NUREG/CR-5988
PNL-8480

Soil Characterization Methods for Unsaturated Low-Level Waste Sites

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Prepared for
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NUREG/CR--5988
TI93 008562

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Manuscript Completed: January 1993
Date Published: February 1993

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Prepared for
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Washington, DC 20555
NRC FIN L1007

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Abstract

To support a license application for the disposal of low-level radioactive waste (LLW), applicants must characterize the unsaturated zone and demonstrate that waste will not migrate from the facility boundary. This demonstration requires an integrated plan to be developed for sampling and analyzing the soil horizons for physical and hydraulic properties. This document provides a strategy for developing this characterization plan. It describes principles of contaminant flow and transport, site characterization and monitoring strategies, and data management. It also discusses methods and practices that are currently used to monitor properties and conditions in the soil profile, how these properties influence water and waste migration, and why they are important to the license application. The methods part of the document is divided into sections on laboratory and field-based properties, then further subdivided into the description of methods for determining 18 physical, flow, and transport properties. Because of the availability of detailed procedures in many texts and journal articles, the reader is often directed for details to the available literature. References are made to experiments performed at the Las Cruces Trench site, New Mexico, that support LLW site characterization activities. A major contribution from the Las Cruces study is the experience gained in handling data sets for site characterization and the subsequent use of these data sets in modeling studies.

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Executive Summary

Applicants for a license permitting disposal of low-level radioactive waste (LLW) must characterize the physical properties of the site, and provide evidence of its suitability for long-term monitoring. Site characterization and monitoring are required by the U.S. Nuclear Regulatory Commission (NRC), as specified in 10 CFR Part 61. This document, developed for unsaturated media, reviews the need for site characterization, discusses principles of contaminant flow and transport, and presents information on site characterization and monitoring strategy. The report also contains a chapter on data management. Frequent references are made to an NRC-funded study performed at the Las Cruces Trench site. This latter study, conducted in the semi-arid area of southern New Mexico, was designed to provide data to test deterministic and stochastic models of vadose zone flow and transport.

A significant contribution of this report is a description of the interaction between data collection and management and subsequent modeling, which is clearly one of the key features of a well-organized site characterization plan. The salient features of such a plan are outlined in this report. Experiences gained from the Las Cruces Trench Experiment in data management have been an invaluable guide to future studies.

A large part of the report is devoted to methods and practices that are currently used to determine the physical properties of unsaturated soils, as well as to monitor the flow of water and transport of contaminants in unsaturated media.

This latter part of the report is divided into laboratory and field methods. It includes descriptions of methods for determining 18 physical properties affecting flow and transport. Where possible, use has been made of existing procedures and methods, and the reader is frequently referred to the applicable references.

Many of the methods described here have been used at the Las Cruces Trench site. This has resulted in what we believe are improvements over existing methods, making them more suitable for site characterization. It has also resulted in recommendations for using these methods for arid- and semi-arid conditions.

Acknowledgements

The authors gratefully acknowledge the financial assistance of the Office of Nuclear Regulatory Research of the U.S. Nuclear Regulatory Commission. Dr. Ralph Cady of the NRC is project manager of the project entitled "Model Validation at the Las Cruces Trench Site" (TD 2049, FIN L1286) conducted by the University of Arizona and New Mexico State University. Mr. Thomas Nicholson of the NRC is project manager of the project entitled "Unsaturated Zone Field Studies for Validation of Models" (TD 2766, FIN L1007) conducted by Pacific Northwest Laboratory. We thank Jan Raffler, administrative assistant of the Department of Soil and Water Science, University of Arizona, for her help in producing this report. We also thank Joe Flynn, Environmental Communications Section, Pacific Northwest Laboratory, for his editorial review.

1 Purpose and Scope

An important part of preparing and reviewing a license application for a low-level radioactive waste (LLW) disposal facility is the characterization of physical conditions at the site, and the observation of environmental conditions which may fluctuate during the year. Site characterization and monitoring are required by the U.S. Nuclear Regulatory Commission (NRC), as specified in 10 CFR Part 61, Licensing Requirements for Land Disposal of Radioactive Waste. Other stipulations in the regulations require the site to meet certain performance objectives, such that site contamination is detected before it migrates off site, and that the site is capable of being characterized and monitored. The license application must include detailed information on the site conditions and environs so that assessments like these, and of the facility performance as a whole, can be made. Therefore, the collection of site specific information for characterizing background and baseline conditions will be critical to the licensing decisions made by NRC staff.

The level of information needed to satisfy NRC regulations will differ at each site. Characteristics of individual sites will dictate the type and number of tests that should be run, and the spatial and temporal distribution of samples that should be collected. Arid and semi-arid sites, specifically discussed in this manual, have characteristics that differ from humid sites. Deeper water tables, lower rainfall rates, thicker sequences of unsaturated material, and fewer perennial water bodies are common in the western United States. Thus, site characterization activities in arid and semi-arid areas must address these attributes by concentrating more heavily on the unsaturated zone.

This report discusses methods of characterizing physical properties in the unsaturated zone at arid and semi-arid zones. It focuses on tests that may be needed to complete an acceptable license application. Whenever possible, and when appropriate, references are made to research completed at the NRC-funded Las Cruces Trench studies at the Jornada Experiment Station near Las Cruces, New Mexico. However, it should be noted that not all tests for site characterization were completed at the trench site. We have also included methods for characterizing several physical and hydraulic properties that were not specifically conducted at the trench, but may be important in a license application for LLW disposal. Moreover, we have attempted to include more than one method, when appropriate, for characterizing each property. References are made to relatively recent texts, journal articles, and government documents to provide the reader with additional information.

It was not the goal of this report to provide step-by-step methods and tests that NRC staff would endorse. Rather, the goal was to discuss those methods that will have to be conducted in many cases to characterize the hydraulic properties of the unsaturated zone. The discussions emphasize theoretical considerations: why each test is important, how the results are used in the overall analysis of water flow and solute transport, and where more information can be obtained on each method. Procedures that are not readily obtainable are discussed in more detail herein. During the development of a characterization plan, decisions on the many samples to collect and which tests to conduct should be determined in consultation with NRC staff, so that the license application conforms to the Standard Format and Content Guide (NRC, 1988a).

It should also be noted that this report discusses methods for characterizing unsaturated, unconsolidated and partially indurated sediments. It does not include methods for characterizing rock. Information on site characterization methods for rock are available from other sources (e.g., Evans, 1983; Rasmussen and Evans, 1987; Evans and Rasmussen, 1991).

This report is organized into the following five chapters that discuss various aspects of site characterization: introduction and regulatory requirements; flow and transport processes; site characterization, modeling, and validation; characterization and monitoring strategies; and data management and processing. Three appendixes are also attached. Appendix A discusses laboratory methods for characterizing the physical, hydraulic, and transport properties of soils. Appendix B includes field methods for characterizing some of the same properties as discussed in Appendix A.

Appendix C presents a sample database that has been useful for storing and managing the large amount of data collected during the characterization and monitoring of the Las Cruces Trench site.

This report is a product of a continuing study of water movement and contaminant transport in heterogeneous unsaturated soils supported by the Office of Nuclear Regulatory Research of the NRC. The purpose of the overall study is to provide regulatory guidance and assistance in the development of low-level waste disposal facilities. Site characterization, field experiments, and numerical simulations have been part of this continuing study. The need to better understand the relationships among site characterization, conceptualization, and simulation efforts for low-level waste disposal sites has become apparent during the course of the study. This report is a product of this multidisciplinary project that has conducted field experiments, performed field and laboratory measurements of physical and hydraulic properties, and interpreted those measurements in efforts to simulate the environment. Contributions to the report came from NRC staff and their contractors at the University of Arizona (UAz), New Mexico State University (NMSU), and Pacific Northwest Laboratory (PNL).

2 Introduction

Guidance and regulation require the license applicant to collect and analyze site characterization data to fulfill a variety of objectives. These objectives require the collection of data enabling the applicant to describe the site, design and determine the survivability of the cover, identify geologic resources, assess the potential for settlement and its influence on local infiltration rates, and forecast groundwater mass transport. Several of these objectives require that the hydrogeologic environment be conceptualized as an integrated system.

2.1 Requirements of 10 CFR Part 61

The licensing requirements for LLW are codified in Chapter 10 of the Code of Federal Regulations (10 CFR Part 61), "Licensing Requirements for Land Disposal of Radioactive Waste." These requirements state that the cornerstone of an LLW disposal system is the stability of the waste and disposal site. This stability of waste and site is to assure minimal access of water to the waste, and to provide confidence in long-term maintenance-free disposal. The groundwater (meaning both the unsaturated zone and aquifer) pathway is among those that must be analyzed to demonstrate protection of the general population. Analyses of the stability of the disposal site examine active natural processes such as erosion, settlement of wastes and backfill, infiltration through covers and adjacent soils, and surface drainage.

Specifically, paragraph 61.12 of 10 CFR Part 61 requires that "... technical information must include ... information needed for demonstration that the performance objectives of Subpart C of this part and the applicable technical requirements of Subpart D of this part will be met: (a) A description of the natural and demographic disposal site characteristics as determined by disposal site selection and characterization activities. The description must include geologic, geotechnical, hydrologic, meteorologic, climatologic, and biotic features of the disposal site and vicinity..." Paragraph 61.50 of Subpart D in Part 61, the technical requirements section, states that "(2) The disposal site shall be capable of being characterized, modeled, analyzed, and monitored." In paragraph 61.51, this section further reinforces the quest for "stability" by requiring "(4) Covers must be designed to minimize to the extent practicable water infiltration, to direct percolating or surface water away from the disposed waste, and to resist degradation by surface geologic processes and biotic activity," and (5) Surface features must direct surface water drainage away from disposal units at velocities and gradients which will not result in erosion..."

The licensing requirements call for characterization efforts to gather sufficient information about a site for preparation of the license application. Monitoring is also required during site construction and operation to provide data for the evaluation of health and environmental impacts during construction and operation, and to enable the evaluation of long-term effects and the need for mitigative measures.

2.2 Guidance from NUREG-1199

To support the Low-Level Waste Policy Act Amendments of 1987, the NRC has issued NUREG-1199, "Standard Format and Content Guide of a License Application for a Low-Level Radioactive Waste Disposal Facility, Safety Analysis Report (Rev 1) (NRC, 1988b)." This document serves two overall purposes: (1) to discuss the information that should be provided in the Safety Analysis Report (i.e., license application), and (2) to establish a uniform format for presenting the data and information. The NRC does not require applicants to follow this format; however, license review time could increase if the format is not followed.

Section 2.4.2 of NUREG-1199, specifically the paragraph on unsaturated zone characterization, describes information about the unsaturated zone to be included in the license application. Within the unsaturated zone the applicant is asked to identify the lateral extent and thickness of permeable and impermeable zones; any potential conduits of anomalously high flux, the spatial and stratigraphic distribution of total and effective porosity, and saturated hydraulic conductivity, the spatial and stratigraphic distribution of water retention and relative permeability relationships, hysteretic behavior during wetting and drying cycles (especially during extreme conditions), water content variations with time, and the direction and velocity of unsaturated flow.

Section 2.5 on Geotechnical Characteristics, and specifically the subsections on Groundwater Conditions and Borrow (Quarry) Materials, request that the applicant identify among other things (a) the hydraulic conductivity and infiltration characteristics of the site and quarry materials, and (b) the physical and engineering properties of quarry materials at the same range of density and moisture content as proposed for construction.

Section 2.7 on Natural Resources requests that known natural resources including geologic and water resources be identified. Geologic resources include industrial mineral deposits such as sand, gravel, clays, aggregate sources, shales, and building stone. If exploited, these natural resources must not result in either inadvertent intrusion into the disposal site or failure to meet the performance objectives of 10 CFR Part 61, Subpart C.

Section 5.1.2, which deals with the stability of engineered covers during site closure, requires the applicant to provide information on the settlement and infiltration monitoring program including the location, type, and typical installation details of the monitoring devices, and proposed methods for analyzing and evaluating the data.

Section 6.1 on the Release of Radioactivity calls for applicants to provide infiltration values based on data or analyses or both. Applicants are to provide estimates of hydrologic infiltration for three purposes: (1) as a key parameter for the design of covers that will minimize to the extent possible water infiltration, water percolation and surface run-on, (2) as input to long-term cover stability/maintenance forecasts, and (3) for the forecast of groundwater mass transport of radionuclides. Infiltration is to be given as a flux per annum, and the applicant is to give the time between deep percolation events and identify zones of potentially high percolation.

2.3 Guidance from NUREG-1200

To further support the Low-Level Waste Policy Act Amendments of 1987, the NRC issued NUREG-1200, "Standard Review Plan for the Review of a License Application for a Low-Level Radioactive Waste Disposal Facility, Safety Analysis Report (Rev 1) (NRC, 1988a)." This document establishes a uniform and impartial process for the review and evaluation of data and information provided in a license application. In Section 2.4.2 of this guidance on Groundwater Characterization, reviewers are instructed to view the unsaturated zone as a transport avenue for water and contamination to reach the groundwater aquifer. The reviewer expects to find under "Characterization of the Unsaturated Zone" the protocol for measurement and sampling, the rationale for selecting sample locations and frequency, the rationale for sampling methods and instruments, the procedures to be used for analysis of field and laboratory data, and a complete conceptual model of unsaturated zone flow and mass transport. Under "Numerical Analysis of the Unsaturated Zone" reviewers should find the rationale for use of particular codes or models, a description of input data and data reduction methods, and simulations of water infiltration rates and water movement. Results of the simulations should reveal the spatial and temporal distributions of deep percolation to the aquifer, quantify any anomalously high or low infiltration, and demonstrate the validity of the model(s) employed. Overall, reviewers are to determine whether the applicant's results are adequately conservative and defensible. This calls for a thorough review of both (1) the characterization protocols and rationale, and (2) the numerical analyses conducted and reported by the applicant.

In Section 6.1.2 on Infiltration in the Standard Review Plan (NRC, 1988a), reviewers are instructed to examine the applicant's characterization of the amount of water infiltrating through the cover system, i.e., the volume of water entering the disposal unit and the temporal and spatial distribution of infiltration. Estimates of infiltration are to be directly related to design-basis meteorological events. The license application should document data analysis and analytical techniques used by the applicant to estimate infiltration. The reviewers are to verify data on the physical character of cover, confirm values are adequately conservative or realistic, and assure manipulations of data are justified and defensible. Reviewers are also charged with reviewing the chosen numerical method, site-specific environmental factors (e.g., evapotranspiration), meteorological events (e.g., maximum precipitation, and temporal distribution of probable rainfall events), subsidence effects on flux of water, differences in infiltration between engineered covers and adjacent undisturbed material, and long-term predictions considering the effects of erosion, burrowing animals, and vegetation.

2.4 Summary

Certainly, all knowledge gained through the characterization and modeling efforts described above contributes substantially to the applicant's ability to describe the site, develop design standards for the performance of covers, assess infiltration into waste deposits and adjacent media, and forecast mass transport. Ultimately, the objective is a reasonable yet conservative assessment of radioactivity that may be released to individual transport pathways for each of five periods of concern: operation, closure, observation and surveillance, active institutional control, and passive institutional control.

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3 Flow and Transport Processes

3.1 Introduction

In 1982 the NRC sponsored a symposium on unsaturated flow and transport modeling (Arnold et al., 1982). The purpose of the symposium was to review the state of knowledge of flow and transport processes in the vadose zone and our ability to model them. These processes are key to understanding the vadose zone as a repository of wastes. It was stated at this symposium, and has since been reinforced in regulatory guidelines (10 CFR 61 Section 61.50) for LLW disposal, that analysis of potential releases of radionuclides from near-surface disposal units must consider the flow and transport in partially-saturated (vadose zone) media. While not relying solely on modeling to determine the suitability of a proposed or existing site, the NRC is requiring that modeling be used to calculate potential migration of radionuclides. What was apparent at this symposium was the relatively mature development of models and the lack of a comprehensive database for the study of flow and transport at the field scale in the vadose zone. Several participants expressed concern that modeling a site could provide a general scoping view of reality, but that data were needed to calibrate and validate the performance of the model for the site conditions.

Since 1982, several other NRC-sponsored workshops and meetings have been held to evaluate the status of our knowledge of the vadose zone. One notable example is the Ruidoso conference held in May of 1988 in Ruidoso, New Mexico (Wierenga and Bachelet, 1988). At this workshop, attended by more than 200 participants, national and international speakers presented papers on flow and transport studies in the vadose zone. While some progress had been made, it also was apparent that issues such as model validation and adequacy and completeness of data were still major topics of discussion and controversy. In addition, several papers presented at the Ruidoso meeting questioned our ability to adequately measure and hydraulically characterize the vadose zone. For example, papers were presented on observed preferential and unstable flow in the vadose zone. A paper by Glass et al. (1988) demonstrated that wetting front instabilities created by layered soil systems could invalidate the convective-dispersion equation. Papers by Kung (1988) and Hendrickx et al. (1988), and more recently Hendrickx and Dekker (1991) illustrate the problems of flow instabilities in the vadose zone under specialized cases of layered, sloping sandy soils and soils with hydrophobic surfaces. Differences in wettability and flow channeling (and funneling) can occur in some soils under certain conditions. Although these phenomena may complicate modeling of solute transport under field conditions, it should be noted that flow channeling and wettability problems have mostly been observed in areas with moderate to high rainfall or under irrigated conditions. These phenomena have not been clearly demonstrated under natural rainfall conditions in arid or semi-arid areas. There is, however, mounting evidence that flow in the unsaturated zone is often chaotic and transport processes ill-defined (Gee, 1991). For sites where such phenomenon have been observed, it would be prudent to modify computer codes to incorporate the flow instabilities and the two- and three-dimensional features needed to describe these phenomena. In the following text, we describe modeling approaches and issues that relate to assessment of transport in the vadose zone. We also provide some information on acceptable approaches to the validation of transport models. Such information will be needed by regulatory agencies when assessing site suitability and licensing at LLW sites.

3.2 Modeling Approaches

A number of approaches have been developed over the years to model transport of chemicals in soils. Sardin et al. (1991) provide an excellent review of models used for transport of linearly interacting solutes in soils. They identify a progression in modeling approaches, from the use of the classical one-dimensional convection-dispersion equation to the use of extended or two-region (mobile-immobile) transport models, and finally to the use of transfer function models. They show that transfer functions can be used to describe both equilibrium properties (e.g., distribution coefficients) and kinetic processes (e.g., convective transport, hydrodynamic dispersion, adsorption-desorption), and they demonstrate that many of the solute transport models used today are essentially identical. A general description of the factors affecting solute transport through soil is provided by Jury et al. (1991).

3.3 Convection-Dispersion Equation

The most common approach in describing solute transport through soils is through the convection-dispersion equation. This equation presents a mechanistic description of solute transport. It states that solutes move by convection, i.e., with the water, and by diffusion. In the absence of diffusion, water and the dissolved tracer move at the same rate, but not at the same rate everywhere. Fluid velocities in a porous medium vary because the fluid conducting pores differ in diameter, shape, and direction. Furthermore, fluid velocities inside a pore vary as a result of frictional forces. In the convection-dispersion approach, this mechanical variation in fluid velocities that actually occurs at a variety of scales results in a solute mixing process called mechanical dispersion (Bear, 1972). The overall effects of mechanical dispersion on solute transport through a porous medium resemble the effects of a large-scale molecular diffusion. Therefore, mechanical dispersion and molecular diffusion are often lumped together in a Fickian diffusion model where a single parameter, D, is used to describe both processes (van Genuchten and Wierenga, 1976).

The resulting equation describing fluid flow by convection, diffusion and dispersion is:

$$J_s = -\theta D \frac{\partial C}{\partial x} + qC \qquad (1)$$

where J_s is solute flux, expressed in units of mass (M), length (L), and time (T), (M/L^2T), θ is the water content per bulk volume (L^3/L^3), D the dispersion coefficient (L^2/T), C the solute concentration (M/L^3), x the distance (L), and q the flux of water (L/T). The coefficient D represents both mechanical dispersion and diffusion. Equation (1) may be combined with the equation of continuity to yield the transport equation for a noninteracting dissolved solute:

$$\frac{\partial \theta C}{\partial t} = \frac{\partial}{\partial x}\left(D\theta \frac{\partial C}{\partial x}\right) - \frac{\partial qC}{\partial x} \qquad (2)$$

Equation (2) is the convection-dispersion equation describing movement of a noninteracting chemical through a porous medium in one direction. For sorbing chemicals the equation is similar to (2), except that a parameter is added which describes the degree of interaction or sorption of the solute with the porous medium. If the sorption process is nearly instantaneous so that there is equilibrium between sorbed and solution concentrations, and the ratio of these two quantities is constant (e.g., independent of concentration), equation (2) becomes:

$$R\frac{\partial \theta C}{\partial t} = \frac{\partial}{\partial x}\left(D\theta \frac{\partial C}{\partial x}\right) - \frac{\partial qC}{\partial x} \qquad (3)$$

where R is the retardation factor. R is a function of the adsorption or distribution coefficient and is defined as:

$$R = 1 + \frac{\rho}{\theta}K_d \qquad (4)$$

where ρ is bulk density (M/L^3), and K_d is the distribution coefficient (L^3/M). If there is no adsorption, $R = 1$. Equation (3) shows that if convective flow is dominant (the second term on the right-hand side of equation (3), then the advance of the solute front will be proportional to 1/R times the velocity or flux.

Equations (2) and (3), or modifications thereof, have been used extensively to describe solute transport through soils and groundwater. In practice, numerical solutions are used because mathematical solutions of the differential equations (2) and (3) are not available for realistic field conditions. There are many such numerical models available in the public domain, as well as in the private domain. These models are used for prediction purposes for a wide variety of field problems. They are often the best tools available for making predictions. Unfortunately, few of these models have been adequately tested under field conditions.

3.4 Two-Region Model

In many soils, the convection-dispersion equation provides an inadequate description of solute movement. This may be caused by a variety of reasons, including inhomogeneous soil, the presence of immobile water, and the occurrence of preferential flow. For the convection-dispersion equation to be applicable it is generally assumed that the soil is homogeneous. This is rarely the case, except in carefully packed laboratory soil columns. Few field soils or aquifers are homogeneous with respect to solute transport properties. Even in carefully packed laboratory columns one sometimes encounters inhomogeneities. Furthermore, in unsaturated soils water may be present in dead-end pores, and inside or between aggregates where fluid flow is very slow to stagnant. In natural soil profiles, especially those with a history of biological activity (roots, worm holes) water may also flow through preferential flow paths during storm related drainage episodes; however, water may preferentially bypass these same large-diameter flow paths during more prevalent unsaturated flow periods.

The conditions under which inhomogeneities, immobile water, or preferential flow affect solute transport are not well understood. What is known is that these phenomena generally result in faster transport than would be predicted on the basis of the convection-dispersion equation and the total volume of water in the soil (Jury et al., 1991). Thus, one generally observes early arrival of the first solute front as a result of by-pass of stagnant water and preferential flow. In addition, with immobile water there will be transverse diffusion of solute into the immobile water while the solute is passing through. Once the solute in the mobile water has passed through, solute will diffuse out of the immobile water into the mainstream, resulting in much longer times for the solute to leach out of the soil column, i.e., a phenomenon known as "tailing" of solute elution curves.

In order to model solute transport in soils with early arrival and tailing, van Genuchten and Wierenga (1976) used a model first described by Coats and Smith (1964). In the model, soil water is divided into mobile water (θ_m) and immobile or stagnant water (θ_{im}). Solute transport is assumed to occur by convection-dispersion in the mobile region only, while transfer of solute between the two regions is by diffusion. The resulting equations for a noninteracting solute are:

$$\theta_m \frac{\partial C_m}{\partial t} + \theta_{im} \frac{\partial C_{im}}{\partial t} = \theta_m D \frac{\partial^2 C_m}{\partial x^2} - q_m \frac{\partial C_m}{\partial x} \qquad (5)$$

$$\theta_m \frac{\partial C_m}{\partial t} = \alpha (C_m - C_{im}) \qquad (6)$$

The subscripts "m" and "im" refer to mobile and immobile or stagnant water, respectively. q_m is the average flux in the mobile region and α is a mass transfer coefficient (with units of inverse time). Analytical and numerical solutions of equations (5) and (6) are available (van Genuchten and Wierenga 1976; de Smedt 1988).

Sardin et al. (1991) and Brusseau and Rao (1989 and 1990) have shown how extensions of equations (5) and (6) may be used to model transport of interacting contaminants, including those subject to decay or degradation through porous media.

3.5 Transfer Function Approach

Jury and Roth (1990) have provided a detailed treatise on the use of transfer functions to describe solute transport in soils. A summary of transfer function theory is also provided by Sardin et al. (1991). Transfer functions are based on the principles of linear system dynamics developed in the chemical engineering literature (e.g., Wen and Fan, 1975; Villermaux, 1987).

Conceptually, one can think of the soil as a reactor through which water flows (the flow may either be saturated or unsaturated). The flow can be thought of as moving convectively in a series of isolated stream tubes. While water flow in soil is generally transient (except at significant depths), one often assumes that the flow in the soil (reactor) is steady, and further, that there are no sources nor sinks within the tubes. If the tubes are of differing lengths and solute is injected into them at a constant rate, then a distribution at the exit point will reflect the range of travel paths for the solute. The net effect is a spreading of the solute input pulse or front.

A typical analysis for transport in soils is to run an experiment in the laboratory or the field, and observe the breakthrough curve of solute being transported through the soil. If the soil is relatively homogeneous then transfer function parameters likely will work well to predict the spreading of the solute front and its advance in the soil profile. However, if the soil is heterogeneous, containing large, conducting macropores, discontinuities, layers, etc., then there is little likelihood that the parameters used to describe the transport at one depth will be useful in predicting transport at other depths in the profile. These complications are serious drawbacks to present modeling and must be evaluated carefully. Jury and Roth (1990) have discussed some of these issues and recommend that tracer tests be conducted to evaluate the effects of the heterogeneities on the transport processes in the vadose zone.

3.6 Issues

A feature, unique to the vadose zone, that can affect transport is the anisotropy in hydraulic properties introduced by water content differences in soils. McCord et al. (1988 and 1991) demonstrate a so-called "state-dependent" anisotropy in a sand dune in New Mexico. Their data show that tracers moved laterally in areas where uniform rainfall was infiltrating into sloping but uniform sands. Water contents were initially nonuniform, as is typical in field soils. After several months of rainfall events, tracers were observed to move laterally, reflecting a distinct two-dimensional flow pattern that was strongly associated with the water content gradients that existed at the site. Modification of a two-dimensional model to incorporate the state-dependent anisotropy was reasonably successful in predicting the tracer plumes.

Work by Hills et al. (1991) at the Las Cruces Trench site also investigated water and solute transport into soil that had water contents that were highly variable. They observed that water contents and tracer movement were reasonably well predicted with a two-dimensional model without consideration to state dependent anisotropy. However, they did observe that bromide moved faster and deeper than the tritium and attributed this to anion exclusion of the bromide. It is likely that the differences between the observations of McCord et al. (1991) and those of Hills et al. (1991) lie in differences of soil types and water infiltration (application) rates, and possibly differences in sloping of soil layers.

Flow and transport parameters have been measured in detail for the Las Cruces Trench (Wierenga et al., 1989; Wierenga et al., 1991). These data are now being used by investigators throughout the world for model validation purposes. The unique features of these data are that they combine both flow and transport properties for water infiltration, redistribution, and drainage in an extended, carefully sampled set of tests. They are perhaps the most complete set of observations from one site that are available for vadose zone model testing and validation. It is unlikely that such a complete set of data will be available at a LLW site. It is expected that over the next several years, as model testing proceeds, researchers will be able to assess the performance of numerical models, from the simple to the complex, by testing them against the Las Cruces data and similar data sets. After these tests are completed we will have a better idea about the success of model validation for vadose zone transport and will be better able to say what level of detail will be required to adequately characterize and model a LLW site in terms of its key hydrologic parameters.

4 Site Technical Requirements: Characterization, Modeling and Validation

4.1 Introduction

Regulation requires pathway simulations and stability analyses that examine the future influence of active natural processes on the site and adjacent environs. It is a technical requirement of a site that it "be capable of being characterized, modeled, analyzed, and monitored" (10 CFR Part 61, paragraph 61.50). Certainly, how well one characterizes a site influences one's ability to model it. Conversely, how well one wishes to model the site influences the level of detail designed into site characterization efforts. Similarly, the level of confidence one wishes to have in the results of detection or monitoring system directly influences the spatial and temporal distribution of observations in the sampling plan for either type of activity. Thus, there exists an obvious relationship between site characterization or monitoring, and modeling or analysis at a waste disposal site.

4.2 Characterization Versus Modeling

While a relationship is obvious (i.e., between characterization and modeling), the relationship is not. Several unresolved issues influence our ability to either characterize or simulate water movement and contaminant transport in the natural environment with great confidence. One issue is the tremendous spatial variability that exists in most unconsolidated deposits that comprise unsaturated zones. Another issue is the temporal variability in the climate; i.e., the segment of the hydrologic cycle that both delivers water as precipitation to the land surface and removes it as evapotranspiration. This spatial and temporal variability, taken with the fact that models are used to extrapolate future events based on short-term present-day records, forces one to acknowledge considerable uncertainty in forecasts of water and contaminant movement. Because of the spatial variability observed in physical and hydraulic properties within most unconsolidated sediment deposits, interpretations of site characterization and monitoring data also must acknowledge significant levels of uncertainty. Methods of analysis are being developed that attempt to quantify this uncertainty and relate characterization requirements to confidence in model-based forecasts , however, initial efforts have focused on the somewhat easier problem of saturated zone or aquifer environments. Peck et al. (1988) provide an excellent summary of the state of the art regarding the accuracy of groundwater aquifer models and their dependence on field data.

For the unsaturated zone, the state of the art is in its infancy. At present, there is an uncertain relationship between the completeness of a characterization effort and the confidence one should have in simulations. However, research is currently addressing this issue in several ways. The overall validity of water flow and contaminant transport models is being studied by national and international programs, particularly those addressing the siting of radioactive waste repositories. The NRC, through research programs conducted at the Massachusetts Institute of Technology, New Mexico State University, the University of Arizona, and Pacific Northwest Laboratory has been at the forefront in developing methodologies to address this complex problem. Methods of quantifying uncertainty in two- and three-dimensional data sets of physical and hydraulic properties (Marsily, 1986), and of quantifying sensitivity and uncertainty in predictions of water movement and contaminant transport, (i.e., Monte Carlo and stochastic methods), have given rise to a probabilistic interpretation of the subsurface environment (Yeh et al., 1985a-c; Mantoglou and Gelhar, 1987a-c; Jury and Roth, 1990; Polmann et al., 1991; Luis, 1991). As in the case of groundwater aquifer analyses, the interdependence of field data resolution and model confidence can be quantified by merging these disciplines; however, initial attempts have revealed that small-scale variations in soil physical and hydraulic properties can have a profound influence on water movement within the unsaturated zone. Thus, the different scales of measurement and modeling of the unsaturated zone present new challenges.

4.3 Validation

In the past decade, a series of international programs have been undertaken to establish confidence in models of the geosphere, i.e., water flow and transport in the subsurface environment. These programs have led to an ongoing project, the INTRAVAL Project (SKi, 1990), which focuses on the validation of field-scale transport models for their use in siting radioactive waste repositories. While not yet completed, this program and those that preceded it have developed widely accepted definitions and an approach to site model validation. These definitions and the approach to model validation are relevant to the issue of characterization and modeling.

The International Atomic Energy Agency (IAEA, 1982) has defined validation as follows:

> "A conceptual model and the computer code derived from it are validated when it is confirmed that the conceptual model and the computer code provide a good representation of the actual processes occurring in the real system."

Definitions have been presented by others; however, all require that we confront three issues; identification of model performance measures and field observations of interest, determination of the necessary accuracy for useful predictions, and selection of the range of conditions anticipated for model application.

Validation is always imperfect, and in a very real sense, can never be achieved in absolute terms, because our knowledge of governing processes and the geologic setting is always incomplete. Though we continue to broaden our understanding through laboratory and field studies, it is widely acknowledged that validation is site-specific. The imperfect and site-specific aspects of validation make the assertion that a model is valid both subjective and relative to existing knowledge. That is, validation can only be perfect relative to what we now know. Whether it is appropriate to apply a validated site-specific model to an adjacent site will always be judged relative to the proximity of the two sites, their similar structure and process conceptualization, and the character of waste disposal practices proposed or applied at each site.

Validation requires that we distinguish between conceptualization of a site and modeling of that site. Conceptualization relies on our understanding of geologic structure, dominant processes, and boundary and initial conditions. Through the validation process, the review of structures and processes should yield insight into additional measurements needed to improve our confidence in a model. Modeling relies on an accurate conceptualization and uses governing equations, numerical methods, computer algorithms, and input data to produce simulations of possible future events.

Modeling of the subsurface environment for a field setting can be viewed as a six-step process (Tsang, 1987 and 1991). First, all available data are reviewed, analyzed, and evaluated. On the basis of this review, the conceptual model and potential scenarios of interest are developed for the site. With a knowledge of the site and the situation at hand, the third step is to adopt performance criteria or measures, and appropriate and realistic standards related to the key issues in the evaluation of alternate actions. Fourth, we adopt, adapt, or develop the needed calculational model and interpret available data to assign process model parameters. Next, modeling calculations are performed, and sensitivity and uncertainty analyses are completed. Finally, the results of modeling are evaluated for acceptability; i.e., we address the question of whether the results with associated uncertainty are satisfactory or unsatisfactory with respect to previously adopted performance criteria. Furthermore, if unsatisfactory, we need to decide future actions and the merit of further investment in either characterization or modeling of the site.

