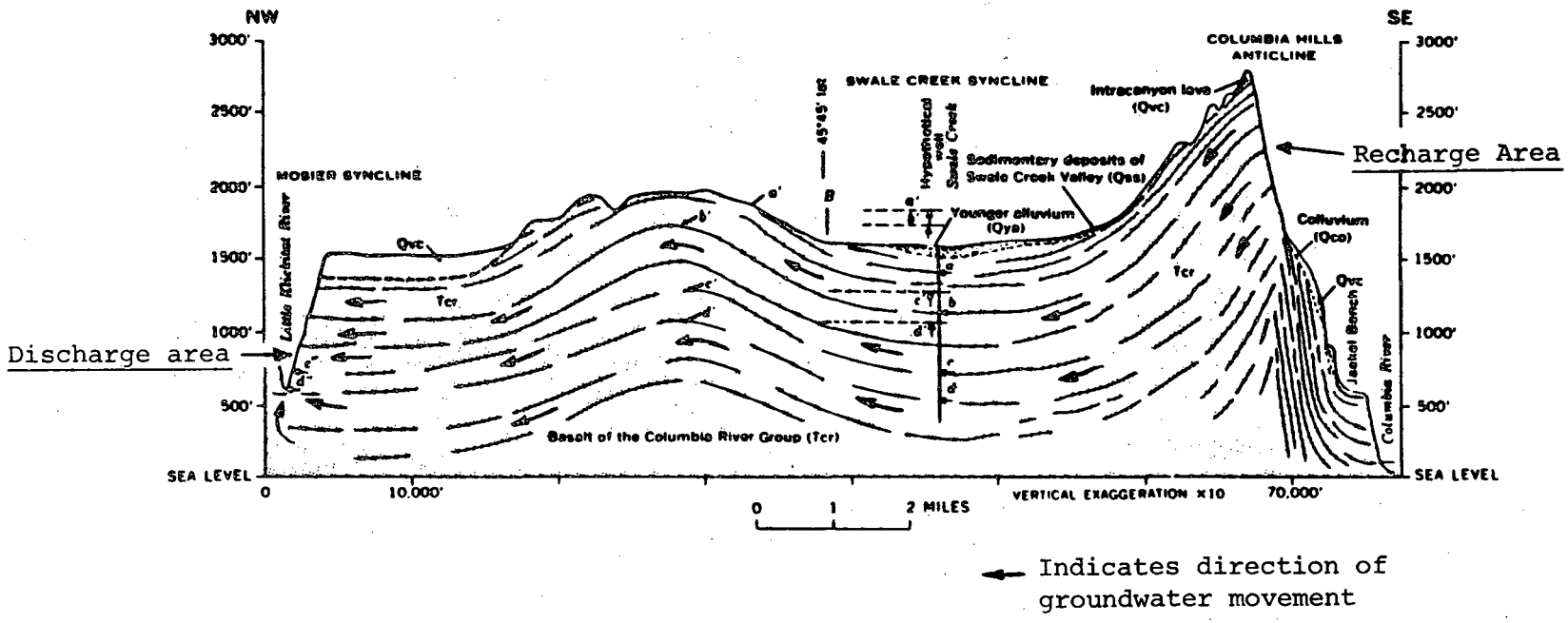


Figure 3.1. Example of groundwater recharge and discharge in the Swale Creek Valley area, Washington (adapted from Newcomb, 1969).

[XBL 826-10491]

2. Hydraulic properties: hydraulic conductivity and specific storage.

3. Initial conditions: regional hydraulic head distribution.

4. Boundary conditions: relationship to adjacent groundwater basins and to shallow groundwater systems; roles of lakes and rivers.

The first two of these data categories apply to the identification of HSU's as well as to development of a regional flow model, and are discussed in Section 2 of this report. Boundary conditions are required to define the relationships between the study area and neighboring hydrologic systems, and initial conditions are required to correlate the initiation of a transient model with a known point in time. Additional discussion on this subject has been presented by Long and Wilson (1978, p. C-5).

Data directly indicative of present patterns of groundwater movement include groundwater head and hydraulic gradient, groundwater chemistry and geochemical gradient, and groundwater age dating. An example of the use of such data to approximate patterns of groundwater movement within the Pasco Basin is given in Appendix D.

3.4.2 Methods of Data Analysis

Application of the theory of groundwater movement to the prediction of areas and mechanisms of recharge and discharge requires selection of an appropriate model, identification of HSU's, assignment of necessary hydraulic properties to those units, and identification of initial and boundary conditions. Models appropriate to the study may range from conceptual models, such as the water budget technique, to highly developed numerical methods. The physical property measurements needed to predict groundwater movement include geologic and stratigraphic data, hydrogeologic measurements including groundwater head, and supplemental measurements by geophysical and hydrochemical techniques from which information on hydrologic conditions can be inferred. Hydrochemical measurements, including groundwater age dating and hydraulic head measurements, provide information on groundwater flow patterns that can be analyzed independent of conclusions based on physical property measurements, and thus may provide independent support to these conclusions.

The basic field data required to evaluate areas and mechanisms of groundwater recharge and discharge are fundamental to most hydrogeologic investigations, including the identification of HSU's. The two basic classes of measurements, those of physical properties and those indicative of present behavior, are discussed in Section 2.

3.5 METHODOLOGIES FOR RESOLUTION OF ISSUE

3.5.1 Standard Approaches and their Limitations

Three primary standard approaches will be discussed here. The first two, water budget and numerical analysis techniques, rely upon two different types of theoretical structures to manipulate the basic data into a form that can more easily be understood in light of the problem to be answered. The third approach involves data that bear directly on the problem and need little or no analysis for interpretation. All data that directly indicate present patterns of groundwater movement fall into this third category.

3.5.1.1 Water budget techniques

The water budget method employs the principle of conservation of mass to evaluate the constituents of water flow into and out of a study area. The method is based on the fundamental relationship

$$Q_{in} - Q_{out} = \Delta S,$$

where

Q_{in} = volume of water entering the study area in a given period of time,

Q_{out} = volume of water leaving the study area in a given period of time,

ΔS = net change in storage of water within the study area during a given period of time.

In applying the water budget technique, each water supply or depletion component of the water budget equation is broken down into its constituent parts. Thus water inflow is treated as the sum of all components of inflow, and water outflow is treated as the sum of all components of outflow. Typically, these components are as follows:

Inflow: Surface Water System

Direct precipitation: Includes both rain and snow.

Surface water inflow: Includes all surface water inflow in natural rivers and streams.

Imported water:	Includes all artificial inflows in man-made conduits, such as canals and pipelines.
Groundwater withdrawal:	Includes all water extracted from the ground by man.
Groundwater discharge:	Includes all water leaving the groundwater system and entering the surface water system by natural means, such as through springs.

Inflow: Groundwater System

Subsurface inflow:	Includes all groundwater entering the system through subsurface inflow from adjacent groundwater systems.
Natural groundwater recharge:	Includes all natural recharge from surface sources, including lakes, rivers, and direct precipitation.
Artificial groundwater recharge:	Includes recharge resulting from the practices of man, such as agricultural irrigation and waste disposal.

Outflow: Surface water system:

Evaporation:	Includes direct evaporation from surface water bodies and that component of the precipitation which is directly evaporated.
Surface Water outflow:	Includes all surface water outflow in natural rivers and streams.
Exported water:	Includes all artificial outflows in man-made conduits, such as canals and pipelines.
Evapotranspiration:	Includes water retained, evaporated, or otherwise removed from the system by natural vegetation.
Consumptive use:	Includes water retained, evaporated, or otherwise removed from the system by municipal, industrial, agricultural, and domestic uses of man.
Natural groundwater recharge:	Includes all natural recharge from surface sources, including lakes, rivers, and direct precipitation.
Artificial groundwater recharge:	Includes recharge resulting from the practices of man, such as agricultural irrigation and waste disposal.

Outflow: Groundwater system

Subsurface outflow:	Includes all groundwater leaving the system through subsurface outflow to adjacent groundwater systems.
Groundwater withdrawal:	Includes all water extracted from the ground by man.
Groundwater discharge:	Includes all water leaving the groundwater system and entering the surface water system by natural means, such as through springs.

The principal components of a water budget are shown schematically in Figure 3.2. For purposes of illustration, the surface water system shown in this figure is treated separately from the groundwater system. These two systems are coupled because the components of outflow that go from the surface water system to the groundwater system are also components of inflow to the groundwater system, and vice versa. It is also possible to consider the groundwater and surface water as a single system, but in such a case the water flow between surface water and groundwater would not enter into the computations. The method can also be adapted to consider inflow and outflow for a single HSU by treating inflow and outflow along the boundaries of that unit. Another point to note is that the subdivision of flow components shown in Figure 3.2 at the boundary between the groundwater and surface water systems occurs beneath the groundwater table and beneath the root zone. Thus the vadose zone is generally ignored, and the use of groundwater by plants is considered by convention to be a surface water phenomenon.

The effects of water storage within each system are sometimes ignored if it is felt that the systems return to essentially the same initial conditions at the end of each study period. Although this approximation may be adequate for surface water systems involving no large reservoirs, it is generally not adequate for studies of unconfined groundwater systems. Moreover, reductions of the amount of water stored in groundwater systems may be irreversible. For example, water held in some types of chemical bonds (e.g., water of hydration) and water held in consolidating clays cannot be restored once released from the system.

Application of the water budget technique involves first identifying the study area and then determining the magnitudes of all significant types of inflows and outflows occurring along its boundaries. The data are obtained from a wide variety of sources. The U.S. Geological Survey, state water resources or agriculture departments, and local water supply agencies are good sources of information on surface water flows, imported and exported water, subsurface water flows, evapotranspiration, and consumptive use. Information on water use by private industry, such as power companies or large agricultural firms, is generally available from the industries involved. Information on reservoir operations is available from the reservoir operators and is generally quite complete.

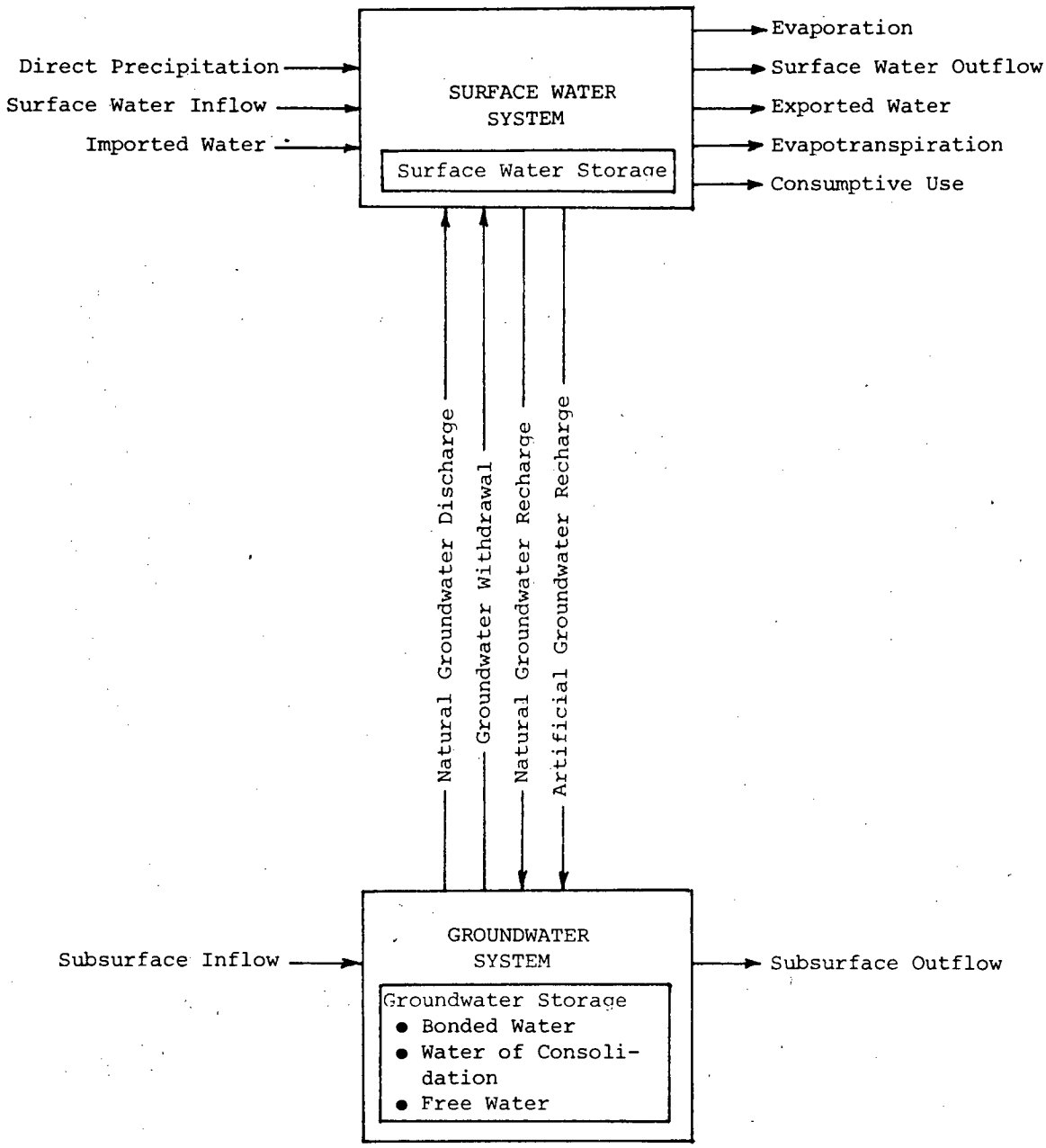


Figure 3.2. Typical components of a water budget. [XBL 826-10489]

The primary difficulties in applying the method involve the quality of available data, which may be only approximate or entirely lacking. The data on subsurface water movement across the boundaries of the system generally fall into the latter category and must be approximated. This is generally done with a simplified application of Darcy's law for steady laminar flow:

$$Q = KIA,$$

where

Q = volumetric flow rate of water crossing the boundary,

K = hydraulic conductivity of the geologic medium at the boundary,

I = component of hydraulic gradient normal to the boundary,

A = cross-sectional area of the flow field at the boundary.

More rigorous techniques are rarely employed to estimate groundwater movement for the water budget technique, because the other available data are usually also approximate and the technique is generally not sufficiently precise to warrant further sophistication. If a great deal of effort is put into developing an excellent data base, more precise analytical techniques involving numerical methods are generally used. These are described in Section 3.5.1.2. Basic data on hydraulic conductivity and hydraulic gradient are normally obtained from the well tests described in Section 2. Cross-sectional areas are obtained from geologic data.

An example of the water budget technique is taken from Gephart et al. (1979, p. II-75). They used the method to estimate the net groundwater recharge by surface waters in the Pasco Basin and neighboring basins. They were therefore confining their study to the surface water system, as shown schematically in Figure 3.2, and computed as their unknown the net amount of natural and artificial groundwater recharge and discharge. It was assumed in their study that the net annual change of surface water in storage was zero. Surface water inflows and outflows were by far the largest single elements in this study, primarily because of the influence of the Columbia River. Thus the locations of the surface gauging stations are of primary importance; in fact, they are the primary factors that were used to define the boundaries of the study area. A schematic drawing of this gauging station network is presented in Figure 3.3.

The results of the study by Gephart et al. are summarized below. The average net contribution of each major source of water to groundwater recharge was found to be as follows:

		Billions of cubic meters per year
1.	Precipitation	0.0
2.	Streamflow	-3.6
3.	Artificial mechanisms	0.3
	Net recharge	-3.3

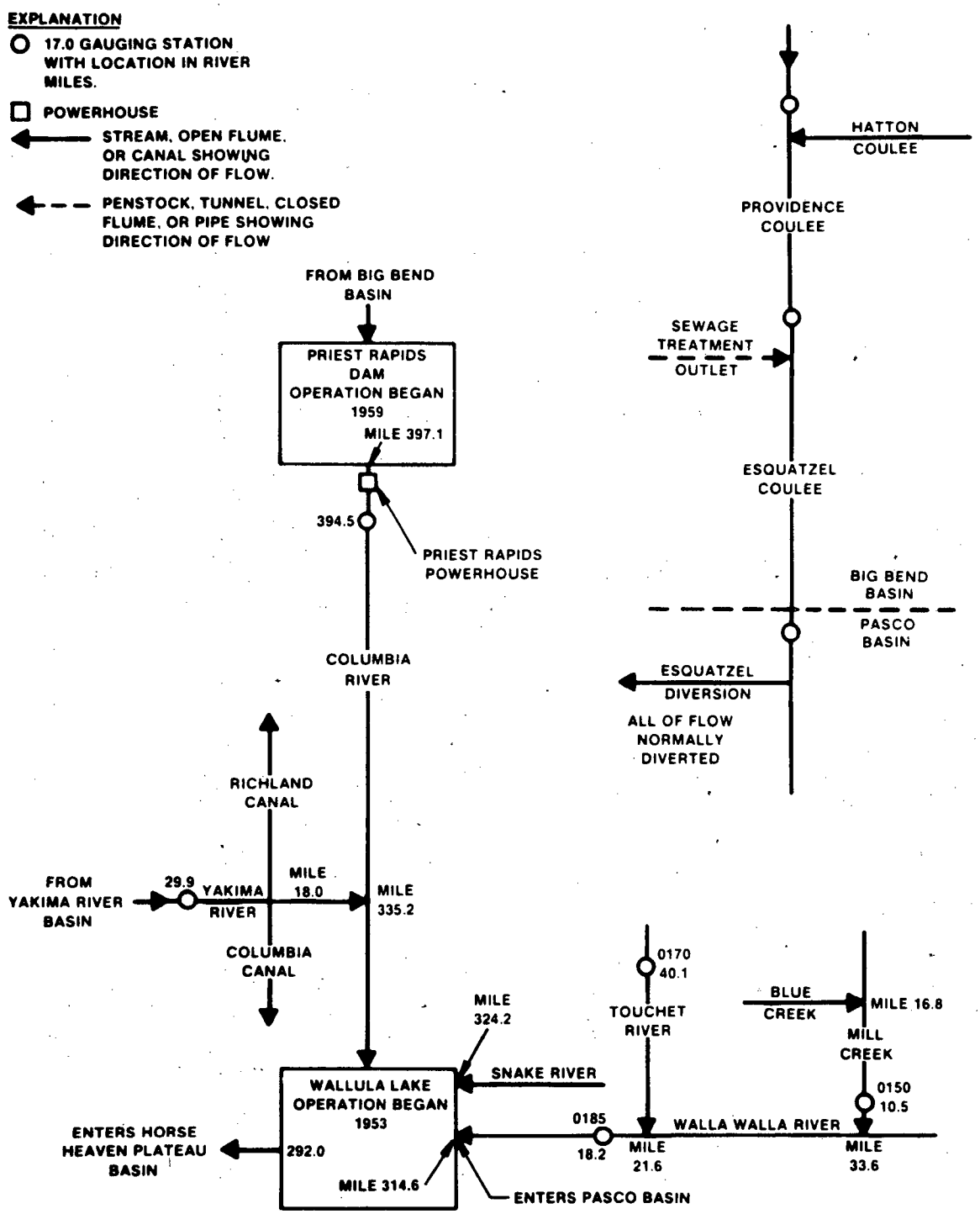


Figure 3.3. Schematic drawing of U.S. Geological Survey stream gauging network for the Pasco Basin (from Gephart et al., 1979, Figure II-18). [XBL 826-10488]

The negative sign on the net value indicates that averge discharge of groundwater to the surface exceeds recharge by some 3.3×10^9 m^3/year. As large as this value may seem, it is very nearly equal to the difference between the inflow and outflow of the major rivers; these amounts are 161.8×10^9 and 165.4×10^9 m^3/year, respectively. The net groundwater discharge represents only about 2% of these surface water flows. Stream gauging techniques are not highly accurate, and data with errors of less than 5% are considered "excellent" in that area (Gephart et al., 1979, p. II-81). The computed net groundwater discharge may therefore be close to the noise level of the basic data, and supporting information from other sources may be required before this result is considered to be quantitatively significant.

This example serves to illustrate the major limitations of the water budget technique. First, the method relies upon flux measurements that are difficult to make with high accuracy. The desired values, which are treated as unknowns in the equations, are often small differences between relatively large numbers, and may fall near or within the error bands of these larger numbers. Thus the conclusions reached with this technique may under certain circumstances be largely qualitative.

Second, the technique treats the hydrologic system as a black box and is concerned only with fluxes across the boundary of the system. It can give no information on water transfer mechanisms within the system. Further, the boundaries of the system are often dictated more by sources of data than by the needs of the study. For example, the topographic boundary of the Pasco Basin is at Sentinel Gap, but because no stream gauging station exists there, a gauging station some 25 km downstream had to be used to measure inflow to the basin. This station is downstream from both Sentinel Gap and Priest Rapids Reservoir, two locations where recharge to the deeper aquifers may be occurring. Installation of a gauging station at Sentinel Gap would eventually resolve this problem, but several years of records would be required before a reliable correlation could be obtained with the older stations. Similar problems exist with rain gauging stations, which are also generally widely spaced. The coarseness of the available data usually makes the water budget technique more amenable to regional rather than local analysis.

Third, the technique in practice is limited in precision when defining the locations of recharge or discharge across a boundary. The primary reason for this is that the technique involves only one equation and therefore can have only one unknown. Although in principle it may be possible to let that one unknown be the net recharge for a specific portion of the boundary, in practice this is not normally tenable because (1) the computed value is often very small and falls within the noise level of the data and (2) the method requires that net recharge for all other portions of the boundary be known, which is generally not the case.

In summary, the water budget technique serves in practice primarily as a reconnaissance technique for obtaining information on the magnitude of water supply data for a particular study area. Although it is rigorously

correct in a technical sense, its limitations with regard to accuracy and precision and its inability to identify flow patterns within the study area limit its usefulness for identifying areas and mechanisms of recharge and discharge.

3.5.1.2 Numerical model techniques

Numerical model techniques employ numerical methods to identify the groundwater flow patterns within a study area. These methods can be highly sophisticated and provide detailed information about rates and directions of transient groundwater movement in three-dimensional space. The methods involve dividing the study area into a large number of interdependent blocks or elements, each of which must satisfy an equation of continuity for transient flow, which is very similar in concept to the governing equation for the water budget method. For numerical models based on the finite difference method, this equation states that the net inflow into the nodal block over a particular period of time is equal to the dynamic change in storage:

$$Q_{in} - Q_{out} = S_s V \frac{\Delta h}{\Delta t} ,$$

where

Q_{in} = volume of water entering the nodal block,

Q_{out} = volume of water leaving the nodal block,

S_s = specific storage of the nodal block,

V = volume of the nodal block,

h = hydraulic head at the node within the nodal block,

t = time.

The numerical model is built up by subdividing the entire study area into a large number of blocks. An example of a two-dimensional array of this type, which was prepared by Rockwell for the Pasco Basin, is shown in Figure 3.4. Each of these blocks is coupled in such a way that outflow from one block becomes inflow to the neighboring blocks. The rates of fluid movement are controlled by the average hydraulic conductivities of the geologic media represented by each block. Inputs normally consist of: (1) the geometry of the system from geologic and topographic data, (2) the average hydraulic conductivity and specific storage for each block, and (3) the initial hydraulic head at each node and the boundary heads or fluxes at boundary nodes. Not all of these data needs are expected to be supplied by direct field measurement because of the high cost and the desire not to impair the integrity of a potential repository site. Data not measured must

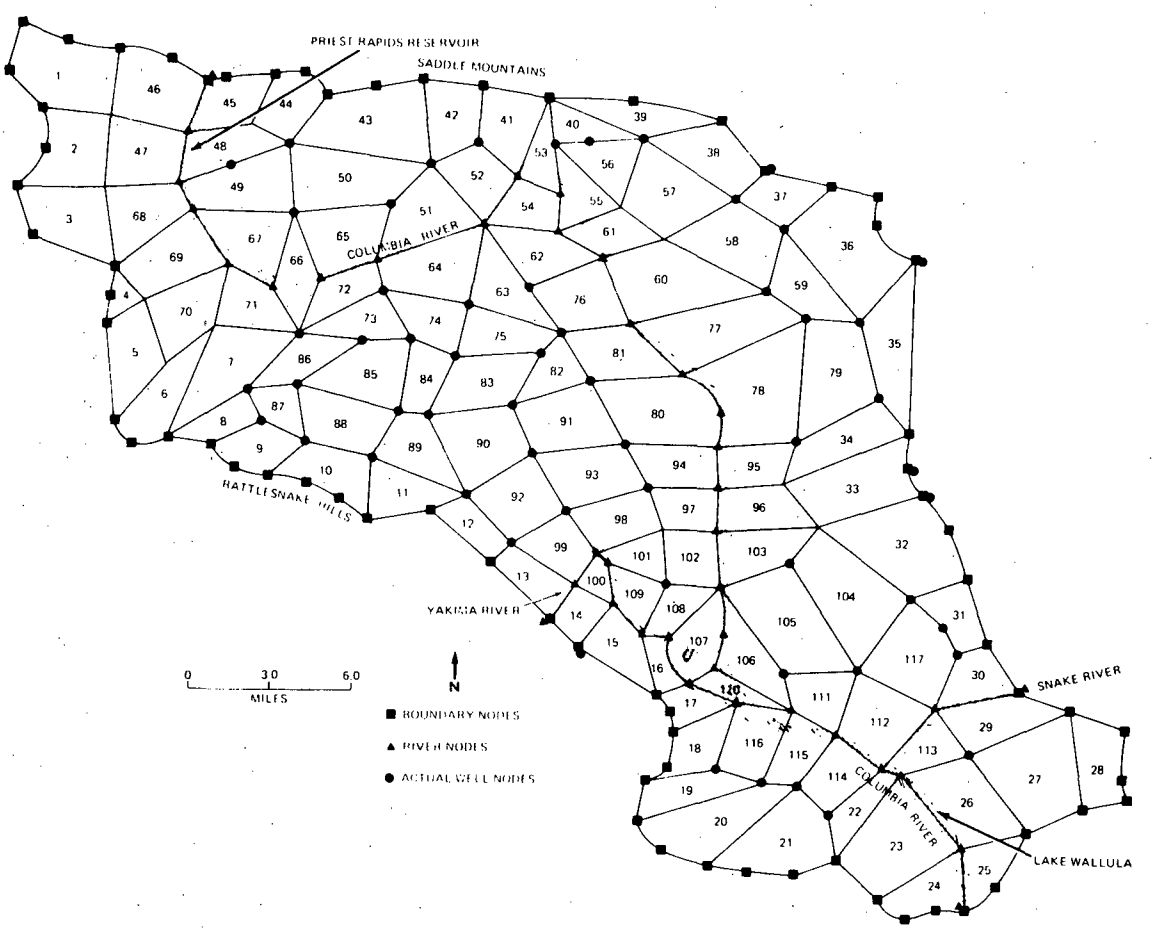


Figure 3.4. Example of the subdivision of a study area into an array of blocks for the purpose of numerical modeling (from Gephart et al., 1979, Figure IV-14). [XBL 826-10487]

be estimated using techniques discussed below. The nodes are generally either in the center of each block, as in finite difference models, or along the boundaries of the blocks, as in finite element models. The example shown in Figure 3.4 is for a finite element model.