Each of the six steps in simulating a site should be validated to ensure that we achieve a good representation of actual processes occurring in the real system. In addition to the prediction-observation comparison, the validation process needs to include a statement of purpose, scope, and objective, the review and evaluation of all available data, and the conceptualization of the site leading to code selection and ultimately to the evaluation of modeling results. Only through evaluating and assuring the validity of each step in the modeling process can one be sure that a validated site-specific model has been created (Tsaug, 1991).

4.4 Scientific and Regulatory Application of Models

A review of the scientific and regulatory applications of groundwater models conducted by the National Research Council (Schwartz et al., 1990) revised the common and narrow definition of modeling to embrace a more holistic view of simulation. Modeling of the subsurface environment was redefined as "a cost-effective way of interpreting all available data, to the extent that the interpretation provided by that modeling effort enables one to be comfortable in making a decision." In this definition all data are either used or explained by our conceptual model of a site, and modeling based on the conceptual model confirms our conceptual model by providing an estimate of the integrated response of the environment. Simulations are required to truly understand the overall effects of complexities in site-specific geologic structure and dominant processes. Thus, data accumulated during characterization or monitoring efforts are related to modeling and analysis through the conceptual model of the site.

As in the case of the international radioactive waste repository programs, the conceptual model provides the linkage needed to view site-specific data and modeling in a single framework. Both characterization data and modeling seek to describe a spatially and temporally varying subsurface environment. Ultimately one wishes to compare the interpretation of field data to the simulation of the field setting. Both field data and simulations contain inherent uncertainty. Uncertainty in simulations can arise from a variety of sources including uncertainty in the field initial condition, the geologic setting, the dominant processes, and future driving forces.

Often, there are clear differences between scientific and regulatory applications of subsurface models. The scientist is most often interested in an ability to <u>accurately</u> describe the subsurface structures and processes such that model forecasts accurately describe future events. These events may even be the subject of confirmatory field experiments. It is often desirable that applications of models made to support regulatory decisions <u>conservatively</u> represent future events. Thus, model results supporting regulatory decisions are frequently biased toward a conservative or worst-case result. Models used to support regulatory decisions are available in a hierarchy of sophistication from simple to complex; the analyses becoming more sophisticated (e.g., incorporating greater dimensional and process complexity) to demonstrate that the environment can tolerate the alternate disposals being considered. Each level of increasing sophistication is believed to exhibit less conservatism while becoming more realistic. Thus the measure of accuracy may not directly apply to the evaluation of model versus observation. This is because a conservatively biased modeling result, and not an accurate result, is often the goal of each phase of the increasingly sophisticated modeling effort. However, the accuracy measure must apply indirectly, otherwise the degree of conservatism in the model can not be determined. Therefore, an assessment of the validity of a regulatory model may be a two-step process of first determining the accuracy of a realistic conceptual model and then determining the degree of conservatism found in the model.

4.5 Relationship Between Characterization and Modeling

Research on the issues of model validation and application have lead to a structure in which to view the merging of site characterization and modeling. Notable among the contributions have been the approaches by McLaughlin and Wood (1988a) and Freeze et al. (1990).

McLaughlin and Wood (1988a) focused on model accuracy measured in terms of prediction error (reference value versus model prediction) because it provided a readily defined measure of model performance, and because they were interested in the influence of modeling decisions on the mean and variance of this error. The authors observed that groundwater model accuracy depended on natural heterogeneity, data availability, model approximations, and methods used to estimate model inputs. They used a stochastic approach based on distributed parameter estimation theory to develop a description of the modeling process, and derived approximate expressions for the first and second moments of the model prediction error. These moments provided a convenient way of examining the interrelationships among sampling design, input estimation, and model performance. The distributed approach to accuracy evaluation also allows spatial variability and uncertainty to be represented in a way that does not depend on a particular simulation scheme.

Such an approach recognizes the dependence of practical modeling studies in field measurements. McLaughlin and Wood (1988a) asserted that the amount of field information needed is a function of "a number of related factors, including the heterogeneity of the actual groundwater system and the procedure used to discretize and estimate the model input." They described a conceptual framework (Figure 4.1) for model accuracy analysis that relates the reference system to the model through the intermediate steps of field sampling and model input estimation.

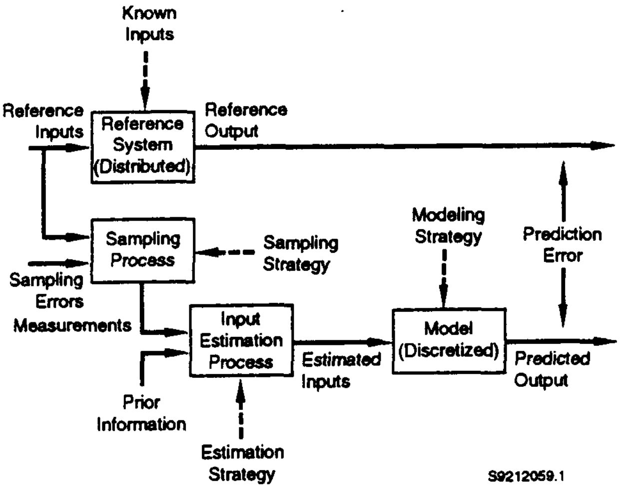

Figure 4.1 Conceptual framework for groundwater model accuracy analysis (Source: McLaughlin and Wood, 1988a)

McLaughlin and Wood (1988a) suggested that prediction errors arise from approximations introduced to compensate for imperfect knowledge of spatially variable physical processes. Acknowledging the computational cost of their approach, the authors believed the best way to address this computational limitation was "to focus on the factors that appear to have the greatest effect on prediction error (e.g., spatial variability, data limitations, model approximations) and to introduce simplifications where they will have minimal impact on the ultimate conclusions."

While their approach acknowledged the potential importance of structural and discretization errors, the authors chose to use an accuracy analysis of flow in a groundwater aquifer simplified by the omission of these terms to demonstrate the influence of spatial variability, sampling strategy, and suboptimal estimation on model prediction accuracy (McLaughlin and Wood, 1988b). While the authors' examples focused on flow fields and steady-state phenomena, they suggested approaches to both transient analyses of flow and groundwater transport.

Luis (1991) and Luis and McLaughlin (1992) presented a stochastic approach to validation of a model of moisture movement in an unsaturated porous medium. The authors distinguished between evaluations of model validation that use field data to determine whether or not model error is "significant," and of model accuracy that use probabilistic methods to project the magnitude of model error resulting from natural heterogeneity, data availability, model approximations, and methods used to estimate model inputs. They noted the following three sources of differences between model prediction and field observation: measurement error, spatial heterogeneity, and model error. These sources of error represent, respectively, the differences between measured and actual small-scale measurements, large-scale trend and actual small-scale measurements, and model predictions and actual large-scale trend. As their measure of validity, the authors adopted the objective of reproducing the ensemble mean of the water content distribution. Thus, once descriptions of soil heterogeneity and measurement error were established, the extent to which the model prediction matched the actual water content distribution would reveal model errors. This approach was illustrated by applying a two-dimensional deterministic model (Bouloutas, 1989) to one of the well-instrumented infiltration experiments conducted at a field site near Las Cruces, New Mexico (Wierenga et al., 1989; Hills and Wierenga, 1991).

In a series of papers that clearly portrayed groundwater modeling in the decision making process, Freeze et al. (1990 and 1992), Massman et al. (1987a,b, and 1991), and Sperling et al. (1992) described a method of decision analysis for engineered systems in which the hydrogeologic environment played a significant role. It was based on a risk-based philosophy of design, and combined three separate models; a decision model based on a risk-cost-benefit objective function, a simulation model for groundwater flow and transport, and an uncertainty model for both geological uncertainty and parameter uncertainty. Such an approach has direct applicability to assessments of the value of additional data in monitoring and characterization efforts. The general theory was presented by Freeze et al. (1990 and 1992) and applications to alternate groundwater remediations were presented by Massmann et al. (1991), Sperling et al. (1992), and Freeze et al. (1992). As shown in Figure 4.2, taken from Freeze et al. (1990), the decision framework acknowledged the need to assess geological (structural) uncertainty as well as parameter (process model) uncertainty as input to the hydrogeologic simulation. This method of decision analysis addresses the amount of characterization data needed to satisfy the modeling effort.

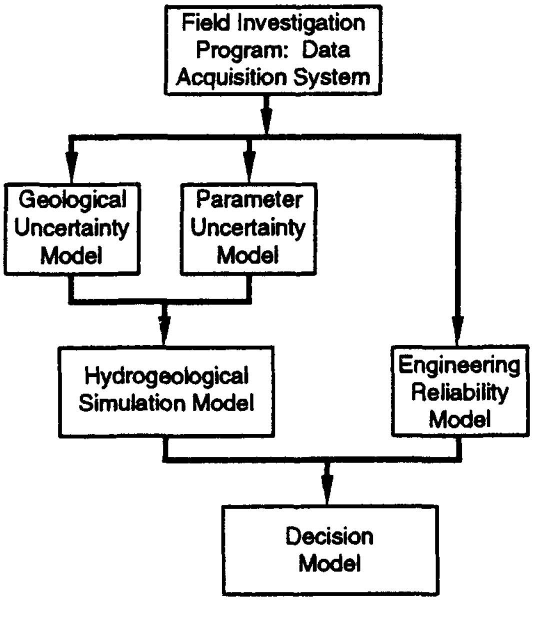

Figure 4.2 Framework for hydrogeological decision analysis (Source: Freeze et al., 1990)

In situations where one has neither the desire to sample exhaustively nor the resources to do so, the method of decision analysis presented by Freeze et al. (1990 and 1992), Massmann et al. (1991), and Sperling et al. (1992) could be used to determine the potential value of additional data collection efforts. For example, one might evaluate the benefit of additional data that are potentially able to discriminate between alternate conceptual models (geometric structure or physical/hydraulic processes) and the risk to site integrity and cost of obtaining field measurements or samples for laboratory analysis. Initial demonstration of this method of decision analysis used a groundwater aquifer model; however, simulation of the unsaturated zone also could use this decision methodology.

4.6 Summary

Clearly the regulatory requirement that a site be capable of being characterized and modeled raises the issue of the relationship between the two. Recent research on the unsaturated zone has focused primarily on model validation or model accuracy, but results also relate to the issue of the amount of site characterization data necessary to provide confidence in simulating the subsurface environment and future events. While a quantitative solution to this issue is not available at this time, researchers have begun to address the issue by first quantifying the uncertainty of site characterization data, and then quantifying the uncertainty in predictions of water flow and contaminant transport that result from uncertain input. In the past decade, geostatistical methods have enabled us to interpolate data to unsampled regions and determine both mean and variance. While no single modeling approach is widely accepted as economically or technically better than others, several methods have been developed and applied to translate the uncertainty in input data into its corresponding uncertainty in model predictions. Thus, the linkage is being developed to address the question of data requirements and model confidence. Currently, a qualitative understanding exists and approaches to linking characterization and modeling have been proposed.

In general a qualitative assessment of the capability to characterize and model a field site must determine whether or not the license applicant has demonstrated a knowledge of dominant structural features and physicochemical phenomena. These features and phenomena will have been revealed by characterization efforts and modeled to produce estimates of various quantities (e.g., infiltration and deep percolation rates, and long-term forecasts of groundwater contamination). The degree to which the modeling effort either uses or explains all of the field observations is the principal indicator of the capability to characterize and model. For example, in a karst hydrologic setting, anomalous flow paths may exist in the subsurface, and they will not be fully identified through characterization efforts. Thus, attempts to simulate the flow of water and migration of contamination are often unsuccessful.

Characterization and modeling efforts are often described as highly coupled and iterative. Knowledge gained through characterization leads directly to greater insight into the conceptual model of the site, and hence, to improved simulations. Similarly, insight gained through simulations, can lead to improved resolution of field data at critical points in space or moments in time. Successive iterations of characterization and modeling efforts ultimately will lead to closure of issues involving the conceptual model, and resolution of the characterization and modeling capability question.

During the site characterization period and over the 50-year (or longer) life of the operational monitoring system, substantial opportunities will exist to iterate between measurement and modeling, and to address any outstanding issue revealed during the license review process. Such an iterative approach to addressing issues is realistic and should lead to greater levels of public confidence in the safety of the disposal site. Taken together, the characterization and monitoring efforts will certainly reveal the dynamic behavior of the system, its dimensionality, any behavior associated with heterogeneous or anisotropic properties, and spatially and temporally varying boundary conditions. While during the license review it is essential to demonstrate a site is capable of being characterized, modeled, analyzed, and monitored, establishing and maintaining confidence in these capabilities will be a continuous and highly integrated activity during the life of the disposal site because of our increasing knowledge of the site and the certain evolution of modeling methods.

5 Site Characterization and Monitoring Strategy

5.1 Introduction

The purpose of this chapter is to discuss characterization and monitoring strategies for LLW disposal sites in arid areas. A number of reports have been prepared by the NRC staff on this matter, but these reports apply to issues of waste disposal across the United States. This report addresses issues that are more specific for arid areas.

Much of the information contained in this chapter can be found, in an expanded form, in the following documents:

> NUREG-0902 - Site Suitability, Selection and Characterization, Branch Technical Position (April, 1982).
>
> NUREG-1199 - Standard Format and Content Guide of a License Application for a Low-Level Radioactive Waste Disposal Facility (January, 1988).
>
> NUREG-1200 - Standard Review Plan for the Review of a License Application for a Low-Level Radioactive Waste Disposal Facility (January, 1988).
>
> NUREG-1300 - Environmental Monitoring of Low-Level Radioactive Waste Disposal Facility, Branch Technical Position (December, 1989).

NUREG-0902 discusses issues related to siting and characterizing a LLW disposal site according to regulations specified in 10 CFR Part 61. NUREG-1199 is intended to provide information and guidance to licensees and their contractors on how the license application is to be formatted for NRC staff review. Although not binding, NRC review may take considerably longer if the format differs from this guidance. NUREG-1200 is intended to provide guidance to NRC staff who are reviewing license applications for an LLW site. It specifies objective and consistent methods of analysis. NUREG-1199 and NUREG-1200 were developed in parallel by the NRC staff to streamline the license review process. NUREG-1388 is a branch technical position paper outlining staff opinions on the essential components of an acceptable environmental monitoring program that must be implemented for site characterization and be maintained throughout the life of the facility into the long-term care period.

This chapter describes site characterization strategies for unsaturated soils at low level waste disposal sites located in arid or semi-arid regions of the country. An example will be used to briefly illustrate the characterization strategy. This chapter will not cover strategies for investigating the saturated zone, the biota at the site, or the monitoring or characterization of engineered barriers that will likely be used to isolate waste. A brief discussion of environmental monitoring that is directly related to site characterization is included at the end of this chapter.

5.2 Site Characterization

Site characterization consists of determining those physical, chemical, and biological properties at a site that directly affect the movement of contaminants from LLW disposal sites. Such characterization is important because, according to regulations found in 10 CFR 61 Subpart 61.53, "the disposal site shall be capable of being characterized, modeled, analyzed and monitored." For this report we assume that the site is located in an arid region and that the groundwater table is relatively deep (e.g., >100 feet). We also assume that the site is not located in high recharge areas such as river beds and playas.

Before site characterization can take place, a site must be selected. Site selection is an important process, and is often affected by technical policy matters. Criteria often employed very early in the site selection are the availability of land; proximity to population centers; prevailing wind and other climatological factors that would strongly bias the outcome of any accident scenarios; proximity to highway, rail and air transportation; and proximity to especially sensitive resources (e.g., a sole-source aquifer), among others. It is prudent to select several candidate sites based on technical criteria, with the possibility of reducing the number of candidate sites to one, based on policy as well as technical criteria.

Large-scale reconnaissance of geographic areas should only be performed after technical criteria have been set with respect to rainfall, depth to groundwater table, elevation, etc. Once geographic areas have been selected, specific sites are chosen, which are further screened against minimum technical requirements listed in 10 CFR Part 61. Site selection may be greatly facilitated by using soil maps prepared by the U.S. Soil Conservation Service (SCS), and by consulting personnel from the SCS. Information on, for example, the depth to the groundwater table is often available from personnel of the SCS and the U.S. Geological Survey (USGS), or from local well drilling companies. Information on the physical properties of soils can be found in SCS soils reports; this information is generally of sufficient detail for initial site selection. Field work to characterize the soils is not envisioned at this stage, but is an important step of the final stages of site selection.

The majority of field activities and laboratory analyses will be performed during characterization of the final site. The goal of this characterization is two-fold: to demonstrate that the site can be characterized, modeled and monitored, and to demonstrate that the performance objectives can be met. The former requirement involves field and laboratory exercises, while the latter requirement mostly involves the subsequent analysis of data and modeling.

Field characterization can be done by in situ testing, or by collecting disturbed and undisturbed samples for analysis in the laboratory. In situ testing is generally preferred because results are directly applicable to the field site, with minimal errors caused by sample disturbance. However, in situ testing is practical only for a limited number of measurements. Furthermore, in situ testing is often very time consuming, especially in unsaturated soils where flow and transport occur at greatly reduced rates in comparison to saturated environs.

It is imperative in designing a characterization effort, to keep in mind the ultimate purpose for which the data and properties are going to be used; i.e., data analysis and subsequent computer modeling for the development of a license application. Full chemical and physical characterization is beneficial if the resulting data can be used for modeling purposes. If, however, no clear need exists for a particular analysis, such an analysis may be deleted in favor of more appropriate measurements. Characterization efforts should, therefore, be designed in cooperation with modelers so that sufficient data are collected for modeling of the site, while at the same time collection of unneeded data is minimized. Note that all data need not be directly associated with parameter identification; some can and should be confirmatory audits for the purpose of checking model results.

Field soils characterization efforts can be organized in the following broad categories: physical properties, chemical properties, flow properties, and transport properties. Physical properties generally considered for soil characterization in arid areas include bulk density, particle density, and particle size distribution. Chemical properties of interest are Ph, cation exchange capacity, total salt concentration of the soil solution, and chloride and sulfate concentrations. Flow properties are soil-water retention curves, saturated hydraulic conductivities, and unsaturated hydraulic conductivities as a function of water content. The main transport property of interest is the dispersivity (or coefficient of mechanical dispersion and diffusion). Details of the methods to be used for soil characterization are listed in the Appendixes. In addition, for a site to be modeled, initial and boundary conditions need to be known. These include the initial depth distributions of water content and soil-water potential in space (i.e., vertical profiles over a depth of interest or in a fully three-dimensional sense). Water flow is the main mechanism for contaminants to move from a disposal site. Thus, the amount of water deposited on the disposal site in the form of rain or snow needs to be well known, as well as the amount of water leaving the disposal site through evapotranspiration, overland flow, or drainage to the subsurface.

For both in situ characterization and for disturbed sampling, the number and location of samples need to be chosen so that spatial variability of the physical and chemical properties of the soils are well defined. However, to date, no definitive method has been presented that provides absolute numbers or locations of samples that need to be collected at a site before it is considered well characterized. This is because of the known potential for spatial variability in property values of heterogeneous soils in both horizontal and vertical directions, and the difficulty in setting forth specific sampling numbers for sites with different soil types. To account for this variability, a representative number of samples must be collected from each distinct lithologic or pedologic unit from ground surface to the depth of interest, e.g., the watertable. Continuous cores should be drilled for the first few boreholes in order to define the continuity, thickness, and inclinations of the major lithologic units. Once the general conceptual model of the subsurface system has been determined, more detailed sampling and in situ characterization can be initiated.

5.3 Las Cruces Trench Site

The Las Cruces Trench experiment (Wierenga et al., 1986, 1989, and 1991) is an example of a characterization effort for a study of water flow and contaminant transport in an arid region. The experiment was supported by the NRC and designed to test deterministic and stochastic models for unsaturated flow and transport in spatially variable soils. The field experiment was designed with input from experimentalists and computer modelers at Pacific Northwest Laboratory, the Massachusetts Institute of Technology, and New Mexico State University.

An experimental site was chosen near Las Cruces, New Mexico, where the annual precipitation is 23 cm/yr, and the Class A pan evaporation 239 cm/yr. The depth to the groundwater table at the site is approximately 100 m. A trench 26.5 m long, 4.8 m wide, and 6.0 m deep was constructed in undisturbed soil to provide horizontal access to experimental plots on both sides of the trench and to provide soil samples. A 4-m x 9-m area was selected on the south side of the trench and a 1.2-m x 12-m area on the north side for controlled application of water containing tracers. Initial exploration at the site had revealed the existence of nine distinct soil horizons between the soil surface and the 6-m depth. It was decided to take replicate samples from each soil horizon, in addition to three continuous cores from 0 to 6 m. To determine the spatial correlation of the soil physical properties, a total of 50 saturated conductivity measurements were made in each soil horizon. The measurements were made along a line transect and were spaced 0.5 m apart. Similarly, 50 core samples and 50 disturbed samples were taken in each horizon, and taken to the laboratory for analysis. To take these measurements and samples, a 1-m-wide strip of soil was removed with hand tools along the north trench wall down to the approximate center of each soil layer. Upon completion of the measurements and sampling, additional soil was removed with hand tools to the center of the next layer, and additional measurements were made. This process was repeated for all nine layers. A total of 594 disturbed and undisturbed soil cores were collected.

The in situ saturated conductivity measurements were made using the borehole permeameter method (Reynolds et al., 1983, and 1985). Bulk densities and water retention curves were determined in the laboratory using the cores. Unsaturated hydraulic conductivities were also determined in the laboratory. The disturbed samples were used to measure the initial distribution of the total salts and selected anions.

Water contents in the soil were measured with a neutron probe, which was lowered into the undisturbed soil through access tubes. Figure 5.1 shows the instrumentation at the trench site. Water contents were measured before water application to establish the initial conditions. Additional measurements were made during and after water application to monitor the advance of the wetting front in the soil and to monitor the redistribution of water. Before application of water, the wetted area, as well as the area around it, was covered with plastic to prevent evaporation and rain from leaving or entering the plot. Vegetation was removed to eliminate transpiration. Thus, the upper boundary was designed to be a no-flow boundary.

The soil matric potential or tension was measured with tensiometers. These were installed to a lateral distance of up to 6 m in a regular grid pattern through the trench face. Tension readings were obtained with a tensimeter, which is a handheld meter with a pressure transducer. The advance of the wetting front could therefore be monitored with either a neutron probe or the tensiometers. The initial soil matric potential distribution was measured on soil samples obtained during installation of the neutron probes. A thermocouple psychrometer was used for these measurements.

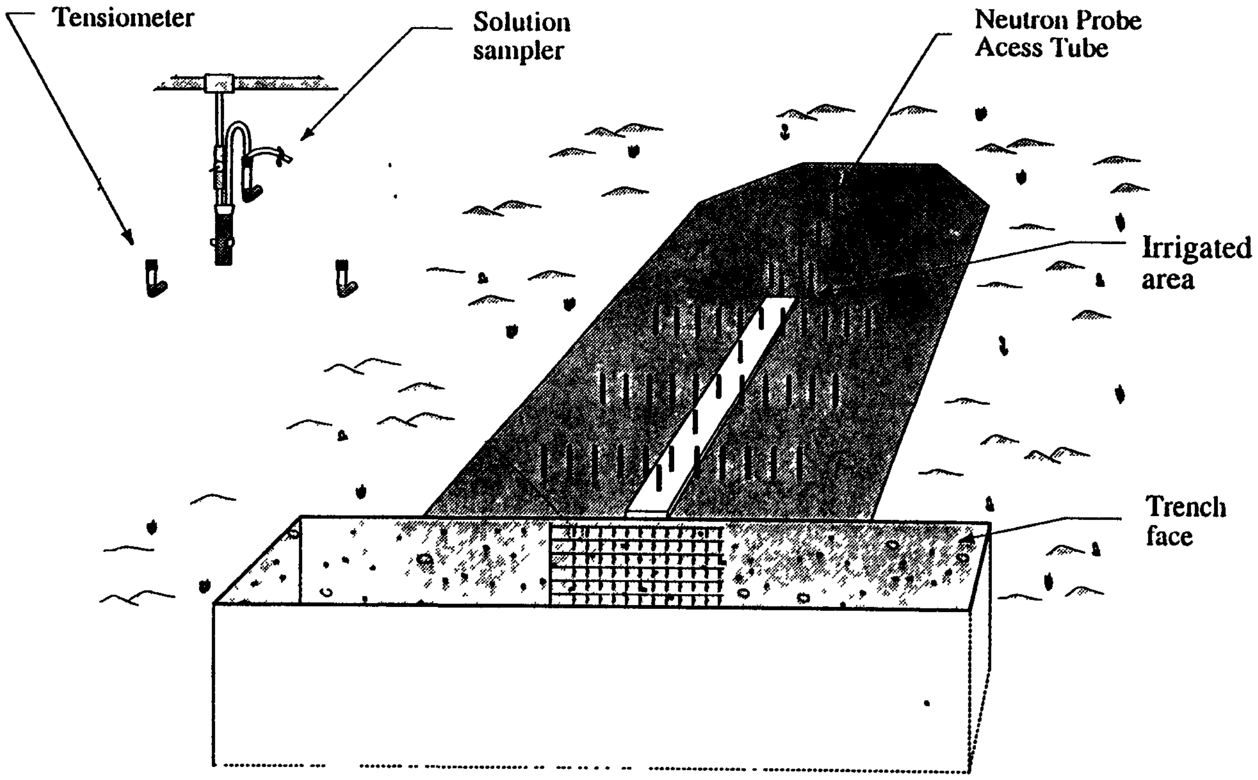

Figure 5.1 Three-dimensional diagram of instrumentation at the Las Cruces Trench Site, Jornada Experiment Station, New Mexico

Solute transport was monitored by withdrawing soil solution samples from the soil. The samples were withdrawn through samplers installed in a grid pattern through the trench wall. The samples were analyzed in the laboratory using standard procedures. Additional data on contaminant transport were obtained by taking core samples from the soil surface down to 6 m, using a manual sampler. The samples were taken to the laboratory for analysis.

The results of laboratory experiments using the soil cores show that the soil is highly heterogeneous with saturated hydraulic conductivities that vary by several orders of magnitude. Despite this variability, wetting fronts on the trench face showed a fairly symmetrical, nearly semicircular infiltration front during the first 34 days of infiltration, with no signs of preferential flow or fingering. The rate of advance of the water front determined with tensiometers was nearly the same as determined from neutron probe measurements, provided measurements were taken in close proximity. In contrast, the rate of advance of the traced water front (labeled with tritiated water) was only half the rate of advance of the wetting front, clearly showing displacement of all resident water by the infiltrating water, even though the initial soil matric potential was a low -40 to -60 bar (-4 to -6 MPa).

The data at the trench site were used in an initial modeling exercise (Wierenga et al., 1991; Hills et al., 1991). Modeling was also done by several other research groups using different approaches (Hills and Wierenga, 1991). This modeling effort is continuing. From these modeling efforts it is clear that among the most important parameters needed for modelling are the initial and boundary conditions and the soil hydraulic properties.

At the trench site, the initial water content distribution was well known through neutron probe measurements. This latter method resulted in detailed and high-quality data sets on water contents before, as well as during and after, the infiltration experiments. For example, the trench site is located in a semi-arid area where minimal changes are expected to occur in the subsoil water content unless a large rainfall event occurs. The neutron probe measurements in the subsoil were indeed very repetitive in that no changes were registered, unless a rain or infiltration event had taken place. At the same time the neutron probe measurements provided an excellent account of the water added to the plots and its distribution in the subsoil. Therefore the neutron probe method may be recommended for determining water contents in deep unsaturated soil profiles.

The initial water tensions were obtained from thermocouple psychrometer measurements. Disturbed soil samples were taken during installation of the neutron access tubes and taken to the laboratory for measurement of the water tension. This method, although somewhat laborious, proved useful for the rather dry soils at the trench site. The method is physically correct and does not require development of calibration curves. However, care has to be taken to not lose water during transportation from the field to the laboratory.

The saturated hydraulic conductivity was determined in the field using a borehole permeameter and in the laboratory with the steady flow method. There were large differences between measurements taken at the individual locations, but the means for each soil horizon and for all 594 measurements were within an order of magnitude (Wierenga et al., 1988). In practice the saturated conductivity is difficult to determine in the field and in the laboratory. Furthermore, its value is of limited interest because arid soils are almost never saturated except below the water table, or in flooded areas, and these sites probably would not be chosen for storage of wastes anyway. Because the main emphasis is on modeling unsaturated flow, it is preferable to determine the unsaturated hydraulic conductivity (though K_{sat} data are needed for most models). This may be done in the field with a tension infiltrometer (Ankeny et al., 1988), which measures the hydraulic conductivity values in the wet range (matric potential between 0 and -30 cm H_2O). However, the method is not readily adaptable to the subsoil unless access isprovided by means of excavation. The tension infiltrometer method is a relatively new approach which was not available at the time of excavation of the trench. Future characterization efforts should consider using the tension infiltrometer for determining the unsaturated conductivity.

The soil water retention properties were determined on soil cores taken to the laboratory. The steady-state method used was very time consuming, making it impractical to analyze a large number of cores. Transient methods are under development for rapid determination of the water-retention properties (Toorman, 1990; Toorman et al., 1992).

Careful control of the boundary conditions is important for model validation. For example, the surface of the soil at the trench was covered with 60-mil pond liner. The material was strong, did not deteriorate in the sun and provided a near zero flux condition at the soil surface. The weight of the material prevented it from blowing off the plot, thus the high cost of the surface cover was more than offset by its effectiveness and low maintenance.

Modeling solute transport requires knowledge of the dispersivity. Field studies on solute transport have shown that the dispersity of field soils generally lies between 1 and 10 cm (Gelhar et al., 1985). At the trench site a value of 5 cm was taken for the initial modeling (Hills et al., 1991). Verification of this value is under way by means of a detailed, well-controlled tracer study. However, in many instances it will not be possible to conduct a detailed tracer study. In these cases, values of dispersivity should be taken from the literature, and computer simulations made with a range of dispersivity values, to determine the sensitivity of model predictions to the chosen dispersivity value.

A major problem with field characterization is to determine how many samples or sample sites to choose. For example, a total of 594 samples were collected at the trench site and analyzed. The time and cost involved in taking and analyzing 594 samples for hydraulic characterization will often be prohibitive. It also may not be necessary. For example, despite the large spatial variability in soil hydraulic properties at the trench site, tensiometer readings, neutron probe measurements, and visual observations on the trench wall suggested that the wetting front moved in a fairly homogeneous fashion during infiltration (Wierenga et al., 1991). Furthermore, predictions using a model that accounted for the different hydraulic properties of each soil layer did not agree with field observations more than predictions with a simpler model in which hydraulic properties were averages over the soil profile. Thus, increasing the spatial resolution of field characterization for this experiment does not always improve model predictions.

The characterization effort at the Las Cruces Trench site was more intense than is generally expected for LLW disposal sites. Yet the experience gained at this site can be useful for designing characterization studies at other sites. For example, the sequence of events included an initial profile description, followed by a coherent sampling and analysis plan. Following the first round of detailed sampling it was determined that additional sampling and analysis needed to be performed on one of the layers. This additional detailed sampling gave a better understanding of small-scale variability at the site. Unfortunately, guidelines are presently missing as to how many samples are required for minimal, adequate, or optimal characterization.*

5.4 Environmental Monitoring

Environmental monitoring, as described by the NRC, is broken up into three distinct phases: pre-operational, operational, and post-operational. Only pre-operational monitoring, which occurs between the time of site selection until the beginning of site construction, is considered relevant to this report. Pre-operational monitoring must be capable of characterizing changes in water content and tension, so that the movement of soil water can be identified and quantified. Data must be collected throughout the year for a period of at least 12 months to define the annual cycle of seasonal variations of these properties. If it is found that seasonal variations are not well defined by the particular 1-year period studied, then additional monitoring will be needed. That is, if the year of the study is not typical (e.g., in terms of climate), then longer term monitoring of the season variations may be necessary.

At the Las Cruces site, a monitoring network was established for characterizing the changes in tension and water content at the trench site. The frequencies of data collection for the three experiments at the trench site were modified depending on the magnitude of change in the water contents and tensions. The changes in this case depended on whether water was being applied to the soil surface, or whether the experiment was in the redistribution phase. Solution samplers were continuously installed ahead of the wetting front to collect soil water for analysis of tracers, cations and anions. In this way, it was possible to plot the movement of the wetting front and the tracer fronts.

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*An insightful discussion on the issue of selection, use and requirements for hydrogeologic data in decision making for waste siting has been presented by Freeze et al. (1992). While the emphasis of the Freeze paper is on saturated flow and transport, the reader is referred to the Freeze discussion and concept on reduction of uncertainties and data worth analysis that may also have application to the unsaturated zone.

6 Data Management and Processing

6.1 Introduction

The characterization and monitoring of LLW sites produce large quantities of raw and processed data. These data originate from many sources and must be accessible to scientists with a variety of interests and backgrounds. The need to access data during site monitoring or for use in updating model calibration parameters will continue well beyond the tenure of those originally charged with characterizing and modeling a site. There is a great need to organize the data into an easily accessible, well-documented, quality-controlled database. The failure to provide sufficient resources to design and manage the database will decrease the usefulness of the data to the end-users, increase the probability that useful data will be lost or misinterpreted, and will lead to a lowering in confidence in the quality of the data by the end-user and the scientific community.