Since one equation is written for each node, it is possible to solve for as many unknowns as there are nodes. Generally, the program is started by specifying a value for the hydraulic head (h) at each node, although for nodes at boundaries the net flux into or out of the boundary could be specified instead. Hydraulic heads for subsequent times are then treated as unknowns and computed at the end of each time step. For steady-state models, initial heads or fluxes must be specified for the boundary nodes, and then the head distribution within the system can be computed. This principle is often used to establish initial conditions for a transient model on the assumption that the flow system is in equilibrium immediately prior to a perturbation. It should be noted that knowing the boundary heads does not necessarily imply that all recharge or discharge areas are known. The areas of highest head will definitely be recharge areas, and those of lowest head will definitely be discharge areas, but the directions of water movement across boundaries of intermediate head will not be known because they depend on the nature of groundwater flow paths within the system.

Because of the expense of obtaining the large amount of input data required for most regional studies of recharge and discharge, it is often necessary to estimate hydrologic parameters for many of the elemental blocks in the model. The validity of these estimates is checked by a procedure known as calibration, where the estimated parameters are varied within reasonable limits until the computed groundwater heads compare with the actual heads to an acceptable degree of accuracy.

Boundary conditions can be inferred from field information or be approximated using numerical models. The most common type of boundary condition inferred from field data is the no-flow boundary that results from a groundwater divide or an impermeable fault zone. Boundaries across which groundwater flows are generally treated as having either constant-head or constant-flow conditions. In either case, a considerable amount of field data, including permeability and head information, must be available on both sides of the boundary. The economic and time constraints, which strictly limit the amount of data available for identifying hydrologic parameters within a study region, also apply to the boundaries of the region.

To help overcome the problems of limited data, numerical models can be used. One approach is to calibrate for the boundary conditions rather than for the internal hydrologic parameters. In this approach, the internal hydrologic parameters are all assumed to be accurately known, and the boundary conditions are varied within reasonable limits until the actual groundwater heads are adequately matched by the computed heads. The method has two principal limitations: (1) use of heads to calibrate

boundary conditions precludes their use to calibrate internal hydrologic parameters; and (2) the boundary conditions derived by this method will not be unique, and therefore their accuracy cannot be assured. An alternative approach is to develop a model of the larger region that encompasses the study area (a "nested" model) and use that model to determine boundary conditions for the study area. The larger model would normally be more approximate than the study area model, but would be expected to produce boundary conditions that are compatible with regional flow patterns. Although either method could produce erroneous results, the latter is normally preferred because it makes use of additional data from beyond the study area in determining boundary conditions; it also frees groundwater head information within the study area for use in calibrating internal hydrologic parameters.

The directions and magnitudes of groundwater flow can be determined from the completed numerical model for either the outer boundaries of the system or for any surface of any elemental block or groups of blocks within the system. Thus the areas and mechanisms of recharge and discharge can be determined for the outer boundary of the system as well as for any arbitrary group of block surfaces representing an inner boundary. If, for example, groups of blocks were designed to represent specific HSU's, as they generally are, the numerical model techniques would allow quantitative identification of areas and mechanisms of recharge and discharge for each individual unit within the system.

Numerical methods are powerful tools for the identification of areas and mechanisms of recharge and discharge. Two basic approaches to groundwater modeling are currently in use: the finite difference formulation and the finite element formulation. Either approach is satisfactory for resolution of this issue. These methods have been described by Remson et al. (1971), Trescott et al. (1976), and Pinder and Gray (1977).

An example of the use of numerical model techniques to identify areas and mechanisms of recharge and discharge is presented for the Pasco Basin in Figures 3.5 and 3.6. This example is presented only for illustration. The results may or may not reflect actual flow conditions. Figure 3.5 is a plan view of the three-dimensional finite element mesh used in the study; Figure 3.6 is a contour plot of the groundwater head computed by the model for the Mabton Interbed at the top of the Wanapum Basalt. These model results, part of a series of calibration tests made by Rockwell, were intended to identify the probable ratio of vertical to horizontal hydraulic conductivity for the HSU's employed in the model (Rockwell Hanford Operations, 1980c, p. III-46). The intent was therefore to compute hydraulic heads that were correct in general pattern but not necessarily quantitatively correct. The result shown in Figure 3.6 was reported by Rockwell to be the closest to the field-observed patterns. Field-observed heads available in 1979 for the part of the Mabton Interbed that underlies Cold Creek Syncline are shown in this report in Figure C.2 and may be used for comparison with these numerical results.

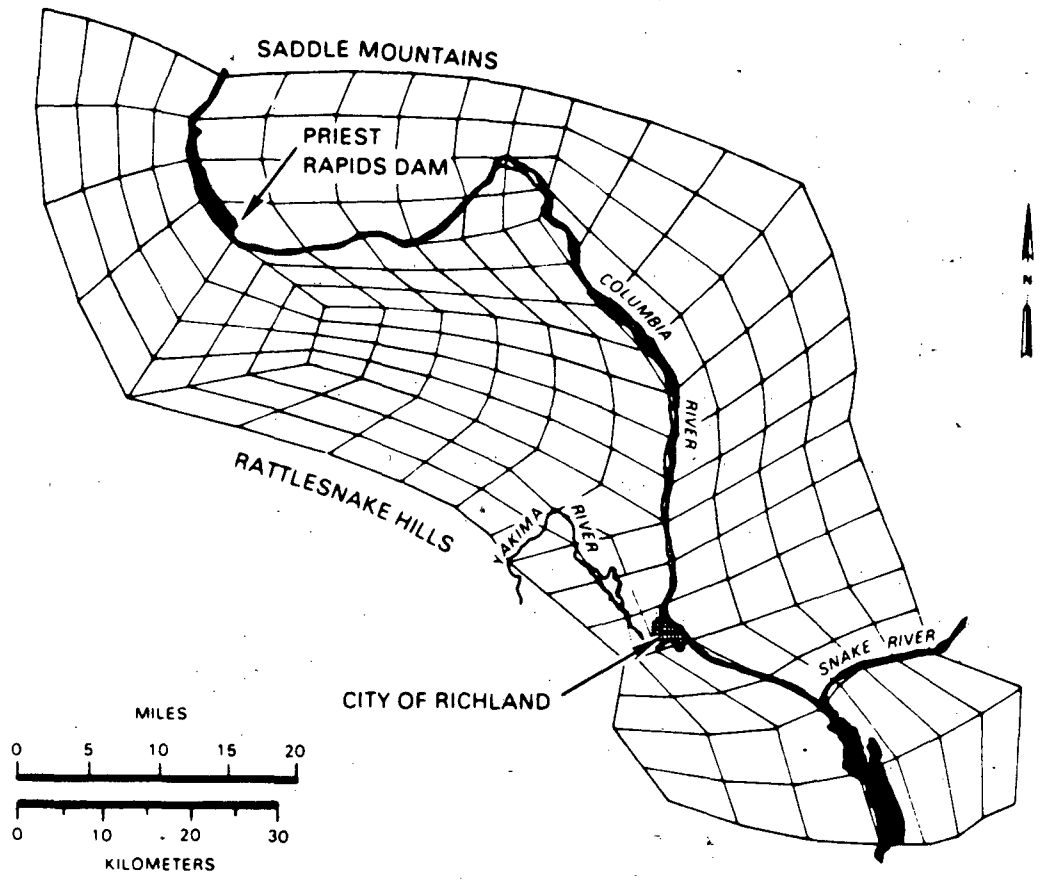


Figure 3.5. Plan view of three-dimensional finite element mesh of the Pasco Basin used to produce the results shown in Figure 3.6 (from Rockwell Hanford Operations, 1980c, p. III-48). [XBL 826-10486]

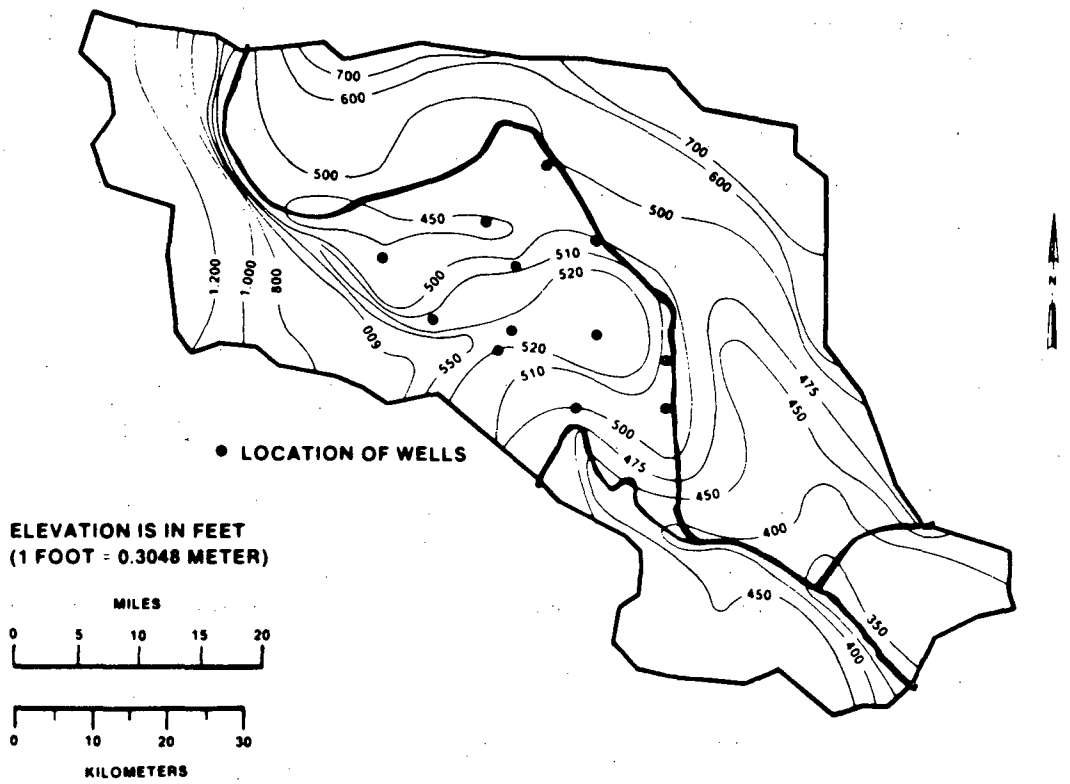


Figure 3.6. Contours of computed hydraulic heads for the Mabton Interbed at the top of the Wanapum Basalt for a model calibration run (from Rockwell Hanford Operations, 1980c, p. III-52). [XBL 826-10485]

Rockwell's studies of the Mabton may be used to illustrate how model results can be applied to the question of areas and mechanisms of recharge and discharge. The results in Figure 3.6 indicate that recharge to the Mabton is occurring primarily from Cold Creek and Dry Valleys to the northwest, the Saddle Mountains to the north, the upland areas to the east, and the Horse Heaven Hills to the south. Some recharge may also be occurring within the Cold Creek Syncline. Discharge is concentrated along the bed of the Columbia River immediately downstream from Priest Rapids Dam and downstream from the city of Richland. The mechanism for recharge appears to be a combination of lateral inflow along the outer boundaries of the model and vertical movement across basalt flows within Cold Creek Syncline. The mechanism for discharge appears to be vertical movement across basalt flows.

The limitations of the numerical modeling techniques are the limitations of numerical approaches in general. These are: (1) the problems of data acquisition, (2) the ability of the algorithm to predict actual system behavior, and (3) the problems of computer system capacities.

Numerical techniques have prodigious data demands, as may be seen from the foregoing discussions. These demands cannot always be met by direct field measurement because of the high cost, the reluctance to drill excessively at a potential repository site, and the inherent limitations of available field techniques to measure the appropriate parameters. A lack of data is by far the greatest limitation in resolving the recharge-discharge issue. Because of this problem, data appropriate to the needs of the problem must often be estimated, particularly in areas where no measurements are made. Errors introduced by insufficient data will affect the accuracy of the model result and are very difficult to evaluate properly.

The ability of the algorithm to predict actual system behavior depends on the degree to which the assumptions used to develop the algorithm match the actual conditions within the system. Of primary concern to the study of recharge and discharge is the degree to which the HSU's used in the model exhibit continuum behavior. The principle requirements for continuum behavior with respect to flux are discussed in Section 2. The assumption of continuum behavior is essentially mandatory for studies of regional flow because the rigorous data requirements of the noncontinuum models cannot hope to be met in the far-field. If the system does not in fact behave as a continuum, the error involved in treating it as a continuum would have to be evaluated.

The capacity of the computer system governs the size of the problem (essentially the number of nodes) that can be treated by the model. This in turn affects the accuracy of the model, because accuracy improves as the elemental blocks become smaller. The computer capacity must in general increase as the square of the number of nodes; thus models with large numbers of nodes become exceptionally difficult and costly to operate.

3.5.1.3 Direct synthesis techniques

Direct synthesis techniques include those methods that do not require evaluation by complex mathematical tools. As applied to the problem of recharge and discharge, this type of technique would require data that directly indicate either the patterns of groundwater flow or the areas of recharge or discharge.

One type of data in this category is that which directly indicates patterns of groundwater flow. Hydraulic head data qualify because groundwater can move only from areas of high head to areas of low head, and flow patterns can be inferred from the data alone or from the results of simple contouring techniques. Hydraulic head data also provide input to the numerical methods discussed in the previous section, and are therefore also amenable to sophisticated analysis. Hydrochemical data that indicate geochemical processes are also capable of providing direct evidence of groundwater flow patterns. Examples of such processes include the progressive change from a calcium-rich to a sodium-rich water as the groundwater migrates farther from the recharge area. Another example is the progressive change with time in the proportions of the various isotopes used in age dating. An advantage of hydrochemical data over head data is that the hydrochemical data provide an independent means of verifying the results of numerical models. Both hydrochemical and head data are also useful in identifying HSU's, and in this context are discussed in detail in Section 2 together with several specific examples from the Pasco Basin.

Another type of data that can provide direct information on areas of recharge and discharge is that derived from direct observation of the surface hydrology of the site. These methods are generally very obvious and are included here for purposes of completeness. They include as indications of recharge areas local measurement of downward hydraulic gradients, observations of significant water sources in topographically and stratigraphically favorable locations, and observations of significant unexplained streamflow depletions over specific reaches. Indications of discharge areas include local measurement of upward hydraulic gradients, the presence of springs or groundwater seeps, abnormal vegetative growth in arid zones, a buildup of chemical precipitates on the soil surface, and significant unexplained streamflow accretions.

Geologic structure can be a direct indicator of either recharge or discharge areas. Outcrops of permeable horizons in topographically high or low areas may be candidate areas for recharge or discharge, respectively. A groundwater barrier that cuts across permeable strata, such as a fault zone or dike, is often associated with discharge areas. Suspected areas of enhanced vertical fracturing, such as at the crests of anticlines, are associated with increased vertical transfer of groundwater. Finally, topographic highs tend to be areas of recharge, and topographic lows tend to be areas of discharge.

The principle limitation of direct synthesis techniques is that they are generally not quantitative without further detailed analysis. Moreover, those methods based on direct observations of surface hydrology provide no information on groundwater flow patterns or on mechanisms of recharge and discharge within the study area.

3.5.2 Alternative Approaches and their Limitations

Alternative approaches to resolving the issue are generally limited to variations of the standard approaches discussed above. Examples of such variations would include the use of numerical methods different from those presented above and the identification of properties of the fluid or of the rock that could be used to supplement hydraulic and hydrochemical data as indicators of the patterns of groundwater movement.

For the issue of recharge and discharge, the primary limitations of both standard and alternative approaches lie in obtaining field data that are both technically appropriate and adequate in areal extent. These limitations are the same for this issue as for the identification of HSU's, and are addressed in Section 2.

Once the field data are collected, the available standard techniques for analyzing these data are considered to be adequate for the resolution of this issue. No new techniques appear to be available that avoid the limitations of standard techniques regarding the needs for input data, thus the consideration of alternative techniques for data analysis does not appear to be required for the resolution of this issue. Rather, effort should be placed upon overcoming the limitations of obtaining technically appropriate data from the field and upon assuring that these data have adequate areal coverage.

3.6 RECOMMENDED APPROACHES AND THEIR LIMITATIONS

Determination of areas and mechanisms of groundwater recharge and discharge will require a field program for basic data collection similar to that required for identification of HSU's. The types of data required to identify HSU's for studies of regional flow patterns are the same as will be required to assign material properties and inital conditions to these units for studies of areas and mechanisms of recharge and discharge.

The identification of HSU's goes hand in hand with identification of areas and mechanisms of recharge and discharge on the basis of those units, thus it is expected that resolution of this issue will benefit from the substantial data base assembled for identification of HSU's. Ideally, it would be expected that resolution of the HSU issue will make available good hydraulic conductivity and specific storage data at the appropriate scale for each HSU within the study area. Similarly, resolution of the

HSU issue should also provide sufficient information on geology and stratigraphy, as well as the areal distributions of hydraulic head and hydrochemistry, for the resolution of the recharge-discharge issue. Since data on boundary conditions and surface water hydrology do not normally strongly influence the choice of HSU's, it will be necessary to provide supplemental field information on these two subjects to satisfactorily resolve this issue.

In developing a strategy for resolution of the recharge-discharge issue, it is recommended that each of the principal techniques described in this section be utilized, but that the degree of effort put into each method be carefully weighed against the accuracy and detail of the probable results. The qualitative and simpler quantitative techniques should be employed first to obtain a reconnaissance level understanding of the issue. This would include applying the water budget technique to readily available surface and groundwater data and reviewing the existing geologic, stratigraphic, hydraulic head, and hydrochemical data to obtain an initial qualitative level of understanding of the net groundwater-surface water exchange and the general patterns of groundwater movement within the study area. The primary benefit of these initial studies, from the standpoint of this issue, will be in the guidance provided by the results in identifying the size of the study area and the most appropriate locations for obtaining additional data. Thus it is important that these studies be initiated during the early stages of the field program.

The numerical model techniques are so powerful in comparison with the reconnaissance techniques mentioned above that it is recommended that most of the emphasis of the later part of the program be placed upon developing good numerical models of the study area. Hydrochemical techniques are valuable for independent confirmation of the hydrologic results, but because these techniques are hydrologically useful by inference and do not provide direct hydrologic information, they must be used with judgement. In general, the numerical model techniques as confirmed by hydrochemical measurements and surface observations form the best combination of tools available for final resolution of this issue.

Following the collection and review of the existing data base, a field program should be planned to provide the additional data needed to refine our understanding of the study area. The strategy to be employed in the field program will be similar in many respects to that described in Section 2 with respect to the identification of HSU's, except that the identification of hydrologic boundary conditions will play a much more significant role. This combination of surface and groundwater data should provide a sufficient base for identification of areas and mechanisms of recharge and discharge using any of the methods for data analysis described above.

The strategy for developing and implementing a field testing program for resolution of this issue should include the following components.

1. Place initial emphasis on collecting and evaluating the existing data base.

2. Apply the qualitative and simpler quantitative techniques early, such as the water budget method, to obtain a reconnaissance level understanding of probable areas and mechanisms of recharge and discharge.

3. Develop the information and techniques needed to prepare refined models of the groundwater flow system; this would include

   (a) identifying the models to be employed in resolving this issue, including their data needs and limitations, and the capabilities and costs of available computing systems;

   (b) performing sensitivity analyses to identify data types and geographic locations that most strongly affect the estimates of radionuclide travel time;

   (c) identifying significant gaps in the types and areal extent of existing data;

   (d) identifying the extent of the hydrologic system that must be studied for identification of groundwater flow patterns and areas of recharge and discharge within the context of the overall issue of safe radioactive waste disposal;

   (e) identifying, to the extent possible, anticipated reference repository locations, so that the appropriate groundwater flow paths can be flagged for detailed study;

   (f) performing direct synthesis tests or analyses (see Section 3.5.1.3) to confirm suspected areas of recharge and discharge;

   (g) identifying other issues related to site characterization, so that all data needs can be integrated into a single program.

4. Develop a comprehensive strategy for field testing based on all available information. The strategy should allow for

   (a) a staged implementation that permits feedback and continuing refinement;

   (b) a dynamic program that can incorporate change as site conditions are revealed;

   (c) a prioritized program that allocates resources to the areas of greatest need.

5. Implement the field testing strategy through the cyclical process of obtaining field data, analyzing that data, and using the results of the analysis to help guide the acquisition of additional field data until the issue is satisfactorily resolved.

It must be recognized that site characterization is an evolutionary process that becomes increasingly refined as more becomes known about the site. The geologic structure and its hydrologic properties can be so highly variable, and contain so many significant unknowns, that it is unwise to attempt to lay out a complete and rigid site characterization scheme either at the beginning of a project or even after considerable information has been obtained. This is particularly true for flood basalts, in which the significant structural variations that can occur due to local cooling history compound the more normal variations of bed thickness, lateral pinch-out, folding, faulting, and so on. As noted in the newly revised British Standard BS 5930 Code of Practice for Site Investigation, site characterization "is a process of discovery, and should not therefore be based on a rigid preconceived programme nor on a slavish adherence to code recommendations" (Meigh, 1981).

The greatest difficulty in collection of field data will be in the cost. Because of this, it will be important to allocate available resources carefully to maximize the benefits of each measurement. The collection of field data in stages, as recommended in Section 2, is intended to serve this function. The use of groundwater models and statistical methods will help to identify the best locations and optimum density for collection of additional data. Field measurements to obtain appropriate boundary conditions are also important. However, their need should be evaluated in light of the confidence that can be placed in boundaries obtained from the larger, regional model and with respect to the sensitivity of the model to the accuracy of a particular boundary. For example, boundaries that carry significant flux or are closest to the reference repository location would command a higher priority for field investigation.

Field investigations of boundary conditions would follow different strategies, depending upon the type of boundary. No-flow boundaries will require a demonstration of negligible groundwater movement across the boundary. The presence of a groundwater divide can be demonstrated by groundwater head measurements. The suspected low permeability of a groundwater barrier can be demonstrated by multiple well, interference type pumping tests in the vicinity of the barrier, as discussed in Section 2. Constant-head boundaries can also be demonstrated by head measurements. Constant-flow boundaries are generally used to model activities of man, such as a pumping well, and would be expected to be unusual in nature except when associated with constant-head conditions. Field investigation of constant-flow boundaries would normally require measurement of the hydraulic gradient across the boundary and the horizontal permeability at the boundary. The standard pumping or injection tests described in Section 2 would be satisfactory for making such measurements.

The limitations to the recommended techniques are both technical and logistical in nature. The principal technical limitation is the degree to which the model parameters are representative of actual conditions in the field; the logistical limitations have to do with costs, time required, and the desire not to impair the integrity of the site by excessive drilling.

The degree to which model parameters represent actual conditions in the rock depends upon (1) the extent to which the flow theory is correctly applied, and (2) the validity of the data. The flow theory will in general be correctly applied if the HSU is identified at a scale appropriate for theoretical treatment as a continuum. Since under current technology the rock must, for practical purposes, be treated as a continuum, an error will be introduced if the actual rock does not, in fact, demonstrate continuum behavior. This limitation is discussed more fully in Section 2.

The data will in general be valid if they correspond to the actual in situ hydrologic properties. The hydraulic properties of basalt that govern groundwater flow are expected to be variable, even within the same HSU. Most numerical models require one (and only one) value of the hydraulic property for each elemental block. Thus at blocks for which measured values are available, there is a question of which measured value to select. At blocks for which no measured values are available, there is a question of how to estimate an accurate value. The identification of initial and boundary conditions also falls into this category. Techniques that are generally statistical in nature are available to respond to these limitations, but are more appropriately treated in studies of model validation and verification and are beyond the scope of this report.

Also falling within the question of data validity is the limited accuracy of surface water data used in the water budget technique. Generally, an error of 5-10% in these data is considered normal, thus the ability of the technique to accurately resolve flow quantities of less than about 5% of the gross inflow or outflow is questionable. This limitation can in part be overcome by working with averages or long-term trends, but this would limit the flexibility of the investigator to establish new gauging stations better suited to the needs of the problem. Establishment of accurate long-term averages can easily require in excess of 20 years of data. This may be partially resolved through correlation of new stations with existing stations.

Logistical limitations are the well-known constraints of time, money, personnel, site integrity, and their impacts on the quantity and areal coverage of the data. These, in turn, increase the significance of the technical limitations related to the identification of hydraulic properties, initial conditions, and boundary conditions, and to the usefulness of hydrochemical data, all of which require good areal availability of data.

3.7 UNCERTAINTIES REMAINING IN RESOLUTION OF THE ISSUE

Given sufficient effort, the approaches described in this report are expected to be able to identify the general flow patterns within the natural groundwater system and the locations and mechanisms of recharge and discharge. Accurate quantification of recharge and discharge in terms of groundwater flux is less certain, however, because of the technical and logistical limitations described above. The numerical model will be the primary tool for this effort, and its accuracy will determine the accuracy with which recharge and discharge can be quantified. Procedures are available for model calibration and verification, the results of which will provide an estimate of model accuracy. The accuracy of the model will depend primarily upon the degree to which continuum behavior is exhibited at the scale of the HSU's and upon the accuracy with which the controlling hydrologic parameters can be identified throughout the basin. The accuracy of the model is the best available indication of the accuracy of the regional hydrologic parameters, and should be used to identify weak points in the data base. Research is required to develop methods for verifying continuum behavior, and time and money will be required for accurate, well-distributed measurements.

3.8 RECOMMENDATIONS FOR RESEARCH

Primary research needs center upon overcoming the principal limitations in data acquistion and interpretation. These needs include

1. Techniques for assessing the amount of data required for site characterization in view of the geologic variability of the site and the accuracy expected of the analysis.

2. Techniques for identifying the optimal locations within the basalt strata for collecting additional data (if required) and for systematically prioritizing specific data needs.

3. Development of refined methods for estimating the values of hydrologic parameters at unmeasured locations within a sequence of flood basalts.

4. Methods for relating the accuracy required in quantification of recharge and discharge to the accuracy required of field measurements and ways of demonstrating whether such accuracy has been achieved.

5. Identification of continuum behavior for intrinsically discontinuous geologic media: analytical and field methods are required to verify continuum behavior on the scale of the HSU's. This research is also required for identification of HSU's.

6. Assessment of the errors involved in mathematical treatment of discontinuous media as if they were continuous media: regional groundwater movement can at present be treated only with continuum models because of the unrealistic data requirements of noncontinuum models. The errors involved in such treatment have not been analyzed.

7. Development of practical techniques for treatment of discontinuous media in studies of regional groundwater flow: realistic methods for modeling a discontinuous medium in a way other than as a simple continuum are required for regional flow. These methods would probably involve some type of stochastic treatment.

4. SOLUBILITY OF RADIONUCLIDES

4.1 STATEMENT OF ISSUE

Moving groundwater is expected to provide the mechanism by which nuclear waste could be transported from an underground storage facility to the accessible environment. In order to predict the rates of radionuclide migration, knowledge is needed of the processes that control residence times of radionuclides in the aqueous and solid phases.

In the event that the canister and waste form fail to contain radioactive waste materials, radionuclides will enter the local groundwater system. They will react with various components of the groundwater, and possibly the host rock, to form relatively insoluble compounds and solution species that can provide major controls on solution concentrations and migration rates. Therefore, appropriate characterization of the groundwaters, as well as thermochemical data on the solubilities of compounds of the waste radionuclides likely to form in the systems, is required to adequately assess and predict the ability of the site to meet established standards for rates of release of radioactive materials to the accessible environment.

4.2 IMPORTANCE OF ISSUE

Many radionuclides can form rather insoluble compounds, as well as solution complexes, with components of basaltic groundwaters. Precipitation of stable solid phases will lower the concentration of radionuclides in the groundwater; on the other hand, formation of aqueous complexes will tend to increase the concentration. Thus knowledge of the solubility of compounds can provide the first step in the assessment of amounts and rates of release of radionuclides from an underground facility. These studies may show that some nuclides could be so insoluble that, with a slow rate of groundwater movement, no other retardation would be required. Knowledge of solution species will also help to define the sorptive properties of the host rock and engineered barrier.

The identities and solubilities of compounds formed by radionuclides will depend on the oxidation states of the radionuclides, the redox properties of the groundwater and surrounding rock and engineered barriers, and the nature and concentrations of precipitating ions and complexing ligands in the groundwater system. Therefore, in order to predict the chemical behavior of the radionuclides, it is essential to obtain representative and uncontaminated samples of groundwater at the depth of the proposed repository and along possible flow paths intersecting the repository. A complete characterization of these waters, including both chemical composition, pH, and redox behavior, is needed to predict possible stable solid phases and solution complexes of the radionuclides of interest. Because temperature

affects chemical equilibria and reaction rates, the effects that increases in repository temperature will have on the chemical composition and redox properties of the groundwater-host rock system must be known. Separate but related problems requiring study are the change in groundwater character with time and the effects of excavation and construction of the repository on the groundwater properties.

Knowledge of the nature and solubility of radionuclide compounds likely to form under existing groundwater conditions at the repository site and under conditions of elevated temperatures is essential for predicting radionuclide release rates. To obtain this information, it will be necessary to identify precipitates that form under the expected groundwater conditions and to either measure their solubilities or demonstrate that sufficient verified thermochemical data are available to calculate that information with confidence.

The significance of this issue is reflected in several sections of 10 CFR Part 60.

1. Section 60.11(a) requires assessment of the site characterization program with respect to investigation activities that address the ability of the site to host a repository and isolate radioactive waste.

2. Section 60.21(c) requires that the Safety Analysis Report contain an analysis of the geochemical aspects of the site that bear significantly on its suitability for disposal of radioactive waste.

3. Section 60.21(a) indicates that the Commission must determine whether the DOE has adequately described the geochemical characteristics of the proposed site prior to construction authorization.

4. Section 60.111(b) requires that the geologic repository and each of its components satisfy specific requirements related to rates of release of radionuclides.

5. Section 60.122 specifies geochemical conditions that may be considered favorable in their effects on the ability of the site to meet performance objectives.

6. Section 60.123 specifies geochemical conditions that would have potentially adverse effects on the ability of the site to meet performance objectives.

7. Section 60.132 specifies additional design requirements for the underground facility that will provide control of radionuclide releases and migration.

The issue of the solubility of radionuclides is related to the following sections of 10 CFR Part 60: 60.11 (a); 60.21 (c) (1), (3); 60.31 (a) (1) (i); 60.111 (b) (1), (2) (ii), (3); 60.122 (d), (h) (1), (2); 60.123 (a) (8), (b) (13), (14); 60.132 (a) (2).

4.3 SITE CHARACTERIZATION METHODS

4.3.1 Characterization of Groundwater

In order to predict the nature of possible precipitates and solution species of radionuclides likely to form in groundwaters, it is necessary to know the chemical composition, pH, and redox properties of representative and uncontaminated groundwater samples. A detailed chemical analysis of major and trace components is necessary. An analysis for particulates in groundwater must also be made to ensure that radionuclides will not be transported by particulates present in the water. Because many radionuclide metal ions form insoluble compounds and solution complexes with the anions of typical groundwater (e.g., hydroxide, sulfide, sulfate, carbonate, phosphate, silicate, chloride, fluoride, and nitrate anions (Katz and Seaborg, 1957)), the identities and concentrations of groundwater anions are needed. The radionuclide anions selenide and iodide can form insoluble compounds and aqueous complexes with several of the heavy metals (e.g., Fe, Mn, Ni, Co, Cu, Ag, Hg, and Pb (Weast, 1977)) found at trace levels in groundwaters at the Hanford site; therefore, trace element concentrations should be determined. In addition, mixed compounds containing radionuclides and major groundwater cations may form (such as $Ca(UO_2)_2(H_2SiO_4)_2$); thus concentrations of the major cations should be measured.

The oxidation states of the waste radionuclides will determine the nature of the precipitates likely to form, and the solubilities of these compounds will in part determine solution concentrations. In order to predict these oxidation states, knowledge of the redox properties of the groundwater-host rock system is required. The pH must be known because solubility and adsorption are functions of pH. Experiments to determine the likely pH in the thermally disturbed zone should also be undertaken.

A rather complete characterization of groundwater will be required as an aid in resolving hydrologic issues, as discussed in Section 2.7.3.1. These data will be used in determining the effects of excavation and construction of the repository on the site properties, in estimating past and future groundwater compositions, and in predicting sorptive interactions of radionuclides with the geochemical environment. The chemical analyses of the groundwaters required for resolution of these issues will normally include measurements of the components needed for resolution of the issues under discussion here. Sampling and analyses should be coordinated to meet the data needs of both the hydrologic and the geochemical issues.

4.3.1.1 Groundwater sampling

A representative, uncontaminated sample is needed of the groundwater that will contact the waste form after loss of canister integrity. It is assumed that contamination resulting from chemical processes occurring within the engineered barriers can be accounted for. If the groundwater system is at a steady state with regard to chemical processes, then samples taken immediately "upstream" from the repository are sufficient for characterization. If, however, compositionally different waters occur far upstream from the repository and may be expected to reach the repository at the time of loss of canister integrity, then it will be necessary to sample those waters and, in addition, account for potential changes in their compositions due to chemical reactions that will occur along the flow path extending from their present locations to the repository site.

Contamination can occur by the introduction of a foreign substance during the drilling process, by the artificial mixing of groundwaters during and after drilling, and by the loss or introduction of chemical components during sample recovery.

Downhole samples are especially susceptible to contamination from drilling muds, detergents, grease, lubrication fluids, and grouting materials. Nonadsorbing tracers should be added to the drilling fluid in order to measure the level of contamination in a groundwater sample. Tritium is commonly used as an indicator of contamination (La Sala and Doty, 1971); stable isotopes have also been used (Fritz et al., 1978), and the use of fluorocarbon compounds, miscible with water, has been suggested (Apps et al., 1979).

The mixing of different groundwaters prior to sampling is a common problem (Newcomb, 1972; La Sala et al., 1973; Apps et al., 1979). The consequences of this problem can be severe in terms of groundwater characterization. Not only is the composition of a "mixed water" obtained, but precipitation or dissolution of solids can occur as a result of the mixing, thus causing changes in concentrations of chemical species dissolved in the aqueous phase.

A sample taken at depth and brought to the surface undergoes changes in pressure and temperature during recovery. These changes can lead to exchange of gaseous components between the sample and the surrounding atmosphere. Such changes can, in turn, lead to changes in pH (CO_2 exchange), changes in the redox state of the system (O_2, CH_4, H_2S exchange), and changes in the amounts of dissolved solids (precipitation and dissolution of solids).

Several methods are available for reduction of sample contamination. To minimize contamination during drilling, the use of air instead of conventional drilling fluids is highly recommended. This procedure has been used successfully in drilling several deep holes at the Nevada Test Site. If conventional drilling fluids are used, hydrologic testing and

groundwater sampling in previously contaminated boreholes generally require time-consuming, expensive cleanout procedures. Estimates of the time necessary to remove contaminants from the rock surrounding a borehole have been made by Apps et al. (1979). The estimates assume contamination inflow at a constant head difference of 75 m into the formation and removal by swabbing at a constant head difference of 1000 m into the well. Figure 4.1 from Apps et al. (1979) shows the number of invasion volumes (volume of drilling fluid that invaded the formation during drilling) that must be removed by swabbing as a function of time. It may not be unusual for 20 invasion volumes to be removed before the water is sufficiently clean for geochemical sampling. Assuming that the sampling zone was exposed to drilling fluid contamination for one month during drilling, it would take about 45 days of constant swabbing to remove 20 invasion volumes and produce an acceptable sample under the above assumptions.

There are three drilling and sampling methodologies that can be employed to minimize contamination due to the mixing of groundwaters: (1) the well can be drilled to completion and adjustable packers can be set above and below each aquifer of interest; (2) the well can be drilled in a discontinuous fashion each time a new aquifer is penetrated, after which the top of the aquifer can be sealed with a packer and the aquifer pumped until an uncontaminated representative sample is obtained; (3) a nest of wells can be drilled, each well being bottomed in a different aquifer. Methods 2 and 3 afford the least potential for contamination and are recommended. However, it should be noted that Method 3 can be quite costly and time consuming. Method 1 is most commonly used, but has often been shown to lead to a significant amount of aquifer mixing (La Sala and Doty, 1971).

To insure that a representative sample of groundwater is obtained from a borehole, the groundwater should be pumped and parameters such as conductivity, pH, temperature, and dissolved oxygen (all of which can be measured potentiometrically) should be measured in a semicontinuous fashion until steady-state conditions are achieved. Samples should then be taken and analyzed for a wider variety of ions and stable isotopes at discrete points in the pumping process until the investigator is reasonably assured that a representative sample of the aquifer under study has been obtained.

To minimize problems associated with changes in pressure and temperature during the recovery process, several procedures should be adopted. The sample should be immediately analyzed (at the well head) for dissolved gas content, alkalinity, pH, and redox state. To decrease the possibility of precipitation, the sample should be diluted with ultrapure, deionized, distilled water. The addition of ultrapure nitric acid can also be used to avoid precipitation. However, the possibility exists for dissolution of suspended colloidal-sized clays. Filtration with 0.10-μm filters can minimize this possibility (Kennedy et al., 1974), although it may be

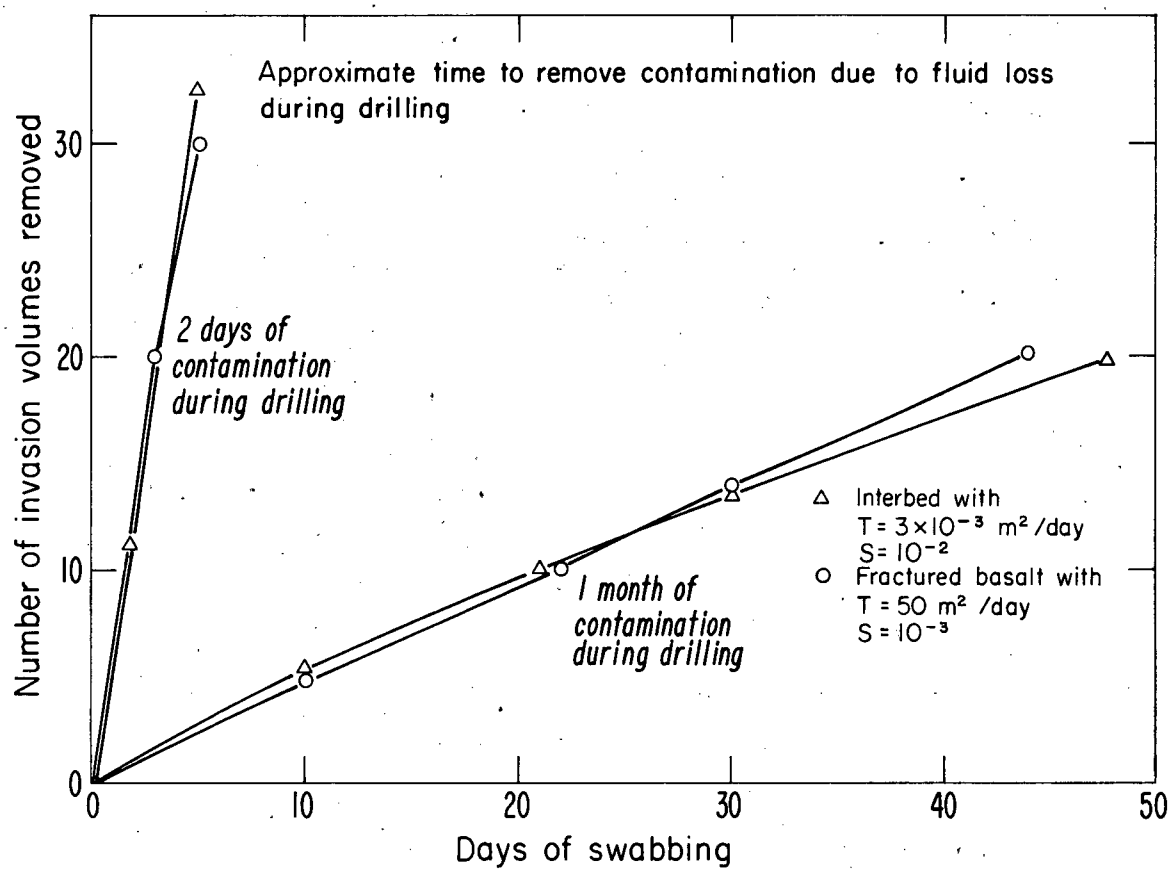


Figure 4.1. Approximate time to remove contamination due to fluid losses during drilling (from Apps et al., 1979, Figure A-2). [XBL 788-2654]

necessary to subject the sample to ultracentrifugation followed by examination of the aqueous phase with a nephelometer to completely avoid the problem. In any case, the sample should be centrifuged and shown to be free of detrital material prior to chemical analysis, even if field acidification has not been accomplished. If significant loss of dissolved gases has occurred during transit up the well, it will be necessary to collect dissolved gases with a special downhole sampling device and determine their amounts and compositions (e.g., see Truesdell and Nehring, 1978).

During excavation of the repository, horizontal boreholes should be drilled for groundwater sampling. Such a system has several advantages over surface sampling of vertical boreholes: the boreholes may be self-cleansing, thus providing an uncontaminated sample of groundwater; and field collection and analysis can be performed under ambient conditions. In addition, the flow distance to the sampling point from the original locations of the fluid should be much smaller than the flow distance of a well; therefore, loss of dissolved gases is minimized. Finally, cross-aquifer contamination can be entirely avoided.

In summary, an adequate sample of groundwater can be obtained if care is taken to minimize the various sources of contamination. Existing sampling methodologies should be sufficient for this purpose. If collection is done at depth in the repository itself, it would be advisable to set up a laboratory in the test facility and perform as many analyses as practicable immediately upon sampling. The laboratory could include facilities for determining effectiveness of various filter sizes and for monitoring elemental composition of the flowing fluid by atomic absorption spectroscopy to insure a representative sample.

4.3.1.2 Analytical methods

4.3.1.2.1 Chemical analyses

A number of analytical methods are available for determining the concentration of major and trace elements, as well as anions, in water samples. They include neutron activation analysis, fluorimetry, emission spectroscopy (particularly inductively coupled plasma), atomic absorption spectroscopy (both flame and nonflame), atomic fluorescence spectroscopy (flame, oven, and x-ray) and wet chemical methods (gravimetry, titration, electrometry, and ion-exchange chromatography). Since the utility, detection limits, and reliability of the various methods differ for different elements, no single method can be recommended for a complete chemical analysis of a water sample. Generally speaking, spectroscopic and neutron activation techniques are used in combination for major and trace metal analysis, and wet chemical methods are used for anion analysis. The choice of methods usually depends on the instruments that are available and on the components to be measured. The analytical methods listed above are well

established and the procedures, advantages, limitations, and precautions have been discussed in a number of publications (Ellis et al., 1968; Brown et al., 1970; Winefordner, 1976; Wood, 1976; Pinta, 1978). The chemical analysis should include the measurement of at least the following components in addition to pH and temperature: B, Li, Na, Mg, Al, K, Ca, Sc, Fe (Fe^{2+}, Fe^{3+}), Mn, Ni, Zn, Co, Cr, Cu, Sr, Mo, Ag, Cd, Sn, Cs, Rb, I, Ba, La, Ce, Pr, Nd, Pb, Th, U, F, Cl, Br, SO_4, S, NO_3, PO_4, H_4SiO_4, CO_3, organic contaminants, and the gases CH_4, O_2, N_2, CO_2, He, and Ar.

Precision and sensitivities of analytical techniques have increased to such an extent in recent years that the weakest links in the analysis are the procurement of uncontaminanted samples and the subsequent handling and preparation of samples. Therefore, certain precautions should be observed and certain procedures followed to insure reliable results (Brown et al., 1970; Ellis et al., 1968; Wood, 1976).

A sufficient number of replicate samples should be analyzed to establish the consistency of sample preparation and the accuracy of measurements. Because discrepancies between different analytical methods for some elements at low concentrations arise from differences in sample preparation techniques, it is desirable to analyze for some elements by two or more alternative methods. For example, in reporting the results of analyses of waters from the Hanford area, Apps et al. (1979) showed that analyses by neutron activation and x-ray fluorescence tend to yield higher values than analysis by atomic absorption. The difference was attributed to the fact that the former methods analyzed for both dissolved and colloidal or suspended material while the atomic absorption method, which employs a preliminary solvent extraction step, measures only the dissolved species. The particular measurement to be made will determine whether the samples require filtration. However, the adequacy of the filtration to separate solid and solution phases, or the degree to which the analytical method is sensitive to suspended solids, should be determined.

Several measurements should be made in the field at the time of sampling. Temperature measurement is, of course, one. Furthermore, laboratory measurement of the pH of a water that is only slightly buffered and not at equilibrium with the atmosphere may differ from measurements made at the time of collection; the difference may be due to loss of dissolved gases, absorption of CO_2 or laboratory fumes, or deposition of salts from solution (Brown et al., 1970). Carbonate and bicarbonate measurements on groundwaters are particularly subject to changes if samples are collected and stored in containers that may be permeable to CO_2 (Wood, 1976). Hydrogen sulfide gas is readily lost from neutral or acid solutions, but in alkaline solutions the rate of oxidation of sulfide by air is very rapid (Ellis et al., 1968). Samples should be taken with a minimum of aeration and stirring and analyzed for pH, carbonate/bicarbonate, and sulfide in the field within minutes of collection.

Checks should be made to test the internal consistency of the analyses. These checks should include tests of chemical and electrical balance, reconciliation of alkalinity titrations with CO_2 measurements and pH, and reconciliation of solution composition with the nature of the contacting geologic media. However, these tests provide only approximate indications of the validity of the analyses. Large deviations can indicate a large error in one or more of the determinations, but consistency is not conclusive proof that each determination is accurate.

4.3.1.2.2 Redox measurements

An important parameter that must be considered in the study of multivalent radionuclides, e.g., Tc, U, Np, and Pu, is the oxidation-reduction potential (Eh) of a groundwater. Eh controls the chemical reactions in which elements undergo a loss or gain of orbital electrons and thus change their valence state. Eh may also affect univalent radionuclides that are sensitive to Eh. Eh has been considered to be a direct indicator of the redox state of a rock-water system and to be a master variable analogous to pH. However, the ability of Eh measurements to accurately describe the redox properties of natural waters has been questioned (Stumm, 1966; Morris and Stumm, 1967). Oxidation-reduction related reactions in natural systems are frequently irreversible and not at equilibrium, so that measured Eh is often a mixed potential resulting from several redox reactions that may not readily couple with each other. A meaningful Eh cannot be defined for such nonequilibrium systems. However, although true equilibrium may not be achieved, partial equilibrium may be approached in many cases, and a metastable system may exist for which a working redox potential can be related to certain redox couples.

The Eh of water samples is frequently measured with a noble metal (usually platinum) electrode and a reference electrode system using a sensitive voltmeter. This type of electrode measurement of Eh for geologic purposes is beset with a number of experimental problems and limitations (Stumm and Morgan, 1970; Langmuir, 1971; Morris and Stumm, 1967; Benson et al., 1980). Direct measurement of Eh values for natural waters involves complex theoretical and practical problems in spite of the apparent simplicity of the electrochemical techniques. Detailed quantitative interpretation is unjustified in most cases. The results of most experiments with electrode measurements of Eh values described in the literature lead to the conclusion that the measurement provides, at best, qualitative results (Stumm, 1966; Morris, and Stumm, 1967; Wood, 1976; Thorstenson and Fisher, 1979). Therefore, Eh measurements by electrodes alone should not in general be relied upon to predict the oxidation states of radionuclides that can exhibit multiple valence states under groundwater conditions.

In theory it is possible to evaluate the redox potential in natural waters by determining the relative concentrations of members of some or all of the redox couples in the system. Normally, only a few elements are major

participants in redox reactions in natural waters, i.e., C, O, N, S, Fe, and Mn. The potential generated by a couple is related to the activities of the components through the Nernst equation,

$$Eh = E^\circ + \frac{RT}{nF} \ln \frac{(\text{oxidized state})}{(\text{reduced state})},$$

where

E° = the standard potential of the half-cell reaction,

R = the gas constant,

T = the absolute temperature,

F = the Faraday constant,

n = the number of electrons involved in the half-cell reaction.

After measuring the concentrations of appropriate components of the couples that are controlling the solution redox properties, e.g., $CH_4 - CO_2$, $H_2O - O_2$, $NH_4^+ - NO_3^-$, $S^{2-} - SO_4$, $Fe^{2+} - Fe^{3+}$, and $Mn^{2+} - Mn^{4+}$, an Eh value can be calculated for each couple. A single Eh value can be assigned to the system if the calculated Eh values for the couples are in reasonable agreement. Thorstenson and Fisher (1979), for example, have analyzed waters from several wells in the Fox Hills-Bosal Hill Creek aquifer region. Redox potentials calculated from the components of the couples $HS^- - SO_4^{2-}$, $CH_4 - CO_2$, and $NH_4^+ - N_2$ agreed to within about 50 mV, indicating that the redox reactions approached, but probably did not achieve, true equilibrium. The calculated values are about 200 mV more negative than the Eh values measured with a platinum electrode. Thus Eh values calculated from the concentrations of the components of the major couples can be used to estimate the redox level of water samples, but may not be reliable in all cases. Such measurements can at least provide limits on the Eh-pH range of the water. Reliability of this method will depend on the particular system and will require verification. In any case, the method is useful for identifying the controlling redox reactions.

At this time, methods for determining the redox potential of groundwater are neither sufficiently reliable nor sufficiently accurate for the prediction of oxidation states of multivalent radionuclides in the groundwater system. Therefore, it may be necessary to determine the oxidation states by direct measurement, either in situ or in very closely related laboratory experiments. This process can be difficult and time-consuming, but there may be no viable alternative. For the initial site characterization study, an attempt should be made to obtain the necessary data on the groundwater composition to calculate Eh values for the major redox couples. If these values are reasonably self-consistent, it may only be necessary to verify the result by direct measurement of the oxidation states of a few selected multivalent radionuclides.