In this chapter, we focus on the organization of site characterization and monitoring data into a digital database. We provide some suggestions as to how the data should be acquired and processed, the use of visualization for quality control, and the organization and management of the data into a functional database. An example of a database designed for model validation is provided in Appendix C.

6.2 Raw Data

Raw data come in many forms. Raw data may be sketches in a workbook, hand recorded measurements on a worksheet, or digitally recorded measurements stored on magnetic media. The data can be static or dynamic in nature. Examples of static data are data obtained from characterization experiments. Once the characterization experiments are complete, the data can be processed and distributed to the end users. In general, the processing of such data does not continue throughout the lifetime of the site. However, experience has shown that even these data may be reexamined in the future; especially if the instruments used to collect raw data are found to be biased in some way, or if the interpretation of what one has measured changes. In contrast, data that are monitored as a function of time is dynamic data. Examples include the continued monitoring of water content and water quality or toxic concentrations. These data must be processed and made accessible to the end-users on a continuous basis.

High-quality, well-documented raw data are the foundation of a successful program. Collecting raw data is usually the most expensive and time-consuming aspect of a data acquisition program because of the costs associated with instruments and labor related to the experimental procedures required to produce the data. Because of the extensive effort expended on data collection, there is often a tendency not to fully document details of the experimental procedures, thus making post-mortem analysis of unusual trends difficult if not impossible. In addition, much of the raw data, such as the *measurement of initial conditions*, cannot be reacquired after the site is operational, leaving all subsequent analysis highly dependent on original interpretations and therefore vulnerable whenever details of experimental procedures are omitted. Information and factors that improve the quality of raw data include the following:

- The goals of the site characterization and monitoring program must be carefully defined, well documented, and supported by *a priori* scientific analysis that includes numerical simulation. This analysis can help define the types of data to acquire, such as initial conditions and boundary conditions, the location and density of the data sampling grids, and the sampling rates for the acquisition of dynamic data. The installation of sampling grids without the numerical simulation of the corresponding dynamic variables will likely lead to an excessive number of sample locations outside the region of influence and sample grids that are too sparse within the region of influence. This can lead to ambiguous results.

- The experimental techniques must also be well defined, well documented, and accepted by the scientific community as appropriate for the task at hand. If new measurement techniques are to be used, these techniques should be backed up by duplicate measurements using conventional techniques at appropriate spatial and/or temporal scales until new techniques are confirmed.

- Personnel performing the experiments must be experienced with the experimental techniques and procedures so that anticipated problems can be avoided and unanticipated problems can be handled in an effective, logical, and timely fashion.

- The acquisition of the raw data must be designed with human imperfection in mind. The process should be automated as much as possible without introducing undue complication. There should be immediate feedback between data acquisition and processing and the experimentalist, especially for the monitoring of dynamic processes. Several levels of quality control should be built into the data acquisition procedures.

The raw data should be digitized as soon as they are acquired. If the data are generated by instrumentation using dense measurement grids, then the raw data should be acquired in digital form through the appropriate use of data acquisition systems and immediately placed in the database. If the data are obtained and processed by hand, the data should be processed immediately and transferred into the digital database. The immediate digitization of the raw data into computerized databases has several advantages:

- The raw data are stored in a central location. This greatly simplifies the access of data by the data manager and, more importantly, by other parties.

- The storage of the raw data in a database allows much of the data processing to be accomplished automatically. This unambiguously defines the actual analysis used for data processing since the formulas used are programmed into the database. In addition, as changes are made to the processing formulas (e.g., changes in calibration constants), the raw data can easily be reprocessed.

- One of the more important advantages of the immediate entry of raw data into the digital form is that the data can be visualized using computer graphics. The data can be visualized in either their raw or processed form. For example, the plotting of breakthrough curves of solute concentrations can be automated using all available data up to the last day the raw data were entered. This greatly enhances the ability of the experimentalist and the database manager to detect problems with the instrumentation, chemical analysis, and data acquisition procedures, and allows these problems to be corrected during experimentation.

Once the raw data are placed in the database and quality assured, they should be made readily accessible to the appropriate scientists and engineers. If only a small group of personnel needs access to the data, then they may be able to access the database directly after the appropriate training. If a larger group of scientists and engineers who are not familiar with the database software must access the data, then it may be more appropriate for the database manager to simply post ASCII files of the data in a protected directory on a computer accessible through computer networks. Most database software allows ASCII files to be easily generated. The use of ASCII files allows the end users to copy only the data they need and to import this data into spreadsheets or databases on their own computer systems.

6.3 Processes Data

Some raw data must be processed before they are useful. Much of the raw data that must be processed can be processed directly in the database. For example, the conversion of neutron probe counts to volumetric water contents can be done through simple calibration formulas. In contrast, the estimation of water retention model parameters from laboratory data involves nonlinear curve fitting, which is usually not possible using standard database software. In this case, the raw data are exported to an appropriate computer software package, the parameters are estimated, and the results imported back into the database.

Processed data can also be static or dynamic. For example, the estimation of the water retention parameters can be done during site characterization with no additional data processing required once site characterization is complete. In contrast, water contents are typically monitored over many years. This requires continuous data processing.

As was the case for its acquisition, the processing of raw data must be done with human imperfection in mind. The processing should be automated as much as possible without introducing undue complication. There should be immediate feedback between the processed data and the experimentalist, especially for the monitoring of dynamic processes. Several levels of quality control should be built into the processing procedures. These include the following:

1. Data processing techniques must be fully documented in reports readily available to the end users. The documentation should be a high-priority item so that the exact procedures used are known to the end users as soon as they have access to the processed data.

2. Computer visualization of the processed data should be built into the data processing system. This greatly enhances the experimentalist's ability to access the quality of the data and to take immediate corrective action.

3. The processed data should be made available immediately to the end users in digital format. The users often see inconsistencies in the data that are not apparent to the experimentalist.

Items 2 and 3 illustrate the importance of including the processed data in the database in a timely fashion. The structure of the data (both raw and processed) in the database should be such that the additional processing can take place as unexpected trends in the data become apparent. Because much of the additional processing will be performed by the end users, the structure of the database must be designed and well documented to simplify access by the end user.

6.4 Databases and Database Management

To design databases with the end user in mind, the database designer must either be familiar with the needs of the end users, or the end user must participate in the early phases of the database design. Databases and database users associated with vadose and saturated zone characterization and LLW site monitoring have several unique characteristics that affect the design of the database. These include the following:

- The typical producers and end users of the data will wish to perform data analysis in addition to that already performed in the database using their own software and computers. This requires that the data be accessible to the end users in a digital form that is compatible with their software. Because most software can import ASCII text files, the database should be capable of exporting data in this format.

- The variety of data associated with site characterization and monitoring is not large and the experimentalist producing the data can organize it into digital format (i.e., ASCII files) before importing it into the database. As a result, most of the data can typically flow into the database through a single control point (i.e., the database manager). In contrast, data flowing into corporate databases go through many channels, which complicates security and requires more expensive database systems.

- All of the data can easily reside on a single small computer system. This greatly simplifies updating, distribution, security, and backup procedures.

Because the database is small and easily manageable, responsibility for its control and maintenance should lie with a single person. This database manager should work with the experimentalist(s) to transform the raw data into appropriate digital form. The manager should document the types of data in the database and serve as a point of contact to the end users. The manager should be experienced with soil and hydrology data so that he or she can provide feedback to the experimentalists and to the end users on the type and quality of the data available.

Databases should be developed using well accepted commercial software. This software has the advantages that it is readily available, is written by professionals familiar with the security needs of entering and storing data, is dependable, and is well documented. The commercial software should provide easy import and export of ASCII files. The database should be relational in nature in the sense that data from different sources in the database can be merged into single files for output. Because it is impossible to anticipate all uses of the data, the database software should allow the manager to easily restructure the data. Generally, the learning curve for database software designed for use on personal computers is much shorter than for software designed for large computer systems. While not as feature laden (nor as expensive), personal computer software is generally easier to use, easier to modify, and generally adequate for the database needs discussed here. An example of a database designed to provide data for the model validation of water flow and solute transport in the vadose zone is provided in Appendix C.

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Appendix A

Laboratory Techniques

Contents

Figures

1 Laboratory Soil Solution Sampling

1.1 Introduction

Characterization of the soil solution chemistry is an important aspect of the license application for low-level waste. The levels of dissolved constituents in the soil solution will be reported in the license application and used, in part, to determine whether site activities have caused any changes to the soil chemistry. Assessing the changes in soil solution after site construction requires that the background and baseline levels of dissolved constituents be known. These levels can be determined from soil solution collected in-situ, as described in Section 2 of Appendix B, or from soil solution collected from soil transported to the laboratory.

Removal of soil samples from the site with subsequent extraction of pore fluids in the laboratory is a standard method for determining solution chemistry. This method has a number of advantages over in-situ extraction of soil solution. They include (1) the soil solution is extracted in a laboratory, where environmental conditions and decontamination of equipment are better controlled, (2) the physical and hydraulic properties of the soil can be measured on the same soil sample from which the solution was extracted, and (3) the solution was extracted from a known volume of soil. A major disadvantage of this method is that the soil sample is removed from the ground, precluding an on-going monitoring program with the same soil. Another disadvantage is that the soil solution may be exposed to different environmental (e.g., temperature, pressure), conditions during transport to the laboratory.

This chapter will describe various methods of sampling soil solution in the laboratory. It will include procedures for preparing extracts from soil and water, soil solution sampling from soil cores, and collection of samples in fraction collectors for retardation studies.

1.2 Principles

1.2.1 Preparation of Extracts from Bulk Soil Samples

Preparation of extracts are useful for determining soil solution chemistry of disturbed soil samples. It can provide a more unbiased assessment of the solution chemistry than removal of the soil water from a soil sample. However, because recovery of sufficient volumes of water for analysis will not be possible unless the soil is saturated or near-saturated at the time of field sampling, it will almost always be necessary to add distilled deionized water to the soil prior to extraction. Then, after the soil water comes to equilibrium with the soil material, it can be extracted. Extracting water from the soil matrix too quickly can hasten the equilibration of the solution with atmospheric CO_2, thus changing the pH and EC of the soil solution (Artiola, 1989). So it is necessary to allow the water and soil mixture to equilibiate before extraction. This point will be discussed later.

1.2.2 Solution Sampling from Soil Cores

Soil solution sampling from either disturbed or undisturbed soils often is performed while other experiments are being conducted. Saturated hydraulic conductivity and retention function experiments both afford the user opportunity to collect discrete solution samples while the sometimes long experiments are underway. It can be advantageous to attempt this type of sampling because the results can indicate how the solution chemistry evolves over time, and whether the evolution affects the property being determined from the primary experiment. Also, the use of an undisturbed soil sample ensures that the soil structure, along with any exposed mineral surfaces, remains intact, thus providing a more accurate assessment of soil solution chemistry within the soil profile.

Collection of soil solution during these experiments is relatively easy. Volumetric flasks often are attached to or placed beneath the bottom of the soil core to capture water already contained in the soil sample. For example, flasks can be connected to the base of soil columns via flexible hoses during a retention function experiment. Or, a flask can be placed beneath the core during saturated hydraulic conductivity experiments to contain water draining from the soil. The constituent concentrations in the solution samples collected in this manner represent average values for the volumes collected. This averaging process may increase the difficulty of determining subtle changes in solution chemistry, particularly when the soil sample is small relative to the solution sample. It is generally desirable to obtain solution samples that are a fraction of a pore volume (i.e., the amount of fluid retained in the sample or column at the test water content). This procedure is discussed in the next section.

1.2.3 Solution Sampling Using a Fraction Collector

A method to overcome the effects of averaging due to large solution sample volumes is the use of a fraction collector during extraction. Fraction collectors are critical instruments during column transport studies, because the user is able to collect solution samples in the milliliter volume range, for a time interval at his/her choosing. van Genuchten and Wierenga (1986) describe a method of collecting soil solution for transport studies in soil cores.

The principle behind this type of sampling is similar to the collection from core samples. The difference is that the user collects a larger number of samples containing smaller volumes, then plots the concentration of the target constituent against either time or pore volume. From this data, dispersion coefficients and retardation factors (in Sections 5.1 and 5.2, respectively) can be calculated.

1.3 Methods

1.3.1 Preparation of Extracts from Bulk Soil Samples

1.3.1.1 Introduction

The procedure for preparing extracts samples from bulk soil samples varies slightly depending on the constituent being analyzed. In all cases, however, extracts are prepared by adding deionized distilled water to a mass of soil, either air-dried or over-dried. Because the amount of water added to the soil affects the level of dissolved constituents found in the extract, it is important that the user record the amounts of soil and water used for the experiment.

Five varieties of extract samples include saturated paste and soil to water mixes, 1:1, 1:2, 1:5, and 1:10. The saturated paste is prepared by adding enough water to create a saturated mixture that glistens in light and has no cohesion. The amount of water needed to make this paste depends on the initial water content, the texture, mineralogy and organic content of the soil. The 1:1 soil to water mix is created by adding equal amounts, by mass, of soil and water. The 1:2 mix is created by adding 1 part soil to 2 parts water, by mass, and so on for the other mixes.

As mentioned above, the amount of water added to the soil affects the concentration of dissolved constituents. For example, it was found[1] that the cation exchange capacity (CEC) increased by 50% for saturated paste samples versus extracts collected from 1:1 mixes. Levels of calcium, magnesium, and other cations also were dependent on the amount of water added to the soil. In theory, the soil solution samples for the saturated paste became saturated with respect to these cations before all the cations dissolved. As the amount of water was increased, the concentration of dissolved constituents increased, until a point when dilution reduced the concentration. This example shows that (1) both the mass of soil and the mass of water must be recorded, and (2) it may be necessary to run several samples of different mixes to ensure that the total amount of dissolvable constituents is removed from the soil without losing accuracy due to dilution effects. When the total mass of the target constituent in the solution sample becomes constant with increased ratio of soil to water in the mix, the proper fixed ratio is found for that constituent in that soil sample.

1.3.1.2 Equipment

(1) Cups, with air tight lids, for storing the soil sample
(2) Stainless steel mixing spatulas or spoons
(3) Buchner funnel
(4) Filter paper, Whatman No. 42, or equivalent
(5) Container for collecting and storing the solution
(6) Source of vacuum (if necessary), and
(7) Other miscellaneous laboratory items.

1.3.1.3 Procedures

The procedures for preparing extract samples are listed in Artiola (1989), and summarized here for convenience.

Saturated Paste Extracts

(1) Weigh about 50-100 g of air or oven-dry soil into a soil paste cup. A lesser mass of soil may be used if the total soil sample is small (e.g., the sample came from an open faced ship auger).

(2) Add small increments of deionized (DI) water to the soil and mix with a spatula until the condition of saturation is reached. Saturation will be evident when the surface of the soil glistens and flows slightly when the container is tipped, and when the soil mass slides freely off the surface of the spatula. Soils with high clay content will not flow cleanly.

(3) After mixing, the soil sample should be covered and allowed to stand for at least one hour, but preferably for four hours. Check the sample and add more water if the glistening is gone. If free water is present, add a small amount of dry soil, mix again, and allow to stand.

(4) Place the soil sample into a Buchner funnel fitted (pre-wetted) with a Whatman No. 42 filter paper (or equivalent). Connect the funnel to a vacuum manifold.

(5) Pass a vacuum through the Buchner funnel, and collect the extract in a suitable sample container until air passes through the filter paper. Remove the sample container, preserve, and store as necessary. Sample preservation, storage and holding periods are available in Standard Methods manual (Greensberg et al., 1985).

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[1] Ali. M. (1991), Unpublished data and personal communication, Department of Soil and Water Science; Soil, Water, and Plant Analysis Laboratory, University of Arizona, Tucson, Arizona.

(6) The water content of the soil can be determined by scraping the soil off the filter paper, weighing it, placing the soil in an oven at 105 C for 24 hours, and weighing again. Remember to tare the container used to dry the soil in the oven. The formula for determining gravimetric water content is as follows:

$$\theta_g = \frac{(\text{weight of wet soil})}{(\text{weight of dry soil})} - 1 \qquad (1)$$

Fixed Ratio Soil/Water Extracts

Fixed ratio extracts are recommended for soils that deviate significantly from a loam texture (Artiola, 1989). The procedure for preparing the extracts are very similar to the saturated paste extract procedure described above. The major differences are noted below:

(1) The amount of water added to the soil is fixed, hence the name, regardless of whether more water is added to the soil than in the saturated paste extract. The air-dry mass of soil in the sample must be known prior to adding any deionized distilled water.

(2) The sample container should be mixed thoroughly, and if extraction through the filter paper is to be achieved via gravity, the flask should be shaken for 30 minutes. The soil water mix is then allowed to stand for four hours to equilibrate.

(3) The soil water mix is transferred to a Buchner funnel, fitted (pre-wetted) with a Whatman No. 42 filter paper (or equivalent), and allowed to drain via gravity. If gravity draining is slowed because of clay in the sample, the funnel can be connected to a vacuum system and pulled through the filter paper.

(4) Sample collection, preservation, and storage are the same as above.

(5) Different soil/water mixes, with replicates, are highly recommended, as the level of dissolved constituents can vary from one sample to the next.

1.3.2 Solution Sampling from Soil Cores

1.3.2.1 Introduction

Sampling of soil solution from cores, either disturbed or undisturbed, requires a method of soil collection different from bulk soil sampling. In all cases, the soil is contained in a sample ring, usually between 5 and 7.5 cm in diameter. The soil ring containing the soil is placed in either a pressure cell or Buchner funnel. The sample is then saturated slowly to remove air in the soil (the method of saturating soil cores is described in Section 4.4, Laboratory Saturated Hydraulic Conductivity). As the hydraulic conductivity or retention function experiments are underway, the water can be collected for analysis. Field Soil Sampling (Appendix B, Section 1) describes methods of collecting undisturbed soil samples.

1.3.2.2 Equipment

Equipment and material needed to collect water samples are the same as those listed in the Section entitled Laboratory Saturated Hydraulic Conductivity.

1.3.2.3 Procedure

The procedure for collecting samples during conductivity or retention function experiments is relatively simple. To collect samples during the conductivity experiments, a volumetric flask or graduated cylinder can be placed beneath the outflow port of the soil core. During the experiment, the user measures the amount of water collected within a specified time period, and analyzes the extract. Evolution of the soil chemistry can be understood by collecting a sample for each pore volume which passes through the core. For a saturated soil column, pore volume, which is simply the total volume of pores contained in a sample, is calculated by the following formula:

$$PV = V_T\left(1 - \frac{\rho_b}{\rho_m}\right) \tag{2}$$

where

ρ_b = bulk density of soil (M/L^3) (M = mass; L = length)
ρ_m = mineral density (M/L^3; usually $2.65 g/cm^3$) (Koorevar et al., 1983).
V_T = total soil volume (L^3)

Thus, the user should monitor the outflow flask, and collect a sample for each pore volume of solution passes through the sample, until the outflow rate reaches a steady state.

During retention function experiments, when the user is attempting to derive the water tension/water content relationship, samples can be collected in sidearm flasks. A stopcock installed on the vacuum or pressure line should be closed between steps so that the sample doesn't depressurize. The outflow flask can then be switched, and the volume of sample measured, preserved and stored.

1.3.3 Solution Sampling Using a Fraction Collector

1.3.3.1 Introduction

A disadvantage of the two aforementioned methods is that the soil chemistry is averaged for a large soil solution sample. Time-dependent sampling can not be readily achieved. However, by using a fraction collector, the user is able to collect small discrete samples which correspond to a particular time interval of the experiment, then plot constituent concentration versus time (or relative pore volume of effluent). This method of soil solution sampling is especially useful when performing transport studies on soils. Transport studies involve the addition of water to the soil during the experiment, where the water is tagged using a tracer exotic to the soil solution. As the water with tracer migrates through the sample, it disperses, with some tracer moving faster than the water and some moving slower. By collecting small fractions of water during the experiment, it is possible to note the increase in tracer concentration. The time necessary for the tracer to migrate through the sample, such that the relative concentration is 0.5 (i.e., the concentration of the tracer in the extract is exactly one half of the concentration of the tracer in the inflow water), is a parameter through which the retardation factor and dispersion coefficient are determined. The complete experiment, and the calculations of retardation factor and dispersion coefficient are described in van Genuchten and Wierenga (1986). The Sections entitled Dispersion Coefficient and Laboratory Retardation Factor, respectively, also discuss when this method of solution sampling is useful.

Soils used for this method are almost always contained in cores, and can be either disturbed or undisturbed.

1.3.3.2 Equipment

Equipment and material necessary to complete this sampling are listed on page 117 of Laboratory Dispersion Coefficient.

1.3.3.3 Procedure

The procedure for collecting soil solution samples is fully described by van Genuchten and Wierenga (1986). The interested reader should consult this reference.

1.3.4 Quality Assurance/Quality Control

The interpretation of saturation when saturated paste extracts are being prepared is susceptible to error. Because each person may interpret when a sample glistens, or when the sample slides easily from a spatula, the amount of water added to the sample will vary. It is therefore important that the same person prepare the extract samples during the project. One way to avoid this problem would be to concentrate on preparing fixed ratio extracts, where this subjectivity is eliminated.

As mentioned in Appendix B, Section 1, Field Soil Solution Sampling, maintaining a proper quality assurance/quality control (QA/QC) program is critical when regulators and the public review data and information in the license application. A laboratory QA/QC program should strive to maintain the highest level of accuracy in the methods of solution sampling, so that cross-contamination of samples is avoided.

The QA/QC program should include provisions such that the date, time and person collecting the sample are recorded into a log book. The method of sample preparation, amounts of water and soil used in extract samples, time of equilibration, and other salient aspects of the extraction procedure must be recorded and checked for accuracy.

Sample tracking protocol should be enforced so that proper preservation, storage, and chain-of-custody can be confirmed from the time of sampling through analysis. Nuclear Regulatory Commission (NRC) staff have published two documents related to QA/QC, NUREG-1293 (U.S. NRC, 1989) and Regulatory Guide 4.15 (U.S. NRC, 1979). In addition, it may be helpful to consult two U.S. Environmental Protection Agency (EPA) reports that each region uses to develop their individual QA/QC programs for the CERCLA program (EPA, az, 1987b).

2 Physical Properties

2.1 Bulk Density

2.1.1 Introduction

Bulk density is the ratio of the mass of the dry solids to the bulk volume of the soil. The mass is determined gravimetrically after the sample has been oven-dried. The bulk volume is that of the sample taken in the field, and it includes the volumes of the solid material and the pores. Total bulk density can be broken into three phases: solid, liquid, and gas.

Bulk density is an important physical parameter because, with it, one can convert mass-based water content to volume-based water content and calculate porosity and void ratio given a particle density. Smaller soil samples usually are collected in cores 5 to 7 cm in length and diameter. Results are then applied to larger areas for site characterization. The weight or volume of large soil masses can also be estimated when conventional methods are infeasible. This technique is not usually recommended for site characterization activities, because more accurate assessments are needed.

Bulk density is expressed in terms of M/L^3, or kg/m^3 in the SI unit of measure. Often, and sometimes more conveniently, it is expressed as g/cm^3. This allows the conversion of values from, for example, 2650 kg/m^3 to 2.65 g/cm^3.

2.1.2 Principles

Bulk density is usually expressed along with the water content because, in some swelling soils, the density changes in response to additions of water. For these soils, it is usually best to weigh the sample at the time of sampling to establish the water content. Methods for determining bulk density vary depending on whether the sample volume is known at the time of collection. Three methods will be discussed herein. The "core method" uses a short sampling tube of known volume. The "clod method" and the "excavation method" involve the collection of sample volumes with an unknown volume. Volumes are determined after the sample is returned to the laboratory. The final method to be discussed is called the "rubber-balloon" method. In this method, the user determines the volume of a small excavation by measuring the amount of water needed to fill the excavation, after placing a flexible plastic liner in the excavation. The volume of water needed to fill the void is the volume of the sample. Gamma attenuation is also used for determining bulk density. It is based on the principle that attenuation of a monoenergetic energy source is dependent on the water content and the density of the material. An equation is available (Gardner, 1986) that relates these variables to the ratio of the returning gamma flux to the incident gamma flux. If the water content is constant in the core, then changes to this ratio are due to changes in density. This method is accurate, but calibration and use of the instrument is difficult, so it won't be discussed further.

The core and rubber-balloon methods are used more commonly in the field; the clod method is used when other methods are inappropriate. These methods will be discussed herein only briefly. The reader is referred to Blake and Hartge (1986a) for a detailed description of these methods.

2.1.3 Methods

2.1.3.1 Core Method

Introduction

The basic principle behind this method is the use of a sampler having a known volume. Samplers come in a variety of designs, some where a soil ring is driven directly into the ground, and others where a sampler containing two or more soil rings is driven into the ground. This is often called the double-cylinder core sampler. In the latter example, the soil is contained in two rings. The person sampling then has the freedom to choose from either of the two soil filled rings as the sample.

Material

The authors have obtained soil samplers from Soilmoisture Equipment Corporation (Santa Barbara, California) and Forestry Suppliers, Inc. (Jackson, Mississippi).

Procedure

Regardless of how the sampler is driven into the ground, the important aspect of sampling is to recover an undisturbed soil sample which has experienced a minimum of compaction. Thus, it is important to drive the sampler into the soil at a relatively slow rate. Each sampler design comes with its own instructions for use. The procedures listed briefly here are for the double-cylinder core sampler most commonly used.

Drive the sampler into soil either vertically or horizontally, if sampling through a trench wall. It is important that the sampler is driven to the top of the sample rings, so that the soil is not compacted in the rings, or that insufficient volumes of soil are collected. Before pulling out the sampler, slowly twist or push it back and forth gently to break the soil column below the sampler. This ensures that the soils cohesion will not be strong enough to pull sample out of the rings when the sampler is extracted. Once the soil rings are removed from the sampler, excess soil must be scraped off both ends of the ring until the soil surface is flush with the ring. The soil sample should be transferred to a soil can as soon as possible to avoid loss of water. The can lid should be sealed with electrical tape to reduce evaporation loss, particularly if the samples need to be stored for longer periods of time, or if the can is left in sunlight.

The sample then can be placed in a drying oven at 105 C until a constant weight is reached. The bulk density is the dry-mass of the sample (minus the weight of the sample ring) divided by the volume of the ring. (This assumes that the sample does not shrink or swell.)

Comments

Undisturbed samples collected for bulk density can be used for other tests. Water retention experiments, hydraulic conductivity tests and pore size distributions can be done on the same sample. In these cases, determination of the dry-mass bulk density is made after completion of other tests.

Very wet samples may be difficult to collect if the sampling process causes the liquefaction of the soil. This can occur especially if a hammer is used to advance the sampler. Very dry soils are also difficult to collect because of compaction. One should observe the top of the soil sample in the ring after collection to determine whether compaction was significant. McIntyre (1974) provides a discussion on analyzing samples collected under either very dry or very wet conditions.

2.1.3.2 Clod Method

The clod method is used for samples with unknown volumes. This can be important for large pod samples or clods. The bulk density determined with this method may be higher than from other methods (Tisdall, 1951). Blake and Hartge (1986) provide a detailed procedure, along with analysis method and additional comments. The reader is referred to this discussion.

2.1.3.3 Rubber-balloon Method

Introduction

The rubber-balloon method, developed at the U.S. Department of Agriculture (USDA), Soil Conservation Services (SCS), Lincoln, Nebraska Laboratory, is a method of collecting a sample and determining the sample volume in the field without the use of a sampling ring. This method was first described by Bradford and Grossman (1982), and more recently by Andraski (1991). Blake and Hartge (1986a) provide the methodology.

Material

Material and equipment for setting up the sampling site are a foam ring approximately 7.5 cm high, an acrylic ring, and three threaded rods used to level the acrylic ring on the foam ring. A thin clear plastic bag, a graduated cylinder, and a hook gauge are needed to determine the volume of the ring. A standard sampling trowel and soil can are used to collect the sample.

Procedure

To prepare the site, place the foam ring onto the soil surface with the acrylic ring on top. The threaded rods are driven into the ground. Nuts and a level are used to level the acrylic ring. After attaching the hook gage, insert the bag into ring, and add a measured amount of water into the bag until the water level reaches the top of the hook. This represents the presample volume of the ring. Sample the soil down to approximately 5 cm, trying to keep the walls of the excavated hole vertical. After collecting a sufficient volume of soil, the bag is reinserted into the ring and water is added. The increase in water necessary for the water level to reach the top of the hook gauge is the volume of the sample collected. Weighing the sample, after drying, allows for the calculation of bulk density.

Comments

The user should be sure that the bag has no leaks before adding water, otherwise the bulk density will be biased low. Also, this will cause an increase in the soil moisture, thus biasing any measurements of water content. The user should check for any burrows or fractures into which the bag could sag. The foam and acrylic rings, and the hook gauge, can be fabricated fairly easily at most machine shops.

2.1.4 Quality Assurance/Quality Control

Areas of quality assurance/quality control which should be noted include the use of a calibrated balance capable of measuring to at least 0.1 grams for samples equal to or greater than 100 g. Most electronic balances sold today are capable of measuring down to 0.01 grams. Some mechanical balances may not have this level of accuracy. It is also important that the sample be dried sufficiently before measuring its weight. Bulk density values will be biased high if the sample retains water. The reader is referred to the Section entitled Laboratory Water Content, or Gardner (1986) for methods of sample drying. When using the core method, the user must be certain that the soil is flush with the top of the sampling core. Soil that hangs over the top of the core, or falls out below the top of the core will lead to erroneous bulk density results, because of the incorrect volume.

2.2 Particle Density

2.2.1 Introduction

Particle density refers to the density of the solid material excluding pore spaces. Particle density is used primarily in porosity and bulk density calculations. It is the ratio of the total mass of solid particles to their total volume, and is usually expressed in units of megagrams per cubic meter (Mg/m^3) or grams per cubic centimeter (g/cm^3).

Methods of determining particle density are discussed by Blake and Hartge (1986b) and American Society for Testing and Materials (ASTM, 1989g). The reader should consult these references for additional information.

2.2.2 Principles

Two methods of measuring particle density are used today: the pycnometer method and the submersion method. The pycnometer method is more accurate than the submersion method (Blake and Hartge, 1986b), so it will be discussed briefly herein.

The pycnometer is a flask with a precisely known volume and a ground glass stop cock with a capillary through the top. The capillary makes it possible for the user to add exactly the same amount of water each time, thereby minimizing errors in the amount of water added to the soil sample.

This method is performed by weighing a pycnometer filled with soil and air, adding water and weighing the pycnometer again, then reweighing the same pycnometer with water only. The difference in mass, taking into account the density of the deionized water, is the mass of the sample. The volume of the sample is the volume of water displaced in the pycnometer. The mass of the soil sample is the oven-dry mass.

2.2.3 Methods

The method used to perform this analysis is discussed in detail be Blake and Hartge (1986b) and by ASTM (1989g), thus it will not be repeated here.

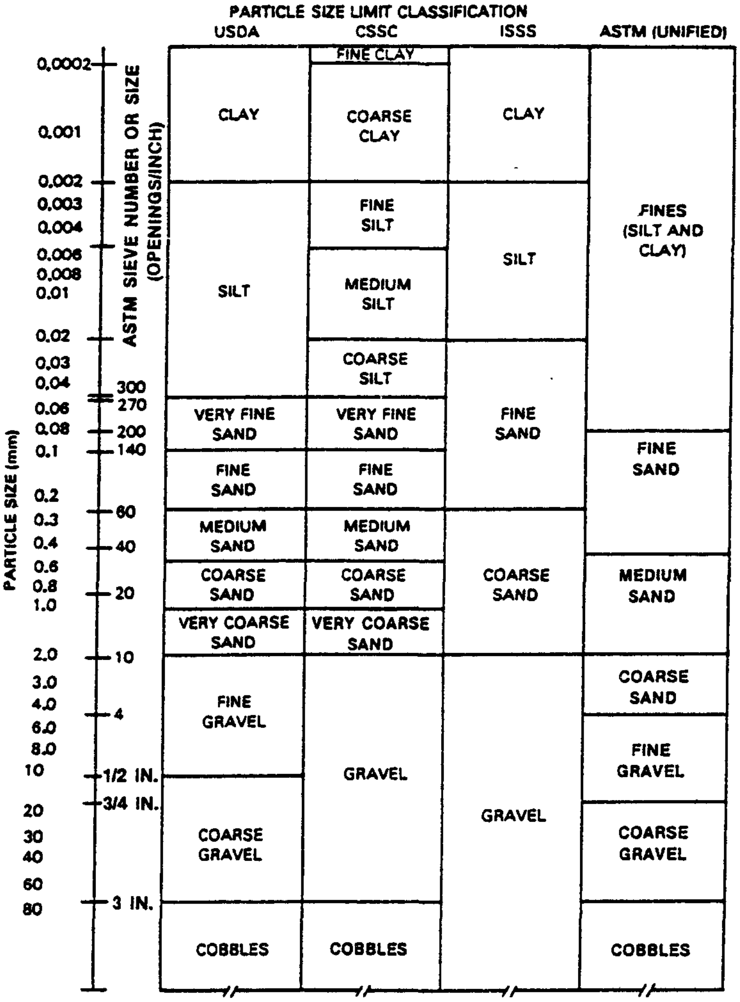
2.2.4 Quality Assurance/Quality Control

The major sources of error that should be accounted for include 1) adding water to a different level in the pycnometer when soil is present, and for water alone, 2) not agitating the sample sufficiently to remove any air pockets, 3) not using the oven-dry mass in the final calculations, and 4) not cleaning off soil and water from the sides of the flask. Even small errors caused by some of the above poor lab procedures can create relatively large errors in particle density results. For example, an error of 10 mg on a 30 g sample will cause a particle density error of 0.001 g/cm^3.