Other possible methods for estimating the redox potential of water samples need further development. Organic dyes that exhibit one color in the oxidized state and another in the reduced state (Zobell, 1946) have been used in estimating the redox potential of systems by colorimetric methods. For example, Bondietti has used indigo carmine as an Eh indicator in studies of the oxidation states of Tc (Bondietti, 1979). Moreover, certain fluorescent dyes, such as triamylmethane and thiozinyl, lose their fluorescence reversibly at particular redox potentials. The fluorescence intensity of such a dye is thus a redox indicator. A combination of dyes may be used to cover the Eh range of interest. This is a particularly interesting technique to explore from the point of view of monitoring of Eh in the field.

4.3.2 Determination of Solubility

Two different approaches can be taken for determining the effect of formation of insoluble compounds on solution concentrations of radionuclides. One method is to calculate solution concentrations from available thermochemical data on solubility product constants and solution complexation constants. The other method is direct measurement.

In order to predict solution concentrations of radionuclides in a repository-groundwater system, the identities and solubilities of the solid phases and identities of the solution species likely to form under geologic conditions are needed. Solubility product constants alone are usually not sufficient to predict solution concentrations because the formation of hydrolysis products and other complexes increases apparent solubilities. For example, one can predict the concentration of the ion UO_2^{2+} in equilibrium with solid $UO_2(OH)_2 \cdot H_2O$ from the solubility constant,

$$UO_2(OH)_2 \cdot H_2O(\text{Solid}) + 2H^+ = UO_2^{2+} + 3H_2O, \quad \log K = 5.40.$$

However, UO_2^{2+} is a minor solution component in the pH range of natural systems, and the formation constants for the following hydrolysis reactions are needed (Lemire and Tremaine, 1980):

$$UO_2^{2+} + H_2O = UO_2(OH)^+ + H^+$$

$$UO_2^{2+} + 2H_2O = UO_2(OH)_2^\circ + 2H^+$$

$$2UO_2^{2+} + 2H_2O = (UO_2)_2(OH)_2^{2+} + 2H^+$$

$$3UO_2^{2+} + 4H_2O = (UO_2)_3(OH)_4^{2+} + 4H^+$$

$$3UO_2^{2+} + 5H_2O = (UO_2)_3(OH)_5^+ + 5H^+$$

$$3UO_2^{2+} + 7H_2O = (UO_2)_3(OH)_7^- + 7H^+$$

$$4UO_2^{2+} + 7H_2O = (UO_2)_4(OH)_7^+ + 7H^+$$

All of these equations must be solved simultaneously in order to calculate the concentrations of the individual solution species, since they can occur together in solution. In addition, if other solution complexes are present, they must be included. For example, if carbonate is present in the uranium system, reactions involving the carbonate complexes of uranyl must be included, i.e.,

$$UO_2^{2+} + CO_3^{2-} = UO_2CO_3^{\circ}$$
$$UO_2^{2+} + 2CO_3^{2-} = UO_2(CO_3)_2^{2-}$$
$$UO_2^{2+} + 3CO_3^{2-} = UO_2(CO_3)_3^{4-}$$

The formation of insoluble phases and their equilibria with solution species are much more complicated processes in the natural systems than in the homogeneous solutions normally encountered in the laboratory. Since the waste radionuclides would most likely be present at low concentrations in the contaminated groundwaters, it is reasonable to expect that they would behave in a manner similar to other trace elements. Trace elements usually occur in nature as mixed cationic compounds, as solid solutions with mineral phases formed by more abundant elements, and as precipitates that form along with those of more abundant elements. Unfortunately, complete thermochemical information on such reactions does not exist for any of the waste radionuclides in natural systems. Therefore, it is not possible at present to calculate the course of such complicated reactions for these radionuclides. In situ experiments with the waste nuclides to obtain the necessary thermochemical data would be extremely difficult, if not impossible, to carry out; indeed, such measurements have seldom been done for even the trace elements usually occurring in natural waters. What can be done more readily is to consider the solubilities of simple or pure compounds of the waste elements that can form with groundwater components under conditions of temperature, Eh, and pressure characteristic of the repository environment. That this is a reasonable approach can be seen from thermodynamic considerations: compounds or minerals of higher free energy tend to convert to compounds or minerals of lower free energy; i.e., solid phases will continuously change to phases having lower solubilities. Thus, in principle, upper limits to radionuclide solubilities could be established. Unfortunately, there are no thermochemical data on even simple compounds and complexes of many of the important radionuclides, e.g., carbonates, phosphates, and silicates of Np, Pu, and Am. Very few data are available on any chemical species at elevated temperatures.

The second approach for determining the effects of the formation of insoluble compounds on solution concentrations of radionuclides is direct measurement of the solution concentrations as functions of the initial

radionuclide concentration over the range of solution compositions, temperature, Eh, pH, and other parameters expected for the groundwater system in the vicinity of the repository. Present technology does not allow such experiments to be conducted in situ, and the actual groundwater-rock system cannot be adequately simulated in the laboratory. An additional problem with this approach is that fundamental thermochemical data would not be obtained to extrapolate to possible future conditions of the repository system beyond the range of parameters studied. Careful characterization of the solid phases and solution species produced in such solubility measurements would greatly enhance the utility of the information for predictive purposes. Characterization of solid phases, e.g., by x-ray crystallography, would present no particular problems. However, characterization of solution species, i.e., hydrolysis products and other complexes, at solution concentrations of 10^{-8} to 10^{-12} M associated with very insoluble compounds, will require further research to resolve.

4.3.2.1 Solubility measurement methods

Measurement of the solubility of a compound in aqueous solution involves basically the following steps: formation or preparation of the solid phase, characterization of the solid phase, separation of the solid and aqueous phases, and analysis of the aqueous phase for the dissolved species. Although this appears to be a straightforward procedure, certain precautions should be observed for reliable results. The most commonly used method for determining solubility consists of the following steps. The compound is first prepared by some standard procedure. After the material is characterized, an excess of the solid is placed in contact with an aqueous solution of the appropriate composition. Some of the solid phase dissolves, and the system is allowed to come to equilibrium before the aqueous phase is analyzed for the concentration of the element of interest and the precipitating counter-ion. From the concentrations, a solubility product can be calculated.

A second, but less commonly used method involves the preparation of an aqueous solution containing both the element of interest and the precipitating counter-ion at concentrations that produce a supersaturated solution with respect to precipitation of the compound. Again, the system is allowed to come to equilibrium and the aqueous phase analyzed.

For reliable results, it should be demonstrated that equilibrium has been achieved in solubility measurements. The most rigorous method of demonstrating that a solubility experiment has reached equilibrium is to approach equilibrium from both undersaturated and supersaturated conditions, i.e., a combination of the two methods discussed above. The value of the solubility product constant should obviously be the same in both cases. However, this method of demonstrating equilibrium is seldom used. More frequently, the concentrations of the components of the solution are measured as functions of time using either one or the other of the preparation methods described above. When the concentrations remain constant for several weeks or months, it is assumed that equilibrium has been established.

4.3.2.1.1 Characterization of solid phase

Careful characterization of the solid phase used in making a solubility determination is of utmost importance, but is frequently omitted. When using a compound prepared under one set of solution conditions to measure solubility under a different set of solution conditions, it cannot be automatically assumed that the prepared compound is the controlling solid phase without confirmation. In complex aqueous solutions such as groundwaters, a second, more stable solid phase may form that could control the solubility of the element of interest. Moreover, when preparing a sparingly soluble compound according to an established procedure, the exact composition and structure of the solid will vary depending on a number of factors, including kinetics, temperature, solution concentrations, and age of the precipitate. Furthermore, the solid phase may change from an "active" to an "inactive" form during the course of the experiment, i.e., a free-energy change is associated with the conversion of an amorphous or finely divided crystal precipitate into a well-crystallized solid. The active form of a precipitate consists of very fine crystals with disordered crystal lattices. Such a precipitate may persist in metastable equilibrium with the solution and may be converted only slowly into a more stable and inactive form (Feitknecht and Schindler, 1963; Stumm and Morgan, 1970). Measurements of the solubility of "active" forms give solubility products that are higher than those of the inactive forms (Zimmerman, 1952; Baes and Mesmer, 1976), and would provide data relevant to a worst-case analysis.

Finally, the particle size of the solid phase is a factor in determining the solubility of a compound. Because the equilibrium concentrations of dissolved products decrease as the average particle size increases, special precautions on this point are sometimes needed (Zimmerman, 1952; Baes and Mesmer, 1976).

From these facts, it follows that determination of the solubility product should be accompanied by a characterization of the solid. X-ray diffraction is recommended for the characterization, and can be acccomplished with microgram amounts of material. Crystal structure and stoichiometry can usually be determined by this method if a sufficiently large single crystal is available. Frequently, only a finely divided crystalline precipitate is available, and characterization is made by comparison of powder patterns with those of known compounds of chemically related elements. Through this method, conclusions can be drawn as to the chemical activity or degree of crystallization of the precipitate from broadening of the lines (Feitknecht, and Schindler, 1963). Amorphous precipitates cannot be analyzed by these means, and characterization is made through elemental analysis of the solid. Although this type of analysis can often identify the nature and stoichiometry of the solid phase, it provides no structural information, and hence no information on the active form of the solid. Elemental analysis usually requires milligram amounts of material, which may not be available during site characterization studies.

Techniques for the characterization of small amounts of precipitates adsorbed on surfaces, as might be the case in natural systems, are not generally available.

4.3.2.1.2 Separation of solid and solution phases

The compounds of many of the long-lived radionuclides that are likely to form in natural systems are very insoluble, and very low solution concentrations of the radionuclides would be expected, e.g., 10^{-8} to 10^{-12} M. However, these radionuclides can form colloidal suspensions which, if included in the analysis of the solution phase, could lead to large errors in the solubility measurement. The separation of solid and solution phases is an important step in the analysis.

The techniques most often employed for separating the solution and solid phase in solubility studies include (1) gravitational settling, (2) centrifugation, (3) filtration, or a combination of the three methods. In the first method, the solid phase is simply allowed to settle for an extended period of time before a portion of the aqueous phase is withdrawn for analysis. This method could allow suspended or colloidal material to be withdrawn as well. In the case of centrifugation, rarely is a discussion given of the minimum time or revolution speed needed to achieve adequate separation, nor is a verification of the effectiveness of the separation made. Finally, filtration is often used as a final or single separation step. Few studies report effects of pore size or filter material. However, increasing use is being made of two or three filters with decreasing pore sizes in the range of 0.4 to 0.15 μm to filter the same sample. Constant concentrations of the components passing each filter are taken as verification of effective separation. However, there is some evidence that the filters themselves may at times adsorb soluble species from solution and that different materials and different filter constructions behave differently in this respect (Polansky and Baer, 1977). No systematic studies or comparisons of these three methods were found in the literature.

4.3.2.1.3 Analysis of the aqueous phases

A number of analytical methods are available for determining the concentrations of the dissolved species. The particular method to be used depends on the element and its expected concentration. Since the radionuclide concentrations may be quite low, rather sensitive methods need to be employed. In the past, the most commonly used methods included radiochemical techniques, potentiometry, polarography, colorimetry, and atomic absorption spectroscopy. Generally speaking, these methods are aequate for concentrations in the range of parts per million. More recently, neutron activation analysis, emission spectroscopy, and fluorescence spectroscopy have lowered the sensitivity range to parts per

billion. All of these methods are well established, and their advantages and limitations have been discussed in detail (Winefordner, 1976; Pinta, 1978). Very recently, enhanced stripping voltammetry (Nurnberg, 1977) and laser fluorescence spectroscopy (Perry et al., 1981) techniques have lowered detection limits for many elements to a few parts per trillion; these methods, however, are still in the developmental stage.

5. PHASE TRANSFORMATION OF FRACTURE FILLING MATERIALS

5.1 STATEMENT OF ISSUE

The retardation of radionuclide transport by natural geologic materials contributes in an important way to the safe disposal of nuclear waste in a repository designed on the multiple barrier approach (Smith et al., 1980, p. 2-6). In the event that radioactive wastes escape the canister and engineered barrier regions, the host rock must provide an effective barrier to transport of the wastes to the accessible environment. In the Hanford basalts, transport would occur in groundwater flowing principally within fractures. The rate of flow of the groundwater would be affected directly by the effective permeability of the fractures, and particularly by the permeability of any material contained in the fractures. Further, the rate at which dissolved radioactive materials move relative to the groundwater flow rate could be affected by the kind of materials that fill fractures. For example, highly sorptive materials could significantly retard the rate of transport of dissolved materials relative to the groundwater flow rate. An assessment of the ability of a repository to meet radionuclide release standards depends, in part, on the ability to predict the nature and magnitude of the effects of changes that may occur in fracture filling materials as a result of the construction and operation of a repository.

5.2 IMPORTANCE OF ISSUE

Fracture systems in the vicinity of a repository may result from either naturally induced processes (thermal cooling, local or regional tectonics) or artificially induced processes (repository construction, waste emplacement). Thermal gradients generated by a repository may create changes in the physical properties of the host rock and thereby affect the geometry and permeability of the fracture system. Thermal conditions can produce interactions between the rock and groundwater, leading to dissolution, precipitation, and phase transformations of minerals adjacent to the fractures; and subsequent radionuclide migration may be affected. For example, the dissolution of fracture filling material may lead to increased permeability of the host rock and enhanced groundwater migration; conversely, the precipitation of secondary phases may lead to fracture and vesicle sealing. Phase transformations that change the mechanical properties of the fracture filling materials will also affect the mechanical properties of the host rock. For example, the elastic characteristics of the rock mass may change, and so may the shear strength of the fractures.

Hydrothermal alteration involves both in situ and mass-transport processes. For example, in the Umtanum flow basalt in the Pasco Basin, thermally induced in situ phase transformations, including dehydration and cation-exchange reactions of smectites and zeolites, are manifested as

layers of secondary minerals lining fractures and vesicles (Teague, 1980). Thermally coupled dissolution and precipitation reactions involve the aqueous transport of ions. In the Umtanum flow, this occurs between the overlying porous flow-top breccia and the denser colonnade and entablature zones (Noonan et al., 1980).

Present knowledge allows identification of reasonable limits to the mineralogical effects of hydrothermal processes induced in the Umtanum basalt by repository conditions. These effects will be influenced also by chemical compositions of the basalt and the associated groundwater. Within these limits are certain characteristic phase changes in the secondary mineralogy that may affect permeability, sorptive properties, compressibility, and strength of fracture fillings. Changes in these properties may have either positive or negative influences on the performance of a waste repository, depending on the magnitudes and directions of the changes relative to prerepository conditions. Thus site characterization to resolve this issue should include not only identification of existing conditions of fracture fillings, but also assessment of the kinds and magnitudes of changes caused in fracture fillings by repository-induced hydrothermal processes.

The significance of this issue is reflected in several sections of 10 CFR Part 60.

1. Section 60.11(a) requires assessment of the site characterization program with respect to investigation activities that address the ability of the site to host a repository and isolate radioactive waste.

2. Section 60.21(c) requires that the Safety Analysis Report contain an analysis of the geochemical aspects of the site that bear significantly on its suitability for disposal of radioactive waste.

3. Section 60.31(a) indicates that the Commission must determine whether the DOE has adequately described the geochemical characteristics of the proposed site prior to construction authorization.

4. Section 60.111(b) requires that the geologic repository and each of its components satisfy specific requirements related to rates of release of radionuclides.

5. Section 60.122 specifies those geochemical conditions at the site that may be considered favorable in their effects on the ability of the site to meet performance objectives.

6. Section 60.123 specifies those geochemical conditions that would have potentially adverse effects on the ability of the site to meet performance objectives.

7. Section 60.132 specifies additional design requirements for the underground facility that will provide control of radionuclide releases and migration.

5.3 HOST ROCK GEOCHEMISTRY

5.3.1 Geologic Setting

The Umtanum flow has been identified as a candidate horizon for studies of the suitability of the Hanford Reservation as a site for construction of a nuclear waste repository (Deju, 1980b, p. 16). This flow is located 900 to 1000 m below the surface in the Grande Ronde Formation and is composed of both highly and moderately vesicular aphyric basalt. The intraflow structure consists of an upper flow-top breccia zone, an upper colonnade and entablature, and a basal colonnade. The breccia zone, comprising about 20% of the member, is composed of roughly equal proportions of nonoxidized vesicular basalt and massive nonvesicular basalt fragments set in a locally palagonitic matrix. The presence of a palagonitic matrix in this zone suggests a mode of formation that included a flooded flow surface and subsequent rapid chilling (Goff, 1981). The matrix of this porous upper zone is characterized by significant alteration to secondary mineral phases. The degree of alteration has been associated with local groundwater dissolution (Noonan, et al., 1980). Textural analyses of the Umtanum units indicate the absence of dissolution features in the colonnade and entablature, and preferential dissolution seems confined to the upper breccia zone, a result of its porous palagonitic matrix (Deju, 1980b, p. 44; Noonan, et al., 1980). As a result, the denser upper colonnade and entablature have been used in all experiments to test host rock properties. The upper colonnade can be distinguished from the entablature by its coarser grain size and lesser amount of groundmass. These textural differences are associated with distinct differences in the chemical composition of the groundmass (Deju, 1980b, p. 45). Chemical analyses of the groundmass material indicate that the colonnade is more fractionated and that it is characterized by higher K_2O and lower Na_2O and FeO contents. The precipitation of secondary minerals that have been observed to seal fractures, vugs, and vesicles in the upper colonnade and entablature is being considered as a means of radionuclide retardation through coprecipitation and/or sorption of the radionuclides (Deju 1980b, p. 44). Reference outcrop samples from Umtanum Ridge are nearly identical to samples correlated at depth in core DC-2 for the Umtanum flow.

5.3.2 Primary Mineralogy

The Umtanum flow is a dense, black, aphyric tholeiitic basalt. It is similar to other flows within the Grande Ronde Formation, which are characterized by the absence of phenocrysts and a matrix or mesostasis that consists of about 80% microphenocrysts and crystallites, 15% glass, and 5-6% alteration products (Smith et al., 1980, p. 2-46). The crystallized portion of the matrix is dominated by plagioclase (An_{49}-An_{51}), augitic clinopyroxene, and titaniferous magnetite (28-32% TiO_2) (Deju, 1980b, p. 42). Accessory minerals include pigeonite, ilmenite, Fe-oxide

apatite, calcite, and pyrite (Foundation Sciences, Inc., 1981, p. 4). The Umtanum colonnade and entablature possess subtle textural differences that can be related to their cooling histories. For example, the larger grain size and euhedral morphology of feldspar and pyroxene crystals in the colonnade suggest a longer cooling history and more fractionated matrix. However, the larger volume of groundmass and abundant microlites of magnetite in the entablature also suggest a more rapid chilling of this zone. These differences can affect the physical properties of the host rock and contribute to uncertainties regarding rock strength and fracture density/distribution characteristics (Myers and Price, 1979, p. III-97). In contrast to the mesostasis, the primary minerals show no particular adverse affects to thermal loading and have not been significantly altered since igneous petrogenesis. Only the mesostasis or groundmass is considered susceptible to alteration upon emplacement of radioactive waste.

Although no volumetric estimates of matrix material have been made for the individual intraflow units of the Umtanum, an average bulk value of 49% has been suggested (Foundation Sciences, Inc., 1981, p. 2-5). No dissolution of the mesostasis is found to occur within the uper colonnade and entablature; yet fractures and vesicles associated with these units in the lower portion of the flow are filled and perhaps sealed with secondary mineral phases. Ames (1980, p. 145) has estimated that 85% of all observed fractures and vesicles are filled in DH-5 core samples.

5.3.3 Secondary Mineralogy

Secondary minerals are found primarily in the matrix of the upper flow-top breccia zone and as fracture, vug, and vesicle fillings in the denser colonnade and entablature units. The alteration sequence most commonly observed is clay, clinoptilolite, silica, and clay (Benson and Teague, 1979, p. 4; Teague, 1980, p. 10). This paragenetic sequence is attributed to long-term, low-temperature diagenetic conditions (Benson and Teague, 1979, p. 19).

Smectite is the primary alteration product of glassy basaltic material and occurs both as single and multiple layers of precipitate in fracture linings and cavity fillings. Single generations tend to be found with fine-grained massive or spheroidal textures. Multiple generations usually appear as morphologically and chemically distinct layers, commonly separated by another mineral phase. Smith et al. (1980, p. 2-54) have reported the following generalized chemical formula for smectites observed in Pasco Basin basalts by Benson and Teague (1979), Ames (1980), and Teague (1980):

$$(Ca,Na)_{0.66}(Al,Mg,Fe^{3+},Fe)_{4-6}(Si,Al)_8O_{22}(OH)_4.nH_2O$$

Chemical compositions vary primarily as functions of Si, Al, Fe, and Mg substitutions. Ames (1980, p. 160) identified the smectite lining the surface of fresh basalt as nontronite-beidellite. His compositional

determinations were based on qualitative x-ray diffraction methods and observations regarding the source terrain. The formation of nontronite has been associated both with in situ hydrothermal alteration and surface weathering of basalt (Weaver and Pollard, 1975, p. 77).

Clinoptilolite is the zeolite most commonly observed in secondary mineral assemblages in Pasco Basin basalts. Although clinoptilolite and heulandite form an isomorphous solid solution series, compositional limits for the end members have been defined by Mason and Sand (1960, p. 341) and Mumpton (1960, p. 351) using silica/alumina ratios and exchangeable cation ratios. Benson and Teague (1979, p. 13) have unequivocally identified clinoptilolite as the primary zeolite phase from electron microprobe analyses. The most commonly observed paragenetic sequence consists in the formation of smectite as a lining in the fractures or cavities of basalt and its subsequent alteration to euhedral clinoptilolite crystals. The zeolite phase is precipitated in a single stage in open-space cavities or fractures and typically displays tabular, blocky, fibrous, or bladed crystal habits.

Zeolite occurrences are more abundant below depths of ~370 m (Benson and Teague, 1979, p. 8). Euhedral mordenite crystals with tabular and fibrous habits at depths below ~900 m (Ames, 1980, p. 161; Benson and Teague, 1979, p. 8) seem to be associated with the disappearance of clinoptilolite. Mordenite is formed during late-stage hydrothermal activity and after most other zeolites. A zonal mineral distribution with depth is probably a function of pressure and temperature. Benson and Teague (1979, p. 19) suggest that the observed mineral assemblages result from diagenetic rather than hydrothermal conditions.

Opal, cristobalite, and quartz are the principal silica phases found in secondary mineral assemblages. Authigenic silica deposited in several generations is present in various forms (Teague, 1980, p. 3). Opal or amorphous opaline silica (identified by a broad diffraction peak at low angles) is often found spatially associated with β-cristobalite either as spherical crystal aggregates, fibrous and botryoidal masses, or as massive coatings on clinoptilolite or clay. Quartz is typically found as discrete crystal clusters filling cavities and fractures. Teague (1980) notes that the mineralogy of cavity fillings is more complex, and that core samples within the Umtanum may contain different relative amounts of secondary phases in the same depth interval. Silica phases are often intergrown and their occurrences compatible with diagenetic conditions. Minor amounts of other secondary minerals (e.g., illite, calcite, pyrite, apatite, and various zeolites) have also been identified in cavity and fracture fillings.

5.4 HYDROTHERMAL CONDITIONS

Estimates of ambient geothermal gradients and potential repository conditions are required to evaluate geochemical controls on the retardation of radionuclides during groundwater migration. Specifically, temperature

variations are important when considering the stability of mineral phases found lining fractures and cavities in basalt.

5.4.1 Pasco Basin Geothermal Gradients

A mean geothermal gradient for the Columbia River Plateau, which encompasses the Hanford Reservation, is 38.25°C/km (Sass et al., 1971, p. 6376). Calculated thermal gradients using measured bottom-hole temperatures range from 35 to 45°C/km (Korosec and Schuster, 1980, p. 33). For a depth of 1000 m below the surface, the ambient temperature is ~65°C and is considered the baseline repository temperature (Wood, 1980, p. 45).

5.4.2 Potential Repository Conditions

To evalute the effects of repository operation on the properties of the host rock, the maximum temperature estimated to be produced by radiogenic heating must be known. Temperature perturbations are a function of the nature and amount of the waste and the thermal conductivity of the host rock (Smith et al., 1980, p. 2-108). Temperature simulations have been performed for a hypothetical repository depth of 1000 m in basalt, and a maximum rock temperature of 250°C is estimated by Hardy and Hocking (1978). Any upper temperature limit is directly related to repository design specifications. Smith et al. (1980, p. 2-13) identifies the temperature range 60-300°C expected during the thermal period of a repository in basalt at a depth of 1000 m. The maximum temperature will be reached years after closure and will occur at the waste package-rock interface (Smith et al., 1980, p. 2-113).

5.4.3 Groundwater-Basalt Interactions

The formation and stability of secondary mineral assemblages is controlled by the surrounding hydrothermal environment. In turn, the solubilities of solid phases affect the pH, Eh, and oxygen fugacity of the groundwater. Hydrothermal experiments have shown that the precipitation of secondary phases from solution and the hydrolysis of silicates have opposing effects on the pH of the solution. When clay or smectites precipitate from solution, the reactions consume hydroxyl ions and the pH is lowered. The hydrolysis by silicates or glass generates hydroxyl ions, which in turn raise the pH of the solution. Because these opposing effects are probably controlled by different kinetics, a significant time will pass before equilibrium is approached. The equilibrium pH varies inversely with temperature. Barnes and Scheetz (1979, p. 384) have empirically determined the dependence of pH on temperature in groundwater in Umtanum basalt for

low water/rock ratios. Groundwater in equilibrium with the Umtanum at 1000 m depth and 45°C is buffered by the dissociation of silicic acid. The following empirical relationship has been formalized:

$$pH = 2640/T(^{o}K) + 1.64$$

(Wood, 1980, p. 45). Although Eh and oxygen fugacity are important solution parameters, they cannot be reliably measured and must be estimated from thermodynamic data, if adequate data are available.

Formation water sampled from the Grande Ronde at the hypothetical reference repository depth coincides with the Umtanum unit and is chemically distinct from the Upper Wanapum and Saddle Mountain Formation water samples. The Grande Ronde water samples have lower decreased concentrations of K^{+}, Mg^{2+}, and Ca^{2+}, a higher concentration of Na^{+}, higher concentrations of CO_3^{2-}, Cl^{-}, SO_4^{2-}, F^{-}, and a higher concentration of total dissolved solids (TDS) relative to the overlying waters (Smith et al., 1980, p. 2-89). In order to provide a common basis for laboratory experiments, simulated groundwater compositions have been standardized, and these simulated compositions are used in the experiments. A comparison of natural groundwater compositions from the Grande Ronde Formation with synthetic formulations is shown in Table 5.1. The concentrations of total dissolved solids, chloride, and sodium increase with distance from recharge area (Gephart et al., 1979, p. III-160). The analytical data indicate that the Grande Ronde groundwater is isolated from major recharge. Additional analyses using theoretical methods are not available because the carbonate/ bicarbonate ratios are reported by Gephart and others to be anomalously high at the given field pH (1979, p. III-180).

Smith et al. (1980, p. 2-131) have summarized the equilibrium solution parameters for a representative groundwater at repository conditions. The summary is shown in Table 5.2. Although Eh and oxygen fugacity cannot be reliably measured, the estimated range corresponds to geologic control with the repository host rock (Smith et al., 1980, p. 2-132).

5.5 PHASE TRANSFORMATIONS

The hydrothermal alteration of basalt at temperatures up to 300°C in laboratory experiments shows that the pH depends on the rock composition and the H_2O/rock ratio (Barnes and Scheetz, 1979, p. 384). The groundmass is most susceptible to alteration, although some primary phases are etched. Secondary minerals may precipitate from hydrothermal solutions or form directly from the alteration of basaltic glass. Temperature and fluid chemistry control the mineral reactions involving smectites, zeolites, and silica. The information available to evaluate phase transformations of fracture filling materials is limited either to bulk basalt/groundwater

Table 5.1. Summary of Repository Equilibrium Conditions.

	Temperature (°C)	Equilibrium pH	Log Oxygen Fugacity (atm)	Eh(V)
Period of Geologic Controls	65	9.4	-64.5 to -67.15	-0.51 to -0.55
Thermal Period	100	8.7	-57.8 to -60.0	-0.49 to -0.53
	150	7.9	-49.6 to -51.8	-0.48 to -0.53
	200	7.2	-43.3 to -45.4	-0.47 to -0.52
	250	6.7	-38.3 to -40.2	-0.48 to -0.52
	300	6.2	-34.1 to -35.9	-0.45 to -0.51
Operating Period	65	9.6	-0.7	+0.54

After Smith et al., 1980, p. 2-131.

Table 5.2. Summary of Groundwater Compositions.

	Grande Ronde Formation					Columbia River Basalt
	Natural Samples		Synthetic Simulations		Average Composition	Average Composition
Na^+	181	250	225	263	225	12
K^+	2	1.9	2.5	1.9	2.5	5.3
Ca^{2+}	0.26	1.3	1.06	1.3	1.1	24
Mg^{2+}	N/A	0.04	0.07	0.04	0.7	15
SiO_2	153	103	108	103	117	50
Cl^-	95	148	131	148	131	15
HCO_3^-	74	70	75	70	66	156
CO_3^{2-}	27	27	75	70	52	N/A
SO_4^{2-}	26	108	72	109	72	1.6
F^-	21	37	29	37	29	0.2
TDS	N/A	N/A	N/A	N/A	648	280
pH	9.8	N/A	10.0	9.92	N/A	N/A
Reference	a	b	d	b	c	e

References: a = Apps, 1979, analysis from DC-2 well 6/26/78 (III-18).
b = Deju, 1980a, 3Q.
c = Gephart et al., 1979.
d = Deju, 1980b, 4Q.
e = White et al., 1963.

N/A = data not available from indicated reference.

experiments or to the evaluation of isolated phases such as clay or zeolites. Hydrothermal and sorption experiments have shown basalt to be a potential radionuclide retardant; this has been attributed to the physical properties of the secondary mineralization (Ames, 1978). The surface area, swelling properties, and cation exchange capacities of clays and zeolites have been documented in controlled laboratory experiments (Breck, 1974; Barrer, 1978; Weaver and Pollard, 1975; Vaughan, 1978). However, their behavior together in an open system as parts of a paragenetic sequence, smectite→clinoptilolite→silica/smectite, has not been investigated. Therefore, each mineral is discussed separately below.

5.5.1 Smectites

Smectite is the dominant secondary phase in layers found lining fractures and cavities in the Umtanum basalt. It is a normal alteration product of basaltic groundmass, and its mode of formation involves the hydration of basaltic glass at temperatures below 100°C. The high water content of smectites, 20-40 wt% (Weaver, 1979, p. 1), limits their stability range to fairly low temperatures. Interlayer water can be removed reversibly at surface temperatures between ~120 and 100°C (Weaver and Pollard, 1975, p. 3) or as low as 50 to 80°C at 1500 to 2000 m depth (Weaver, 1979, p. 59); removal of this water can result in chemical and physical changes that may be important to the control of radionuclide transport in groundwater. Smectites found in cores in the Pasco Basin vary widely in chemical composition (Benson and Teague, 1979, p. 50). The effect of the proposed thermal interval, 60 to 300°C, on clay minerals should be investigated using a bentonite analogue. Bentonite is a soft, porous rock composed essentially of montmorillonite and colloidal silica. It is being considered as a primary backfill component because its low permeability and large swelling capacity are expected to minimize contact of the canister with groundwaters (Smith et al., 1980, p. 2-279). Other clay minerals are also being considered as sealants. Although the thermal stability of montmorillonite has not been thoroughly investigated, Smith et al. (1980, p. 2-281) have suggested that this clay would not be affected to any significant extent at temperatures up to 300°C. This recommendation is based on DTA techniques that indicate no loss of structural water until ~450-500°C (Deer et al., 1967).

The thermal alteration of clay minerals has also been recognized from field data. With increasing temperature and depth, smectite is transformed to mixed-layer illite-montmorillonite. The transformation is associated with the collapse of 17-Å montmorillonite layers to 10-Å illite layers as detected by x-ray diffraction methods. The formation of illite requires the incorporation of potassium into interlayer sites. It is suggested that the groundwaters from the Grande Ronde Formation do not contain enough potassium for this reaction to occur (Smith et al., 1980, p. 2-281). If significant alteration to mixed-layer clay does occur, the effectiveness of the backfill or fracture sealing materials will be reduced. Controlled laboratory experiments indicate that temperatures of ~150° are sufficient

for some mixed-layer transformations (Weaver, 1979, p. 35). Complete conversion to illite has been observed in active geothermal areas at 200°C (Weaver, 1979, p. 30). The low-grade metamorphism of shale is expected to experience similar thermal conditions. These observations suggest that at temperatures above 100°C, more importantly between 200 and 300°C, some layer contraction will occur in the smectite or clay phases. These contractions create a volume reduction that increases pore space, reduces the cation exchange capacity, and decreases the swelling capacity of the material. These textural changes caused by heating may affect the migration of groundwater, an important consideration to the design of the repository. To date, no experiments to investigate the stability of secondary mineral assemblages have been reported. Bulk basalt/groundwater interactions have been studied at 300°C and ~140 bars (Ames, 1978, p. 138). After 15 days, silica and potassium contents declined, and quartz, microcline, and talc were deposited. The investigator used only fresh basalt as starting materials, and the secondary phases were selectively removed prior to heating. Guillemette et al. (1980, p. 168) determined that with both glass and crystalline starting materials at high pH conditions, smectite is the first phase to form. These hydrothermal experiments indicate that the stability of smectite at temperatures up to 300°C must be investigated further.

5.5.2 Zeolites

The zeolites in the Umtanum are clinoptilolite (Benson and Teague, 1979). Zeolites form readily at surface conditions in alkaline environments. Hay (1977, p. 62) has determined that zeolite assemblages found in upper zones of burial diagenesis are mineralogically similar to those found in open hydrologic systems. Thick zones of clinoptilolite or mordenite are not uncommon in open-system environments (Hay and Sheppard, 1977, p. 93). Field evidence suggests that the hydrolysis of glass to clay may actually be a precursor to zeolite formation by removing hydrogen ions and raising the pH of the solution (Hay and Sheppard, 1977, p. 95). This is precisely the alteration assemblage observed in the Umtanum. Although little is known about the dependence of zeolite stability on pressure and temperature, five burial metamorphic zones have been identified (Boles, 1977, p. 108).

Zone 1: fresh glass

2: alkali clinoptilolite

3: clinoptilolite and mordenite

4: analcime

5: albite

Judging from the approximate temperature and depth limits associated with each zone, a temperature increase to 300°C in the Umtanum does not seem to correspond to a burial metamorphic environment. Holler and Wirsching (1978, p. 335) have determined that an open-system environment with a sufficiently large temperature gradient can produce zoned zeolitic and subsequent alteration assemblages observed in active geothermal systems. On the other hand, in these natural hydrothermal areas, propylitic or potassium silicate alteration assemblages are commonly produced (Ellis and Mahon, 1977, p. 90). In geothermal areas where the source rocks are basaltic, zeolite occurrences have been identified up to temperatures of ~190°C from drill-hole data (Kristmannsdottir and Tomasson, 1978, p. 281). Occurrences have been associated also with slightly higher temperatures, 200 to 230°C, as estimated from geothermal gradients. No hydrothermal experiments have been performed to investigate the stability of clinoptilolite or any heulandite group minerals. Temperatures of crystallization have been found to be between 25 and 65°C with the initial removal of zeolitic water occurring between 350 and 400°C, and total dehydration at ~700°C (Breck, 1974).

5.5.3 Silica Minerals

Authigenic silica is often associated with zeolites in secondary mineral assemblages. The only phase transformations that need to be considered up to 300°C are the dissolution and reprecipitation of various phases. The precipitation of silica phases in fractures and cavities can reduce the host rock permeability. Elders (1978) observed fractures sealed by silica phases in areas of the Salton trough where the temperatures are now less than 100°C. Temperatures of 200 to 300° are adequate to dissolve quartz in granite and granodiorite cores (Charles, 1978, 1979). The anticipated thermal perturbations generated by repository conditions seem to be sufficient to mobilize silica, dissolving it at higher temperatures and precipitating it at lower temperatures. Since Grande Ronde groundwaters are saturated with silica, possibly controlled by amorphous silica solubility (White and Claassen, 1979, p. 45), it seems reasonable to assume that no significant increase in permeability will be caused by silica dissolution occurring at the higher end of the thermal plume.

5.6 SITE CHARACTERIZATION METHODOLOGIES

At the Hanford site, basalt is being considered both as host rock and as backfill material. Many studies have evaluated basalt and its potential to retard radionuclide migration through sorption, chemical reaction, or diffusion (Smith et al., 1980, p. 2-260). It has been noted that the sorptive capacity of basalt may be attributed to its secondary mineralization. Since basalts from different flows have shown different sorptive properties (for summary, see Smith et al., 1980, p. 2-332), it is important to investigate geochemical factors explicitly for the Umtanum

flow. However, the principal issue to be resolved in the context of nuclear waste disposal pertains to potential thermal conditions and subsequent phase transformations. Since little is known about the response of natural assemblages of minerals to changes in thermal conditions, resolution of the issue will rely almost entirely on future research. As a result, the methodologies for site characterization that can presently be recommended are limited to routine collection of site-specific data from field experiments and boreholes. Laboratory experiments and theoretical modeling techniques have not been developed for low-temperature authigenic phases to the extent that they could provide any definite criteria for the site characterization process. The development of additional methodologies is required for the resolution of this issue. These developments are hampered by the complexity of the authigenic phases (both chemically and structurally), sluggish reaction rates, and kinetic barriers. However, the site characterization methodologies described below should provide a preliminary data base that could serve as a framework for research directed toward resolution of the issue.

5.6.1 Host Rock Field Studies

An important means of characterizing a medium for a repository involves investigation of the existing material at depth. In this respect, preliminary site characterization analysis has already been performed using cores from boreholes located within the Hanford site. The analytical results have been summarized in previous sections of this report; these results indicate that secondary minerals within the Umtanum show wide compositional variation, a variety of habits, and definite paragenetic sequencing. In addition, the properties of fracture filling materials have been found to vary locally as a function of depth and hydrologic setting. The two types of reactions important to identify with regard to this issue are (1) the conditions of dehydration for smectites and zeolites, and (2) mineralogical phase transformations, including dissolution and precipitation of phases. At low temperatures, the dehydration of smectites is reversible, causing minor dehydration effects (less than 2% water loss at temperatures below 100°C), which may be important to fracture development and propagation in the host rock. Zeolites can release significant amounts of water without increasing the effective rock permeability, although this can lead to increased fluid pressures and cause physical and chemical changes in the host rock.

As a preliminary step in site characterization, in situ heater experiments should be carried out within the Hanford site at the Near-Surface Test Facility (NSTF). Although the facility is constructed within the Pomona flow (stratigraphically above the Umtanum), it would be possible to assess the response of both groundwater and pore water in a dense basalt flow to a thermal source. Short-term, controlled experiments utilizing the electric heaters of NSTF-Phase 1 (Foundation Sciences, Inc., 1980) could yield information on the kinetics of phase transformations. The results of these experiments can be used to define requirements for the construction of a deep test facility within the Umtanum.

The design of in situ experiments should take into account regional features such as the secondary phases found in the fracture system of the Umtanum flow. The fracture pattern throughout the Umtanum flow generally consists of vertical and planar patterns in the colonnade, with a more irregular distribution in the entablature. Both the colonnade and entablature would provide direct determination of the effects of temperature on fracture filling material. Field observations also permit these zones to be analyzed separately from the porous, flow-top breccia. Because fractures are easily disturbed, experiments should consist of heating the host rock at depth, taking samples, and analyzing the samples to observe any mineralogical changes.

The experiments should be designed so that the effects of elevated temperature can be determined in both wet and dry downhole environments. At elevated temperatures, dry environments would presumably tend to become progressively wet as a result of dehydration of solid phases. However, the variations in the host rock and hydrologic environments may produce distinctly different paragenetic assemblages in the alteration/phase transformation/fracture filling sequence. It is necessary to characterize the material at depth prior to any temperature increase. The following properties should be considered: mineralogy and petrology (x-ray and thin section analysis), thermal expansion, density, porosity, permeability, compressive strength, and thermal conditions (see Johnstone and Wolfsberg, 1980, for similar experiments designed for use with tuff). The duration of a thermal pulse necessary to cause characteristic changes in the above mineral properties cannot be estimated a priori. This type of approach seems to be the only available methodology with which to obtain model data on authigenic fracture sealing at elevated temperatures.

5.6.2 Laboratory Experiments

Laboratory experiments should be used in the site characterization process to identify possible limits on reaction conditions that may occur in the host-rock environment. The evaluation of phase transformations of secondary mineral assemblages in basalt is difficult for several reasons: the quantities of secondary phases available are small, compositional variations are large, and the reaction rates at low temperatures are sluggish. Laboratory techniques are useful for accelerating natural processes within reasonably short time intervals. Commonly, bench experiments are run with finely ground starting materials and at elevated thermal conditions on the assumption that such modifications serve only to increase reaction rates. A limitation is that these methods typically have used bulk basalt as starting materials rather than the secondary phases.

An important aspect of laboratory techniques is that secondary phases can be studied under controlled conditions--either individually, in mixed form, or in mixtures with the host rock. Differences in the physical and

chemical properties of smectite, clinoptilolite, and silica warrant individual experiments. For example, smectite has a high swelling capacity; its attendant high volume increase has been cited as a mechanism for sealing fractures and fissures. However, in the presence of sufficiently high concentrations of potassium, smectite layers collapse to form illite. It has been suggested that illite formation may be inhibited in the Umtanum by low concentrations of potassium in Grande Ronde groundwaters. This conjecture should be tested by laboratory experiments.

Although the dehydration temperatures of smectites and zeolites have been estimated, their lower limits have not been measured. Experiments using thermal gravimetric analysis and differential thermal analysis should be conducted to delineate more definite boundaries for the dehydration conditions of individual secondary minerals and of their assemblages. Moreover, the effects of pressure on phase transformations in these minerals should be investigated by means of hydrothermal experiments.

Silica has been observed to act as a natural cement in stirred autoclave experiments at 250°C with crushed basalt and simulated Hanford groundwaters (Smith et al., 1980, p. 3-83). Limits of temperature, pressure, and compositional variables should be measured in order to define ranges of conditions under which this effect may reduce radionuclide transport.

5.6.3 Theoretical Modeling Techniques

Theoretical models of geochemical systems have provided valuable insight into processes occurring in relatively simple, closed systems whose behavior can be approximated closely by the assumption of equilibrium conditions. Existing models incorporate many simplifying assumptions in their descriptions of natural systems, leading to a relative insensitivity to minor variations of input parameters. Typically, these models simulate interphase mass transfer and evolution of an aqueous phase by a series of steps, each step representing the addition of a definite amount of reactive material. Equilibrium is assumed within each step, and the evolution of a geochemical system is thus modeled through a series of equilibrium states, as depicted schematically in Figure 5.1 (Smith et al., 1980, p. 2-345).

Modeling of the behavior of fracture filling materials under repository conditions would, if successful, complement and provide guidance to field and laboratory investigations, and would provide useful information for assessment of effects on repository integrity. However, several studies (Apps et al., 1978; Benson et al., 1980; Deutsch, 1980) have had little success in applying equilibrium step models to the generation of existing secondary phase assemblages in the Pasco Basin basalts--the necessary first step in the theoretical prediction of the long-term behavior of these systems under repository conditions. This lack of success can be attributed to several limitations on the applicability of the models to complex, open, natural systems.

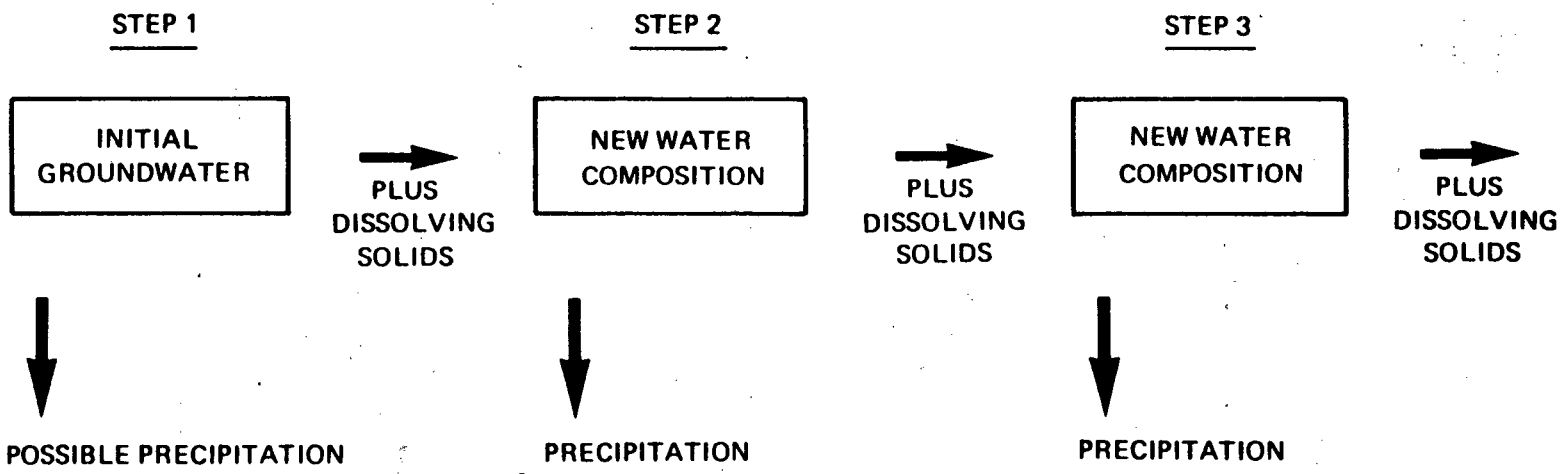


Figure 5.1. Local equilibrium mass-transport as modeled by the EQ3/EQ6 Mass Transfer Simulation Code developed by Wolery (1979). Figure from Smith et al. (1980, p. 2-347). [XBL 826-10484]

The chemical reactions that can be modeled by this method are limited to those involving solid phases and solution species for which accurate thermodynamic data are available. Such data are limited for the secondary mineral phases observed in fracture and cavity fillings.

Existing models do not have the capability, nor are the necessary data available, to simulate the extensive compositional variations, metastability, and steady-state, nonequilibrium processes that undoubtedly exist in low-temperature geochemical systems.

Finally, equilibrium models cannot simulate systems in which kinetic effects dominate evolution of the systems. Time-dependent, kinetic processes are significant at temperatures below 300°C, and their treatment is made even more difficult by the possible occurrence of metastability of solid phases and aqueous species. Experimental data necessary for simulation of such systems are not available.

Existing methodologies of the site characterization provide assessment of present conditions and identities of fracture filling materials. Additional research is required to extend these methodologies to the prediction of possible effects--either positive or negative with respect to retardation of radionuclide migration--under hydrothermal conditions imposed by construction of a waste repository.

5.7 RESEARCH NEEDS AND LIMITATIONS

The most significant limitations to existing methodologies for resolution of this issue are the lack of data pertaining to compositional variations of smectite, clinoptilolite, and silica phases as functions of repository conditions, and the lack of data to characterize the time dependence of these variations.

Primary research needs are development and design of in situ field tests and laboratory experiments that can become part of the site characterization process. Further laboratory research should investigate behavior of secondary phases in saturated, open-system environments and the extent of their departure from equilibrium. These data can be used to determine criteria for the collection of site-specific data and future modeling capabilities. As a first approximation, complex geochemical conditions require the investigation of simplified systems with reduced numbers of components (i.e., synthetic stoichiometric phases). This research would be primarily hydrothermal in nature and should be specifically restricted to smectite, clinoptilolite, and silica phases. There does not appear to be any further need for data from crushed bulk basalt experiments except for consideration as backfill materials. An experimental research program should be directed at interpreting the behavior of the physical and chemical properties of the fracture filling materials at elevated thermal conditions.

Research needed to overcome existing limitations to theoretical modeling can be divided into two general categories that are mutually interactive.

Modeling capabilities should be extended to include nonequilibrium (both steady-state and time-dependent) processes and metastability effects in low-temperature geochemical systems. This will require prior extension of theoretical concepts, and will be critically dependent on acquisition of experimental data for use in model verification and in data bases for predictive modeling.

Experimental data should be acquired on stabilities, as functions of pressure, temperature, and solution composition of secondary solid phases constituting the fracture filling materials. Precise thermochemical data (e.g., heats of solution) are needed for construction of data bases both in equilibrium and nonequilibrium codes. Extensive data (e.g., reaction mechanisms and kinetic rate constants) on time-dependent systems are needed for use with (as yet undeveloped) nonequilibrium models.

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APPENDIX A. GEOLOGIC HETEROGENEITIES IN FLOOD BASALTS

A hydrostratigraphic unit (HSU) was defined earlier as a body of rock that performs a distinct hydrologic function within the hydrologic system being studied. The nature of geologic heterogeneities in sequences of flood basalts is presented to provide a geologic foundation for the role of heterogeneities in the identification of HSU's.

Flood basalts behave hydrologically as a peculiar blend of igneous and sedimentary rocks. In a microscopic sense, basalt is an igneous crystalline rock with a matrix of such low permeability that essentially all of the groundwater movement occurs in fractures. In this respect, basalt is much like igneous intrusives, such as granite. In a macroscopic sense, however, basalts are systems of layered rock, and, like sediments, they have hydrologic properties that vary considerably from flow to flow as well as within single flows. If sufficient time has elapsed between successive flows, a nonvolcanic sedimentary horizon of alluvial deposits and weathering products can occur within a basalt sequence. Thick sequences of flood basalts exhibit much of the hydrologic behavior of sedimentary rocks.

A.1 HETEROGENEITIES WITHIN SINGLE BASALT FLOWS

Heterogeneity in hydraulic properties within a single basalt flow is primarily due to the different types of fractures that form as the flow cools. Vesicles formed by gas bubbles trapped in solidifying lava are not normally interconnected and thus do not form significant conduits for fluid movement. Fractures normally are interconnected and are formed by contraction upon cooling and by rupture of the solidified surface skin due to movement of the liquid lava beneath.

A schematic diagram showing the structural features found in a typical basalt flow is presented in Figure A.1. Four principal zones are usually encountered.

1. The flow top: A thin layer of potentially weathered, scoriaceous lava and rubble over a thicker layer of highly vesicular lava.

2. The upper colonnade: A region containing large warped or twisted vertical hexagonal columns that may be 2-3 m in diameter. Some cross-fracturing occurs and frequently coincides with horizontal elliptical vesicles.

3. The entablature: An intermediate zone characterized by the occurrence of slender columns that seem to form fan or radiating joint patterns. Large columns in the upper colonnade may continue in the entablature as bundles of small hexagonal columns.