2.3 Particle-size Analysis

2.3.1 Introduction

The particle-size distribution is a measure of sand, silt and clay fractions in soil. Knowing this distribution and the bulk density allows one to make rough estimates of soil hydraulic properties (Arya and Paris, 1981) of the sample. Knowing the soil hydraulic properties is crucial for predicting movement of water and contaminants in soil. The distribution is also used by geomorphologists to evaluate alluvial processes, and by engineers to evaluate foundation materials for construction. In soil science, the particle-size distribution is often used to classify soil texture. The SCS and ASTM both support different, though similar, classification schemes for soils, based on percentages of sand, silt and clay fractions. Figure A.1 presents the different classification systems presently used.



USDA—U.S. DEPARTMENT OF AGRICULTURE, (SOIL SURVEY STAFF, 1975)
CSSC—CANADA SOIL SURVEY. COMMITTEE, (McKEAGUE, 1978)
ISSS—INTERNATIONAL SOIL SCI. SOC. (YONG AND WARKENTIN, 1966)
ASTM (UNIFIED)—AMERICAN SOCIETY FOR TESTING & MATERIALS (ASTM, D-2487, 1985a)

Figure A.1 Particle-size limits according to several classification schemes (after Gee and Bauder, 1986)

The particle-size analysis (PSA) technique has been standardized by the ASTM, and the American Society of Agronomy (ASA). Thus, the discussion presented below only briefly describes this technique. The reader is directed to Gee and Bauder (1986), ASTM (1989e).

2.3.2 Principles

Two basic procedures need to be considered for completing this analysis: sample pretreatment and dispersion, and the actual analysis. Sample pretreatment and dispersion is such an important step in this test, that the particle-size distribution data should not be used if the pretreatment methods are not reported (Gee, 1991). In fact, Gee (1991) stated that the pretreatment methods probably affect the distribution more than the specific method (e.g., pipet, hydrometer, etc.). Four components of soils are often removed from the soil mass prior to dispersing the sample. These include organic material, iron oxide, carbonates, and soluble salts. Soil type and morphology dictate whether these components are abundant, or whether they can be neglected in the pretreatment. According to Gee and Bauder (1986), organic material is most often removed with hydrogen peroxide; iron oxide is removed with a bicarbonate-buffered, sodium dithionite-citrate system; carbonates can be removed by acidification; and soluble salts are commonly removed by flushing with deionized water.

Following pretreatment, the samples need to be dispersed. This can be accomplished either by chemical, physical or ultrasonic methods. Chemical dispersion of soils is usually done by adding Na-hexametaphosphate (HMP), commonly known as Instant-Calgon (Veneman, 1977). Physical dispersion generally uses standard electric mixers, though shakers are also used. Ultrasonic dispersion uses the principle of vibrating sound waves to break up soil aggregates into primary particles.

It is important to note that pretreatment and dispersion methods are not standardized. Soil chemistry must be considered when deciding upon a particular method of sample preparation. For example, it would not be advisable to remove iron oxide from soils where iron is a dominant fraction, because many primary particles could be lost. Likewise, leaching of carbonates from caliche-rich soils could cause errors in the particle-size distribution curve. Therefore, it is important to select methods of pretreatment and dispersion which accomplish the task of breaking down the sample to primary particles without destroying crystal structures of the primary particles.

After pretreatment and dispersion of the soil, the particle size analysis can be performed. The pipet and hydrometer are the most commonly used methods. Both use the principle of settling velocity (Stokes' Law) to determine the time interval for sampling the next smaller-sized fraction. Both require that the sample be passed through sieves to capture particles that fall into sieves of size 1000-, 500-, 250-, 106-, 53-µm, and pan. The mass of the sample captured by these sieves is then weighed and plotted as a percentage of the sample passing through that sieve. The material passing through the smallest sieve into the pan, comprises the silt and clay fractions, which is then analyzed using either the pipet or hydrometer method.

2.3.3 Methods

The presence of methods standardized by ASTM and ASA obviates the need to repeat them here. Thus, the reader is referred to ASTM method D 422-63 (1972) (ASTM, 1989e), and to Gee and Bauder (1986). These references provide procedures, discussions and calculations for generating the particle-size distribution curves.

2.3.4 Quality Assurance/Quality Control

Significant errors can be realized if the silt and clay fraction is sampled too early or too late. Fine sand will be included in the silt fraction if the sample is collected early, and the silt fraction will be biased low if the sample is collected too late. The sample weight measured before fractionation should be the same, or close, to the final integrated weight of the individual fractions. Also, errors can be significant if the sample fluctuates during sedimentation. This can be caused by high carbonates, gypsum, or excessive salts in the soil. Additional dispersant may be required for such soils, or special pretreatment to remove excess salts or carbonates. Recovery of 99%, or better, is achievable and should be the criterion for acceptability of results. Gee and Bauder (1986) should be consulted for additional information on quality control procedures.

2.4 Porosity

2.4.1 Introduction

Porosity is the ratio of the total volume of pores to the total volume of the sample. It is expressed as a dimensionless number. Porosity is a very important soil physical parameter because it is used in calculations of bulk density, water content, and eventually the velocity of soil water movement. The total porosity does not, however, provide an indication of the pore size distribution, the connectivity of the pores with each other, or the overall structure of the soil sample. These characteristics of a soil are extremely complex, and usually are altered or destroyed during sampling and subsequent analysis. This chapter does not attempt to describe how to determine connectiveness or soil structure. It will concentrate on the total porosity only.

The pore size distribution, often determined along with total porosity, is useful in understanding which pore size classes dominate the sample. The distribution can be inferred fairly accurately from the water release curve, as discussed in Section 4.3, in Water Retention Function. Danielson and Sutherland (1986) provide a discussion of how to determine porosity. ASTM Method D4404-84 (ASTM, 1989f) also provides a method of determining porosity. The reader should consult these references for more information.

2.4.2 Principles

Two methods of determining porosity are commonly in use: calculation from particle and bulk densities, and the Gas Pycnometer Method. Calculation from particle and bulk density is more commonly used, primarily because bulk density is a relatively easy laboratory procedure, and because particle density is constant over time for a given soil sample. The gas pycnometer method works on the principle of being able to determine the volume of air added to the sample for a given temperature and pressure. Thus, the total volume of air in the soil at the end of the experiment minus the volume added to soil during the experiment represents the air-filled porosity. Of course the moisture content of the soil must also be accounted for when calculating the total porosity.

2.4.3 Methods

2.4.3.1 Calculations from Particle and Bulk Densities

Porosity is calculated from bulk and particle densities (ρ_b and ρ_m, respectively) via the following equation:

$$\phi = 1 - \frac{\rho_b}{\rho_m} \qquad (3)$$

Dry bulk density is determined using the method described in Section 2.1, in Bulk Density. Particle density is determined using the method is described in Section 2.2. If very precise measurements of porosity are not required, then particle density can be estimated. A common estimate of particle density is 2.65 Mg/m^3 (or 2.65 g/cm^3) (Danielson and Sutherland, 1986).

2.4.3.2 Gas Pycnometer Method

The gas pycnometer method is fully described in Danielson and Sutherland (1986), along with a description of the apparatus which must be manufactured for the analysis.

2.4.4 Quality Assurance/Quality Control

Sources of error for calculating porosity using densities are usually found in estimating the particle density. The user should understand the level of accuracy needed for the porosity results before deciding on whether an estimated particle density is sufficient. For the gas pycnometer method, air leaks around the sample container will cause errors in the final volume of air added to the sample. The pycnometer should be pressure tested before use with samples.

3 Soil Temperature

3.1 Introduction

Soil temperature is a condition which affects biological systems (plant growth, seed germination, microbial activity) and the volatilization and movement of organic and some inorganic contaminants. Soil temperature varies with the changes in thermal, radiant and latent heat exchange processes which occur mostly at the soil surface. Propagation of energy into the soil profile is influenced by complex transport processes, which are in turn influenced by water content, thermal conductivity and specific heat capacity. These physical properties cause diurnal and seasonal temperature cycles deeper in the soil profile to lag behind cycles at the soil surface. Jury et al. (1991) provide examples of this lagging phenomenon, and Hillel (1980) describes other factors which affect soil temperature and heat flow.

This chapter describes the methods of measuring soil temperature in the field. These techniques can also be applied to laboratory environments, but it is anticipated that most applications will be field oriented. Three general methods of determining soil temperature exist: thermometers, thermistors and thermocouples. Accuracy, response time, and ease of installation are important factors to consider when deciding on the appropriate method. Taylor and Jackson (1986) provide a more in-depth discussion on the methods listed above. The interested reader should consult this reference.

3.2 Principles

Soil temperature is determined indirectly after measuring its influence on another property or condition in the soil. The volume of mercury in a glass, the electrical resistance of platinum wires or wires made of other material, or the pressure change of gas maintained at a constant volume can be examples of properties which are measured to infer temperature. Similar to the indirect measurement of water content, calibration curves must be developed before the technique can be applied in the field. Calibration is often done in the laboratory where environmental conditions can be controlled better. Some standard references have been agreed upon by the scientific community.

3.3 Methods

3.3.1 Thermometers

3.3.1.1 Introduction

A number of thermometers have been developed for measuring soil temperature. However, because their theoretical bases are described by Taylor and Jackson (1986), they will be discussed only briefly herein.

Commonly used thermometers include mercury or other liquid in a glass, bimetallic, and electrical thermometers. Mercury and other liquid thermometers are identical to standard air thermometers. Changes in temperature cause the liquid to expand or contract inside a small diameter capillary. The change in volume is calibrated against temperature and the glass container is marked accordingly. Bimetallic thermometers are used often in the lab to regulate constant temperature baths. They operate on the theory that two different metal strips, welded together, expand differently with temperature causing the strip to deflect. A pointer is used to indicate the amount of deflection. Two types of electrical resistance thermometers are available. The first type depends upon measuring the resistance of metal wire, either platinum, copper, or silver. A bridge or potentiometer measures the changes. The second type of resistance thermometer is called a thermistor. Thermistors are semiconductors with very high negative temperature coefficients of resistance, on the order of 4% per centigrade degree (Taylor and Jackson, 1986). These temperature sensitive resistors can be contained in a porous material for field installation. Thermistors are available in different shapes and sizes, so they must be calibrated separately. Generally, thermistors are calibrated in three steps: (1) each thermistor is exposed to several known temperatures, (2) the current output is converted to resistance using a preestablished standard curve, and (3) the temperature is plotted against log resistance. Thermistors are useful in the field because they can be recorded continuously using any analog recorder.

3.3.1.2 Material

The authors have obtained liquid in glass and bimetallic thermometers from Weathermeasure (Sacramento, California) and Forestry Suppliers, Inc. (Jackson, Mississippi). Platinum resistance thermometers have been obtained from Weathermeasure and thermistors from Campbell Scientific, Inc. (Logan, Utah).

3.3.1.3 Procedure

Calibration procedures are described somewhat by Taylor and Jackson (1986). Instructions for use are available from the respective manufacturers or vendors.

3.3.2 Thermocouple Method

3.3.2.1 Introduction

Thermocouples, also called thermoelectric junctions, are composed of two dissimilar metals joined in two different places. Because the junction is made of two different metals, the total electromotive force is proportional to the difference in temperature between the two junctions. One junction is used for measuring and is called the hot junction, and the other junction is the reference and is called the cold junction. The reference junction must be kept at a constant temperature, such as an ice bath. However, electronic reference junction compensation is most often used. Calibration is achieved by recording the total electromotive force for a range of known temperatures. An advantage of using thermocouples, similar to the use of thermistors, is that data collection can be automated.

3.3.2.2 Material

Thermocouples and a variety of data loggers have been obtained by the authors from Campbell Scientific, Inc. (Logan, Utah). Data loggers are used extensively for remote field data collection.

3.4 Quality Assurance/Quality Control

Quality control issues center around the accuracy of calibration, and the ability of the instrument to function over time according to the calibration curve. Calibration of thermometers is fully described by Taylor and Jackson (1986). Calibration of thermistors and thermocouples is relatively straightforward. In general, however, accuracy will depend on the ability of the user to accurately quantify the temperature which corresponds to the electrical response. Thus, the thermometer used during the calibration process itself must be accurate. Recalibration may be necessary depending on the history of the individual devices. The user should determine whether drift of the calibration curve falls within manufacturers specification.

4 FLOW PROPERTIES

4.1 Laboratory Water Content

4.1.1 Introduction

Water content is one of the most important soil parameters, because it affects soil hydraulic properties, solute transport, heat flow, and vapor transport of contaminants. Field determination of water content is an important indicator of possible failures of a containment system or long-term deep recharge into disposal units or surrounding soil. Accurate estimates or determinations of water content in the laboratory is necessary for assessing energy levels of water in the soil, sorptivity of the soil at given water contents, and points on the water content-hydraulic conductivity curve.

This chapter discusses the laboratory determinations of water content, both direct and indirect. Some methods discussed herein have been developed many decades ago. A thorough review of the theory and importance of water content, methods for calculating water content, and determinations of error associated with these methods are included in Gardner (1986), so they will be included here only briefly.

4.1.2 Principles

Methods for determining water content in soils can be broken down into two broad categories: direct and indirect. Direct methods include those where water is physically removed from the soil sample via evaporation, leaching or chemical reaction. Indirect methods involve the measurement of a physical or chemical property that is affected by water content. These usually involve the measurement of (1) the energy status of the water in the pores using some sort of water absorber (e.g., a porous cup of a tensiometer), (2) the electrical properties, using e.g., a Time Domain Reflectometer, or (3) the neutron scattering or gamma-ray attenuation. Indirect methods have the advantage over direct methods in that they allow the use of automated data collection systems for non-destructive determinations of water content. A disadvantage of indirect methods is the need, in most cases, for calibration. This requirement can be very challenging when using some instruments (e.g., neutron probe) that measure larger volumes of soil, and the need to control precisely the amount of water present in the soil volume. Also, instrument response is often affected by the wetting history of the soil. This phenomenon, known as hysteresis, can cause significant errors in the calibration curves which are difficult to quantify. Hysteresis may, for example, require the user to generate one calibration curve for drying soil, and one for wetting soil.

4.1.3 Methods

It should be noted here that the following discussion applies to the laboratory determination of water content. Field determinations of water content are discussed in Appendix B, Section 5, Field Water Content.

4.1.3.1 Direct Methods

Introduction

Although direct measurement of water content is relatively simple, defining when the soil is dry is not always so straightforward. The definition of dry soil may or may not include water contained in colloidal particles, organic material or structural water derived from the crystal lattices of clay. Thus, including structural water in the water content calculations may not be appropriate. Adsorbed water, on the other hand, is water that actively takes place in the processes of flow and transport, and is of primary importance to flow processes.

Also, water is found as part of the organic fraction of soil. When soil is heated to 105°C, this water is removed. Since water contained in plant material does not actively participate in soil water flow, including this portion of water loss in water content calculations yields a value biased high. Conversely, soil samples with water high in dissolved salts may be difficult to analyze for water content, because of the added mass of the salts when the water is driven off. This process yields water contents biased low; however, for most soils, organic content is less than a few percent and the salt content is negligible. Many of these uncertainties have not been resolved fully.

Material

For most applications, the following materials are needed for direct determinations of water content: a constant temperature oven capable of accurate adjustments between 100 and 110°C, a desiccator with desiccant, and a balance. In cases where the soil sample is collected in the field, a soil can or other container will be needed. Highly accurate determinations of water content may require a special oven, such as a convective, forced-draft or vacuum oven (Gardner, 1986).

Procedure

The direct method of determining soil water content may vary depending on the circumstances or precision needed. However, for most applications the procedure is as follows. The tare weight of the soil can, with lid, must be determined. Place the soil (from 1 to 100 g) into the can and replace the lid tightly to prevent evaporation. Electrical tape to seal the lid can be used; taping the lid has been found to greatly reduce evaporation loss if the samples need to be stored for longer periods of time, even if the can is left in sunlight. Remove the lid and place the soil can into the oven. The time necessary for the sample to reach a constant weight can take from 10 hours in a forced-draft oven, to 24 hours in a convection oven (Gardner, 1986). Immediately after removing the dry sample from the oven, replace the lid and put the soil can into a desiccating jar, with desiccant, until the sample cools. The desiccant creates a very low humidity environment so that the soil does not remove water from the air. Weigh the sample again, with the lid, and determine water content using any of the following equations:

$$\theta_g = \frac{(\text{weight of wet soil + tare}) - (\text{weight of dry soil + tare})}{(\text{weight of dry soil + tare}) - (\text{tare})} \tag{4}$$

$$= \frac{(\text{weight of wet soil + tare}) - (\text{tare})}{(\text{weight of dry soil + tare}) - (\text{tare})} - 1 \tag{5}$$

$$= \frac{(\text{weight of wet soil})}{(\text{weight of dry soil})} - 1 \tag{6}$$

Multiplying these values by 100 gives the percentage on a dry-mass basis.

Comments

Soil samples collected in the field must be quickly sealed to prevent water loss prior to the initial weighing. Also, due to loss of water during transfer of the sample to a drying oven, it may be prudent to record the tare weight before placing the sample in the can. Microwave ovens can also be used to dry the sample; however, because the length of time to dry a sample depends on the amount of organic material in the soil, initial water content, and sample size, it is not possible to provide a specific drying time for all samples. Gee and Dodson (1981) show that for small samples, a wide range of soils (sands to clays) can be dried in a microwave oven when set at full power (650 W). For example, a microwave oven dries a 20 g sample in 20 minutes as thoroughly as a convection oven (set at 105°C) for more than 16 hours. Also, non-uniform drying in the microwave may increase the errors of water content (Gardner, 1986). Precise determinations of water content may require special precautions, such as performing additional analyses to check for uniformity of drying.

Water content on a volume basis is often needed to perform mass-balances of soil water for modeling purposes. It is also needed for determining transport parameters (Parker and van Genuchten, 1984). In these cases, the volume of the sample needs to be known accurately so that bulk density can be calculated. Collection of samples in rings of known volume and weight are useful in this regard. Volumetric water content is determined using the following formula:

$$\theta_v = \theta_g\left(\frac{\rho_b}{\rho_w}\right) \qquad (7)$$

where

ρ_b = is the bulk density of the soil sample (M/L^3)
ρ_w = is the bulk density of water (M/L^3)

4.1.3.2 Indirect Methods

As mentioned above, indirect methods of determining water content are based on the measurement of a soil property which is dependent on water content. Although the relationship between a soil property and water content may be complicated, it is usually possible to generate a reasonably accurate calibration curve so that changes in water content can be approximated. Further, because the methods are usually not destructive, repetitive measurements can be collected on the same soil sample in real-time. Thus, movement of wetting fronts through a soil profile or changes in water content caused by evapotranspiration, as examples, can be monitored.

Given the variety of physical and electrical properties which are dependent on water content, and the ability to monitor changes in these properties, it is not surprising that many texts and articles have been published on this subject. Therefore, it is not necessary to review the theory behind each technique in this document. Rather, a brief discussion on how these properties can be measured in the laboratory will be included here, with references on more in-depth discussions. In this document, the following techniques will be included: soil water tension, and electrical conductivity and capacitance (time domain reflectometry). Gamma ray attenuation will also be mentioned, though only briefly. The procedures for indirect methods of water content are discussed in Gardner (1986). They will not be reproduced herein.

Soil Water Tension

Introduction

One of the most common methods of calculating water content is by determining soil water tension. This because of the strong dependence between soil water tension and water content. Soil water tension (also known as potential) has been defined as "the amount of work that must be done per unit quantity of pure water in order to transport reversibly and isothermally an infinitesimal quantity of water from a pool of pure water at a specified elevation at atmospheric pressure to the soil water (at the point under consideration)" (Aslyng, 1963). Matric potential is a function of the physical properties of the soil material. When the soil is saturated, the matric potential is zero. This is the case below the water table. However, when force is applied on a saturated soil, water will be released. This force can be the pumping of groundwater from a well or pressure applied to a soil sample in a pressure cell. The amount of water released is dependent on the properties of the soil (mainly pore size) and the properties of the liquid (surface tension, density, and viscosity). It is possible, therefore, to measure the amount of water released from the soil for each increment of force, and calculate the water content. A water content-water tension curve then can be generated for a given soil sample. This curve defines one of the most important relationships that govern the movement of soil water, and is therefore considered to be a critical parameter that must be determined to support a license application for low-level radioactive waste disposal in the unsaturated zone (U.S. NRC, 1988).

Because of the importance of soil water tension, two chapters in this document are devoted to its measurement, so it will be discussed only briefly here. It is important to note that, in order to obtain water contents from tension measurements, a calibration curve must be generated. Soil water tension is measured either by tensiometers connected to pressure transducers or manometers, pressure vessels through which a specified pressure (or tension) is applied to a soil sample, or thermocouple psychrometers which can measure the tension in a small volume of dry soil. In each case, however, the soil sample must eventually be oven-dried to determine the actual water content. Generating the water content-water tension curve is relatively easy, once the amount of water removed for each pressure step is determined. The user simply back-calculates the water content by adding the water removed from each pressure step to the water content for the previous step. In this way, individual water content-water tension points are found, and the curve can be generated.

The water tension method of determining water content has a few disadvantages. Firstly, the resulting water content-water tension curve can only be applied to that soil sample, because of the potential for very large spatial variability of soil hydraulic properties. Secondly, the length of time needed to accurately determine points on the water content-water tension can be excessive, sometimes on the order of weeks. Transient methods are being developed to reduce this time frame. See Section 4.2 titled Laboratory Water Tension, which provides more information on methods to determine water tension.

Material

Materials necessary to perform measurements of soil water tension can be obtained from a number of vendors such as may be listed in the Thomas Register. The authors have obtained tensiometers from Soilmoisture Equipment Corporation (Santa Barbara, California), Irrometer Company, Inc. (Riverside, California), and Soil Measurement Systems (Tucson, Arizona). Pressure chambers have been obtained from Soilmoisture Equipment Corporation and laboratory-type thermocouple psychrometers have been obtained from Decagon Devices Inc. (Pullman, Washington).

Electrical Conductivity and Capacitance

Introduction

Electrical conductivity and capacitance of soils vary with water content. Therefore, by measuring the changes in electrical response to changes in water content, a relatively quick and non-destructive technique is available. However, as Gardner (1986) points out, it has not been possible to make unique correlations between electrical responses and water content, because of (1) the effects of salinity and ionic constituents on electrical conductivity, (2) poor contact of the sensors with the soil, and (3) heterogeneities within the soil that restrict current flow. Porous blocks (i.e., gypsum blocks) with imbedded electrodes have been found to be useful. A source of error with these devices is that equilibrium between the porous blocks and the soil is a matric potential equilibrium, not a water content equilibrium. Thus, two calibration curves need to be developed: one for the electrical response-matric tension relationship, and one for the matric tension-water content relationship. Although the matric tension-water content relationship (water release curve) can be relatively well defined, it increases the potential for error. In fact, Gardner (1986) states that precision better than ±2% should not be expected, and errors can reach as high as 100%. Heterogeneity within the soil profile also limits the use of point measurements on larger areas of soil.

Time domain reflectometry (TDR) recently has been given widespread attention as a method of determining water content. Briefly, TDR measures the propagation velocity of a high-frequency voltage impulse down two or more parallel metal probes inserted into the soil (Figure A.2). The return velocity of the voltage impulse is dependent on the dielectric constant of the medium into which the probes have been inserted. Because of large differences in the dielectric constants between soil and water, determination of this constant is an excellent measure of volumetric water content. Automated, real-time data collection of the dielectric constant (and hence the water content) is possible with TDR. Recently, researchers have begun to publish articles describing their experiments (Herkelrath et al., 1991; Baker and Allmaras, 1990; de Jonge and Simpson, 1990; Heimovaara and Bouten, 1990). Topp et al. (1980) published some of the first articles on TDR use and application. Though TDR has many applications, it has a couple disadvantages: (1) it has not been fully determined whether TDR needs to be calibrated for each soil type, and (2) methods to automate the measurement correction have not been fully perfected.

Material

Wheatstone bridges are used for measuring resistance. Porous blocks made of gypsum, fiberglass or nylon cloth can be used with imbedded electrodes. The authors have obtained TDR equipment from Tektronix Corporation (Beaverton, Oregon), Soilmoisture Equipment Corporation (Santa Barbara, California), and Campbell Scientific, Inc. (Logan, Utah).

Gamma Ray Attenuation

Gamma ray attenuation is, in principle, similar to neutron thermalization (see Appendix B, Section 5, Field Water Content). A monoenergetic beam of gamma rays is directed through a soil core where it is attenuated to a degree dependent on the bulk density of the soil and the water content. If the soil core has a constant bulk density, then changes in attenuation are caused by changes in water content. An attenuation equation, which relates the ratio of the returning flux to the incident flux to the bulk density of the soil and water content, is used to solve for water content. Dual gamma sources have been used to measure attenuation through the core using two sources of radiation. This technique provides two equations relating attenuation of density and water to radiation intensity of the two sources. They can be solved simultaneously for water content and density (Gardner et al., 1972).

Because gamma ray attenuation is not used extensively to measure water content in the lab, it will not be discussed further.

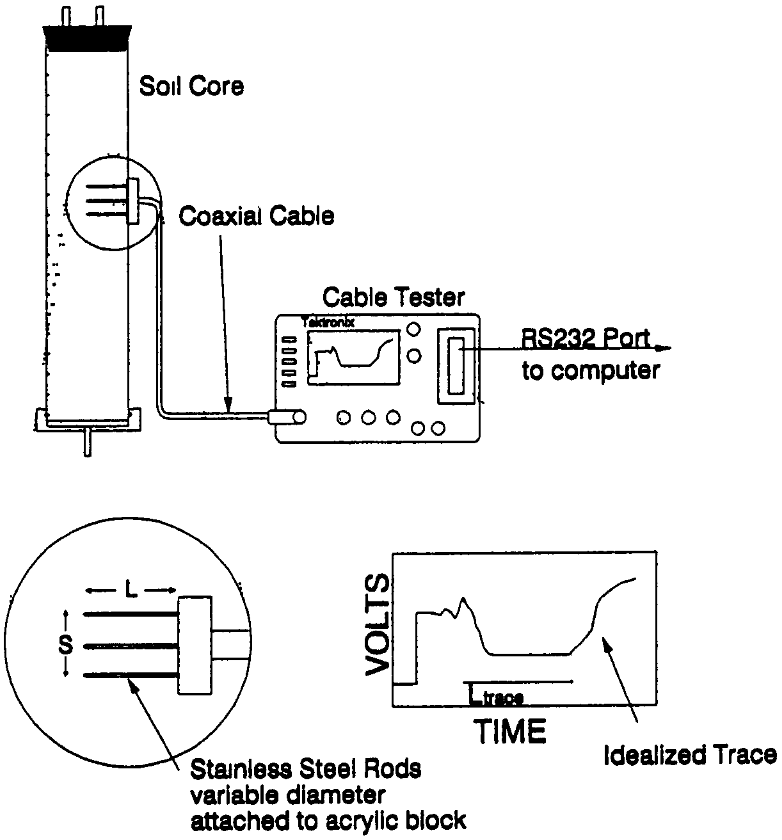


Figure A.2 Diagram of experiment using time domain reflectometry to measure laboratory water content

4.1.4 Quality Assurance/Quality Control

Possible sources of error using direct determinations of water content usually center around not allowing sufficient time for oven drying. The user should be sure that the oven is stable at a temperature of 105°C before using. Balances should be capable of reading to 0.1 grams or better, depending on the mass of water involved.

Possible errors associated with indirect methods can be numerous. This is because calibration curves are used to convert physical or electronic responses to water content. In some agricultural applications, these calibration curves need not be as accurate, because the resolution required for the water content is low. However, this is usually not the case in environmental applications, where errors in water contents on the order of tenths of percents can affect the hydraulic conductivity by several times. It will be experienced by many that the majority of time devoted to indirect methods of determining water content will go towards developing calibration curves. However, the rewards for solving these problems will be realized in greatly reduced staff time requirements and increased experimental efficiency. Obviously, the scope of this text falls short of providing methods to generate calibration curves. The user is directed to manufacturers' data sheets for a list of possible errors for their respective instruments, and to the references for additional information.

4.2 Laboratory Water Tension

4.2.1 Introduction

This section discusses laboratory measurements of soil water tension, (also called pressure potential or potential). Water tension is one of the most important parameters determining how water moves through soils. Soil water tension varies with water content, being 0 at saturation and as high as 30 bar in dry soils. The relationship between tension and water content is called the water retention function (or the water release curve). It may be used to predict water movement in the unsaturated zone. The accuracy of predictions from computer modelers therefore depends on the ability of the laboratory experimenter to generate accurate soil water retention functions. Several mathematical expressions have been developed to fit single values of water content and water tension (e.g., Brooks and Corey, 1964; Mualem, 1976; van Genuchten, 1980). The accuracy of these fitted curves is based, in part, on the accuracy of the tension-water content data determined through experimentation. The ability to measure water tension, therefore, strongly affects the retention curve.

Two methods of measuring water tension will be discussed in this section: tensiometry and thermocouple psychrometry. Tensiometry measures soil tension from essentially saturation to a tension of 0.8 bar (800 cm), and psychrometry is used to measure tension in soils where tension is from 0.8 bar to 100 bars. Both methods are considered essential for generating the complete retention curve, or for determining point values in soil when the entire curve is not required. Point values are useful for defining initial conditions prior to beginning experiments.

The principles behind soil water tension have been discussed in the literature since Buckingham (1907), and many texts, or portions thereof, have been devoted to this subject. Thus, the theory of potential will be discussed here only briefly. Cassel and Klute (1986) include a good discussion of potential and its measurement, as well as a substantial number of references. The reader should consult Cassel and Klute (1986) for additional information.

4.4.2 Principles

The water potential is a measure of the energy status of water in soil. Hillel (1980) defines potential energy as "a measure of the amount of work a body can perform by virtue of the energy stored in it." The potential is measured relative to water in a standard reference state. The energy status is expressed in units of J/kg (as energy/mass), MPa (as energy/volume), or m (as energy/weight or head). Soil water potential can be expressed as a sum of matric (capillary and surface), gravity and osmotic forces. Expressing water potential in terms of head allows for easy addition of the matric and gravity potential to get total head. Soil water under zero or positive pressure is considered saturated, such as below the water table. In soils which are unsaturated, pressure will be negative. Larger negative numbers indicate that the soil is dryer. Soil water tension is equal to the matric potential but opposite in sign. Tension normally will be used in this text rather than potential.

Tension is often measured with tensiometers for soils which have a tension less than 0.8 bar. A tensiometer consists of a water-saturated porous ceramic cup connected to a manometer, vacuum gage or pressure transducer. Tensiometers work on the principle that, as soil water is removed from the soil, water in the tensiometers will no longer be in hydraulic equilibrium with the soil. Because the tension of the water in the tensiometer is higher (less negative) than in the soil, water will flow from the tensiometer into the soil until equilibrium is achieved. This change in energy status can be measured using a simple vacuum gauge, water or mercury manometer, or an electrical pressure transducer. The range of measurements possible with tensiometers is 0 to approximately 0.8 bar. Above 0.8 bar, tensiometers do not function because gases dissolved in the water will begin to form bubbles and the liquid column will break up (Cassel and Klute, 1986). The user should understand that, as the water content decreases, the hydraulic conductivity decreases. This decrease in conductivity will increase the time necessary for a tensiometer to come to equilibrium with the soil.

Solute potential, sometimes called osmotic potential, can be important if the porous material transmits water more readily than solutes, which causes a higher (less negative) pressure to develop on the side of lower solute concentration (e.g., in plant roots). Solute potential is usually neglected because the pore sizes of the porous material separating water inside the tensiometer from water in the soil often do not constrict the movement of solutes. Only the gravitational and pressure potentials are normally considered significant to include in the total head calculations. Gravitational potential is measured relative to a datum elevation.

Thermocouple psychrometry is the second method of determining tension in soils. With thermocouple psychrometers, the relative humidity or vapor pressure of the soil atmosphere in equilibrium with the liquid soil water is measured. The vapor pressure is usually measured inside a thin-walled ceramic cup buried in the soil. There are two thermocouples inside the ceramic cup, one to measure the actual air temperature ("dry bulb temperature") and the other, with a drop of water on its tip, to measure the "wet bulb temperature." The temperature of the wet thermocouple depends on the rate of evaporation from the wet junction, which in turn depends on the vapor pressure inside the ceramic cup. From the difference between the wet and dry bulb temperatures, the vapor pressure can be calculated directly. Vapor pressure can be related to the total water potential of a soil (Rawlins and Campbell, 1986). When soil is relatively salt free, the tension (negative matric potential) can be approximated by the total water potential, thus:

$$h(\theta) = -\frac{RT}{\rho g m}\ln\left(\frac{e}{e_o}\right) = -47.11T\ln\left(\frac{e}{e_o}\right) \tag{8}$$

where

$h(\theta)$ = tension
R = universal gas constant (0.008314 kJ/mole K)
T = temperature (K)
m = molecular weight of water (0.018 kg/mole)
e = water vapor pressure (m/L^3)
e_o = saturated water vapor pressure (m/L^3)
g = gravity (mL/T^2)
ρ = bulk density of water (m/L^3).