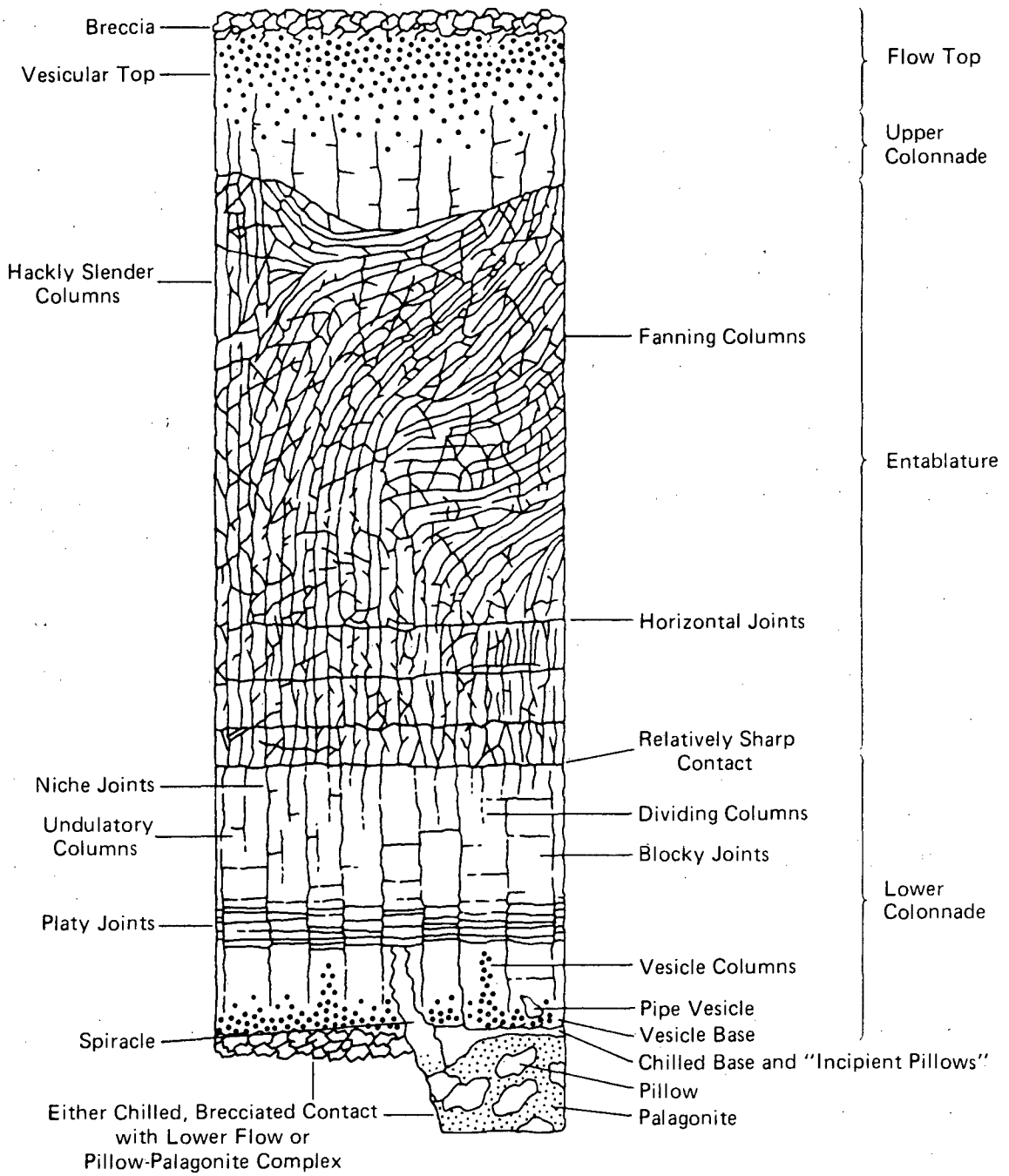


Figure A.1. Schematic diagram showing structure of a basalt flow (modified from Atlantic Richfield Hanford Company, 1976, Figure 5). [XBL 8110-12137]

4. The lower colonnade: A zone that is sharply divided from the entablature and which contains long symmetrical hexagonal columns formed by a very regular pattern of vertical joints (Isherwood, 1980; Agapito and Stanley, 1977).

Below the lower colonnade is the flow base, which contains small vesicles resulting from gas bubbles formed along the lower contact of the flow. Spiracles--hollow "chimneys" formed by steam explosions--would indicate that the lava may have flowed onto wet sediments. If the lava was extruded under water, pillow lava with palagonite (altered basaltic glass) might be found in this zone.

Each of these cooling features produces a distinctive fracturing pattern that results in different hydraulic properties. Examples of nominal hydraulic properties for selected portions of the Umtanum flow in the Pasco Basin are given in Table A.1. This table shows a variation of three to four orders of magnitude in hydraulic conductivity as measured in borehole tests between the more permeable flow-top breccia and the less permeable entablature and colonnade. This large variation demonstrates the magnitude of the hydrologic heterogeneities that can exist within single basalt flows.

Although individual basalt flows can be traced as chemical or stratigraphic entities over many square kilometers, these flows may not be single sheets that were instantaneously deposited over a basin. Rather, flows may be made up of many smaller lobate features, each of which may contain some or all of the cooling features described above (Newcomb, 1969). An example of structural variation over distance is provided by a fence diagram of the Umtanum flow, shown in Figure A.2. The thickness and general flow structure is seen from this figure to be different in each of the nine wells used as data sources. In some wells the entablature is continuous; in others it is interrupted by intermediate zones of columnar basalt. Of interest from a hydrologic point of view is the variable thickness of the more permeable flow-top breccia, which, according to Figure A.2, varies over an order of magnitude.

From the foregoing discussion, it is evident that hydrologically significant heterogeneities can exist within a single basalt flow. Heterogeneities occur vertically because of variations in the hydraulic properties of the various structural components of the individual flows, and heterogeneities occur laterally because of variations in thickness or depositional environment of these structural components. Although vertical variations are generally more pronounced than lateral variations, changes in hydraulic properties may be several orders of magnitude in either case.

A.2 HETEROGENEITIES WITHIN A SEQUENCE OF BASALT FLOWS

In consideration of the hydrologic heterogeneities that can occur within a single basalt flow, a thick sequence of such flows may be considered as a nonsystematic repetition of the heterogeneities of individual

Table A.1. Nominal Hydrologic Properties of Umtanum Flow in the Pasco Basin.[a]

Flow Structure	Primary Porosity (volume percent)	Hydraulic Conductivity Horizontal (m/s)	Hydraulic Conductivity Vertical (m/s)
Flow-Top Breccia	10	10^{-7}	10^{-7}
Entablature, Colonnade	5	10^{-11}	10^{-10}
Flow-Base Breccia	5	10^{-9}	10^{-10}

[a] Data from King et al., 1981, Tables 4-1 and 4-6. Range of values is generally $\pm$ 1 to 2 orders of magnitude.

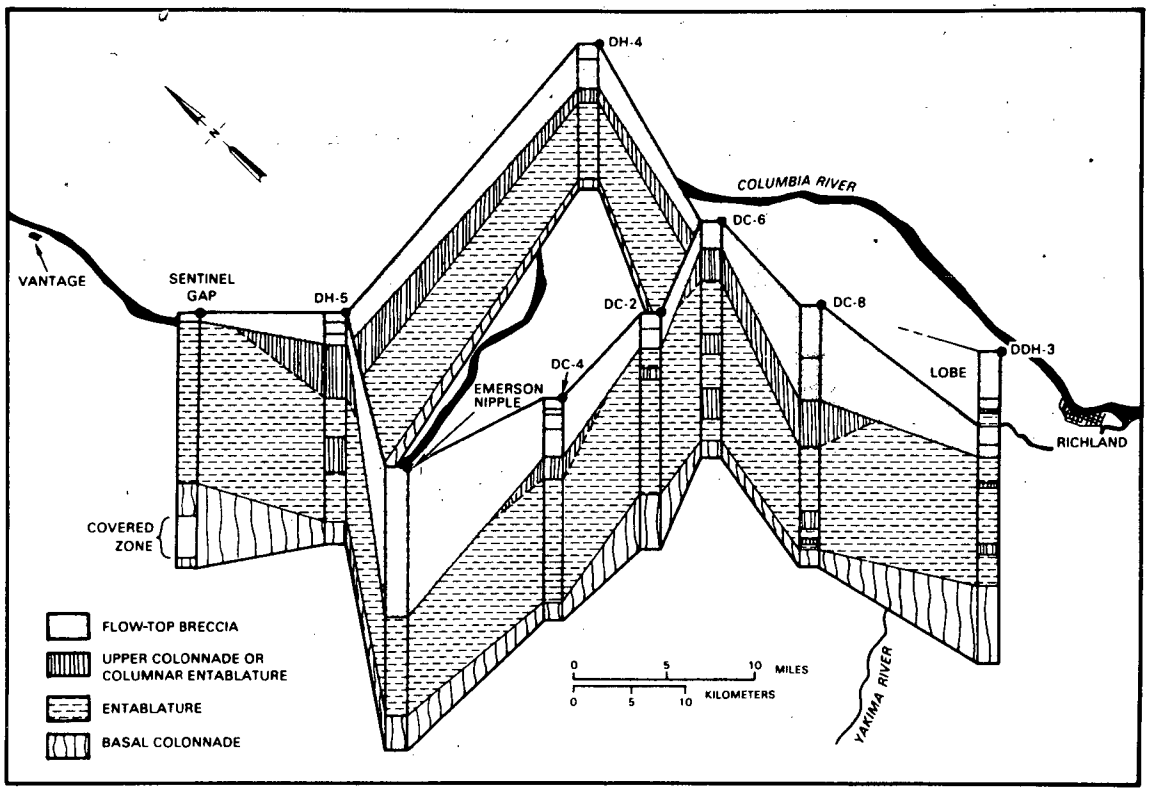


Figure A.2. Fence diagram of the Umtanum flow in the Pasco Basin (from Deju, 1980b, Figure 6). [XBL 826-10492]

flows. The magnitude of the problem is evidenced by the complexity of the complete vertical section presented in Figure 1.4. This figure indicates 50-100 individual flows between the Umtanum flow unit and the surface, each of which may be quite different from its neighbor.

A more detailed representation of the flow units within the upper Grande Ronde Basalt is shown in Figure 1.5. Some 12 flow units were encountered in any particular borehole within the upper 360 m of the Grande Ronde, but these units do not necessarily correspond stratigraphically on a one-to-one basis with those observed in another borehole. Flows are seen to vary in thickness and to pinch out laterally across the basin. The ensemble of flows is heterogeneous on a large scale, and each individual flow is internally heterogeneous on a smaller scale.

In addition to the structural features related to deposition of the basalts, other regional tectonically related features have been superposed that generally increase the degree of heterogeneity. The Pasco Basin basalts, for example, have been locally faulted and folded, and contain regional joint sets (Myers and Price, 1979).

APPENDIX B. TECHNICAL BASIS FOR IDENTIFYING HYDROSTRATIGRAPHIC UNITS IN HETEROGENEOUS MEDIA

B.1 KINEMATIC CONSIDERATIONS FOR HYDROSTRATIGRAPHIC UNITS DEFINED ON THE BASIS OF CONTINUUM BEHAVIOR

Kinematic effects of groundwater flow paths are important for the identification of HSU's on the basis of hydraulic properties and continuum behavior. Kinematic effects determine the size of the REV that may be appropriate for solution of a given problem, and thus affect the size of the appropriate HSU (Long et al., 1981). Problems due to kinematic effects arise when flow paths undergo rapid changes in direction within a single HSU. Rapid changes in flow-path direction are most strongly associated with natural or man-made underground features with high permeability contrasts, such as the cutoff wall of a dam, or with high head contrasts, such as those generated by underground openings. For the "control zone" model, the kinematic effects, and therefore the HSU's, are strongly linked with repository design.

The problem introduced by rapidly changing flow-path directions is that the nonuniform hydraulic gradients associated with such changes may concentrate groundwater movement within a part of the HSU that is smaller than the REV and does not have the same average properties as the unit as a whole. Thus accurate prediction of groundwater flow will require analysis on a scale such that the average gradient appears constant.

The domain of multiple flows used in Figure 2.1 as an example of an HSU is modified in Figure B.1 to illustrate two alternative kinematic situations. In Case A, a uniform, steady gradient exists across the entire unit, and flow lines are parallel. Under these conditions, the unit as a whole can be treated as a homogeneous hydrologic entity in response to a uniform gradient in any direction.

In Case B, however, the hydraulic gradient across the unit is interrupted by an underground opening at a lower head. Groundwater flow will be redirected toward this opening. Because of the higher gradient, the rates of groundwater movement in the upper three strata will increase, but the rate of movement in the lower stratum will not significantly change. Groundwater movement is now concentrated in the upper strata, and if the hydrologic properties of these strata are different from the average properties of the unit, as they are likely to be, then average properties will no longer adequately predict groundwater flow. In such cases, the HSU will have to be locally redefined on a smaller scale, perhaps on the scale of the structural components (entablature, flow top, etc.) of individual flows. An example to illustrate this concept is shown in Figure B.2, where the basis for identifying HSU's varies from the components of individual flows near the hypothetical repository to multiple sequences of flows farther from the repository. Hydrostratigraphic units with the same number in this figure are assigned the same material properties.

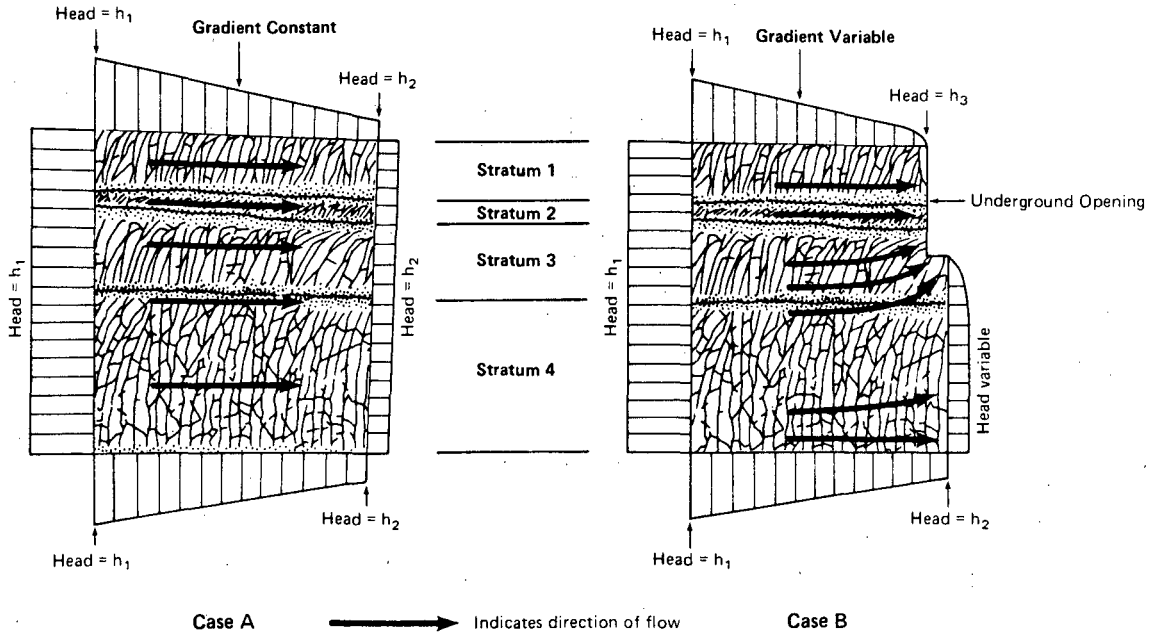


Figure B.1. Example of the kinematic effect, showing parallel flow lines under a uniform hydraulic gradient (Case A) and converging flow lines under a nonuniform hydraulic gradient (Case B). [XBL 8111-4810]

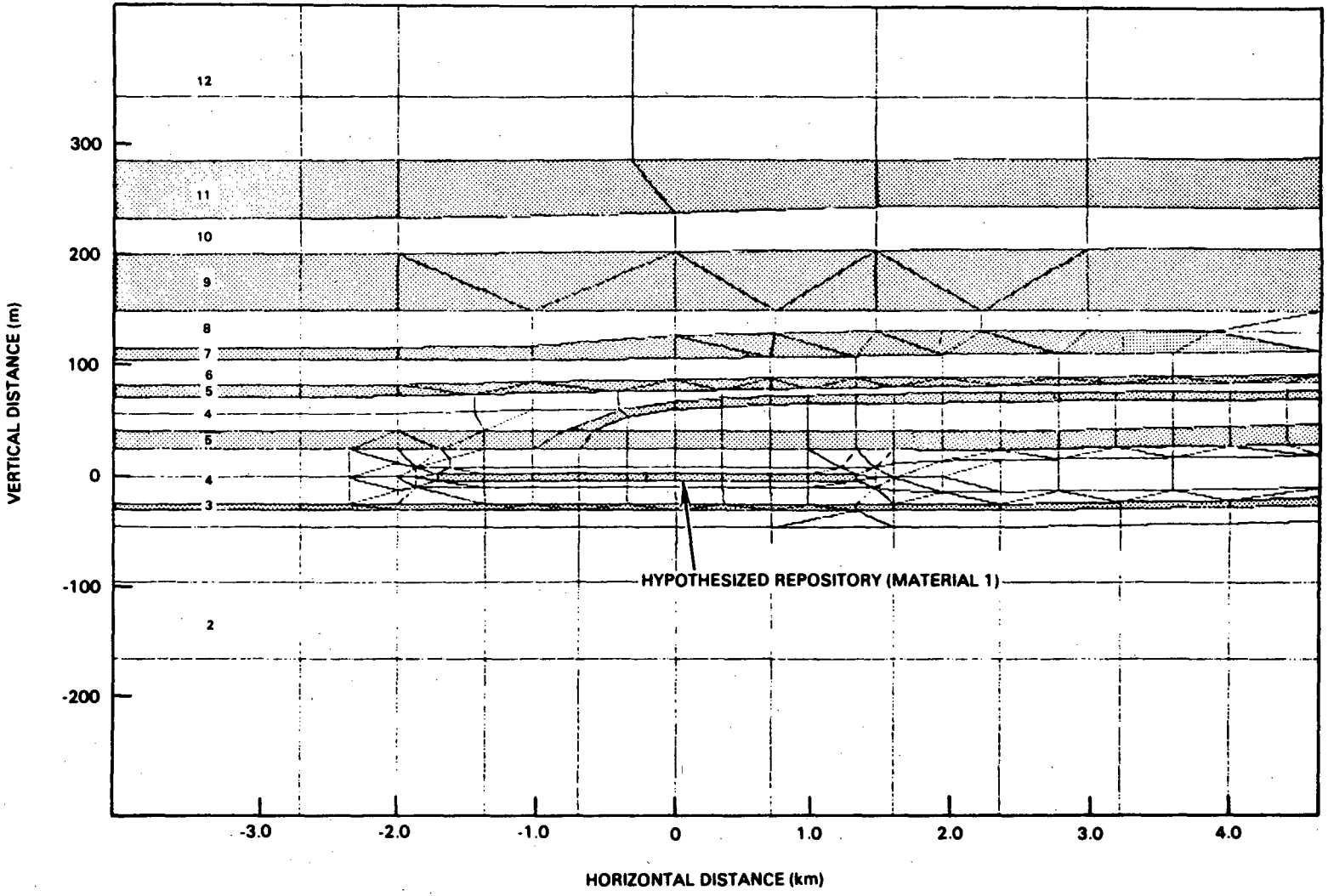


Figure B.2. Example of hydrostratigraphic units identified for the purpose of numerical modeling in the vicinity of a repository in a sequence of flood basalts (modified from King et al., 1981, Figure 4-3).
[XBL 826-10493]

B.2 IDENTIFICATION OF HYDROSTRATIGRAPHIC UNITS DEFINED ON THE BASIS OF HYDRAULIC PROPERTIES AND CONTINUUM BEHAVIOR

An HSU defined on the basis of hydraulic properties and continuum behavior must exhibit statistical similarity and continuum behavior relative to the hydraulic nature of the problem being studied. The minimum size of such a unit would be the REV; the maximum size would be governed by the physical limits of the statistically similar rock mass. For bedded media, the upper limit would be the lateral extent of the relatively homogeneous stratum or sequence of strata.

B.2.1 Identification in the Far-Field

The appropriate scale of an HSU will vary from place to place within the study area, depending upon the nature of the flow patterns to be studied and on the hydraulic properties of the rock. Looking first at the far-field, where flow patterns are not expected to change significantly in response to repository-induced perturbations, one sees that the appropriate scales of measurement are determined both by the existing distribution of head and by the distribution of heterogeneities in hydraulic properties. The head distribution has a direct influence on the appropriate size of the REV, because this distribution determines hydraulic gradients. The appropriate REV must be small enough to experience a relatively constant gradient, as previously described. Thus smaller REV volumes should be sought where the hydraulic gradient is changing rapidly rather than where the gradient is fairly constant. The nature of the gradient field then dictates the maximum appropriate volumes for which representative behavior should be sought.

The distribution of heterogeneities in the rock itself determines the minimum size a representative volume can have, which is the size of the REV. If, in some part of the study area, the size of the REV as determined by the heterogeneities is larger than the maximum size as determined by the gradient field, then continuum techniques cannot be accurately applied at that location. For these locations, either discrete or stochastic analysis will be necessary.

Suppose a head distribution has been measured in a part of the study area, such as that shown in Figure B.3. Suppose that the fractures in this subdomain are pervasive, small-scale features, as shown in Case A. A size for the appropriate REV in terms of the isopotentials is shown in the figure. In Case A, this volume behaves as a continuum because it contains many small fractures. Therefore, the scale of the REV for Case A will be kinematically consistent with the gradient, so that an accurate continuum analysis is possible. If the fractures are large-scale features such as those in Case B, the REV will be much larger than for Case A. This REV is not appropriate for analysis of the true isopotentials, since the gradient within it is not constant. However, if a detailed flow analysis is not necessary in this part of the study area, it may be possible to use

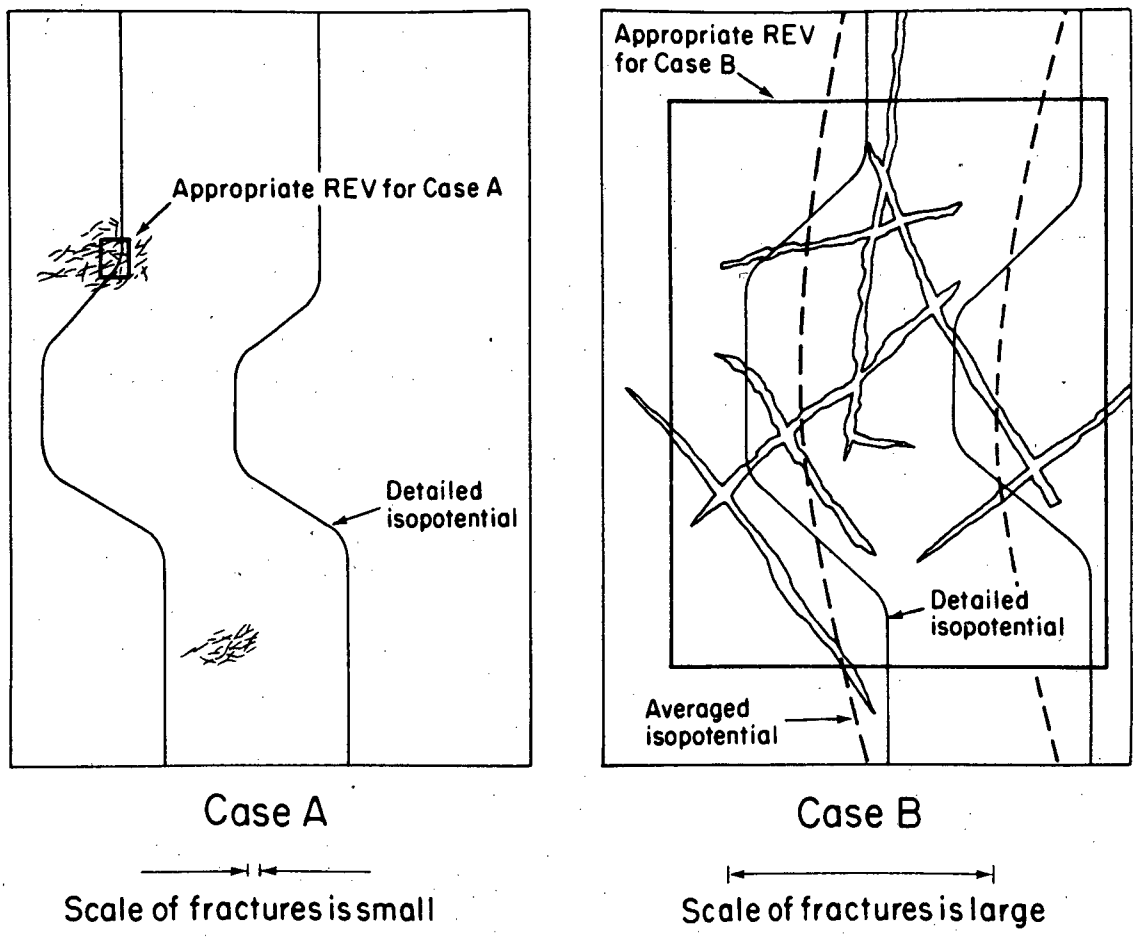


Figure B.3. The relationship between REV's, scale of fractures (or other heterogeneities), and scale of isopotentials for two different constant scales of continuum flow analysis. [XBL 8110-12146]

more grossly defined average isopotentials consistent with the size of the REV for Case B. Such averaged isopotentials are shown with broken lines in the figure. If a detailed flow analysis were also not needed in Case A, and if volumes on a larger scale than the REV for Case A were also shown to be representative, then the rock in Case A could be studied on either a large or a small scale.

The kinematically appropriate scale of measurement will define the minimum size of the HSU. For example, in Case A of Figure B.3, an HSU can be defined either on the scale of the appropriate REV shown or on a larger scale, provided that the hydraulic properties remain representative and the level of detail remains appropriate to the problem being studied. In Case B, however, it would not be possible to identify an HSU on a scale smaller than the appropriate REV shown, nor would it be possible to treat the problem at the level of detail possible in Case A while assuming continuum behavior. The process of finding the appropriate scale of measurement and analysis is iterative. The more data that are available, the more clearly the appropriate scale of measurement and analysis can be identified.

Averaged isopotentials, such as those shown in Figure B.3, cannot always be conveniently found. Figure B.4 shows a case in which averaging the isopotentials does not help. Volume A is an REV but is too large for the gradient field; accurate continuum analysis is not possible on this scale because the volume is not kinematically appropriate. Volume B is appropriate kinematically but is not statistically representative. It behaves neither like a continuum nor like a discrete fracture. Volume C is appropriate kinematically but behaves as a discrete fracture rather than a continuum. In this case, either discrete fracture analysis or stochastic analysis must be used. These types of analyses may often be required to adequately model behavior in the immediate vicinity of the repository.

If the analysis were attempted on the basis of using an REV of the size of Volume A, the problem would be indeterminant. Since Volume A is intrinsically heterogeneous, the hydrologic behavior of that volume will depend on the gradient field. However, the gradient field itself depends on the behavior. As a result, there is no a priori way to assign appropriate hydraulic properties to that volume, and any treatment of it by continuum techniques must be considered approximate.

If a porous medium analysis is attempted on the scale shown in Volume B, which is not a representative volume, continuum behavior cannot be expected, and the values of the hydraulic properties are likely to vary unpredictably at different locations in the rock mass. Neither does this volume behave like a single fracture. Reliable results cannot be expected from analysis on this scale.

The only theoretically appropriate analysis that can be performed on the problem shown in Figure B.4 must be done on the scale of Volume C. Volume C is on the scale of the individual fracture and, as previously stated, is theoretically amenable to either a discrete fracture analysis or

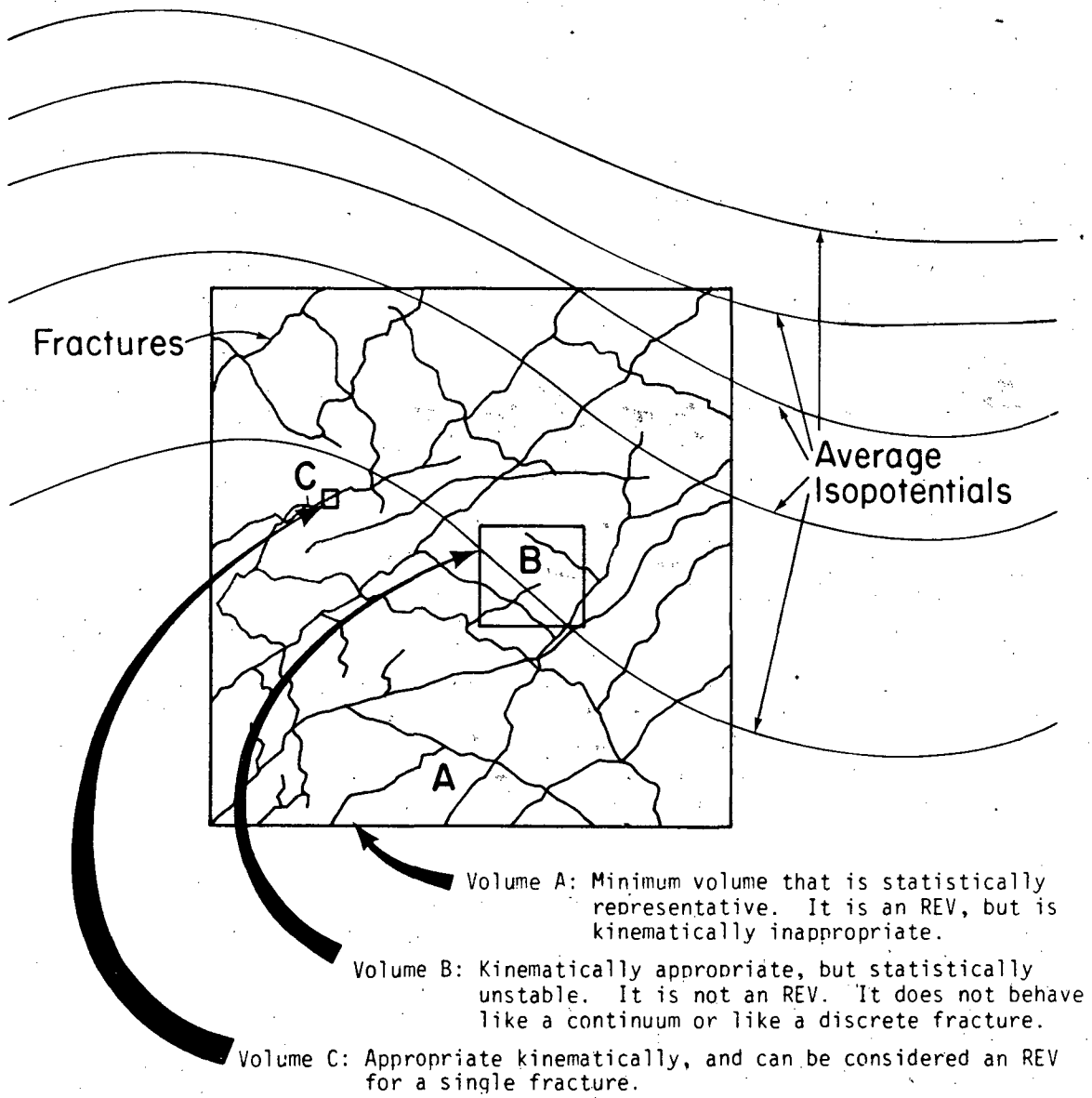


Figure B.4. Example of inconsistent relationship between the REV and the gradient field. [XBL 826-2287]

a stochastic analysis. If a discrete analysis were attempted, every fracture would have to be characterized. This is, in general, impossible. An alternative is a stochastic analysis, which could be conducted either by synthesizing discrete fractures or by random treatment of a large number of small REV's. In applying the stochastic approach, however, the variability in hydraulic properties can be quite high, and the confidence level for the results can be quite low (Smith and Freeze, 1979).

B.2.2 Identification in the Disturbed Zone

Identification of HSU's within the disturbed zone of a repository depends upon the kinematic effects developed during repository construction and waste emplacement. Flow patterns in the disturbed zone should therefore be predicted and the HSU's scaled appropriately. Then the HSU's are re-examined and flow patterns are again refined until proper balance is attained. In general, smaller units will be required in the disturbed zone than in the far-field because of the rapidly converging flow lines found there.

After the repository is backfilled and resaturates, the flow lines will change to reflect thermal loading of the waste rather than drainage into an underground opening. In time the thermally induced flow lines will also change as thermal loading declines and regional flow patterns again predominate. Although HSU's appropriate for analysis of each of these phases must be identified, it is likely that more than one phase can be studied using the same HSU's.

An example of the identification of HSU's within the disturbed zone was developed by King et al. (1981) to study thermal loading and is given in Figure B.2. The use of this sequence of HSU's as an example in this report is not intended to constitute an evaluation of this particular selection of units, but to illustrate one possible approach to the identification of HSU's to study a given problem. The units are identified by number in Figure B.2; the shading of alternate units is to make them easy to distinguish. The individual units were selected to study repository-induced perturbations within the disturbed zone for a repository within the Umtanum unit in the Pasco Basin, and are seen to become generally smaller in the vicinity of the repository in order to satisfy kinematic requirements. These units are:

1. repository backfill,
2. colonnade and entablature of flow immediately beneath repository,
3. interflow breccia,
4. colonnade and entablature of Umtanum unit (containing repository),
5. interflow breccia for Umtanum flow top,
6. colonnade and entablature of flow immediately above Umtanum unit,

7. interflow breccia,

8. colonnade, entablature, and flow top of next major flow above repository,

9. lower colonnade and entablature of Middle Sentinel Bluffs "through runner,"

10. interflow breccia,

11. upper colonnade and entablature of Middle Sentinel Bluffs "through runner,"

12. colonnades, entablatures, and flow tops of Upper Sentinel Bluffs Sequence.

These HSU's were intended by King et al. (1981) to represent a portion of the stratigraphic units shown schematically in Figure 1.5. Comparison of that figure with Figure B.2 will provide an example of the relationship of these HSU's to the existing stratigraphic units.

The finite element mesh used by King et al. (1981) to study repository-induced perturbations has been superposed on the HSU's shown in Figure B.2 and can serve as an indication of the maximum allowable size for REV's. Taking HSU 11 as an example, it can be seen that this unit has been divided into six elements for the purpose of numerical modeling. If the smallest of these elements contains a statistically representative sample of the heterogeneities within that HSU (i.e., if it lies within a flat part of the curve in Figure 2.1), then all elements within the unit will have statistically homogeneous hydraulic properties. The hydraulic properties will all belong to the same statistical distribution. If the standard deviation of that distribution is small, it is reasonable to assign all elements the same hydraulic properties. If the standard deviation is large, however, then a stochastic approach such as that suggested by Smith and Freeze (1979) will be required.

B.3 IDENTIFICATION OF HYDROSTRATIGRAPHIC UNITS DEFINED ON THE BASIS OF NONCONTINUUM BEHAVIOR

The REV for certain sequences of stratigraphic units may either be nonexistent or be larger than the smallest element or nodal that must be treated. Whenever the volume to be treated is smaller than the REV, the continuum approach cannot be relied upon to predict groundwater flux accurately, because such volumes do not contain representative samples of the geologic medium. Volumes smaller than the REV can, in theory, be accurately treated only with noncontinuum, discrete models that take into account the actual heterogeneities of the rock. Each such volume may be expected to have widely varying material properties, which must either be measured independently for each volume or be treated stochastically. From

a practical standpoint, the material properties of each volume cannot be measured independently because of the cost and because the necessary boreholes could seriously impair the ability of the basalt strata to contain the waste. Instead, random samples are taken and stochastic techniques are applied to develop either discrete models, as in Long et al. (1981), or continuum models, as in Smith and Freeze (1979). In practice, however, continuum models are used almost exclusively because of their greater simplicity. The errors involved in the treatment of heterogeneous media by stochastic methods could be large, and have not been fully evaluated. The worst-case approach is considered to be a variant of the stochastic approach, which can also be used for heterogeneous media.

B.4 KINEMATIC CONSIDERATIONS IN CHOOSING HYDROSTRATIGRAPHIC UNITS FOR TRANSPORT MODELING

All of the above discussion applies equally to the identification of HSU's for both flux and velocity modeling. However, in the case of velocity modeling, additional restrictions must be considered. Hydraulic conductivity, the ratio of hydraulic conductivity to effective porosity, and dispersion must each satisfy the requirements of an REV as previously described. Furthermore, not only must the hydraulic gradient be constant over the REV, the average contaminant concentration gradient must also be constant for similar reasons. Thus an appropriate REV for transport modeling will always be at least as small as the appropriate REV for flux. As a result, identification of HSU's for transport will be more difficult than for flux and the models will require more data. Research on the equivalent transport properties of systems of fractures is currently underway at LBL. The topic is not presently well understood, and the results of this research should be helpful in more clearly defining the requirements of HSU's for transport.

APPENDIX C. IDENTIFICATION OF HYDROSTRATIGRAPHIC UNITS IN FLOOD BASALTS: AN ILLUSTRATIVE EXAMPLE

Data from the Pasco Basin will be employed to illustrate the methods of identifying HSU's for treating regional groundwater flux. The use of this data as an example in this report is not intended to constitute an evaluation of its adequacy or accuracy, nor is it intended to suggest that the HSU's that may be derived are the best ones to use in studying groundwater movement. Rather, the purpose here is to illustrate one possible approach to identification of HSU's within a particular hydrologic basin. The analytical techniques will be discussed generally in the order in which they were presented in Section 2.4.

C.1 GROUNDWATER HEAD

Available data on hydraulic head, though quite abundant for the shallower aquifers, decreases rapidly with depth because of the relative scarcity of deep boreholes (Gephart et al., 1979, Table II-11). An additional problem is that available data show considerable scatter, and the degree to which this scatter represents actual conditions rather than measurement error is uncertain. In addition, some of the data represent observed heads, uncorrected for density and temperature variations. Sample head profiles are shown in Figure C.1 for the deeper basalts in boreholes DC-1/DC-2, DC-6, and DC-8. These boreholes were selected to provide examples for HSU identification on the basis of groundwater head because they show a more complex vertical profile than has generally been observed in the deep wells of the Pasco Basin. A location map for these boreholes is shown in Figure C.3.

Available data on hydraulic head would suggest the following HSU's for regional flux.

1. Upper Saddle Mountains Basalt, above and including the Selah unit, shows steadily increasing head.

2. Lower Saddle Mountains, Wanapum, and Grande Ronde to top of Umtanum unit show relatively constant head.

3. Umtanum unit, which appears to behave as a partial barrier to vertical groundwater flow.

4. Higher permeability basalts, extending about 300 m beneath the Umtanum. These basalt flows appear to act as a drain for the regional flow system.

5. Deep basalts underlying HSU 4.

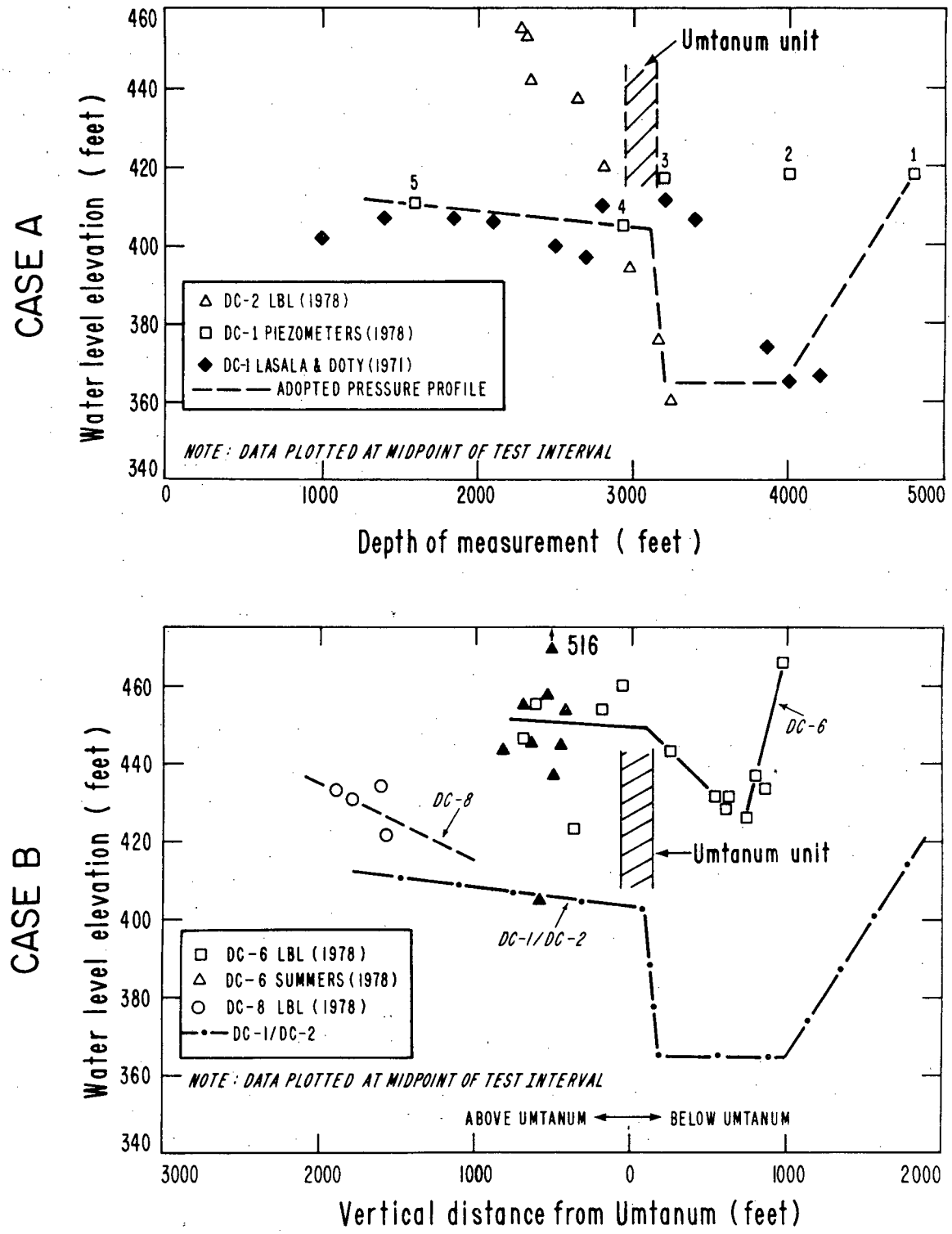


Figure C.1. Variations of hydraulic head with depth. Case A: boreholes DC-1 and DC-2; Case B: DC-1/DC-2, DC-6, and DC-8 (modified from Apps et al., 1979, Figures II-9 and II-12).

[XBL 8110-11692]

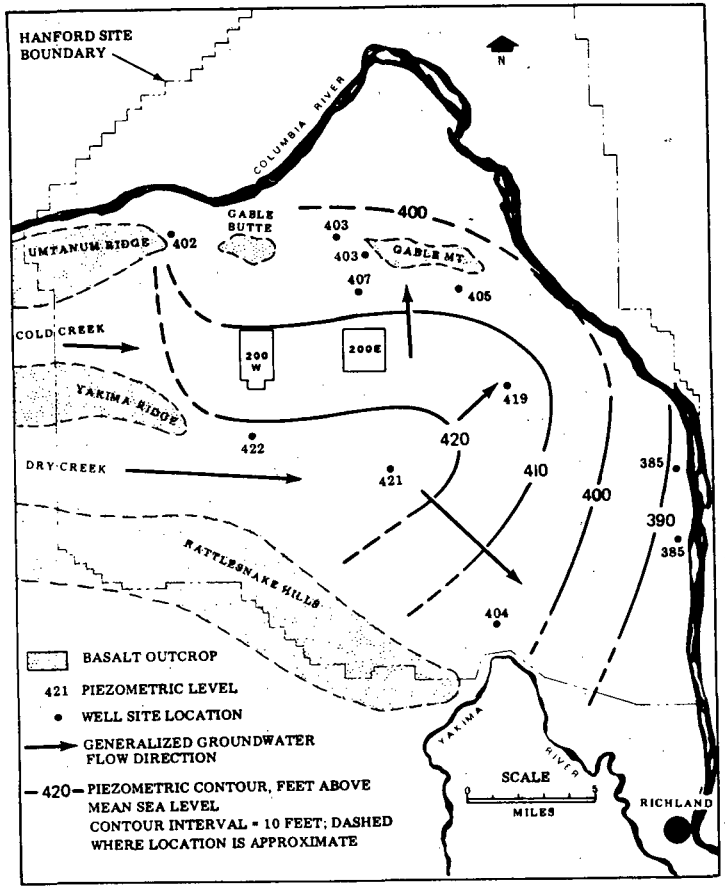
Available hydraulic head data also provide indications of the lateral extent of HSU's and the possible presence of barriers to lateral flow. On the basis of this type of data, Apps et al. (1979, p. II-38) have suggested the presence of two such barriers within the Pasco Basin. One barrier follows the Umtanum Ridge-Gable Mountain anticline, and the other appears to cut across the mouths of Cold Creek Valley and possibly Dry Creek Valley.

C.2 GROUNDWATER CHEMISTRY AND AGE DATING

The areal distribution of published hydrochemical and isotope data for the deep basalts of the Pasco Basin is insufficient to support a quantitative analysis of geohydrologic conditions (Gephart et al., 1979, p. III-154). Available data for the shallower basalts generally support the conclusions made on the basis of hydraulic head measurements discussed earlier. The distribution of total dissolved solids within the Mabton interbed, for example, is shown by Gephart et al. (1979, p. III-161) to be in substantial agreement with the the hydraulic head data. This agreement may be seen by comparing the two contour maps in Figure C.2. Both data sets indicate that the Mabton Interbed is laterally continuous within the Cold Creek Syncline portion of the Pasco Basin. Additional support for the general flow patterns observed in the Mabton are provided by ^{14}C age dating (Gephart et al., 1979, p. III-168).

Early studies of vertical variations in groundwater chemistry have indicated close hydrochemical similarity between waters of the lower Saddle Mountains Basalt and upper Wanapum Basalt (Gephart et al., 1979, p. III-170). Data on the deep basalts is very limited, and some of the reported water samples are suspected to have been contaminated by drilling fluids or by cross-aquifer flow. Three reliable water samples from below the Umtanum in boreholes DC-1 and DC-6 are reported by Gephart et al. (1979, p. III-180) to be chemically similar to one another but distinctly different from reliable samples taken at shallower depths. Each of these samples was taken within 300 m below the Umtanum.

Data obtained since these earlier studies have indicated a somewhat more complicated picture. Boreholes DB-13, DB-15, and DC-12, all within the Cold Creek Syncline, are reported to show a significant hydrochemical break near the Saddle Mountains-Wanapum Basalt contact, whereas data from DC-14 and DC-15, both near the Columbia River and outside of Cold Creek Syncline, are reported to show no hydrochemical break at that contact (Deju, 1980b, p. 38). Moreover, two samples taken in DC-14 show a hydrochemical break progressively occurring within the upper 100 m of the Grande Ronde Basalt (Deju, 1981, Figure 7). Hydrochemical evidence tends to support identification of the Saddle Mountains and Wanapum Basalts as separate HSU's at some locations but not at other locations within the basin. This may be indicative of variations in vertical permeability or vertical hydraulic gradients in various parts of the basin, but these indications should be



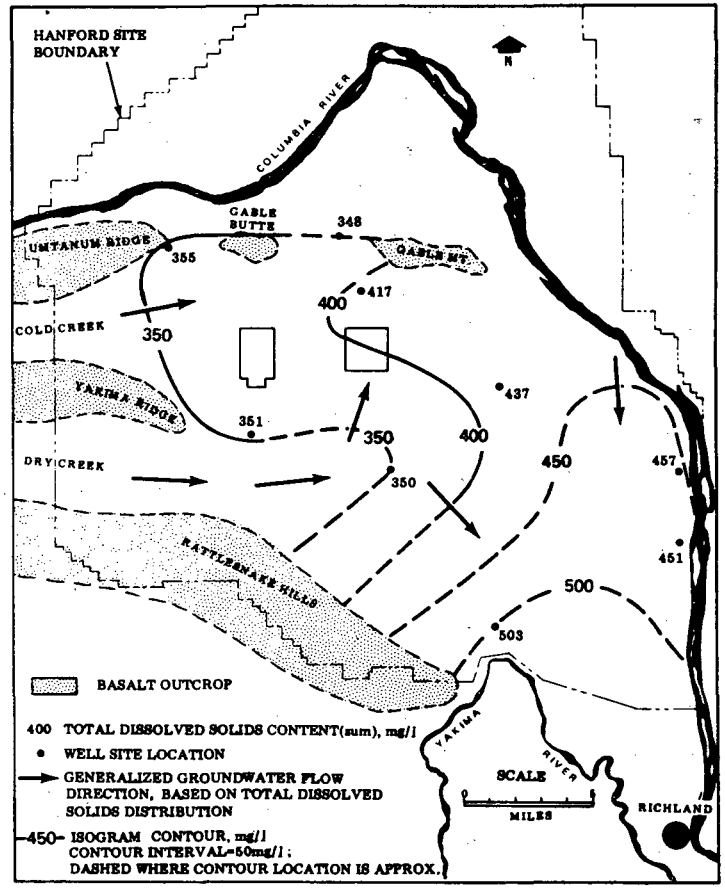


Figure C.2. Comparison of directions of groundwater movements within the Mabton Interbed as inferred by hydraulic head (Case A) and total dissolved solids (Case B) (from Gephart et al., 1979, Figures III-22 and III-42). [XBL 826-10494]

supported by direct measurement. Hydrochemical data also support identification of parts of the Grande Ronde Formation as a separate HSU from the Wanapum; however, additional data are required to more precisely identify the hydrologic factors associated with this hydrochemical break.

C.3 GEOLOGIC AND STRATIGRAPHIC METHODS

Stratigraphic units are not necessarily the same as HSU's. However, in many cases they are strongly related. With this understanding, alternative HSU's will be identified essentially on the basis of geologic and stratgraphic information in this section.

C.3.1 Single-Layer Case: Entire Basalt Section

This is perhaps the most simple conceptual model for an HSU, where all basalt flows are combined into one single essentially homogeneous unit. This approach has obvious limitations, particularly when attempting to understand groundwater movement within the basalt to any detailed extent. The approach also has advantages, the principle one being the relative ease of application to numerical models.

This definition of an HSU was employed by Rockwell Hanford Operations in its first three-dimensional model of the Pasco Basin (Gephart et al., 1979, p. IV-103). It was considered by Rockwell to be a preliminary test model, and has since been superseded by a more refined representation of the basin.

C.3.2 Multiple-Layer Case: Principal Basalt Formations

The principal basalt formations within the upper 1500 m of bedrock in the Pasco Basin are the Saddle Mountains, the Wanapum, and the Grande Ronde. These formations are shown in schematic section in Figure C.3. An alternative identification of HSU's is to correlate them with the principal basalt formations.

This method of correlation is largely stratigraphic rather than hydrologic. As shown in Figure C.3, the units are defined by the surface of the basalt and by the locations of two laterally extensive sandstone interbeds, the Mabton and the Vantage. These interbeds serve as easily identifiable markers of the basalt surface at particular times in history, and are therefore good stratigraphic indicators.