In the laboratory, the wet junction can be wetted by dipping it in water, or by feeding a small direct current through the junction. The temperature of the thermocouple is reduced to the dew point by Peltier cooling and water condenses on the junction.

4.2.3 Methods

4.2.3.1 Tensiometry

Introduction

Tensiometers are useful for measuring tension from 0 to approximately 0.8 bars. Tensiometers generally have ceramic cups and plastic bodies.

Material

Material needed to construct and operate tensiometers can be broken down into two broad categories: the tensiometer itself, and the method of recording the tension. The tensiometer is composed of the porous cup, an acrylic or PVC pipe onto which the porous cup is attached, and a measuring device on the other end of the pipe to record the tension. The porous cup is attached to the pipe using epoxy/hardener, solvent welding or other acrylate bonding solution. The user is advised to check that the adhesive used is compatible with both the porous material and the pipe. Some adhesives have been found to weaken the pipe material to a point where failure occurs. In some cases, hot glue guns do bond the materials together better than regular solvent welding, because with glue guns, air bubbles are more readily eliminated and gaps, which may be present after machining the parts, are filled up. Numerous miscellaneous products can be purchased for modifying stock tensiometers. For example, a user can purchase lengths of pipe for extending the length of the tensiometer, or elbows can be installed at the end of the tensiometer pipe for horizontal installation. Gauges are obtained either with the purchase of the tensiometer or through local vendors. Septum stoppers are used to seal tensiometers for use with hand-held transducer-type Tensiometers.

The devices used to measure tension in the tensiometers range from mercury/water manometers to simple vacuum gages to pressure transducers. Mercury manometers are no longer recommended because of the danger of mercury spills. Water manometers may be used in the laboratory. However, for drier soils, manometers need to be too long to be practical. Also, the use of manometers requires that larger volumes of water be transmitted through the porous cup, increasing the time for equilibration. Vacuum gages are often used in tensiometers in the field, given their relative ease of use but are notable for their lack of precision (seldom better than ± 20 cm). For more precise measurements, and where larger numbers of tensiometers are required, hand-held transducers (Marthaler et al., 1983) are recommended, instead of vacuum gages or manometers. Pressure transducers are used for their ability in automated data collection systems and for their precision.

Transducers are available without power sources or recording devices, or they can be purchased with their own power sources and data storage modules. The authors have obtained tensiometers and associated recording equipment from Soilmoisture Equipment Corporation (Santa Barbara, California), Irrometer Company, Inc. (Riverside, California), and Soil Measurement Systems (Tucson, Arizona). Over 100 tensiometers were used at the Las Cruces Trench site (Wierenga et al., 1990).

Procedures

Tensiometers often are purchased whole though they can be purchased in pieces. Assembly instructions should accompany the components, especially with regard to the adhesive, or bonding material. A number of different epoxies, solvent welders, and even heated glue guns can effect a sufficient bonding for the range of tensions expected during the experiment. As mentioned above, the user should be aware that some epoxies that contain MEK (methyl ethyl ketone) can cause plastic to degrade over time until failure. This type of failure has been experienced at the Las Cruces Trench site, New Mexico.

Installation of the tensiometer involves inserting the porous cup into the soil zone to be monitored. For loose moist soil, the tensiometer can be pushed directly into place. For stony soil, or compacted horizons, it may be necessary to bore out a hole of similar diameter as the tensiometer. The cup should be placed in a slurry of soil and water, so that a good contact between the soil and the cup is established. In some cases, silica flour is used, and in others sieved natural material is used (Wierenga and Young, 1991). Because of the possibility that dissolved constituents will interact with the silica flour, sieved natural material is preferred. Cassel and Klute (1986) provide a lengthy discussion about issues that should be addressed during the installation of tensiometers.

Procedures for data collection vary with the method (i.e., manometer, gauges, or pressure transducer). The user should be cognizant of time for equilibrium if manometers or gauges are used, given that more water must move through the porous material before it is in equilibrium with the soil. Gauges may require significant time for equilibrating, as well as calibration. Pressure transducers require very little time to reach equilibrium, but they must be calibrated, sometimes extensively, before they can be used with confidence. The user is advised to consult with the transducer manufacturer, or with the technical data sheets that accompany each transducer, for a quantitative assessment of the possible errors. Tandeske (1991) provides a manual on the selection and application of transducers, with a good discussion on the different types of transducers.

Comments

During assembly and installation, care should be taken to avoid touching the porous material. Oil and dirt from handling affects the conductivity of the cup. It is important to test the tensiometer for air leaks prior to installation in the soil core. One practical method is to place the tensiometers with their tip in a bucket of water for 12 to 24 hours. Then drain all water from the tensiometers and apply a 1 bar air pressure on the tensiometers. Place the cup under water and look for air bubbles from the tip or any other place where parts are glued together. If bubbles appear, the tensiometer leaks and needs to be repaired.

4.2.3.2 Thermocouple Psychrometry

Thermocouple psychrometers can be purchased as single or multiple chamber models. The Wescor, Inc. (Logan, Utah) Model C-52, a single chamber model, is capable of measuring tension by the psychrometric or dew-point method. The Decagon Devices, Inc. (Pullman, Washington) Model SC-lOA holds up to 9 or 10 samples, and can use either a Peltier-type thermocouple or a modified Richards junction. Rawlins and Campbell (1986) provide a thorough discussion on the use of these thermocouple psychrometers, as well as on calibration and temperature correction issues that the user will face. The user is advised to consult this reference.

4.2.4 Quality Assurance/Quality Control

Major issues of quality assurance/quality control center around the use of equipment calibration curves, and how these curves drift over time. Prior to use of pressure transducers and psychrometers, both must be accurately calibrated. Both devices must be calibrated at the temperatures expected during the experiments and for the range of outputs. Pressure transducers generally have temperature compensation, however, for resolution down to the cm water pressure level, the compensation is often not sufficient and changes in the null offset value (y-intercept) may occur. For the majority of applications null offset shifts do not affect the results significantly. However, if tensiometers are used to calculate gradients on soil cores, even small offset errors can lead to large errors in hydraulic conductivity.

Also, because output resolution is dependent on the pressure rating of the transducers, the user should choose transducers that are rated for the full range of expected outputs, but not much more. It may even be possible to overpressure the transducer by more than 50% of the rated value without damage to the unit. The user can then obtain readings with more precision than possible with transducers that have wider ranges than needed for particular applications. Considering these potential sources of error is important.

Long-term use of tensiometers may cause a decrease in the conductivity of the cup, especially if the unit is not serviced properly between experiments. Plugging of the ceramic cup by microbial slime or by fine silts and clays occurs over time. Porous cups can be cleaned with an ultrasonic cleaner using a mild acidic solution. Manufacturers' guidelines should be followed closely.

4.3 Laboratory Water Retention Function

4.3.1 Introduction

An important soil hydraulic property is the relationship between soil water content and soil water tension. This relationship is described by various names, including soil water release curve, soil water retention function, soil moisture characteristic, and the capillary pressure-saturation curve. The term "soil water" is commonly used for the solution or liquid phase of the soil. The water retention is expressed in terms of soil water content that is in equilibrium with the capillary pressure (or soil water tension or suction).

This chapter will discuss laboratory methods of determining the water retention function. Field methods are discussed by Bruce and Luxmoore (1986) for the interested reader. The Buchner funnel, Pressure Cell, and Pressure Chamber methods are common laboratory methods used today, so they will be discussed here. Klute (1986) provides a very good discussion on the theory behind these laboratory procedures, and some of the issues that the user will likely face during the experiment.

4.3.2 Principles

The soil water retention function is valuable for understanding hydraulic characteristics of a given soil sample as well as the pore-size distribution. The function provides paired values of water content and the corresponding potential, and when plotted on an XY graph, it can be used to estimate the potential at any water content. The pore-size distribution also can be estimated using the soil water retention function, by knowing the amount of water removed from a given volume of soil for a given increase in tension (Koorevaar et al., 1983).

4.3.3 Methods

Soil water retention in the low-suction range (0-1 bar) depends primarily on capillary forces and is strongly influenced by soil structure and pore-size distribution. Thus, measurements made with disturbed samples (e.g., dried, screened, and artificially packed) cannot be expected to represent field conditions because the soil structure is destroyed. The use of undisturbed soil cores is therefore preferable. At tensions greater than 1 bar (0.1 MPa), water is held progressively by adsorptive forces and, therefore, is influenced more by the texture and specific surface of the soil material than by the structure. Thus, at higher tensions, use of disturbed samples may be justified.

The soil water retention function can be determined in the laboratory by placing soil samples on porous plates equipped with drainage outflow tubes, or by placing the soil sample inside pressure cells. Saturated porous plates allow water to flow through them, but not air. This is a function of the surface tension of water, or whatever fluid is being used. The porous plates upon which the saturated soil samples rest, are usually part of a Buchner funnel, pressure cell or pressure chamber. The saturated soil on top of the porous plate is subjected to either suction (Buchner funnel) or positive air pressure (pressure cell and pressure chamber), although suction can be applied using pressure cells and pressure can be applied to Buchner funnels. This causes water to flow out of the soil sample, through the porous plate and into the drainage tubes. Equilibrium at the applied suction or pressure is attained when water no longer flows out of the soil.

At equilibrium, the amount of outflow is recorded and the process is repeated at a higher suction or pressure. The gravimetric water content of the soil sample is computed at each applied suction or pressure by adding up the total amount of water drained from the sample for each applied suction, using the following equation:

$$\theta_g = \frac{(\text{weight of wet soil} + \text{tare}) - (\text{weight of dry soil} + \text{tare})}{(\text{weight of dry soil} + \text{tare}) - (\text{tare})} \qquad (9)$$

In this way, a range of paired values of water contents and suctions are obtained. Figure A.3 presents an example water release curve, including the effects of hysteresis, which are discussed below.

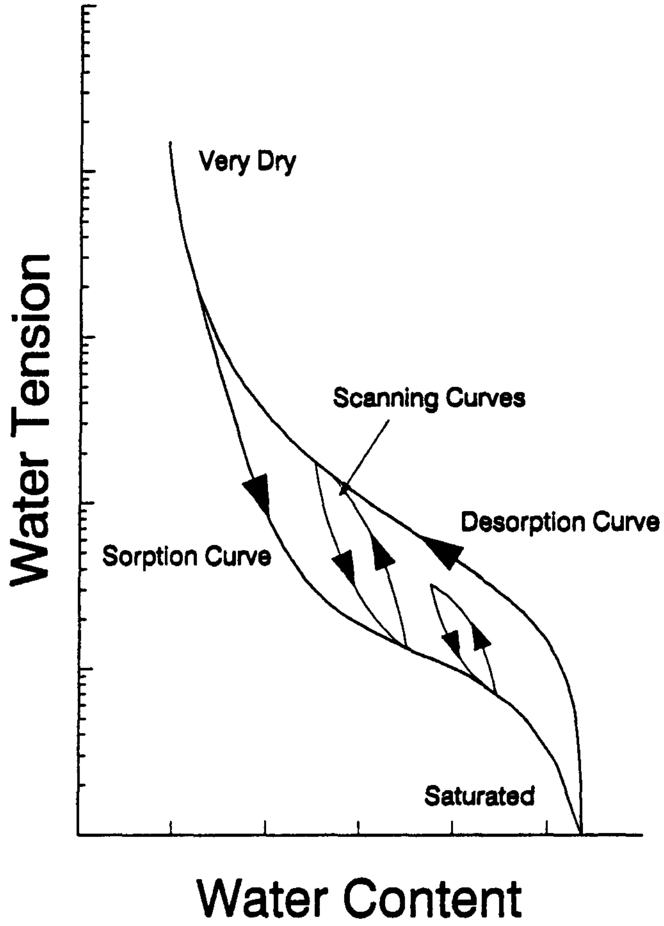


Figure A.3 Water retention curve showing hysteretic relationships between sorption and desorption curves

A commonly ignored phenomenon in soil characterization is hysteresis. Hysteresis occurs when water contents at the same tension differ depending on whether one is conducting a desorption (draining) or sorption (wetting) experiment. The soil water retention curve can be determined under either draining or wetting conditions. The draining curve is determined by extracting water from saturated soil samples. The wetting curve is determined by wetting soil samples from a low water content or low pressure head (large negative value). The equilibrium water content at a given suction is greater in desorption than in sorption (Hillel, 1980).

The bubbling pressure of the porous plate is a very important limiting factor in water release experiments which can be easily overlooked. The bubbling pressure, also called the air entry value, is that pressure (or vacuum) which, when exceeded, allows air to enter the pores of the porous material. It is mostly a function of the surface tension of the liquid and the pore size of the plate. When air enters the porous plate, the conductivity of the plate begins to drop quickly, air starts to leak through, and the experimental results become dependent on the experimental set-up. It is important that the bubbling pressure of the plate be determined before the experiment begins, so that the user knows the upper limit of pressure or vacuum that can be applied to the soil.

The hydraulic conductivity of the porous plate should also be determined prior to running the experiment where soil conductivity is needed or is important. This can be done either by the falling head or constant head method (see Klute and Dirksen, 1986) as it applies to the experimental setup. The hydraulic conductivity of the porous material must be higher than the soil material itself, or the plate characteristics will define the velocity of water movement. Thus, the goal is to choose a porous plate which has a high hydraulic conductivity and a high bubbling pressure.

4.3.3.1 Buchner Funnel Method

Introduction

In this method, the soil core with its metal retaining ring is placed on a Buchner funnel, saturated, and then subjected to increasing tensions through a hanging water column. The Buchner funnel has a fritted glass porous plate ranging from coarse (bubbling pressure less than 50 cm) to fine (F) porosity (approaching 0.5 bar). There is also an ultra-fine (UF) Buchner funnel which has smaller pores and consequently would allow higher tensions. It is strongly recommended that a funnel just slightly larger in diameter than soil sample is used to reduce potential evaporation problems. Two variations of the Buchner funnel method exist. The first variation involves the use of a buret attached to a hanging water column, and the second uses a graduated cylinder also attached to a hanging water column. In both cases, a tension is imposed on the soil sample by lowering the buret or graduated cylinder so that the water level is below a preestablished datum point (usually the base of the soil core). The gradient imposed on the sample causes water to flow out of the soil sample and into the collection vessel. Water continues to flow from the sample until the energy level of soil water is in equilibrium with the tension. The amount of water removed from the sample is then recorded, and used in the calculation of water content for that tension imposed on the sample.

Material

A number of experimental set-ups can be developed to accomplish the same objective; however, the Buchner funnel is needed in each case. When possible, the experiment should be performed on undisturbed soil contained in a sample ring (see Appendix B, Section 1 Field Soil Sampling). Equipment needed to perform the experiments include either a buret or graduated cylinder, flexible tubing for connecting with the Buchner funnel, and several clamps. Choosing a tubing that retards air flow is advisable. Some tubing is permeable to air, and eventually, large air bubbles form beneath the porous plate increasing the potential for error.

Procedure

The Buchner funnel method is not fully described by Klute (1986), who concentrates on the pressure methods. Thus, a procedure is described below.

(1) Place the Buchner funnel upside down in a large pan and fill the funnel with water. Attach the hose to the funnel and the buret. Fill the hose and about half the buret with water. Avoid having air trapped in the hose. Particularly check the joints where the various pieces fit together. It is helpful to use de-aired water to help prevent air problems (Figure A.4).

(2) Clamp the buret and the upright Buchner funnel to a stand. The water level in the buret should be just above the Buchner funnel porous plate.

(3) Prepare the undisturbed soil sample by shaving the open soil surface that will be placed on the porous plate until it is perfectly level with the sides of the ring (see Field Soil Sampling for a discussion on collection of undisturbed soil samples). This step is very important because it ensures good contact between the soil and the porous plate to allow the water to pass through. The volume of sample can be determined accurately, which is then used to calculate bulk density.

(4) Remove the Buchner funnel from the stand, invert it and place the soil sample with the surface against the porous plate. It may be helpful to place the sample upside-down on a soil can lid when moving it around to prevent soil from falling out of the ring. Turn the funnel upright and clamp funnel to stand. Cover the tops of the funnel and buret with Parafilm (thin waxed plastic sheet) or foil to prevent evaporation. Punch a small hole in each piece of Parafilm to allow air pressures to equilibrate.

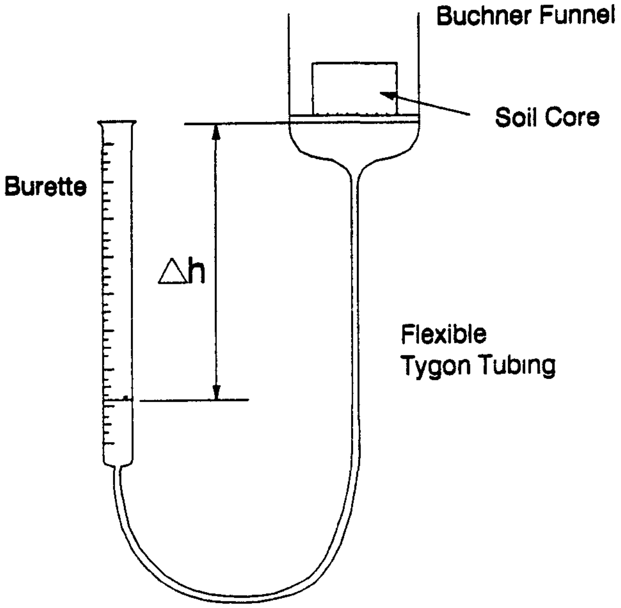


Figure A.4 Diagram of experimental setup of buchner funnel method for determining water retention function

(5) Saturate the soil sample from below by keeping a positive head in the funnel (i.e., keep the water level in the buret several inches above the top of the soil). If water builds up on top of the porous plate, decrease the positive head slightly. Be sure that excess soil doesn't seep out onto the porous plate. If this begins to happen, immediately reduce the positive head of water. It may take 20 minutes to overnight to reach saturation. This is dependent on the soil texture and initial water content.

(6) Determine the reference level used during the experiment. Ideally this is the bottom of the soil ring, but the center of the ring can also be used. Once the reference point is set, it cannot be changed.

(7) Just before applying suction, adjust the water level to the bottom of the buret. The idea is to have the water level in the readable part of the buret, with enough room for the water that will come out of the soil sample. If excess water is on top of the porous plate, remove it with a syringe.

(8) Tension from 0 to about 150 cm can be applied to the soil sample. The tension refers to distance between the water level in the buret and the chosen reference level. The water in the buret is below the reference level. Allow the system to equilibrate. Remeasure the distance and the change in the amount of water in the buret. Equilibrium times should be an hour or more for the first steps and increasing at higher tensions. This will vary with different soils.

For example: Assume the reference level is the center of the ring. Move the buret down (or the Buchner funnel up) so that the initial "height" or distance between the reference level and the water in the buret is 25 cm. Immediately note the buret reading. Allow the system to equilibrate until the water level in the buret has stabilized. Measure the equilibrium height, which will be less than 25 cm, and note the equilibrium water level. The change of water level in the buret is the amount of water drained from the soil under the equilibrium tension. The equilibrium tension (less than 25 cm) and the volume of outflow are used in all calculations.

Ideally, the equilibrium water volume should be the same as the initial volume for the next tension, but realistically it may not be the same because of volume changes in the tubing as the tension increases between readings. The initial water level must be read each time before changing pressure steps.

(9) Repeat step 8 for all tensions. Note that air may enter the system at high suctions. This can be avoided by choosing the proper flexible tubing, and by ensuring that the fritted plate is fully saturated with water prior to starting the experiment.

(10) After taking the last reading, remove the sample from the funnel without changing the water tension. Be sure to remove all the sample from the funnel and determine its wet weight and oven dry weight. Also, determine the volume of the sample in the ring in order to compute bulk density.

(11) Calculate the volumetric soil water content for each equilibrium tension by using the final water content obtained under step 10, and working backwards. This method is preferable because the initial saturation may not be 100%.

Comments

Use of soil cores contained in a sampling ring usually will yield results more representative of field conditions. Once placed on the fritted glass plate, soil in the sampling ring tends to have better contact with the porous plate than loose soil. Another advantage to using a sampling ring is that the volume, bulk density, and porosity sample are more easily calculated. Experiments using soil without the sampling ring are less controlled and more subject to error. Soils that swell upon wetting (i.e., those containing smectite clays, etc.) require special precautions. The volume changes of the sample for swelling soils can be significant and should be accounted for or controlled. Klute (1986) has shown how to manage swelling by loading the sample with a weight on the top to confine the sample during wetting and drying. Such loading may reasonably represent all but unconfined surface soils, because most soils experience some confining pressure in the field due to overburden loads.

4.3.3.2 Pressure Cell Method

Introduction

This method is similar to the above, except that a pressure cell is used. A pressure cell is a device which allows undisturbed soils to be tested under pressure, or under higher vacuums than can be easily applied using the Buchner funnel. Figures A.5 and A.6 show an exploded view of a pressure cell, and a sample experimental setup. The soil core is fully contained inside the cell, which is surrounded on the bottom by a porous plastic or ceramic plate, and on the top either by another plate or slotted acrylic. The soil in the cell is usually saturated at the beginning of the experiment when regulated pressure (or vacuum) is applied. Water content is calculated by measuring the outflow volume from the cell and knowing the initial water content. Alternatively, the weight of the pressure cell containing the soil can be measured and used to determine the water content of the soil at each pressure step used.

Material

The authors have obtained pressure cells, Tempe cells, or flow cells from Soilmoisture Equipment Corp, (Santa Barbara, California) and Soil Measurement Systems (Tucson, Arizona). A variety of pressure cells are available to accommodate different sized soil cores and alternative types of porous plates.

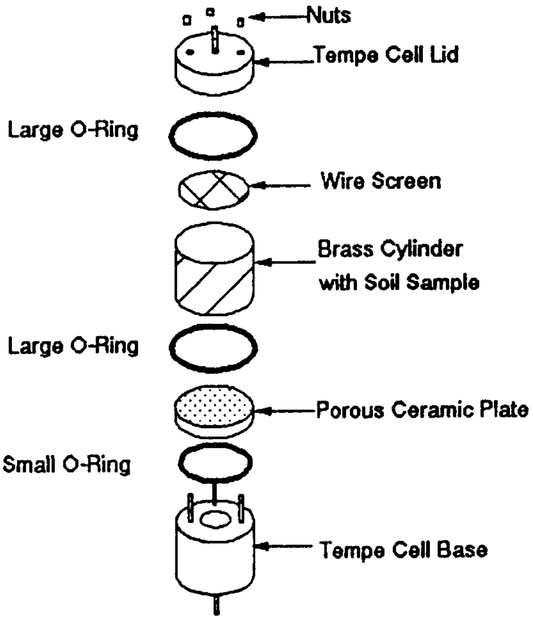


Figure A.5 Exploded view of tempe cell

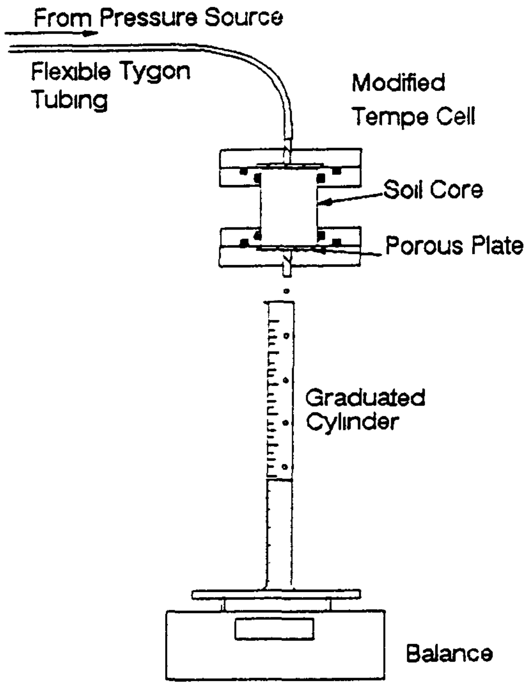


Figure A.6 **Diagram of experimental setup using modified tempe cell and pressure source for determining water retention function (soil measurement systems, Tucson, Arizona)**

Procedure

The procedure for this type of analysis is fully described by Klute (1986), as well as several comments about soil test solution, sample wetting, and temperature effects. The interested reader should consult this reference.

4.3.3.3 Pressure Chamber Method

Introduction

This method is a combination of the Buchner funnel and pressure cell methods. Samples are placed on a porous plate, like Method 4.3.3.1, but instead of using a hanging water column, a pressure chamber is used. An advantage of the pressure chamber is that several samples can be analyzed at one time, and, depending on the limits of the porous plate, pressures up to 15 bar (1.5 MPa) can be applied. The overall concept is exactly the same as the two previously described methods, and the length of time for completing the experiment depends on the soil and pressure ranges desired.

Material

Equipment needed for this method includes a pressure chamber, a ceramic plate with a bubbling pressure of at least 15 bar (1.5 MPa) (or the upper pressure level to be applied to the sample), and a pressure system with a regulator. The authors have obtained pressure chambers, ceramic plates, pressure systems, and regulators from Soilmoisture Equipment Corporation (Santa Barbara, California); however, pressure systems and regulators can be obtained from hardware stores.

Procedure

The method varies slightly for undisturbed and disturbed samples. Undisturbed samples are treated exactly as above in the previously described methods. Disturbed samples are prepared by pouring the sample into a sample retaining ring placed on a prewetted porous plate. The samples are then saturated using a squirt bottle. Water is applied to the soil near the side of the ring, and allowed to saturate the bulk of the sample from below. Between each pressure step, a small subsample should be taken and weighed. This provides the water content corresponding to the pressure.

The complete procedure for this type of analysis is described by Klute (1986).

4.3.4 Quality Assurance/Quality Control

A quality assurance/quality control (QA/QC) program for ensuring accurate and reproducible results from laboratory procedures is becoming more important as these procedures are used to support remedial actions at, or license applications for disposal sites. Several items should be considered when the QA/QC program is developed for performing water release experiments.

(1) Of particular importance is the condition of equilibrium for each pressure step. Although not standardized, a general guideline can be used where equilibrium is established when outflow is less than .1 ml in a 24 hour time period. This criterion ensures that the outflow rate is essentially zero.

(2) The experimenter must ensure that no pressure or vacuum leaks exist when using the Pressure cell or pressure chamber. Leaks will render the experimental results useless because the pressure or vacuum inside the core will not be the same as that recorded on the pressure gages. Leaks can also dry the soil, depending on where the leak is, and on the type of equipment used.

(3) It is critical that good contact be established between the soil core and the porous plate. A poor contact will preclude accurate results because only a percentage of the soil core is involved in the flow processes.

(4) The test fluid used during the test can have a profound affect on the test results. Low salt solutions can cause clay particles to defloculate and migrate through the soil in such a way that pores clog, thus affecting the water retention. This problem is more important for finer textured soils that contain significant amounts of swelling clays. Soil solution concentration is not usually an issue for coarse textured soils because swelling clays are not present. It is recommended that a deaerated 0.005 M $CaS0_4$ solution be used as a general test fluid (Klute, 1986). This concentration should be modified if necessary.

Another aspect of the test fluid which may or may not be important is the presence of a bacterial inhibitor, such as thymol or mercuric chloride. Long-term experiments could lead to bacterial growth, which will affect the retention results.

(5) The behavior of ceramic plates changes over time. Variability of the plates is caused by uneven plugging of pores, and possibly the presence of bacteria. To test the variability of plates, it is recommended that 10 to 15 samples be placed on the plate, so that the water content can be determined at 1 bar (0.1 MPa). (1 bar is suggested because it can be a standard pressure for testing plates with differing porosities and bubbling pressures). Take the average, standard deviation and CV (coefficient of variation) for each plate. Plates with high CV should be cleaned and retested, or retired from use. This test becomes especially important when using multiple plates for testing a larger number of samples. This occurs when, due to time constraints, several plates of different

bubbling pressures are used. Differences in plate behavior can affect the final results, because suction on certain areas of the plates will be much lower. Plate should be tested over time. There is mounting evidence that, even when care is taken to ensure correct plate hygiene and cleanliness, that the 15 bar plates either have exceedingly low conductivities, or plug with use.

(6) Plate manufacturers will rate the plates according to the highest pressure recommended for use (some value below the plate bubbling pressure). Typical ratings are expressed in bars, thus plates of 1 bar, 5 bar and 15 bar maximum pressure are used. The result is that water contents obtained on 15 bar plates at 15 bar (1.5 MPa) applied pressure are often equal to or higher than those obtained on 5 bar plates at 5 bar (0.5 MPa) applied pressure. Such was the experience of laboratory experiments during the analysis of the 595 samples collected from the Las Cruces Trench site. Others (Jones et al., 1990) have tested the "equilibrium" water potential of samples taken from 15 bar pressure plates and found that in the majority of cases (more than 80% of all tests), equilibrium was not obtained and the sample was generally at a lower suction than the applied pressure. The phenomenon could be caused by plate impedance (Valiantsaz, 1990), causing significant energy loss through the porous plate. This error causes water contents at 15 bar (1.5 MPa) to be overestimated. Based on these observations, we recommend that, if 15 bar plates are used selected samples from each 15 bar plate test not only be measured for water content but also be sampled for water potential. Laboratory thermocouple psychrometers are available for this measurement (Jones et al., 1990).

(7) It is also recommended that, in the pressure chamber method, a known sample be run to detect a faulty run. Small leaks are difficult to detect and the final water content may not be reflective of true conditions. If the water content of the known sample falls outside of a predetermined range of acceptable values, then all the samples can be rerun at the appropriate pressure.

4.4 Laboratory Saturated Hydraulic Conductivity

4.4.1 Introduction

Hydraulic conductivity is a measure of the ease with which water can flow through soil. Having the units of flux (L/T), it is the slope of the flux versus gradient curve. The hydraulic conductivity is one of the most important hydraulic parameters to be characterized in the soil, because of its' effect on the movement of water and contaminants in soil. Zones with higher conductivity, such as sand lenses or buried stream channels, can concentrate the bulk of soil water flow, creating significant difficulties when characterizing these areas.

The hydraulic conductivity is of major interest to hydrologists, soil physicists, and engineers, especially above the water table, in partially to near saturated material, because of the strong dependence of conductivity on water content. This non-linear relationship is so difficult to characterize, that most practitioners choose to estimate it, rather than attempt to determine it experimentally. Unsaturated hydraulic conductivity is discussed in detail on page 105.

Saturated hydraulic conductivity is used in Darcy's Law to determine rate of movement of water and, ultimately, contaminants:

$$v = -K\frac{dh}{dl} \tag{10}$$

where

v = Darcy velocity (L/T)
K = saturated hydraulic conductivity (L/T)
$\frac{dh}{dl}$ = hydraulic gradient (dimensionless)

For saturated systems, conductivity is constant in time, for any point in the flow field, though not necessarily equal from point to point. Differences in the physical structure of the porous material cause heterogeneities and anisotropy in conductivity. The hydraulic conductivity used in this equation is analogous to electrical conductivity and thermal conductivity in electrical and heat transfer problems, respectively. From the above equation, it can be seen that the hydraulic gradient needs to be determined before calculating conductivity. For laboratory experiments, the gradient is found by monitoring the hydraulic head at two locations. In most cases, these are the upper and lower boundaries of the soil core. For saturated experiments, it is customary to assume that the matric potential of the soil is zero. Thus, the flux divided by the gradient, taking into account only the elevation head, results in the conductivity.

Determination of saturated hydraulic conductivity (K_{sat}) in the laboratory has been performed for decades (in fact Darcy looked at this problem in 1856). Since that time, many papers and texts have been written to describe procedures for determining conductivity, though many concentrate of theory rather than step-by-step descriptions. Klute and Dirksen (1986) provide an in-depth discussion on the different methods, as well as a large reference section. The reader should consult this reference before deciding on a particular method.

4.4.2 Principles

The value of saturated hydraulic conductivity measured through experimentation implies that all the pores within the soil core are filled with water and contribute to flow. If tension is applied to the soil sample and water is removed, the largest pores will drain first and only the smaller pores will be available for transporting fluids. Because of this phenomenon, the saturated cross-sectional area of the sample will decrease very rapidly at first, then, depending on the pore size distribution, the rate of decrease will change. Indeed, Poiseuille's Law states that the flow rate through a capillary tube is proportional to r^4. Very small changes in the cross-sectional area lead to large changes in flow. This section deals with saturated conditions only.

The principles behind both laboratory procedures discussed in this chapter are the same. The experimenter is attempting to measure both the hydraulic head difference across the core, and the flow rate of fluid from the core. In the case of the constant head method, the hydraulic head above the core remains constant, either through the use of a mariotte tube, lab pump or a system of siphoning with a lab pump. By isolating the head, a relatively simple calculation is used, where the user solves for the hydraulic conductivity, and divides flux rate by the gradient. Average values can be obtained by taking a series of measurements over time. The falling head method is similar, except that the head above the sample is allowed to decrease during the experiment. The user monitors the change in water level in the reservoir above the sample. The flux rate and the head can be calculated from this information; these data are then used in a formula for determining hydraulic conductivity.