This correlation of HSU's with the principal basalt formations represents an increased level of detail over the single-layer case and is a logical step in the process of evolving increasingly refined models. Rockwell Hanford Operations has used a slightly more complex correlation of this general

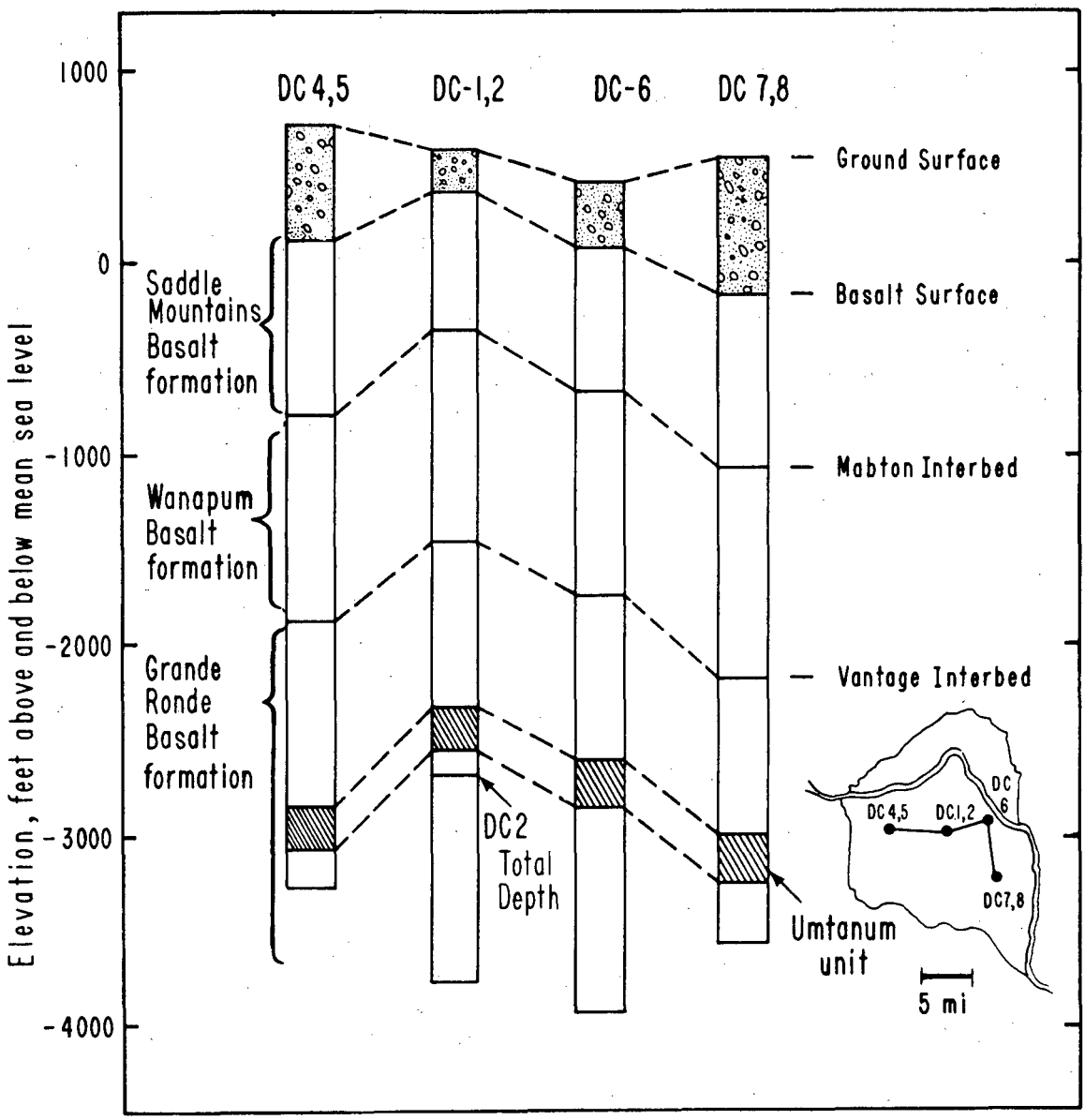


Figure C.3. Generalized basalt stratigraphy within the Pasco Basin (from Apps et al., 1979, Figure I-2). [XBL 792-7372]

type in developing its second-stage basin model (Rockwell Hanford Operations, 1980c, p. III-49), and some preliminary results have been reported by Deju (1980a, p. 22; 1981, p. 28). To function successfully as HSU's for the purpose of basin modeling, the major geologic formations must be shown to have distinct hydrologic functions, and the hydrologic criteria for continuum behavior must be met for the particular applications. Provided that these criteria are met, HSU's identified on the scale of major formations can be useful in studying regional patterns of groundwater movement.

C.3.3 Multiple-Layer Case: Structural Components of Individual Flows

Each individual basalt flow is generally separable into the structural components of flow top, entablature, and colonnade, as discussed in Appendix A. Structurally and stratigraphically, these components offer the smallest likely HSU's of interest to nuclear waste isolation. These structural components are likely to provide relatively consistent hydrologic functions throughout their lateral extent and are therefore good candidates for trial HSU's. Confirmation of such units will require field testing. An additional advantage of identifying these structural components as HSU's is that they generally occur in nature on a scale that is convenient to test under current technology.

Hydrostratigraphic units identified on the basis of structural components of individual flows have been used by King et al. (1981) for analysis of the disturbed zone around a repository in Pasco Basin flood basalts. The configuration of units selected by King and co-workers is shown in Figure B.2 and discussed in Appendix B. Identifying structural components of individual flows as HSU's may not be practical for far-field use because of the high degree of geologic knowledge required and the large number of units that would have to be treated. For such applications, HSU's must be sought on a larger scale.

C.4 HYDROGEOLOGIC METHODS

Hydrologic data combine with stratigraphic data to provide the complete spectrum of information basic to the identification of HSU's. In this section, the data available from hydrogeologic tests in the Pasco Basin will be used in combination with stratigraphic data to identify alternative HSU's.

C.4.1 Hydraulic Conductivity Basis for Unit Identification

Hydraulic conductivity is the key material property governing mass flux in regional flow, where dynamic effects are not normally significant. Gephart et al. (1979) have summarized all pertinent conductivity data available as of June 1979 in a comprehensive report that integrates hydrologic knowledge for the Pasco Basin. Although additional information has since been available from both new and existing boreholes, this more recent data has generally fallen into the ranges previously observed.

Conductivity data available for the Pasco Basin are insufficient to attempt to verify continuum behavior or identify the possible size of an REV. Available data in fact show a scatter of two to three orders of magnitude in test results within the same stratigraphic unit, and even greater scatter within comparable stratigraphic units. This is exemplified by the data in Figure C.4, which show a range of five orders of magnitude for the horizontal hydraulic conductivity of columnnar zones within the Grande Ronde Basalt.

Despite the evidence for considerable scatter in field data, a consistent contrast is evident in the hydraulic properties of the various structural components of the flows. This provides evidence of distinct hydrologic function. For example, hydraulic conductivities of entablatures are typically lower than those of flow-top breccias. Available data on hydraulic conductivity therefore supports the correlation of HSU's with the components of individual flows. However, available conductivity data are not sufficient to provide information on the presence of HSU's on a larger scale.

It may be noted that the foregoing discussion is based entirely on horizontal permeability measurements. At this time no direct measurements of vertical permeability have been reported. In considering the nature of the structural features that give rise to permeability in basalt, however, there is reason to believe that just as much variability will be found in vertical permeability as in horizontal permeability.

C.4.2 Storage Coefficient, Effective Porosity, and Diffusion Basis for Unit Identification

Field data for storage coefficient are very limited as compared with data for horizontal permeability. The data that are available have been summarized by Gephart et al. for the deeper basalts (1979, Table III-36). These data are representative of the more permeable brecciated zones and include two measurements from the Wanapum and four measurements from the Grande Ronde. Dimensionless values of storage coefficient range over three orders of magnitude from 1.8×10^{-3} to 1×10^{-6}.

No published field data were found for effective porosity and diffusion from the deeper basalts of the Pasco Basin. However, these parameters are, like hydraulic conductivity, related to the geometry of the pore volumes. Thus, given the observed high degree of variability in conductivity, considerable variability might also be expected for effective porosity and diffusion.

Insufficient data now exist for the identification of HSU's on the basis of storage coefficient, effective porosity, or diffusion. Each of these parameters is considerably more difficult to measure accurately in the field than horizontal hydraulic conductivity, because present techniques require multiple boreholes and, in the case of effective

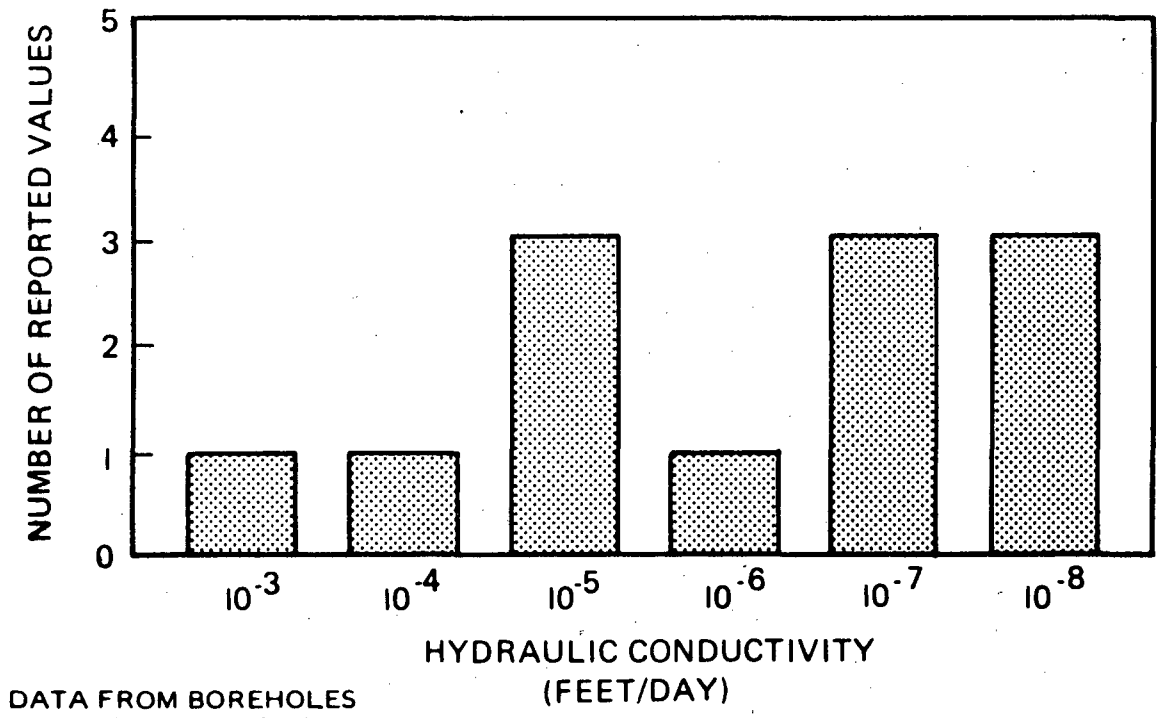


Figure C.4. Observed range of hydraulic conductivity across columnar zones within the Grande Ronde Basalt (from Gephart et al., 1979, Figure III-39). [XBL 826-10497]

porosity and diffusion, a great deal of time. A good data base for any of these parameters would not normally be expected for deep strata in low-permeability rock. Thus, although they are very important to transient flow and solute transport analyses, the use of measured values of these parameters in identifying HSU's may be limited to verifying contrasts in hydrologic function.

C.5 GEOPHYSICAL METHODS

Geophysical techniques are of primary value in providing supporting information for the stratigraphic and hydrologic tests. Geophysical tests are by their nature indirect measurements of the stratigraphic and hydrologic parameters of interest. Geophysical tests rely upon a response to a perturbation that must in turn be related to hydrologic or stratigraphic parameters. For example, electrical resistivity logs provide good information on the electrical resistivity of the host rock, but to relate that measurement to hydrologic or stratigraphic properties requires either that additional assumptions be made or that the technique be calibrated against hydrologic or stratigraphic data obtained by other means. The advantage of geophysical techniques is their speed and ease of field use. Good summaries of the application of geophysics to hydrology have been prepared by Keys and MacCary (1971) and Nelson (1979).

Geophysical techniques have been found to be most useful in the Pasco Basin as indicators of stratigraphy and structure. For example, they have been relied upon by Gephart et al. to provide an indication of rock density (1979, p. III-132). This in turn has been correlated with the structural components of basalt flows. The primary role of geophysics in the identification of HSU's has been in supporting the geologic and stratigraphic bases for unit identification discussed in Section C.3. Without proven correlation with hydrologic or geologic measurements, geophysical measurements in themselves should not be considered as the basis for identifying HSU's.

C.6 SYNTHESIS OF AVAILABLE INFORMATION

The identification of HSU's should be based primarily on direct stratigraphic and hydrologic data. Indirect data from geophysical and geochemical techniques should have stratigraphic and hydrologic support before they are strongly considered.

The data presently available for the Pasco Basin indicate a considerable degree of heterogeneity in both horizontal and vertical hydrogeologic properties. Because of this variability, the primary use of the measured hydraulic properties now available is in identifying distinctions in hydrologic function. These data therefore tend to support the identification of HSU's on the basis of the structural components of individual flows. Further, the hydraulic head and geochemical data provide a basis

for identifying HSU's on a scale larger than the structural components of individual flows. For the purpose of illustrating preliminary HSU's for a study of regional groundwater flux, our present understanding of these data suggest separation of the groundwater regime into the units shown in Table C.1. Within the disturbed zone, stratigraphic and permeability data tend to support the identification of HSU's with the structural components of individual flows.

Table C.1. Example of Preliminary Regional Hydrostratigraphic Units for Studies of Groundwater Flux Within the Pasco Basin

Hydrostratigraphic Unit	Principal Supporting Data
Undifferentiated alluvium	Stratigraphy
Basalt surface to Selah Interbed (upper Saddle Mountains Basalt)	Stratigraphy and head
Bottom of Selah Interbed to Mabton Interbed (lower Saddle Mountains Basalt)	Hydrochemistry
Bottom of Mabton Interbed to top of Umtanum entablature (Wanapum and upper Grande Ronde Basalts)	Stratigraphy, hydrochemistry, head
Umtanum entablature (Grande Ronde Basalt)	Stratigraphy, head, hydrochemistry, permeability
Bottom of Umtanum entablature to point 300 m beneath (Grande Ronde Basalt)	Head, hydrochemistry, permeability
Deeper basalts (Grande Ronde Basalt)	Head

APPENDIX D. MECHANISMS OF RECHARGE AND DISCHARGE IN FLOOD BASALTS: AN ILLUSTRATION FROM THE PASCO BASIN

For the purpose of illustrating the various mechanisms of recharge and discharge that may be encountered in flood basalts, available data from the Pasco Basin will be employed.

The data used in this example are taken from the published literature and have not been reviewed for accuracy by LBL staff. The conclusions presented here are therefore intended only to illustrate the application of field data to the issue of groundwater movement in flood basalts, and are not intended to imply either acceptance or rejection of the basic data. The hydrostratigraphy of the Pasco Basin is considerably more complex than that of Swale Creek Valley, used as an example in Section 3. Being considerably larger than Swale Creek Valley, the Pasco Basin appears to have a wider range of structural features that affect groundwater flow. Also being both structurally and topographically the lowest point in the Columbia Plateau, it serves as the terminus for much of the surface and groundwater drainage of the Plateau.

Presented in Figure 1.3 are geologic cross sections of the Pasco Basin, showing the three principal basalt formations, the Saddle Mountains, Wanapum, and Grande Ronde. These drawings are highly schematic and do not show the extreme complexity of the layering and folding that have been encountered. The reader is referred to Myers et al. (1979) for a more complete understanding of the stratigraphy of this basin. Figure 1.3 does indicate, however, the general layering of the strata and the comparatively large lateral dimensions of the basin. The basin is about 70 km wide in each cross section.

D.1 LATERAL TRANSFER MECHANISMS

Studies made within the Pasco Basin to date have yielded a fair amount of information that can be used to study the probable mechanisms of recharge and discharge. Water budget studies of surface water-groundwater interrelationships have been made by Rockwell for the Pasco and surrounding basins (Gephart et al., 1979, p. II-75). These studies have indicated that the Yakima and Big Bend Basins to the west and north of the Pasco Basin, and the Walla Walla Basin to the southeast, all show net recharge of groundwaters by surface waters, whereas the Palouse/Snake, Pasco, and Horse Heaven Basins all show net discharge of groundwaters into surface waters. The locations of these basins relative to the Pasco Basin are shown in Figure D.1. Although the results of the Rockwell studies are quantitatively approximate, they indicate a pattern of significant regional groundwater movement toward the topographically lower basins. The total discharge of groundwater to surface water for the Palouse/Snake, Pasco, and Horse Heaven Basins was estimated by this technique to average some 10 billion m^3 (9.5 million acre-ft) per year, which is nearly 7% of the average annual flow of the Columbia River at the Dalles Dam.

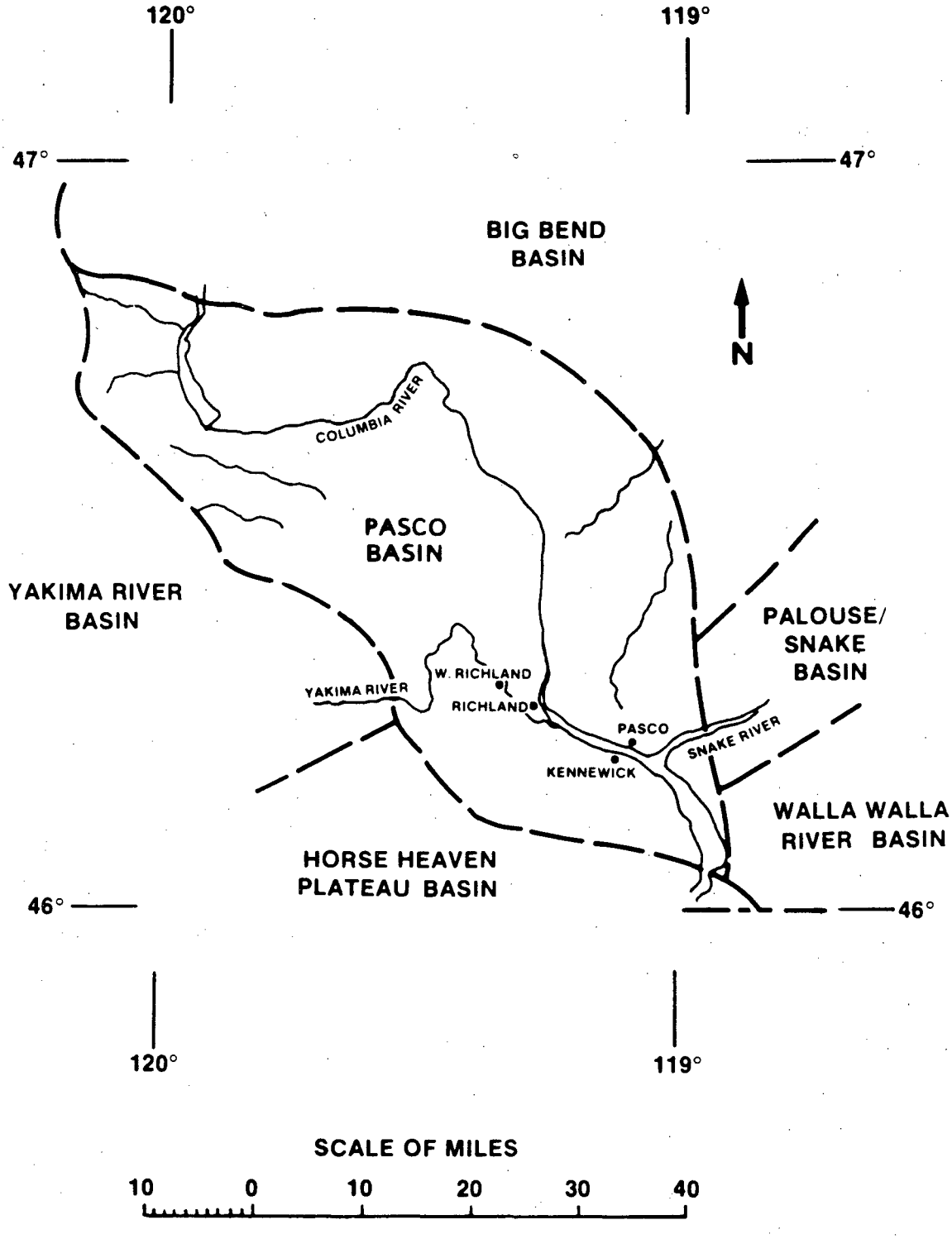


Figure D.1. Map of the Pasco Basin and vicinity, showing neighboring groundwater basins (from Gephart et al., 1979, Figure II-17). [XBL 8210-3031]

The results of Rockwell's water budget studies indicate that lateral movement of groundwater across the Columbia Plateau could be a substantial means of recharging the deeper aquifers within the Pasco Basin. These studies were made on a basin-wide basis, however. They cannot be used to indicate locations of recharge or discharge within basins, but only the net values.

Additional indications of mechanisms of groundwater recharge and discharge within the Pasco Basin may be obtained from the results of numerical model studies or inferred from hydraulic head measurements and hydrochemical data. These studies are largely limited to the Wanapum and Saddle Mountains Basalts, however, where the data are more abundant. Detailed studies have also been made in the unconfined sediments overlying the basalts, and are summarized by Gephart et al. (1979, p. III-57).

Figures 2.3 and C.2 show flow patterns within the Mabton Interbed beneath Cold Creek Syncline, as indicated by hydraulic head and hydrochemical data. These patterns indicate primary recharge of the interbed by lateral flow from Dry Creek and Cold Creek Valleys to the west. Primary discharge areas appear to be along the Columbia River, both to the northwest and to the southeast of Gable Mountain, although data are sparse in these areas. The Mabton Interbed separates the Saddle Mountains and Wanapum Basalts (see Figure C.3), and these general flow patterns are considered by Rockwell to be representative of the Saddle Mountains Basalt (Gephart et al., 1979, p. III-93). The same general flow pattern was also evident in the results of numerical modeling of the upper basalt strata (Deju, 1980a, p. 22). Evidence exists that a flow barrier cuts across the west side of Cold Creek Syncline; such a barrier would limit the importance of this recharge mechanism for the deeper basalts (Gephart et al., 1979, p. II-103). Most of the above place names are shown on the location map in Figure 1.2.

Available data from the deeper basalts are insufficient to evaluate groundwater movement to the same extent as for the Mabton Interbed. Hydraulic head measurements from several wells appear to indicate higher pressures in the deeper aquifers within the Wahluke Syncline (north and east of the Umtanum Ridge-Gable Mountain Anticline) than within the Cold Creek Syncline. These data were interpreted by Apps et al. (1979, p. II-38) to indicate possible recharge of the deeper aquifers from the Columbia River in the vicinity of Sentinel Gap and Priest Rapids Reservoir, where the Wanapum and Grande Ronde Basalts outcrop at the surface. Significant recharge may also be possible through regional subsurface groundwater flow from the northeast. The lower heads found at depth in Cold Creek Syncline may result from barriers to significant lateral flow along the Rattlesnake Hills and the Umtanum Ridge-Gable Mountain Anticline. Recharge and discharge by lateral movement of groundwater would be expected to be significant in the absence of flow barriers, but may be quite restricted where such barriers exist.

D.2 VERTICAL TRANSFER MECHANISMS

Recharge or discharge through vertical leakage across basalt horizons is probably less significant than by lateral flow along basalt horizons, except in areas where barriers exist to lateral flow or where vertical movement may be enhanced by increased vertical permeability, such as along the axes of anticlines. Relatively low vertical groundwater leakage is demonstrated by the artesian conditions encountered at well DC-6 in the deeper basalts within the Wahluke Syncline, indicating the presence of relatively tight confining beds (Apps et al., 1979, p. II-32). Further, groundwater head measurements made in both Cold Creek and Wahluke Synclines indicate relatively little vertical groundwater movement above the Umtanum.

Discharge from the deeper aquifers, however, may occur through vertical movement of groundwater across the basalt strata and into the Columbia River above Wallula Gap if the Horse Heaven Hills present a sufficient barrier to lateral groundwater movement. Vertical movement of groundwater would also be expected to be enhanced in localized areas where regional tectonic deformation has enhanced vertical fracturing, such as along the Umtanum Ridge-Gable Mountain anticline. If no significant barrier to lateral movement exists in the Horse Heaven Hills, primary discharge could be to the Columbia River downstream of Wallula Gap, where outcrops of the Grande Ronde Formation are found.

Measurements of vertical permeability and gradient will be required to evaluate the extent of vertical flow into the Columbia River above Wallula Gap and the extent of vertical transfer along the Umtanum Ridge-Gable Mountain Anticline. To date, the available information on vertical permeability is insufficient to identify the extent to which vertical transfer mechanisms are significant for discharge or recharge of the deeper basalts. The greater the vertical permeability and gradient, the more significant vertical transfer will be as a mechanism for discharge. Information on vertical permeability will be essential to the ultimate resolution of this issue.

D.3 GROUNDWATER EXTRACTION MECHANISMS

The remaining mechanism for significant groundwater discharge or recharge is through groundwater extraction (or injection) in wells. The groundwater well can be thought of hydraulically as a sink or source that is artifically introduced into an aquifer and which can act to significantly discharge or recharge that aquifer. This mechanism of discharge or recharge is not presently significant within the Pasco Basin. The average annual groundwater extractions for municipal, industrial, and agricultural uses are only about 90 million m^3 (72,000 acre-ft) per year, which is less than 3% of the estimated net groundwater discharge from the basin. The

total water use within the basin results in an average net groundwater recharge of about 300 million m^3 (250,000 acre-ft) per year, but this is primarily to the unconfined aquifers and probably has little effect on the deeper basalts (Gephart et al., 1979, p. II-87).

D.4 SYNTHESIS OF ALTERNATIVES

This brief summary of possible mechanisms for groundwater recharge and discharge has demonstrated that, although all mechanisms are active to a greater or lesser extent, the mechanisms that prevail are governed primarily by hydrostratigraphy and by the actions of man. Further, different mechanisms may predominate for recharge than discharge, different mechanisms may predominate in different parts of the basin, and different mechanisms may predominate for different HSU's. A three-dimensional groundwater system with its multitude of time variant mechanisms and locations of recharge and discharge can obviously be quite complex, and substantial amounts of data can be required to sort them out.

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