The methods discussed below, and the associated theory, are fully described by Klute and Dirksen (1986). The interested reader should consult this reference.

4.4.3 Methods

4.4.3.1 Constant Head Method

Introduction

The constant head method is effective for determining saturated hydraulic conductivity of soils. It may be more effective than the falling head method because, during the test, the soil core is, more or less, in steady state; steady state conditions are never achieved in the falling head method. Experimentally, setting up this test may be tedious, depending on the amount of automated data collection desired by the user. However, with little effort, the experiment can proceed without the need for the user to stand-by and collect data. Several issues which the user will face during the experimental setup and during data analysis include: determining the correct concentration of salts in the soil test solution, interpreting changes in saturated hydraulic conductivity with time, maintaining saturated conditions throughout and at the bottom of the core, and showing that unit gradient conditions exist in the core. These issues will be discussed briefly below in the comments section.

Material

The experiment will require a soil core filled with soil to the approximate field bulk density found at the site, or with undisturbed sample. Care should be taken to exclude larger stones in the sample, and cracks or fissures which will lead to preferential flow. Material will be needed to retain the soil in the core. Klute and Dirksen (1986) recommend the use of cheesecloth, or finer material for silty soil. Porous stainless steel, with very large pores, can be used for this purpose. Also, cheesecloth with a screen to prevent swelling can be used. In any case, it is important that the sample not be disturbed during the saturation process. A system for maintaining constant head must be developed. Several set-ups can be envisioned for this type of test: a siphoning system, mariotte tube, small water bath or constant head using a lab pump, are all effective. The user may require laboratory stands, a pressure cell apparatus, and tensiometers, if the sample is not fully saturated.

Procedures

The soil sample should be saturated prior to performing the experiment. Saturating the sample is done by placing the soil core into a tank with the bottom of the core near a water surface. Saturating the sample from below allows entrapped air to escape from the core; saturating the sample from above will not be effective in removing entrapped air. The water in the tank should be increased slowly until the water level is equal to the top of the core. It is important to keep the water level from rising too fast, or above the top of the soil core, unless the soil is well contained. Klute and Dirksen (1986) mention the occasional need to prepare the sample to "natural saturation," the state of saturation achieved when the sample is saturated from above. This may be desired given that under natural conditions, soil usually is flooded from above and not from below. Although not specified explicitly by Klute and Dirksen, allowing the sample to saturate for 24 hours should be sufficient to remove air bubbles. Another method to remove entrapped air bubbles is to flush the sample with CO_2 prior to wetting.

As mentioned above, three methods of setting up the constant head system are commonly used. The siphoning system, and the constant head using a lab pump are described in Klute and Dirksen (1986). The third method not discussed therein is the use of a mariotte tube. Figure A.7 shows a schematic of this method. Theoretically, atmospheric pressure is maintained at the bottom of the mariotte tube, and at the bottom of the core. Pressure applied on the water entering the soil remains constant, regardless of the amount of water in the reservoir column. Gradient is established by adjusting the height of the bottom of the tube with respect to the top of the soil sample. Outflow can be measured on an electronic balance, or simply with a graduated cylinder. A disadvantage of this method is the limited amount of water that can reasonably be added to the

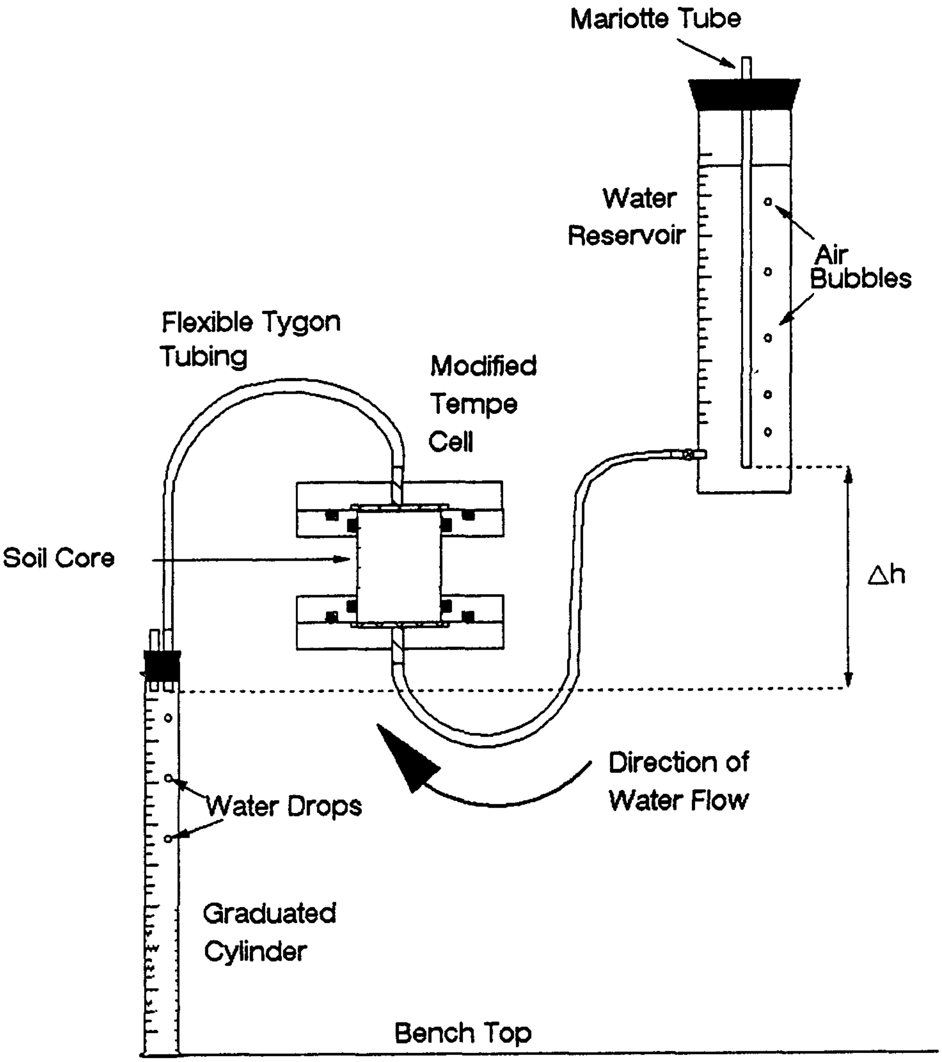


Figure A.7 Diagram of setup using mariotte tube for saturated hydraulic conductivity experiments

reservoir column. Large volumes of water become tedious to use, and adding additional water to the reservoir may disturb the experiment. For coarser-grained soils, conductivity may be high enough to preclude a long term test (the water may flow through the core too fast). Figure A.8 shows a diagram of the water bath method, wherein the gradient across the soil core is measured from the water level in the beaker to the opening of the outflow tube. Constant water levels are maintained in the large beaker using a lab pump and siphon. An advantage of this method is that air bubbles cannot enter through any of the connections, and the test can be conducted for long time periods. The user should choose the test method that best fits the soil type being analyzed.

The test should be run, in theory, until the conductivity results stabilize. If the sample is fully saturated at the beginning of the experiment, steady state should be achieved fairly rapidly. Several issues must be addressed during this experiment. They are discussed below.

Comments

The user may find the conductivity fluctuating during the experiment, either to higher or lower values. For example, the use of a soil solution too low in dissolved salts may cause clay in the soil sample to defloculate and clog larger pores (Dane and Klute, 1977). Conductivity can be reduced essentially to zero if sufficient clay defloculates. It is recommended by Klute and Dirksen (1986) that the test fluid used for the experiment resemble the composition of the original soil water. In this way, geochemical affects are minimized. However, it may not be possible or practical to sample and analyze preexisting soil solution, and obtaining one as an

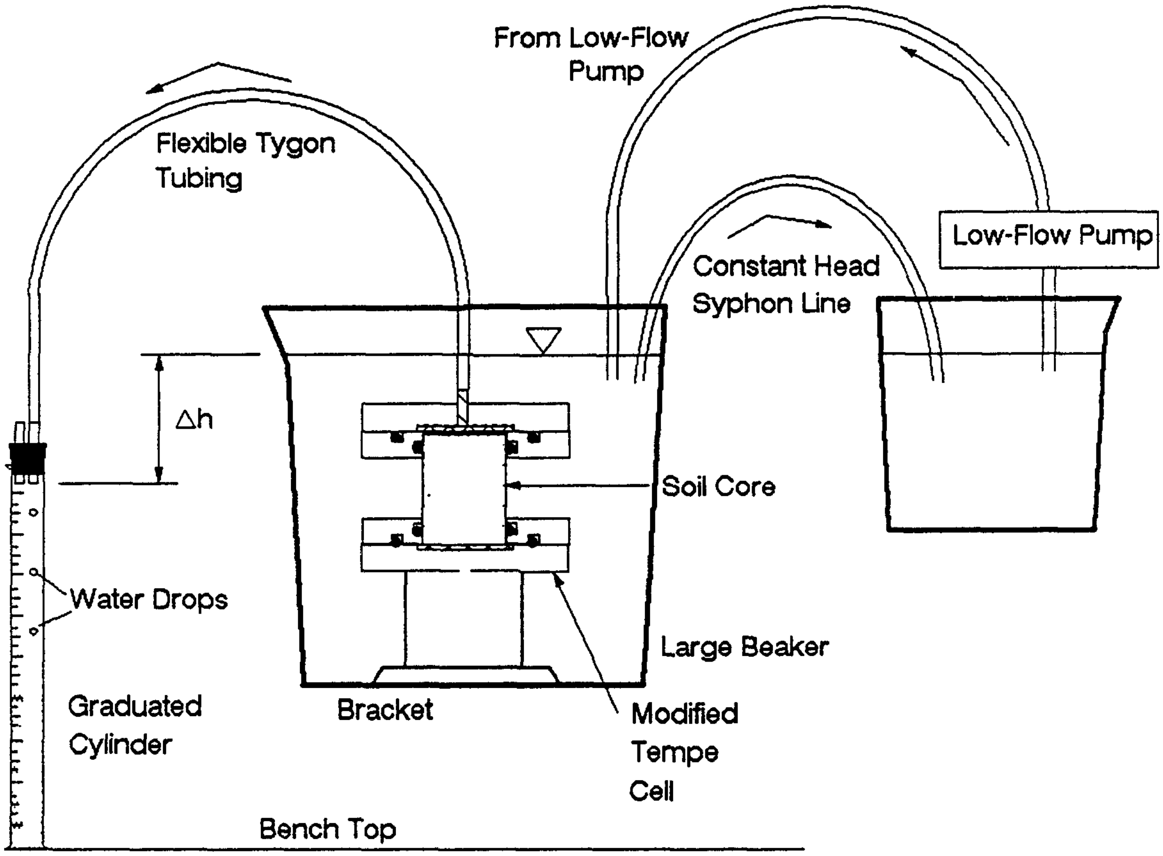


Figure A.8 Diagram of setup using water bath for K_{sat} experiments extract may not be accurate either. Thus, if the soil water can be sampled and analyzed prior to performing the experiment, the conductivity results should more accurately reflect field conditions. If soil water cannot be sampled, the user should use deaerated 0.005 M $CaSO_4$ solution. An antibacterial agent, such as thymol mercuric chloride, or cupric chloride, should be considered, because of the rapid nature that bacteria can multiply in the soil and clog pores. Short term tests may not require biological inhibitors.

Laboratory procedures can also results in abnormally high conductivity values. If, for example, a large gradient is imposed on a coarser soil sample, fine particles from the sample can be removed, resulting in incorrect conductivity values. For this reason, and also because of difficulties in keeping the sample saturated at the base of the core, the user should consider using a gradient of less than unity.

It is important to maintain saturated conditions at the base of the core. Coarser samples lead to such rapid dewatering, that water cannot be transmitted fast enough to maintain a constant cross-sectional area contributing to flow. As mentioned above, desaturation of soil causes a rapid decrease of hydraulic conductivity; thus, the final conductivity values for the sample will reflect that experienced at the bottom of the core. The user may consider the use of tensiometers to monitor hydraulic gradient during the experiment. Though it is normally assumed that unit conditions exist in the core, partial saturation or differences in material properties may lead to a deviation from unity. The use of tensiometers, with either manometers or pressure transducers, will allow the user to more accurately calculate conductivity.

4.4.3.2 Falling Head Method

Introduction

The falling head method is similar in principle to the constant head method, except that in this case, the gradient imposed on the sample decreases with time. The equation for calculating hydraulic conductivity is similar to Darcy's Law, except that the change in volume of water flowing from the soil core is integrated over time and the change in head. The resulting equation is

$$K = \left(\frac{aL}{At}\right)\ln\left(\frac{H_1}{H_2}\right) \tag{11}$$

where

A = the cross-sectional area of the sample (L^2)
L = the length of the sample (L)
a = the cross-sectional area of the reservoir (L^2)
H = the head measured at different times (L)
t = time difference between H_1 and H_2

The issues that need to be addressed which may result in experimental errors are the same as for the constant head test. Desaturation of the soil at the base of the core, test fluid composition, and determining the gradient in the core must be addressed prior to performing the experiment.

Material

The equipment required for this test is similar to that used for the constant head test. A lab pump would not be necessary since water is not added to the reservoir after the experiment begins.

Procedures

Klute and Dirksen (1986) provide a thorough discussion of the procedures for this test, and provide several references.

4.4.4 Quality Assurance/Quality Control

A number of experimental errors can develop which will affect conductivity results. These include ensuring that the conductivity value is somewhat stable before ending the experiment, the fines within the sample are not being removed, and the outflow volume is being measured accurately. Measurement of outflow is critical for low conductivity samples where outflow is 50 ml/day or lower. It may be necessary, in these cases, to use an electronic balance connected to a computer to automate these measurements. Automation will also be useful in calculating hydraulic conductivity in real time, so that an assessment of steady conductivity measurements can be made. The user may need pressure transducers connected with tensiometers if the conductivity of the sample leads to desaturation of soil. Then the conductivity is evaluated for the soil between the tensiometers (operated in the piezometer (positive pressure) mode), rather than for the entire soil sample. Applying a gradient on the sample which is too high can lead to the translocation and removal of fines from the sample. The outflow test fluid should be checked for significant amounts of silt or clay-sized particles. Even small percentages of these fractions (3-4%) will significantly reduce the conductivity of the sample.

4.5 Laboratory Unsaturated Hydraulic Conductivity

4.5.1 Introduction

Research has been conducted on various techniques to minimize the time and labor needed to determine the relationships between hydraulic conductivity ($K(\theta)$) and soil tension ($h(\theta)$) to soil water content. The reason for this effort lies in understanding how water and dissolved constituents (for example, hazardous materials, nitrates, etc.) move downward through the soil profile to the water table. The rate, direction and volumes of water which migrate through the soil are dependent in large part on the hydraulic conductivity, which in turn is dependent on the water content of the soil. However, this relationship is not mathematically or physically well understood, leading to errors in predicting how quickly or slowly water and dissolved constituents move with time.

Depending on the texture of the soil, the procedure used, and the range of water contents included in the experiment, the time required for determining the $K(\theta)$ relationship may be longer than several months. Such a long time-frame precludes adequate characterization of soils for permits and licenses. Therefore, newer, faster methods need to be used that efficiently determine this hydraulic relationship.

The methods described herein will be categorized into steady-state and transient. Steady state experiments usually involve the collection of data on the hydraulic conditions of the sample after they are stable. Steady state experiments, though time consuming, can be used to determine multiple points on the $K(\theta)$ curve. Transient experiments, on the other hand, involve the collection of parameter values collected while they are changing with time. These experiments have not been perfected yet, and they invariably require the use of parameter estimation techniques and water flow modeling to predict the shape of the $K(\theta)$ and $K(h)$ functions. However, their great advantage is that the functions can be predicted after a very short experimental procedure lasting on the order of days, rather than weeks or longer.

This chapter will present several methods of determining the K(θ) and K(h) relationships, including steady state and transient methods. It will describe briefly several methods documented more extensively by Klute and Dirksen (1986), and Dirksen (1991). Other references will be provided when appropriate.

4.5.2 Principles

4.5.2.1 Steady State Experiments

Determining the hydraulic conductivity of soil cores involves extending Darcy's law to unsaturated material. This extension assumes that the hydraulic conductivity is a function of water content and that it can still be used as a proportionality constant between flux and hydraulic gradient. The governing equation for flow in the unsaturated zone is

$$q = -K(\theta)\left(\frac{dH}{dl}\right) \tag{12}$$

where

q = flux density (L/T)
H = total hydraulic head (L)
l = length of the sample (L)
$K(\theta)$ = hydraulic conductivity (L/T)

The gradient in hydraulic head provides a measure of the change in the energy status of the soil water along the length of the core sample. The hydraulic head is a function of elevation head and matric potential or tension. It is determined by summing the height of the point of interest (elevation head) above a preestablished datum point and the soil water tension at that point. A unit gradient indicates that the total hydraulic head changes at the same rate as the elevation head, or that the soil water tension is the same everywhere in the core. Because of the strong relationship between water content and tension (see Section 4.3 for a discussion of Water Retention Function), a tension that is constant in space indicates a uniform water content, which implies that the hydraulic conductivity is also constant. This is important because the hydraulic conductivity value determined through experimentation is averaged for the soil sample.

The relationship between hydraulic conductivity and water content is highly non-linear, and thus it can not be defined by determining the conductivity at one or two water contents. For example, Hills et al. (1989) presented laboratory data showing the non-linear relationship between conductivity and water content for clay loam and sand. They also presented results from seven different estimation techniques for predicting the relationship between these parameters. Though many of the fits were close, none of the methods were able to match the observed data exactly. This example shows that simple mathematical techniques are not able to fully predict the entire conductivity curve found using steady state experiments.

Steady state experiments work on the principle that hydraulic conditions within the core are no longer a function of time. Flux is applied to the core at a constant rate, and vacuum is applied at the bottom of the core to remove water that may be accumulating, thus allowing the water content and hydraulic gradient to reach equilibrium. At this point in the experiment, the user solves equation (12) for the hydraulic conductivity and determines the water content of the core, thus providing a point on the K(θ) curve. Water content is determined by weighing the core between flux steps, by using TDR, or by estimating water content from the water retention curve. The Section on Laboratory Water Content discusses the various methods of determining water content in soil.

4.5.2.2 Transient Experiments

Determining conductivity from transient experiments requires data collection while the hydraulic parameters (i.e., water content, water tension) are changing. Experiments of this type require more intensive data collection and more complicated experimental procedures. The reason behind this additional need for data collection is that water content, water tension and hydraulic gradient are changing rapidly during the experiment. Thus, when a 'snapshot' of these conditions is needed to calculate hydraulic conductivity, the frequency of data collection becomes very important.

Almost all transient experiments provide a measure of sorptivity, from which the hydraulic conductivity is determined (Dirksen, 1991). The sorptivity is a measure of the ability of water to diffuse through soil, and is dependent on the water content and hydraulic gradient. During transient experiments, water moves through soil largely under the forces of the tension gradient. As the soil water conditions reach steady state, the tension gradient approaches zero and gravity becomes the dominant driving force (steady state implies that hydraulic conditions in the core are not changing with time). Using the sorptivity and the Boltzman transformation (Kirkham and Powers, 1972), soil water diffusivity is determined, from which the hydraulic conductivity is calculated via the following equation:

$$K(\theta) = D(\theta)\frac{d\theta}{dh} \tag{13}$$

where

$D(\theta)$ = soil water diffusivity as a function of water content (L^2/T)

$\frac{d\theta}{dh}$ = $c(\theta)$ = specific water capacity as a function of moisture content (L^{-1})

Although determining hydraulic conductivity from transient experiments is more difficult, these experiments have the advantage over steady state experiments of being much more efficient and less time consuming. Thus, more samples could be analyzed in the same time period, especially when automated techniques are used. For example, Chung et al. (1988) discussed a way to automate the data collection of up to 16 soil cores using the one-step outflow method.

For the analysis of transient experiments, one frequently uses parameter estimation techniques. Parameter estimation provides a method of determining the hydraulic conductivity function after performing a single transient experiment. With parameter estimation, the user chooses a mathematical expression or function that describes the water retention data and includes one or more empirical parameters (for example van Genuchten's equation (1980)). The user then makes an educated guess of these parameter values, uses a flow model to simulate movement of water, compares the predicted results with observed experimental results, then optimizes the parameter values to obtain a better fit with the observed data.

Parameter estimation techniques can be effective for understanding flow in similar soils, or soils within the same profile, without the need to run long-term laboratory experiments. Hudson et al. (1991) showed that when water content and tension were collected accurately during transient experiments lasting several days, retention and conductivity functions could be estimated successfully.

4.5.3 Procedures

4.5.3.1 Steady-State Experiments

Constant Head Method

It was discussed earlier that Darcy's Law is the governing equation for determining the flux density of water, which is equal to the product of the conductivity and hydraulic gradient. Thus, by keeping the hydraulic gradient stable during experiments, flux through the core will be equal to the hydraulic conductivity times the gradient. Experimentally, this requires the head to be fixed at the top and bottom of the soil core. The soil core is normally contained in a pressure cell between two porous plates. Once the pressure head is made equal on both ends of the core, only the gravitational head varies with elevation, and unit gradient should be obtained.

The range of measurements that can be achieved with this method depends on the equipment used. The bubbling pressure of the porous plate, for example, represents the lower range of tensions that can be applied to the core before the column of water is broken between the soil and porous plate. Also, because of the need to perform these experiments within a reasonable time frame, experiments at tensions greater than about 300 cm could take a prohibitive amount of time.

A potential problem with this experimental setup can be poor contact between the soil core and the porous plates. Poor contact leads to resistance between the two materials and energy loss. If this becomes significant, the effective pressure head imposed on the soil will be less than expected, leading to an actual hydraulic gradient different from unity. Therefore, it is recommended that, at least for soil columns less than about 10-15 cm in length, tensiometers be installed to measure actual soil water tension during the experiment (Klute and Dirksen, 1986). Tensiometers can be connected to either manometers or pressure transducers. It can be assumed that the contact resistance is nominal or near zero if the tension measured in the soil with the tensiometer approximately equals the tension applied to the soil core from the vacuum. Gradients should be calculated from the tensiometer readings.

By measuring the output volume from the bottom of the core, the user can determine when the core has reached steady outflow. True steady-state is reached when the outflow and the tension are constant, and the tension is the same everywhere in the core. Gravity then becomes the driving force for flow in the soil column. If flux in equals flux out, but unit gradient is not observed in the core, it may be necessary to adjust the vacuum on the bottom of the column. When unit gradient is achieved, the water content of the core can be determined. At this point, the user has knowledge of the tension (from the tensiometers), water content (from the weight of the soil column), and hydraulic conductivity (from the flux). Tension is then adjusted on the top and bottom of the column, and flux is monitored until another data point can be obtained. These data can be plotted to yield the $K(\theta)$ and $h(\theta)$ curves.

Klute and Dirksen (1986) discuss this method in detail, including diagrams of the experimental set-up and calculations, so they will not be included herein. The reader should consult this reference for further information.

Constant Flux Method

The constant flux method endeavors to achieve steady-state conditions by fixing the flux into the core. Thus, when unit gradient is observed, the applied flux equals the conductivity. In theory, this method should provide the same level of accuracy as the constant head method.

The experimental setup varies from the constant head method in that a porous plate is used only on the bottom of the core where the vacuum source is attached. The top of the core does not have a porous plate because of the need for the core to be open during water application. During the experiment, water is applied to the core at a specified flux, and the vacuum source is adjusted until a unit gradient is observed. Steady state is achieved when the flux into the core equals the flux out, and the tension remains constant everywhere in the core.

The range of fluxes which can be applied to the core is somewhat limited due to experimental constraints. The upper limit of flux is, of course, the saturated hydraulic conductivity. The lower flux is not as straightforward. Because steady state experiments require a 'constant' influx of water, very low fluxes can not be applied uniformly. For example, a flux of 1 cm/day (i.e., 1.2 E-05 cm/sec) with a core of 7.62 cm diameter requires the steady application of 14.5 ml over 24 hours. This low flux is difficult to achieve without the use of special water application systems.

Constant head and constant flux experiments have both advantages and disadvantages. Constant head experiments, while well suited for steady application of very low fluxes, have the disadvantage of requiring two porous plates. Two plates increases potential error due to contact resistance. This resistance cannot be readily quantified, nor is it possible to track potential changes in the resistance during the experiment. Thus, it may be very difficult to measure exactly the tension applied to the soil core and subsequent gradient calculations. The constant flux experiments have the advantage of experimentally fixing the flux, which can be measured easily. Also, the use of a single porous plate reduces uncertainty of resistance losses. However, it is difficult with these experiments to apply a low flux uniformly over soil columns.

4.5.3.2 Transients Experiments

The experimental set-up for transient experiments is similar to the one for steady-state experiments. Soil cores are contained in a pressure cell, with both ends closed off with porous plates. The bottom of the core is connected to a vacuum system for some experiments (i.e., one-step outflow) or to a water application system for others (i.e., slow upward infiltration). Tensiometers are used in at least two places for calculating hydraulic gradient. A balance is required for measuring either the change in weight of the core, or the amount of water added to the soil.

The difference between steady-state and transient experiments is the need for much more accurate data for transient experiments. Results of transient experiments are used directly in computer models to compare with simulations. These comparisons are extremely important when determining the hydraulic parameters used to generate the retention and conductivity functions. For example, Hudson et al. (1991) found that water content measurements using TDR needed to be accurate to within about 0.5% in order for his computer algorithm to converge to a unique solution of van Genuchten's parameters.

Several transient experiments are used to evaluate the hydraulic conductivity of soils. Dirksen (1991) listed these methods, and described their procedures and calculations to some detail. However, many of these methods are being refined significantly following the results of laboratory experiments. For this reason, procedures for the methods listed below will not be presented in detail. References will be provided when appropriate. The interested reader is recommended to consult these references and/or contact the authors. Five procedures will be listed below and briefly discussed. They include: One-Step Outflow, Multi-Step Outflow, Stepwise Inflow, Evaporation from a Core, and Upward Infiltration.

One Step Outflow The One-Step Outflow Method (Kool and Parker, 1985; Parker et al., 1985) is performed by connecting a vacuum or pressure source to a saturated soil column inside a pressure cell. The vacuum source can include either a hanging water column and buret or a vacuum pump connected to a manometer. The pressure source can be a small compressor. Pressure is applied to the top of the cell, or vacuum applied to the bottom of the cell, and the cumulative outflow is measured as a function of time. Outflow can be measured accurately using a pressure transducer placed near the bottom of a buret, or with a flask resting on an electronic balance connected to a computer. Soil tension is measured using tensiometers installed in the core. The volume of water removed is the cumulative discharge.

Multi-Step Outflow The Multi-Step Outflow Method is similar to the One-Step Outflow Method, except that multiple pressure or vacuum steps are applied to the top of the pressure cell from near zero (saturation) to close to one bar (the maximum tension before rendering the tensiometers useless). Soil tensions, cumulative outflow, and the time interval are recorded for each pressure step.

Multi-Step Inflow The Multi-Step Inflow Method is begun by placing the core in equilibrium with a given negative pressure. After reaching equilibrium, the negative pressure is increased (less negative pressure) and water flows back into the core until the water content is at equilibrium with the given pressure. Water flow and the time interval are recorded. The time for equilibrium to be reached, the volume of water added, and the soil tension are all recorded for each subsequent step This method has been developed because the use of several steady-state parameter values apparently improves the estimation of the hydraulic conductivity function (Hornung, 1983).

Evaporation from a Core The Evaporation from a Core Method was originally proposed by Wind (1966), and improved by Boels et al. (1978). The experiment is performed by placing a soil core in equilibrium with a free water surface. The soil core is then sealed at the lower end and allowed to evaporate at the upper end. Tension is measured with tensiometers installed along the core, and the discharge is measured by placing the apparatus on a balance and recording the change in weight. For evaporation into a constantly dry atmosphere (e.g., 0% humidity created by a desiccant placed over the soils), the only unknown is the unsaturated hydraulic conductivity function.

Upward Infiltration The Upward Infiltration Method was proposed by Toorman (1990), and developed in the laboratory by Hudson et al. (1991). The original proposed method involved hanging a soil core on a platform connected to a balance. The soil core is lowered until the base breaks the water surface of a constant level reservoir, allowing water to flow into the core via capillarity. Tension of the soil and weight of the core are recorded continuously until steady-state is achieved. However, flow into the soil occurred so rapidly, Hudson et al. (1991) found that the data could not be collected at a rate sufficient to perform the parameter estimation. He modified this method by adding water with a low-flow syringe pump obtained from Soil Measurement Systems. This application system can be sufficiently regulated to achieve steady flux into the core. Because the flux rate was slowed considerably, data could be collected more accurately and the hydraulic parameters could be estimated.

In all of the above experiments, the resultant data sets of tension, water content, and water fluxes are used as input to computer programs that can estimate the conductivity function.

4.5.4 Quality Assurance/Quality Control

A large number of quality control issues exist when performing hydraulic conductivity experiments. These experiments are the culmination of many other experiments which may need to be performed to evaluate the best methods of measuring water content, water tension and the retention function. The bulk of potential quality control issues have been discussed already in the appendices that describe measurement of water content, water tension and the retention function, so they will not be repeated herein.

However, it should be mentioned that replication of experiments is strongly encouraged given the nature of the experiments and possible influences of the experimental set-up on the results.

5 Transport Properties

5.1 Laboratory Dispersion Coefficient

5.1.1 Introduction

The dispersion coefficient is a measure of the extent of "mixing" that a slug or contaminant plume will undergo as it migrates through porous media. This mixing is called hydrodynamic dispersion, and is the sum of molecular diffusion and mechanical dispersion (Javandel et al., 1984). Molecular diffusion is a phenomenon that causes contaminants to spread out due to thermal (or kinematic) activity of dissolved species and random motion. Molecular diffusion is an active process, especially in a static fluid. Mechanical dispersion occurs in a non-static fluid when contaminant particles travel through pores of different radii, shapes, and directions, causing macroscopic velocities to differ depending on the pore size and pathway constraining the molecules. The deviation of these individual particle velocities from the average pore water velocity causes the molecules to migrate at different rates, and mix among themselves.

Manifestation of hydrodynamic dispersion (hereafter called dispersion) is seen by the smearing of sharp contaminant fronts downgradient of a point source. This smearing of a plume in groundwater systems is analogous to the spreading of a plume of smoke from a smokestack, or the spreading of a plume of waste water into an open body of water. This action of dispersion is responsible for the contamination of large volumes of soil and aquifer material from relatively small point sources.

The estimation of dispersion is extremely important when predicting the direction and rate of contaminant plume migration. Areas adjacent and cross-gradient to point sources may be contaminated if the lateral dispersion is high enough. More importantly, dispersion causes some contaminants to travel faster than the average pore water velocity leading to contamination of water supplies faster than predicted. On the positive side, dispersion reduces the concentration as the plume spreads. Solute transport models based on the convective dispersion equation rely heavily on the dispersion coefficient to simulate future contaminant concentrations in groundwater flow systems.

For these reasons, measurement of the dispersion coefficient in soils is important in a license application for LLW disposal. Performance assessment modeling, which attempts to create worst-case scenarios of possible contamination from LLW sites, uses dispersion coefficients (Kozak et al., 1989). Laboratory soil column experiments have been used to estimate field dispersion. However, there is mounting evidence that laboratory column data often fail to predict field dispersion, which has been found to be scale-dependent. The performance assessment activities are reviewed by state and Federal regulatory agencies who must either approve or disapprove the license application. Licensees, however, may choose to perform column experiments to obtain an idea of the dispersion in disturbed (backfill) soils that may surround the waste.

This section will describe how to determine dispersion coefficients for use in predictive calculations and models. Much of the discussion will be taken from van Genuchten and Wierenga (1986) who describe in detail the set-up of column experiments and derivation of the governing equations. Interested readers should consult this reference.

5.1.2 Principles

The spreading of contaminants in the downgradient direction (either hydraulically downgradient in saturated media or towards an area with a lower (more negative) potential) can be quantified by considering three components of transport: convective transport, molecular diffusion, and dispersive transport.

Convective transport describes the passive migration of contaminants with fluid movement in the absence of diffusion. It is not considered dispersion per se, but it is presented here because of it's influence on the migration of contaminants in ground and soil water.

Convective transport is determined by the following equation:

$$J_m = qC \tag{14}$$

where

J_m = solute flux density (M/TL^2)
q = volumetric fluid flux density (L^3/TL^2)
C = volume averaged concentration (M/L^3)

Molecular diffusion describes the motion of molecules, in a static fluid, due to random and natural thermal motion. The random component of diffusion is called Brownian movement, which describes the random path taken by molecules after colliding with one another. The theoretical framework of Brownian movement was developed by Einstein (1908), but more recently discussed by Csanady (1973). Briefly, Brownian motion can be described as a process in which the movement of molecules after a collision is assumed to be truly random. Given this assumption, the distribution of particles after a time period approximates a bell shaped curve whose shape is described by the mean and variance of the position of the particles. External impulses maintain this random movement. Natural thermal motion is also a driving force for molecules to diffuse away from one another. The phenomenon of random and thermal motion is described by Fick's Law, which states:

$$J_d = -D_m\left(\frac{\partial C}{\partial x}\right) \tag{15}$$

where

J_d = solute flux density due to diffusion (M/TL^3)
D_m = molecular diffusion coefficient (L^2/T)
x = distance (L)

Generally, diffusion is considered negligible for non-static groundwater conditions. However, diffusion is a significant process in stagnant ground or soil water systems, and must be considered when characterizing sites for LLW disposal (Federal Register, 1990).

Dispersive transport, the third component of transport, is caused by the tortuous path taken by the individual particles as they migrate through pores of different sizes, shapes, and directions. This tortuosity causes the effective velocity to be slower than the average pore velocity for some particles, and faster for others. Dispersive transport is considered to be a macroscopic phenomenon and occurs only when the fluid is moving. Given this requirement, we may write the governing equation for dispersive transport as,

$$J_h = -D_h\left(\frac{\partial C}{\partial x}\right) \tag{16}$$

where

J_h = solute flux density due to dispersive transport (M/TL^2)
D_h = (mechanical) dispersion coefficient (L^2/T).

The dispersion coefficient generally increases with velocity as follows:

$$D_h = \alpha v^n \tag{17}$$

where

α = dispersivity (L)
v = average pore water velocity (L/T)
n = empirical constant, often taken equal to 1.0

For simplicity, the diffusion and mechanical dispersion coefficients are usually grouped as a single parameter, the dispersion coefficient. It can be seen from equation (17) that the dispersion coefficient is dependent on velocity. It is also dependent on direction. When two and three-dimensional flows are considered, the dispersion coefficient is further broken down into longitudinal and transverse dispersion. Freeze and Cherry (1979) state that the longitudinal dispersivity (i.e., in the direction of flow) and the transverse dispersivity (i.e., normal to the direction of flow) can be significantly different, thus explaining the elongated shape of contaminant plumes. The differences between these components is considered insignificant only when diffusion is the dominant transport process. Because of the difficulty in measuring the components of dispersivity from field experiments, longitudinal and transverse dispersivity often are used as fitting parameters in flow models.

A related dimensionless parameter that incorporates the average pore water velocity and dispersion coefficient is the Peclet number. It is defined as:

$$P = \frac{vL}{D} \tag{18}$$

where

L = length of the column used in the experiment (L)

The Peclet number is often the initial parameter determined from the laboratory experiment and the dispersion coefficient is solved for afterwards. Section 3.0 provides additional information.

5.1.3 Methods

5.1.3.1 Introduction

This section will describe briefly the experimental set-up used to determine dispersion. Only laboratory methods will be considered in this discussion since large scale field experiments to determine dispersion are beyond the scope of this manual. van Genuchten and Wierenga (1986) describe the laboratory procedures in detail.

5.1.3.2 Material

The material and equipment needed for laboratory determination of dispersion are similar to those used for laboratory unsaturated hydraulic conductivity experiments. A soil core, closed on the bottom with a porous plate, is attached to a vacuum source with the soil water outflow directed to a fraction collector (Figure A.9). Tensiometers are installed along the soil core so that the hydraulic gradient can be determined, and the vacuum source is adjusted until unit gradient is achieved. A water application system is used to apply a specified flux onto the top of the soil core.

The test fluid initially used to obtain steady state conditions should, if possible, be compatible in salt content to the original soil solution. Otherwise, Klute and Dirksen (1986) recommend the use of 0.005 M $CaS0_4$ solution. After reaching steady state, the test fluid is switched for a fluid of the same salt concentration, but with a tracer added. The tracer can be either conservative and non-reacting, for example bromide or tritium, or it can be a contaminant expected to be disposed of at the proposed site.

Several variations of the experimental set-up described by van Genuchten and Wierenga (1986) can be used. The user should choose the set-up that best meets his/her requirements for the soil type, length of the column and tracer used.

5.1.3.3 Procedure

The procedures are listed in van Genuchten and Wierenga (1986). They also include potential vendors of several pieces of laboratory equipment which can be used to set up this experiment, and references for further information.

5.1.3.4 Comments

Once the experiment is completed, and the soil solution is analyzed, there are several methods available for interpreting the data. These methods have in common the need to plot the concentration, or the relative concentration (effluent concentration divided by the input concentration) of the effluent versus either time or the number of pore volumes. Figure A.10 is an example breakthrough curve for tritium, which shows how the dispersion smears the front as it approaches the outlet.

Three methods listed by van Genuchten and Wierenga (1986) for analyzing effluent data include Trial and Error, Least-Squares Analysis of the Effluent Curve, and Slope of the Effluent Curve. They also include the procedures for several other methods, for example determining dispersion from a log-normal plot of the effluent curve, and from sectioning soil columns after a specified time period to obtain a snapshot of the concentration gradient with respect to distance from the inlet. Another frequently used method is the Method of Moments (Jury et al., 1991). This method will not be discussed here.

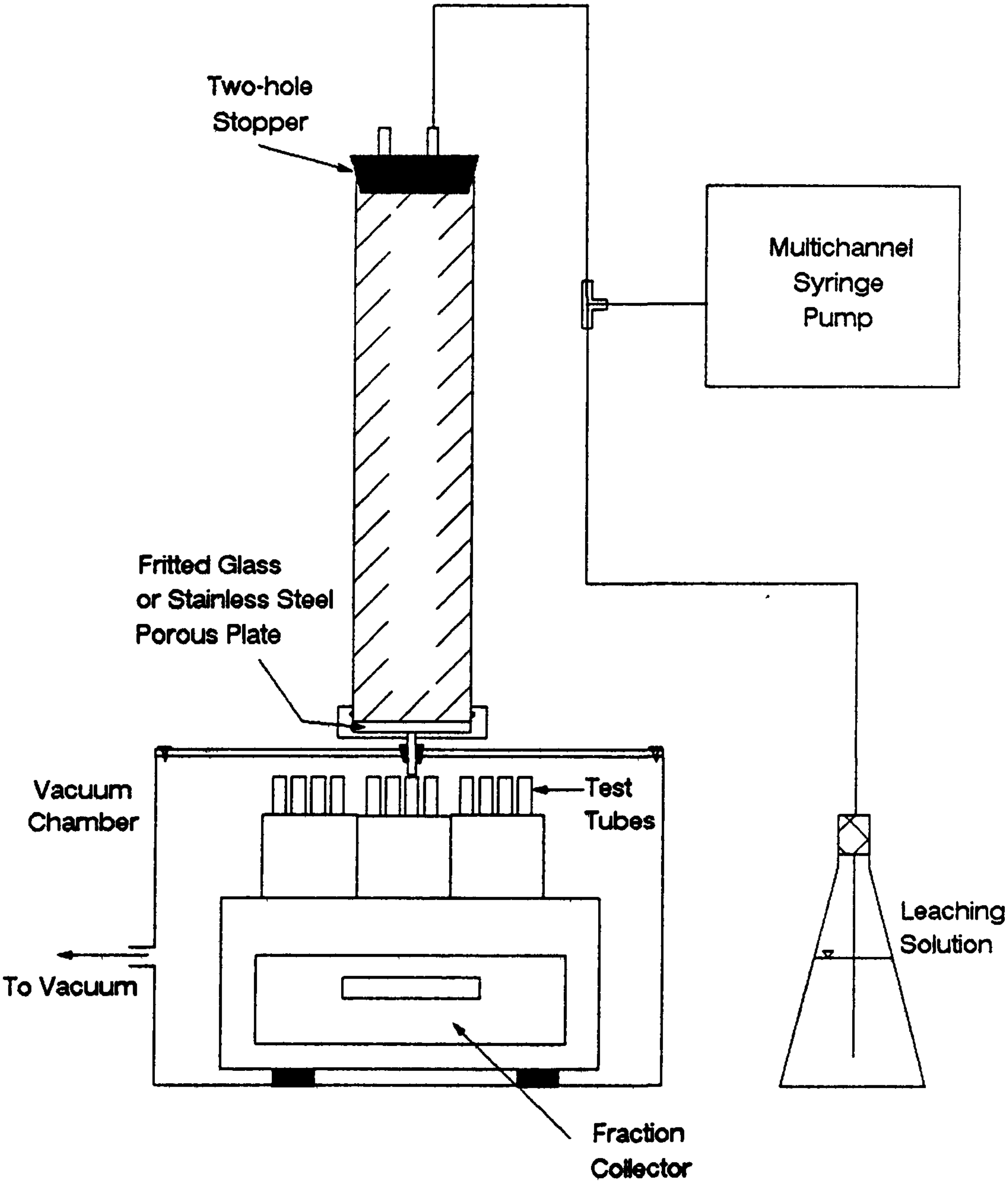


Figure A.9 Diagram of column experiment for determining dispersion coefficient(s)

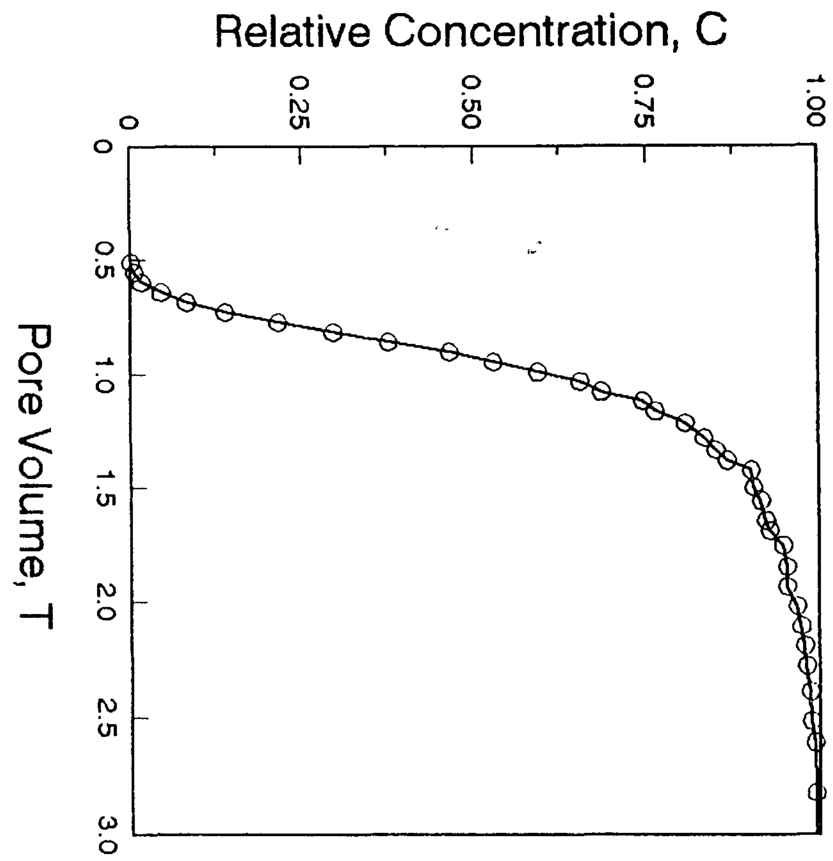


Figure A.10 Example breakthrough curve of tritium

The Trial and Error method determines the retardation factor (R) and the Peclet number (P) by comparing the observed data with a family of curves generated from various R and P values. The equation to generate these curves is a reduction of the solution to the differential equation originally proposed by Lapidus and Amundson (1952), and is

$$C(T) = 0.5\,\mathrm{erfc}\left[\left(\frac{P}{4RT}\right)^{0.5}(R-T)\right] \qquad (19)$$

where

T = pore volume

The dispersion coefficient is then determined by solving for D in equation (18). This method can be time-consuming because of the need to manually fit the P and R to obtain the best fit.

A logical extension of the Trial and Error method is the Least-Squares Analysis of the Effluent Curve method. In this case, P and R are adjusted until a best fit is achieved with the observed data. A residual sum of squares is calculated between the observed concentration at specific pore volumes and the concentration estimated from P and R and equation (19). van Genuchten and Wierenga (1986) consider this to be the most accurate and by far the most convenient method.

The Slope of the Effluent Curve method requires the differentiation of (17) with respect to T, then evaluation of the solution at T = R to yield the following equation:

$$P = 4\pi R^2 S_T^2 \tag{20}$$

where S_T is the slope of the effluent curve after R pore volumes. The dispersion coefficient is then calculated using (18). This method can only yield approximate values because of the approximate nature of (19). The user must determine the pore volume when C/Co = 0.5, calculate the Peclet number, then use Figure 44-6 from van Genuchten and Wierenga (1986) to update the relative concentration. This method provides a relatively easy and accurate estimate with a minimum number of calculations.

5.1.4 Quality Assurance/Quality Control

Many of the QA/QC issues with respect to determining dispersion coefficient have been discussed in the Section on Laboratory Unsaturated Hydraulic Conductivity. It is considered that experiments listed herein are an extension of experiments that will be completed for determining the unsaturated hydraulic conductivity, because the only differences are the addition of a tracer after reaching steady state, along with a modified effluent collection scheme. Thus, measurement of flux, water tension, and water content still must be made accurately.

The tracer used in the experiment must be fully mixed prior to adding it to the core. Care must be taken to quickly change test fluids so that a sharp front exists at the inlet boundary. In this way, dispersion will not be an experimental artifact. It is important to choose the tracer wisely, and with the goals of the experiment in mind. For example, it will not be appropriate to choose a tracer which is known to adsorb onto soil particles, if the goal of the experiment is to determine only the dispersion coefficient.

The method of analysis, and all the QA/QC issues relating to laboratory analyses of water samples must be followed.

5.2 Laboratory Retardation Factors

5.2.1 Introduction

Retardation of contaminants in soil and ground water refers to the chemical reactions between the water phase of the contaminants and the porous material that cause chemical migration rates to become less than groundwater migration rates. Retardation only affects reactive species, causing their concentrations in the fluid phase to decrease. Several chemical and biochemical processes contribute to retardation reactions. They include adsorption-desorption reactions, acid-base reactions, solution-precipitation reactions, oxidation-reduction reactions, ion pairing or complexation, and microbial cell synthesis (Freeze and Cherry, 1979). However, quantifying the magnitude of these individual processes generally will not be possible, because of our lack of understanding of how they change with temperature, pH, organic material in the soil and a host of other competing factors. The retardation factor (R) lumps these individual processes into a single parameter that can be measured experimentally, or determined from computer models.

Experimental determination of retardation can be accomplished two ways: column experiments or batch experiments. Column experiments for determining retardation factors are performed the same as described in Laboratory Dispersion Coefficient. Retardation factors are determined directly from the breakthrough curves. Batch experiments are performed for evaluating the amount of contaminant that sorbs onto soil particles. Retardation factors are then computed using simple equations.

Retardation of contaminants is an important process which removes, either permanently or temporarily, dissolved species from the fluid phase. Precipitation caused by reaction with highly sorbing porous material, such as some clay minerals, can permanently reduce the mass of the dissolved species. If the contaminant becomes immobile due to changes in pH, oxidation state of the soil environment or other geochemical factors which are subject to change, then contaminant migration may be impeded only for a short time. Remobilization of contaminants could cause concentrations to exceed the numerical standards for longer than predicted. The effect of retardation on the shape of a breakthrough curve is the tailing of concentrations after the center of mass passes the outlet point (Figure A.11) and a retardation of the solute plume relative to the water velocity. Although the concentration at a given time period is less than for a non-retarding species, contaminant concentrations are elevated for a longer time period.

An estimate of retardation factors, in the form of the distribution coefficient, is to be included in the license application in an overall database of geochemical conditions (U.S. NRC, 1988). Therefore, this section will

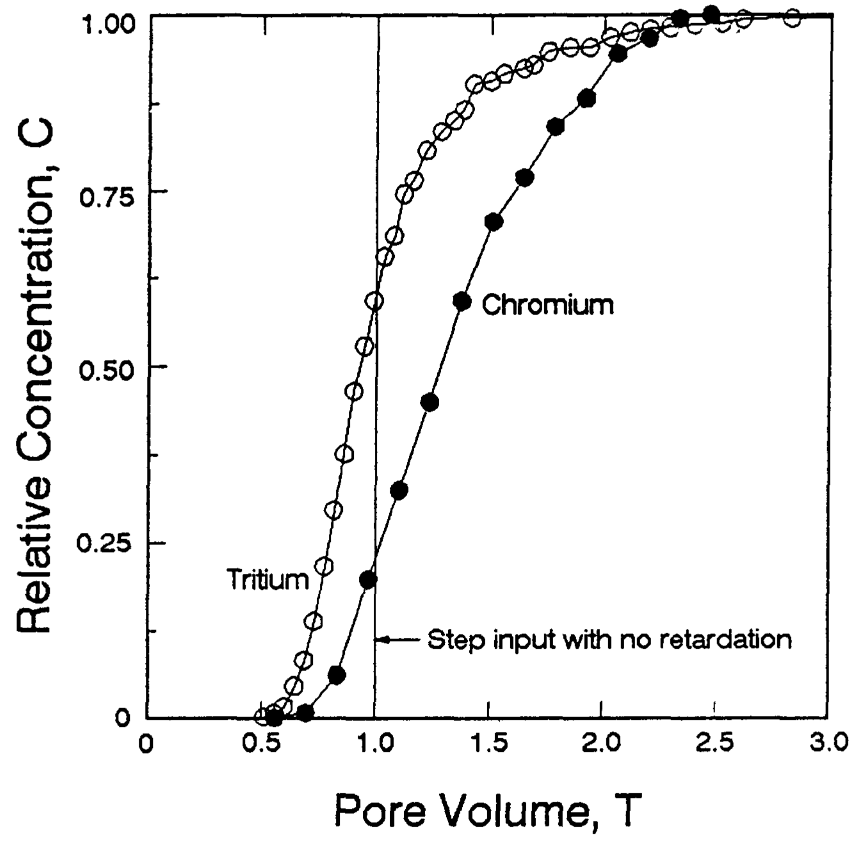


Figure A.11 **Example breakthrough curves illustrating the effects of retardation on step inputs of tritium and chromium, and input functions with no retardation or dispersion**

discuss some theory behind the retardation factor, and the methods used to determine it. References will be made to other appendices in this manual, and to van Genuchten and Wierenga (1986), who provide additional information on this subject.

5.2.2 Principles

As mentioned in Section 5.2.1, two methods exist for estimating the retardation factor: use of breakthrough curves from column experiments and use of batch soil experiments.

5.2.2.1 Use of Breakthrough Curves

The principle behind this method is based on a solution to the governing differential equation for evaluating the change of concentration with time. This equation is:

$$R\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x} \tag{21}$$

where

R = retardation factor (dimensionless)
C = contaminant concentration (M/L^3)
D = dispersion coefficient (L^2/T)
v = average pore velocity (L/T)
x = Distance in the downgradient direction (L)

A reduced form of the solution to this equation was proposed by Lapidus and Amundson (1956). The solution in terms of the Peclet number (P) and R is:

$$C_e(T) = 0.5\,\mathrm{erfc}\left[\left(\frac{P}{4\pi T}\right)^{0.5}(R-T)\right] \tag{22}$$

where

T = pore volume
P = Peclet number
C_e = relative concentration (C/C_O)

for the following boundary conditions:

$C(0,t) = C_O$ and
$C(\infty,t) = 0.$

These specific boundary conditions generally apply to many hydrologic situations where the inlet boundary to the soil core is analogous to a point source, and the concentration is zero at some far distance from the source. The Peclet number, as defined previously, is a dimensionless parameter that relates the pore water velocity, dispersion coefficient (also determined from the column experiment), and the length of the column.

Using equation (22), estimates of R can be obtained by equating R and T (causing erfc(0) = 1.0), and determining the point in the experiment when the relative concentration = 0.5 (i.e., $C_e(R) = 0.5$). Therefore, the time, T, at which the breakthrough curve crosses 0.5 is estimated to be the retardation factor. Figure A.12 provides an example of this method. Note that in Figure 13, S_t is the slope of the effluent curve at R = T pore volume (R and Pore defined previously).

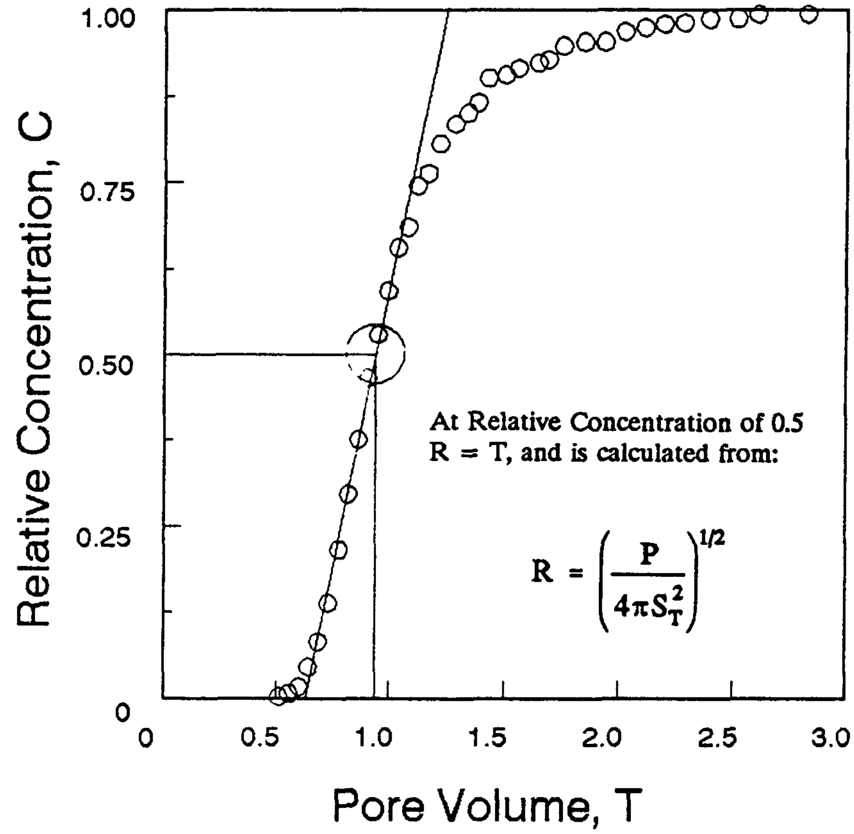
5.2.2.2 Use of Batch Experiments

Batch experiments are used to determine the equilibrium sorption of contaminants onto the soil material. The more sorption of dissolved species onto the soil, the higher the retardation. By changing the concentration of dissolved species in solution, and observing the amount that sorbs onto the soil, it is possible to derive a graphical relationship relating the concentration of solute in the solid phase bound by the soil (S),with the concentration of solute in the liquid phase (C). The line representing these data is called an isotherm. The linear isotherm is represented by:

$$S = K_d C \qquad (23)$$

where

K_d = distribution coefficient (slope of the adsorption isotherm)(L^3/M)



At Relative Concentration of 0.5 R = T, and is calculated from:

$$R = \left(\frac{P}{4\pi S_T^2}\right)^{1/2}$$

Figure A.12 Example of how to use breakthrough curves to determine retardation factor

Linear isotherm models lead to retardation factors which are independent of concentration, as will be discussed below. When the relationship between S and C is non-linear the isotherm equation is represented by:

$$S = K_f C^n \tag{24}$$

where

n = dimensionless parameter
K_f = Freundlich partition coefficient (L^3/m)

By differentiating (24) with respect to time, we get

$$\frac{\partial S}{\partial t} = K_f n C^{n-1} \frac{\partial C}{\partial t} = K_d \frac{\partial C}{\partial t} \tag{25}$$

Thus, K_d and R are dependent on concentration.

The retardation factor is determined from K_d by plugging the right-hand term of equation (23) or (25) into the governing differential equation. After rearranging the terms and assuming linear adsorption ($n = 1$), one obtains:

$$R = 1 + \frac{\rho K_d}{\theta} \tag{26}$$

where

ρ = bulk density of the soil (M/L^3)
θ = water content (L^3/L^3)
K_d = distribution coefficient (L^3/M)

The complete derivation is available in most hydrologic texts. See Brusseau and Rao (1989) for a discussion.

These two reasonably simple methods for estimating R can be completed on a number of soil samples, both on disturbed bulk samples, or undisturbed core samples, in a reasonable amount of time. The laboratory estimates can be used in computer models to predict contaminant concentrations downgradient of a source.

5.2.3 Methods

5.2.3.1 Use of Breakthrough Curves

Column experiments are used to produce breakthrough curves for soils and contaminants. The description for setting up these experiments is fully discussed in van Genuchten and Wierenga (1986), and briefly in the Section on Laboratory Dispersion Coefficient of this manual. The interested reader should consult these references.

5.2.3.2 Batch Experiments

Introduction

Batch experiments are widely used for determining adsorptive behavior of compounds on soils (Green et al. 1980), and the distribution coefficient (K_d). Once K_d is known, it can be used to predict the amount of adsorption onto soil that will occur given a soil solution concentration and a soil type, or the concentration of a compound in the soil solution given the concentration in the solid phase. The plot of S versus C can follow a linear, log-linear, or other functional relationship (Bohn et al., 1985).

Material

Equipment and material needed for carrying out these experiments are listed in Laboratory Soil Solution Sampling.

Procedures

The procedure for preparing extract samples to be used in the determination of the distribution coefficient and retardation factor are similar to those listed in Laboratory Soil Solution Sampling. Because the K_d requires several points to define the functional relationship, a number of experiments must be conducted. These experiments are run in two stages, which are discussed below.

Determination of Equilibrium

Results of batch experiments have to reflect conditions in which the precipitation and dissolution of contaminants are in equilibrium. Because the kinetic behavior of contaminants likely will depend on the soil properties as well as the chemical properties of the contaminants, time to reach equilibrium will vary. A procedure to determine this equilibrium time requires that solution samples be taken at different times from several batch experiments and analyzed for contaminant concentrations. By plotting the concentration versus time, it should be possible to note where the increase of concentration begins to level off. It is important that a separate mixture be prepared for each data point. Removal of solution will alter the estimated mass of contaminant in the soil, and possibly the concentration. Enough mixtures should be prepared to adequately describe the functional relationships, especially if linearity is in question.

Determination of Distribution Coefficient

Once the time to reach equilibrium is known, experiments can be performed for progressively higher concentrations in the solution phase. The maximum concentrations should reflect a value much higher than anticipated in the waste stream, ensuring that extrapolation to higher concentrations will not be necessary. Bohn et al. (1985) stated that extrapolation of K_d to concentrations greater than those performed experimentally could be in error because of non-linear sorption behavior for some pesticides at high levels.

Once the experiments have been performed, the concentration in liquid phase versus the concentration in solid phase should be plotted, and the retardation factor calculated using equation (26).

Comments

A major assumption of the batch method for determining the retardation factor is that of linearity. As seen in equation (25), R is calculated directly from the K_d and physical properties of the soil. Given that the physical properties are constant, a non-linear K_d function will lead to a concentration-dependent retardation factor. Retardation defined by (26) is not considered to be concentration dependent, but rather it is a single value dependent on the contaminant and soil properties only. Adsorption experiments may often lead to isotherms and sorption coefficients which change with increasing or decreasing concentrations in the fluid phase. Non-unique sorption coefficients may increase the difficulty in modeling contaminant migration. Bohn et al. (1985) describe the theory of multi-layer adsorption where non-linear isotherms can be linearized for small segments of the function.

Groundwater and transport models which use the K_d and R approach for predicting migration rates generally do not incorporate non-linear isotherms. Only linear isotherms with unique adsorption rates can be used in most models. However, more recently, models have been developed where non-linear sorption isotherms are taken into account (Brusseau et al., 1989; Brusseau and Rao, 1989). Brusseau and Rao (1989 and 1990) review current approaches to modeling non-ideal systems. The interested reader should consult these references.

5.2.4 Quality Assurance/Quality Control

Quality assurance/quality control (QA/QC) issues for performing column experiments are listed in the Section on Laboratory Unsaturated Hydraulic Conductivity. It is considered that experiments listed herein are an extension of experiments that will be completed for determining the unsaturated hydraulic conductivity, because the only differences are the addition of a tracer after reaching steady state, and a modified effluent collection scheme.

QA/QC issues for preparing batch samples are listed in the Section on Laboratory Soil Solution Sampling.

Appendix B

Field Techniques

Contents

Figures

Tables

1 Field Soil Sampling

1.1 Introduction

Soil samples are collected in the field and analyzed for properties which are used to predict water and solute movement in the vadose zone. It is the goal of the person who collects the samples to collect a sufficient number of soil samples, within a predetermined sampling program, such that the properties of the samples can accurately represent the properties of a much larger area of soil. Highly variable soil properties in some areas of the study site could require more or less intensive sampling, but the degree of variability cannot be estimated until the first round of sampling and analysis is completed. The problem of representativeness of test results is compounded by issues of whether the soil itself was sampled properly, or whether the action of sampling could have affected the soil itself, and hence the test results.

Two major issues in soil sampling will be discussed in this chapter. The first issue will be on developing a program for soil sampling, including different types of random sampling schemes, and analyses. However, this chapter will not provide hard numbers of how many soil samples need to be collected from each soil horizon or laterally across the site, because spatial variability of properties are different at every site. U.S. Nuclear Regulatory Commission (NRC) guidance on these matters leaves open the number of samples that should be collected at each site (Shum et al., 1989). In this way, licensees can use data collected during the site selection process as a guideline for where and how many samples should be collected for their license application. Therefore, given the complexity of problems with determining how many samples should be collected, and the amount of material already available to the general public, this chapter will include only a brief explanation of the problems that practitioners will confront, possible solutions, and some references for further information.

The second major issue to be discussed involves various techniques for collecting soil. The method chosen must depend, of course, on how the sample is going to be analyzed. The need for undisturbed samples, or for specific volumes of soil, for example, will dictate the requirement for sampling protocols. This chapter will discuss briefly the more commonly used methods of soil collection near ground surface and at depth. References will be provided, when necessary, for a complete discussion on methodology.

1.2 Principles

1.2.1 Statistical Aspects of Soil Sampling

Soil profiles are heterogeneous masses of material. Properties such as hydraulic conductivity, bulk density, cation exchange capacity vary both laterally and with depth. The magnitude of these variations is very difficult to characterize. Soil forming processes create this variability. Types of vegetation, proximity to surface water bodies, and differences in parent material all lead to the formation of soils with different properties. Unless the entire soil mass is sampled and analyzed, errors in characterizing these different properties are inevitable. It is the goal of the practitioner who must characterize a soil profile to develop a sampling and analysis program which reduces these errors to acceptable levels. From a statistical standpoint, a sufficient number of samples must be collected so that the properties of the "population" can be described. A number of different sampling plans are described fully by Petersen and Calvin (1986), so they will only be summarized.

1.2.1.1 Judgement Sample

Judgement sampling programs are developed and implemented based on the judgement of the sampler. The sampler supposedly has a priori knowledge about the soil characteristics (i.e., from the activities during site selection), and thus is able to use this knowledge when deciding the location and number of samples that must be collected. The statistical accuracy of the data set rests upon the ability of the sampler to collect representative samples. A small dataset may be void of outlier values which the samplers deemed nonrepresentative, whereas his/her desire to include extreme values could skew the variability of the results. Potential error can increase significantly if the sampling area is large. This may be the case when preparing a license application for low-level waste disposal sites, since the buffer zone must be included, and possibly the area outside the buffer zone. Therefore, unless the sampler has a very good understanding of the soil characteristics in the vicinity of the disposal site, a more rigorous sampling plan may be needed.

1.2.1.2 Simple Random Sample

A simple random sampling plan uses a coordinate system and an origin located along a boundary of the site. Sampling sites are determined by choosing two numbers, at random, and pacing off these numbers using a predetermined scale interval (i.e., 100 meters, 10 meters, etc.). The scale interval used for this sampling plan is chosen to provide a reasonable number of intervals that span the site. After the sample is collected, the origin of the coordinate system is updated to the new sampling location, and two new numbers are collected. Assuming that the numbers are chosen at random, then the location from which the samples are collected are also chosen at random. Analysis results can be compiled and used to determine population mean, variance and confidence intervals. A variation on the sampling scheme would be to choose a fixed origin, and randomly sample from there. In this case, choosing the origin somewhere near the center of the site ensures that each quadrant of the site has an equal chance of being sampled. Using equations and the method described by Petersen and Calvin (1986), it can be determined if the sampling size was sufficient to characterize the variances in properties values, or whether additional samples need to be collected.

1.2.1.3 Stratified Random Sample

Stratified random sampling plans take into account known subpopulations from which unrelated property characteristics exist. For example, if a soil profile existed with nine different horizons, it would be reasonable to assume that property values within each horizon could be related, but not necessarily across boundaries into different horizons. Random sampling, as described in Section 1.2.1.2 is performed for every "strata," regardless if the strata is a new horizon, a different transect, or a different site altogether. The characteristics of that property can be averaged for the entire site by taking into account the percentage of the total area contained within a particular sample and calculating both "within-strata" and "among-strata" statistical characteristics. Determining sufficiency of sample size is performed the same as in Section 1.2.1.2.

1.2.1.4 Systematic Sample

Systematic sampling plans require that samples be collected along specific intervals, like on a grid pattern for two-dimensional sampling. A specified interval of the grids is chosen for sampling. A variation on this would be to randomly sample from the established grid, thus using only a subset of grid points. The sampler also determines whether the center of the grid is sampled, or the intersection of the grid lines. The origin of the grid can be chosen as either the center or corner of the study area. A number of studies have been conducted which compare theoretical and empirical aspects of systematic sampling vs. simple and stratified sampling plans. Petersen and Calvin (1986) list these studies. In almost every case, systematic sampling produced more favorable results. The only notable exception occurs where periodic trends exist. For example, where topographic effects altered the tops of soil horizons, or where a stream channel meandered across the study area. In these cases, specifically sampling these features will be critical to predicting migration patterns of water and solutes.

1.2.1.5 Comments

Errors will be present whenever a set of samples is used to characterize the properties of a population. However, given that characterizing the entire population is not possible, the practitioners need to understand the sources of error so that they can be minimized. Sampling errors are caused when the samples collected do not represent the characteristics of the population. Selection errors occur when outlier or extreme values are removed from the sample set, or when physical conditions of the site require that the location be modified (e.g., a particular site is avoided because of the presence of subsurface caliche layers). Lastly, measurement errors are present when the analytical results do not represent the true value of the sample. Measurement error is calculated by assessing both random error and biases, which are dependent and independent of the sample size, respectively. The practitioners should define these sources of error, to the extent possible, by carefully evaluating each sample result for accuracy and acceptable variability, and by checking manufacturer's equipment specifications for associated error.

The strategies listed above are used in the field to sample small volumes of soil so that the properties can be applied to much larger volumes. Data analysis follows field work and laboratory analysis, and it is this step where the experience or inexperience of the practitioner can lead to increased biases and incorrect interpretations. Applying the results of samples to the entire population can be done by interpolation, extrapolation, or other geostatistical techniques. An advantage of using geostatistical techniques over interpolation or averaging is that geostatistical techniques take into account trends, and periodicities that would be otherwise hidden. Geostatistical techniques, kriging for example, use the theory that property values of samples collected in close proximity to one another will be related. Depending on the variability of the property, that distance can be relatively long or very short. The relationship between property values becomes statistically random past a distance known as the range (Davis, 1973). The variability of property values within the range can be subdivided into pure variability, and a variability which is dependent on the distance separating the samples (Warrick et al., 1986). This type of analysis uses a variogram, or a graph of variability vs. distances between sampling stations. The variogram can indicate when the variability of property values requires that more intensive samples be taken, or when additional sampling is not warranted. Use of geostatistics can reduce the uncertainty of the merits of the sampling program, thus saving time and financial resources. Warrick et al. (1986) provide a number of excellent examples of how this concept is used in soils analysis, as well as a thorough set of references.

1.2.2 Physical Collection of Soil Samples

In order to reduce measurement error associated with soil sampling, it is important that the sampling procedure not bias the results of the subsequent tests. For example, bulk samples cannot be used for determining undisturbed hydraulic conductivity, because the soil structure is disrupted during collection. On the other hand, undisturbed samples are not needed to characterize grain-size analysis, only the location and depth must be determined accurately. The sampler thus needs to be aware of the test to be run on the sample, then choose the sampling method appropriately. The samplers to be described herein include auger samplers, tube samplers and bulk samplers. Table B.1 contains a compilation of suggested sampling types for corresponding property determination.

1.3 Methods of Soil Sampling

Much has been written on the different methods of soil collection, a large portion by the individual manufacturers themselves. However, a compendium of available methods is available by Dorrance et al. (1991), which discusses the methods to be listed below. Driscoll (1986) provides an excellent discussion on sampling and drilling methods, including a number of diagrams and photographs. The American Society for Testing and Materials (ASTM, 1989b, 1989c, and 1989d) has published a number of standardized methods for soil sampling with

Table B.1 Soil sample types for various physical measurements

Property	Preferred Sample Type	Page Number
Bulk Density	Undisturbed core	41
Particle Density	Ground and sieved < 2.0 mm	44
Particle-size Analysis	Ground and sieved	45
Porosity	< 2.0 mm	47
Water Retention Function	Undisturbed core	61
Saturated Hydraulic Conductivity	Undisturbed core or sieved < 2.0 mm and repacked	69
Unsaturated Hydraulic Conductivity	Undisturbed core or sieved < 2.0 mm and repacked	75
Dispersion Coefficient	Undisturbed core or sieved < 2.0 mm and repacked	81
Retardation Factor	Undisturbed core or sieved < 2.0 mm and repacked	87

(Modified from McIntyre, 1974)

augers (D-1452), split-barrel samplers (D-1586), and thin-walled (Shelby) tubes (D-1587). McIntyre (1974) includes a table of recommended sample types for various physical measurements. The interested reader should consult these references.

1.3.1 Auger Samplers

Auger samplers are essentially solid or hollow drilling stems with cutting flanges welded to the outside of the stem. The auger tip usually consists of two metal tips, 180° from one another, pointed downwards. A wide variety of auger types are available, depending on the depth of drilling, type of soil, and need for collection of soil samples (see Dorrance, 1991 and ASTM, 1989d) The augers are advanced to the desired depth either by hand, truck mounted drilling rigs, or larger rigs which can advance augers down several hundred feet. The samples generally are recovered by two methods. The first method is collection from the auger flights as the bit is advancing, and the second method is collection with a sampling tube driven down inside the stem of the augers, slightly ahead of the bit. The former method is useful for collecting bulk samples where the exact depth of collection is not critical. Accurately determining the depth of collection becomes very difficult because of the time lag from when the bit reaches a certain depth to when the sample finally arrives at the surface. The latter method is useful for collecting "undisturbed" samples, sometimes in S-foot barrel samplers, several meters below ground surface. Split-barrel sampling, which is also used extensively during environmental investigations, will be discussed below.

A number of hand-augers are available for near-surface sampling. The augers range from simple screw augers (similar to drilling bits) to barrel augers where the soil remains inside a short solid metal tube until extracted. Hand augers can be advanced down to 5 meters, or more, but drilling deeper than that can be unwieldy. Hand auger samples are almost always disturbed.

Augers work best in moist cohesive soils. Very dry, cohesionless soils may not be removed efficiently from the auger flights, potentially causing the augers to lock up in the borehole. Cobbles and larger pebbles may be too large to be removed from the flights. Eventually these accumulate in the borehole, thereby locking up the augers, or causing the augers to be deflected from vertical drilling. Soils with high clay content can be very difficult to remove from the flights, or the inside of a hollow stem, especially if the clay is moist and swelling.

1.3.2 Tube Samplers

Tube samplers are usually longer than auger samplers, but have smaller diameters. Tube samplers are rarely rotated downwards to retrieve soil. Instead, hammer mechanisms are used to force, or pound, the cutting tip into the soil profile. Four examples of tube samplers include soil sampling tubes, Veihmeyer (King) tubes, thin-walled (Shelby) tubes and split-barrel drive samplers, more commonly known as split spoon samplers. Soil sampling tubes are hand-driven samplers and consist of a hollow metal rod, 2.54 cm (l-inch) in diameter, with a cut-away section for extracting the soil. The cut-away section allows the soil to be removed in sections. A welded metal stand is used so that the person sampling can add extra weight to the sampler assembly.

Veihmeyer tubes are similar to the soil sampling tubes, without the cut-away section. The cutting head is advanced with a driving hammer, usually by hand. The tube is extracted with the soil by inserting the drilling rods into a key-hole in the hammer and lifting. Soil is removed as a bulk sample by turning the tube upside down or by banging the tube with a hammer to dislodge soil. The boreholes used with Veihmeyer and soil sampling tubes are not usually reamed out as the sampler is used. Thus, the borehole may become too tight to sample with depth. A Veihmeyer type hand driven auger, successfully used at the Las Cruces trench site was obtained from Clements Associates, Inc. (Newton, Iowa) and manufactured by JMC Soil Investigation Equipment.

Thin walled sampling tubes (i.e., Shelby tubes) are used in finer-grained cohesive soils, and are usually used with machine drilling rigs. The length and diameter of the tubes vary, but are usually .61 m (2 feet) in length and 7.6 cm (3-inches) in diameter. Because of the fragility of the sampler, Shelby tubes cannot be pounded into the soil. Instead, the weight of the drilling rods, or with added pull-down pressure from the rig, pushes the tube into the soil. Coarser-grained soils, or soils with cobbles or large pebbles, generally cannot be sampled with Shelby tubes because the cutting surface of the tube will become warped, leading to a complete failure of the tube. Shelby tubes are useful for collecting undisturbed cores at depths up to several hundred feet. Their disadvantage is the limited range of grain sizes that can be sampled.

Split barrel samplers, more commonly known as split-spoon samplers, are perhaps the most commonly used tube samplers. They are used extensively for sampling soils during environmental investigations and geotechnical explorations, and almost always require machine drilling rigs. Split spoons consist of two barrel halves, a cutting head, and sampler head. The sampler head is threaded to drilling rods on one end, and to the barrel halves on the other. Generally, split spoon samplers are used to collect grab samples from relatively specific depths, though liners can be used on the inside of the spoons to retrieve "undisturbed" core samples. The sampler is normally inserted through hollow drilling rods, or hollow-stem augers, and advanced using a hammer which is dropped 0.61 m (24-inches) from the masthead of the drilling rig. The weight of the hammer depends on the outside diameter of the sampler. Split spoon samplers can be used in any soil type, though sampling in very cobble-rich soil may not be effective. Dry cohesionless soil can be retained in the sampler by using a plastic or metal trap installed in the cutting head.

It is important to note that a problem with each of the tube samplers is that of secondary compaction during sampling. This problem is compounded when the sampler is driven with a hammer. The undisturbed core samples collected may have incorrectly high bulk densities. The depth of sampling determined for each subsample within the tube will also be affected. In field testing at the Las Cruces Trench site, compaction was found to be up to 25% in some cases when using 1.52 m (5-foot) spoon samplers inside of a hollow stem auger, making it very difficult to calculate the exact depth of collection. Very dry unconsolidated soils are susceptible to this problem. The depths of collection can be approximated by normalizing the recovery by the total length of the sampler. Each depth is then multiplied by the normalizing factor for that particular sampler.

1.3.3 Bulk Samplers

Bulk sampling of soils usually refers to digging up volumes of soil either by hand or with a backhoe. These samples can be used for determining physical and chemical properties such as particle size analysis, particle density analysis, cation exchange capacity, or routine mineralogical analysis. Soils can be homogenized and repacked into columns to simulated undisturbed samples, but this is not very accurate.

As mentioned above, auger drilling is useful for collecting bulk samples at depth. Also, bucket augers, very large diameter buckets with cutting blades and an open bottom can be used for collecting samples.

1.4 Quality Assurance/Quality Control

Quality assurance/quality control (QA/QC) issues with respect to soil sampling can be divided into two major areas, accuracy of choosing the location for sampling and data analysis, and the action of collecting the soil sample.

A number of statistical studies have been conducted to analyze for sources of uncertainty when determining the physical property of soils. As discussed above, geostatistical methods can be used to subdivide sources of uncertainty of the property fields, thus increasing the efficiency in the sampling and analysis program. Thus, components of error should be quantified and reported in the license application, so that the need for further sampling can be evaluated.

Quality control programs are used extensively during environmental investigations, especially for the investigations under the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) (Superfund) program. In these cases, the Federal government takes control of the site investigation for the purpose of identifying parties responsible for reducing risks to the environment and to the public from cleaning up abandoned uncontrolled hazardous waste sites. The QA/QC program is implemented for all stages of these investigations, covering decontamination procedures of sampling equipment, sample tracking, laboratory QA/QC, and data analysis (EPA, 1987a and 1987b). Though this program may not be needed for some investigations, the overall structure of the program should be considered when designing a sampling and analysis plan for investigating sites for radioactive waste disposal facilities. Each site activity should be accompanied by a QA/QC procedure. It may appear, at first, that the umbrella of an overall QA/QC plan is unwarranted. However, given the need for assurances that the data were collected and analyzed properly, and the time and monetary investment in characterizing a site for radioactive waste disposal, a QA/QC program would be prudent.

2 Field Soil Solution Sampling

2.1 Introduction

Field sampling and analysis of soil solution allows for the characterization of soil solution chemistry before site activity, and detection of changes in solution chemistry during operations and after closure. The requirement for disposal site monitoring in the vadose zone during and after waste emplacement is described in NRC regulation 10 CFR 61.53, which states that the monitoring network shall be capable of detecting early releases of contaminants before they leave the facility boundary.

This chapter describes the various methods of sampling soil solution that commonly are being used for characterizing the soil solution chemistry. It covers only those methods used to extract solution from unsaturated soils, and does not include saturated zone sampling, regardless of whether the saturated zone is contained in a perched water table in the larger vadose zone. The methods described herein are categorized into two major classes: physical soil sampling with subsequent extraction of pore water and analysis, and the use of suction samplers for removing pore water from soil in-situ. The term used throughout this text for describing these sampling devices will be soil solution samplers, as opposed to suction lysimeters. Lysimeters are considered in this text to be related to meteorological measuring devices. Each method will be described and appropriate references provided, so that the user can determine which method will meet his/her requirements for site characterization and longer-term monitoring. One relevant reference is Wilson (1990), which reviews available methods of soil solution sampling for the American Society for Testing and Materials.

2.2 Principles

2.2.1 Soil Sampling and Pore Water Extraction

Removal of soil samples with subsequent extraction of pore fluids in the laboratory is a standard method for determining solution chemistry. This method has a number of advantages over in-situ extraction of soil solution. They include, (1) the soil solution is extracted in a laboratory, where environmental conditions and decontamination of equipment are better controlled, (2) the physical and hydraulic properties of the soil can be measured on the same soil sample from which the solution was extracted, and (3) the solution was extracted from a known volume of soil. Interpretations of results could be affected if solution samples were extracted from uncharacterized soils. The major disadvantage of this method is that the soil sample is removed from the ground, precluding an on-going monitoring program with the same soil. Another disadvantage is that changes may occur in the soil sample containing the solution during sampling and transportation to the laboratory.

This method can be very useful during site characterization activities to support site selection and license applications. Physical removal of the soil allows the user to run a larger number of tests which would not be possible if the soil itself was not sampled. For example, an entire suite of tests can be run for determining physical characteristics of the soil, including bulk density, particle-size analysis and density, pore-size distribution and retention function. If the sample is undisturbed, additional analyses can be performed. The tests listed above eventually must be performed on the soils during site characterization, and thus it would be prudent to include the extraction and analysis of pore fluids on the same soil samples. After the soil solution chemistry has been characterized, locations can be chosen for placement of tensiometers and solution samplers for long-term monitoring.

2.2.2 Soil Solution Samplers

Four types of soil solution samplers will be discussed in this section: vacuum suction samplers, pressure-vacuum suction samplers and dual chamber pressure-vacuum samplers and wick samplers. These soil solution samplers all work under the same basic principal; that is, a gradient is imposed across the boundary of a porous cup (or wick) where the energy inside the cup is more negative than the energy of water in the soil. This gradient causes water to flow from the soil into the sampler. The water content of the soil determines the amount of the vacuum needed to cause movement of water into the cup; wetter soil requires a lower vacuum, and drier soil requires a higher vacuum. Water will flow into the porous cup until the energy levels inside and outside of the cup, usually expressed in units of length, are equal.

The vacuum suction sampler operates by creating a vacuum inside the porous cup, allowing water to migrate through the porous material (Figure B.1). If the sampler has two tubes, the second tube is closed off. To remove water from the cup, the vacuum is released, and water is pulled from the sampler either by a second line extending to the bottom of the cup, or by the vacuum line which in that case also extends to the bottom of the cup. These samplers are effective down to depths of about 25 feet (Dorrance, 1991), and are fairly simple to use. For example, over 100 solution samplers of this type have been installed at the Las Cruces Trench site, near Las Cruces, New Mexico (Wierenga et al. 1989), and their performance has been acceptable (Elabd et al., 1988).

Pressure-vacuum samplers necessarily have two lines, a vacuum-pressure line and a water discharge line. To obtain a sample, the body tube is placed under vacuum using the vacuum-pressure line, with the discharge line closed. When a sufficient amount of sample is obtained, the discharge line is opened, and pressure is applied on the vacuum-pressure line, causing water to evacuate the cup via the discharge line. Because of the external pressure source, these devices can be used to greater depths than if the sample is removed by suction only. Note that solution can exit via the cup if too much pressure is applied to force the solution to the surface.

Dual chamber pressure-vacuum samplers operate the same as pressure-vacuum samplers. The difference between the two is that a separate reservoir exists in the dual chamber pressure samplers into which the solution sample is stored. A one-way check valve keeps the pressure inside the second reservoir, thus preventing backflow of air or water through the porous cup and allowing water to be lifted from great depths.

It is also possible to use tensiometers as solution samplers. Tensiometers, as described in Lab Water Tension of this text, are constructed the same as solution samplers, with the exception that vacuum and discharge lines are not used. Thus, if a different stopper is used containing these lines, the tensiometer can be converted to a solution sampler. This convenience, however, is tempered by the fact that the tensiometer must be fully drained and decontaminated before is can be used as a solution sampler. And it may not be possible to fully decontaminate tensiometers given that pores in the cup will contain water not compatible with the soil solution.

It should be noted that a number of solution samplers other than those found in porous cup form can be used to collect discrete samples. Monitoring wells, perched ground water samplers and pan -Type solution samplers are examples of what are known as free-draining solution samplers. Free-draining solution samplers are commonly used in perched or below water table conditions. These conditions are not common in arid and semi-arid environments, though they can be useful as indicators of background soil chemistry or possible leaks in disposal cells. This section will not cover these types of samplers because the text is restricted to unsaturated zone samplers where water is not free draining. Dorrance et al. (1991) describe a number of examples of free-draining solution samplers for near surface sampling. The interested reader should consult this text, if necessary.

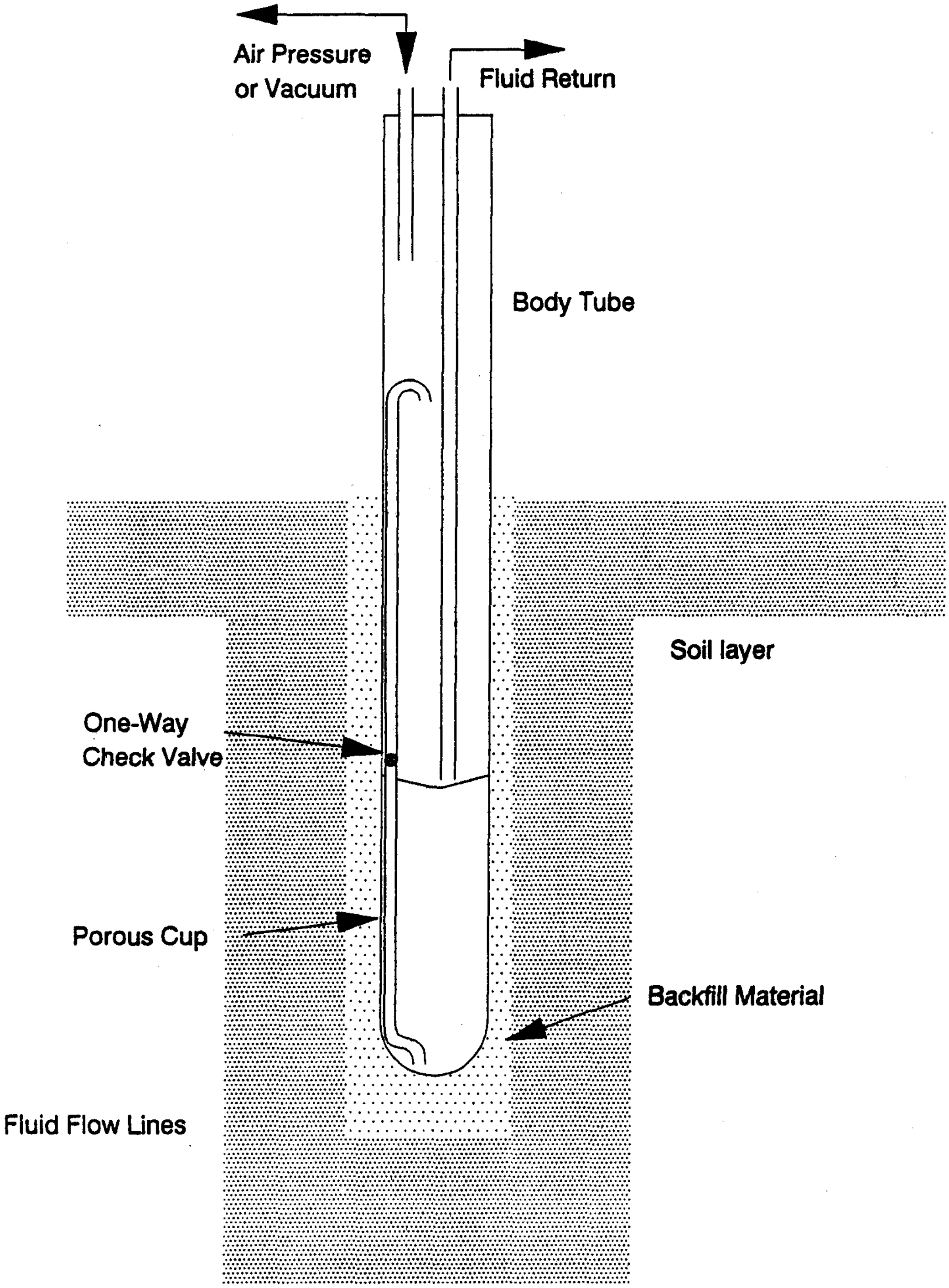


Figure B.1 Diagram of dual-chamber solution sampler

2.3 Methods

2.3.1 Pore Water Extraction

Pore water extraction and analysis first requires that a volume of soil be collected. The section entitled Field Soil Sampling describes soil collection. The collection of pore water from bulk soil samples almost always occurs in the laboratory. Laboratory conditions allow for more accurate measurements of the masses and volumes of soil, and of the volume of deionized water added to the sample to prepare the extracts. More importantly, laboratory environments are cleaner and more versatile for setting up the vacuum systems necessary to extract the sample. Therefore, pore water extraction discussions will be included in the section entitled Laboratory Soil Solution Sampling.

A recent innovation in pore water sampling is the use of fiberglass rope (acting as a wick) to pull solution from the soil (Holder et al., 1991; Boll et al., 1992). The device is restricted to low suctions but has the advantage over pan -Type solution samplers that the solution is removed under tension. In areas where soil tensions range from 0 to 100 cm or less, such devices can prove very useful. The major advantage over vacuum samplers is that they are passive systems and require little or no maintenance. However, because the wicks act as a hanging water column, the sampling jar must be below the wick filaments. This may be logistically difficult to set up in the field, especially for pre-existing disposal units. Further work is being performed to better understand this new sampling technique. The reader should consult the aforementioned references for further information.

2.3.2 Soil Solution Samplers

Three of the four types of soil solution samplers mentioned herein, vacuum suction samplers, pressure-vacuum samplers, and dual chamber pressure vacuum samplers, all have similar installation procedures. Procedures for their use are also very similar. Thus, this section will group all discussions together, and indicate differences where appropriate.

2.3.2.1 Introduction

Soil solution samplers often are purchased ready to install. Manufacturers supply a variety of porous cup designs, riser pipe lengths and methods of applying vacuum to the sampler.

Installation of the solution samplers is accomplished in much the same way as for tensiometers. For installation closer to the soil surface and in loose moist soil, the solution sampler can be pushed directly into place. For stony soil, or compacted horizons, it may be necessary to bore out a hole of a diameter similar to that of the sampler. This borehole is advanced either by hand with an auger or core sampler, or by machine for deeper depths. The borehole diameter should not be much greater than the outside diameter of the sampler because contact with the walls of the borehole will be difficult to achieve. The cup should be placed in a slurry of sieved natural material and water, so that a good contact between the soil and the cup is established. The sieved material, which has been found to work very well in field situations (Wierenga and Young, 1991), ensures that coarse-grained sediments that can reduce contact with the borehole are removed from the slurry. The slurry is useful in filling air gaps between the soil material and the sampling cup. Use of natural material is preferred over silica flour because of possible interaction between dissolved constituents and the silica flour. Of course, interaction of constituents with fine-grained material surrounding the cup is also possible, but the use of material indigenous to the area should reduce deleterious effects.

Once the solution sampler is installed, a vacuum system is required to create the hydraulic gradient that causes soil solution to flow into the cup. The vacuum is applied in one of two ways. In the first method, the vacuum line acts as the discharge line, forcing solution out of the porous cup as soon as it accumulates. The second method uses separate vacuum and discharge lines. The vacuum line creates the gradient, causing the water to enter the cup, where it is stored until a sufficient volume of solution has been collected. The vacuum line is then pressurized, and the discharge line, which extends to the bottom of the cup, is opened up. Solution flows through the discharge line to the sample bottle.

Reliable performance of solution samplers requires that the bubbling pressure of the porous cup should not be exceeded. Exceeding the bubbling pressure leads to poor efficiency of the sampler. In addition, maintaining the integrity of the sample during collection is critical to the integrity of the laboratory results and subsequent analysis. Forcing water to flow through the porous cup, and the solution in the cup itself can affect the concentrations of volatile organic compounds and possibly inorganic constituents (Palmer, 1991). The extent to which the sample can be affected is not fully known and should be researched further. Given this unknown, the user should apply a vacuum necessary to remove a sufficient volume of sample, without applying too high a vacuum.

All components of the solution samplers should be decontaminated between samples, if the porous cup or components of the sampler (i.e., vacuum lines, discharge lines) are not dedicated to a particular borehole. Cross-contamination is a problem which can lead to incorrect conclusions about geochemical conditions prior to waste emplacement, and, more importantly, about possible leaks from the disposal cells. Most samplers are sold with dedicated lines which may not be removable for routine cleaning or replacement. For these types of instruments, the user should consult with the manufacturer regarding their recommended decontamination procedures.

2.3.2.2 Equipment

Soil solution samplers, though slightly different in design from one another, all have the same basic components. A porous cup, made of ceramic, stainless steel, or PTFE (Teflon) is glued or otherwise attached to a hollow tube. The tube is closed at the other end, except that one or two tubes are inserted through it, one tube extending down to the end of the cup, the other extending a short distance. This latter tube acts as both the vacuum line and the pressure line. The second tube acts as the conveyance line for the soil solution. Dorrance et al. (1991) provide diagrams of several types of solution samplers.

Several types of porous materials are used today to form these porous cups, though ceramic is the most widely used. Cups can be purchased for a specific range of anticipated vacuums and different sizes, depending on the specifications of the user. The authors have obtained ceramic porous cups from Soilmoisture Equipment Corporation (Santa Barbara, California), solution samplers made of stainless steel from Soil Measurement Systems (Tucson, Arizona), and solution samplers made of teflon material from Timco Manufacturing (Prairie du Sac, Wisconsin).

The use of wick sampler to collect soil solution is gaining popularity. Holder et al. (1991), and Boll et al. (1992) provide the details for construction and installation of these devices for sampling contaminants in soil pore water. The wick samplers are extremely simple and apparently quite reliable. The basic principle of the sampler is the use of a wettable rope material (generally an inert, non-degradable material) such as fiberglass as the wick. The wick is placed into the soil through an access hole. The wick is made into a hanging column to create a tension in the soil at the point of contact. The tension created is equal to the length of the water column, in an manner very similar to the buchner funnel procedure for water retention described in Section 4.3.3, Water Retention Function. Figure B.2 shows the salient feature of the wick sampler. Holder et al. (1991) show that wick samplers are inert (do not interact with solutes), and are easy to install and maintain. The distinct advantage is that these devices require no external source, relying on the passive nature of the wick to maintain the tension in the sampling fibers of the wick. They are also self-priming. In other words, they avoid the difficulties of air entrapment and purging - often found in porous cup samplers.

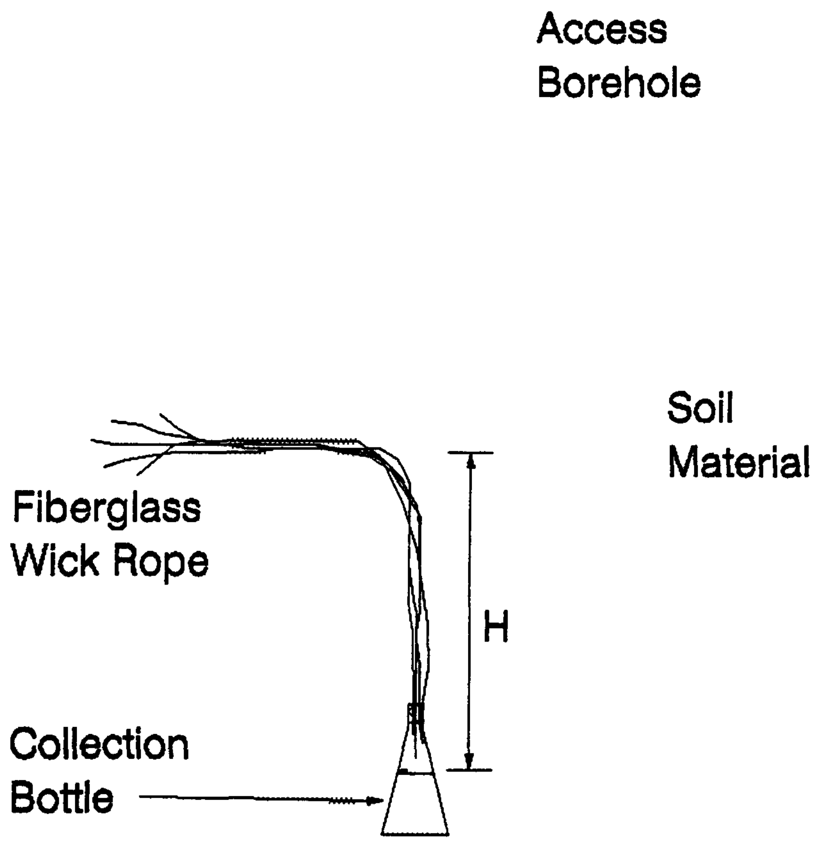


Figure B.2 Salient feature of a wick sampler

Where solution is draining in relatively coarse soils, tensions are generally 100 cm or less. Under these conditions, wick samplers appear to be suited as pore water collectors.

2.4 Quality Assurance/Quality Control

A quality assurance/quality control (QA/QC) program should be developed and maintained which spans instrument installation through sample tracking. It is important that logs be maintained which outline how each sampler was installed, including but not limited to, the sampler manufacturer and model number, method of installation, depth of the porous cup, porous cup material, backfill and slurry composition, and final completion. A description of how the sampler was installed will be used to determine the credibility of the analytical results to describe geochemical conditions at the time of sampling.

During sampling, the date, time and person collecting the sample should be recorded into the log book. Also of importance is the amount of vacuum applied to the porous cup, length of time that the vacuum was applied, volume of sample collected, type of analysis to be completed on each sample, and decontamination procedures.

Sample tracking, though seemingly unimportant against the problems of collecting the sample itself, is extremely important when using the results in a license application for low-level waste disposal. The scrutiny that the results will be given by regulatory officials, and members of the public and their consultants, almost requires that sample tracking be implemented and strictly maintained. Maintaining a QA/QC framework for sample tracking in the CERCLA program (i.e., Superfund), for example, is meant to ensure that the results will be admissible in court. Samples collected outside of the program, even those collected in earlier investigations often are not used in the final analyses of environmental impacts because EPA can not be guaranteed of the integrity of the results. These data are useful, however, in estimating the extent of contamination and in proposing future investigations.

NRC staff have published two documents related to QC/QA, NUREG-1293 (U.S. NRC 1989) and Regulatory Guide 4.15 (U.S. NRC, 1979). In addition, it may be helpful to consult two U.S. Environmental Protection Agency reports that each region uses to develop their individual QA/QC programs (EPA, 1987a and 1987b).

3 Field Saturated Hydraulic Conductivity

3.1 Introduction

Hydraulic conductivity is a measure of the ease with which water can flow through soil. Having the units of flux (L/T), it is the slope of the flux versus gradient curve. The hydraulic conductivity is one of the most important hydraulic parameters to be characterized in the soil, because of its' effect on the movement of water and contaminants in soil. Zones of soil material with higher conductivity, such as sand lens or buried stream channels, can concentrate the bulk of soil water flow, creating significant difficulties when attempting to monitor soil water for contaminant migration. Characterizing the physical properties of soil at sites which have highly variable materials is difficult.

The hydraulic conductivity is of major interest to hydrologists, soil physicists, and engineers, especially above the water table, in partially to near saturated material. The hydraulic conductivity is strongly dependent on the water content. This relationship, however, is highly non-linear and is difficult to characterize. Most practitioners choose to estimate it, rather than attempt to determine it experimentally. However, the saturated conductivity is more readily estimated, and is the upper limit of the capacity of the soil to transmit water (higher flow rates will occur if the gradient is greater than unity). It is a function of the soil structure and composition, and of the fluid properties (viscosity, density, and surface tension).

Saturated hydraulic conductivity is used in Darcy's equation to determine rate of movement of water and, ultimately, contaminants in saturated systems:

$$q = -K_{sat}\left(\frac{dH}{dl}\right) \tag{27}$$

where q = flux density (L/T)
K_{sat} = saturated hydraulic conductivity (L/T)
H = total hydraulic head (L)
l = distance (L)

For saturated systems, conductivity is assumed constant in time, for a location in the flow field. Differences in the physical structure of the porous material cause heterogeneities and anisotropy in conductivity. The hydraulic conductivity used in this equation is analogous to electrical conductivity and thermal conductivity in electrical and heat transfer problems, respectively. From the above equation, it can be seen that the hydraulic gradient needs to be determined before predictions can be made. The gradient is found by monitoring the hydraulic head at a minimum of two locations, then dividing the differences of the heads by the distance between the monitored zones. Vertical and horizontal gradients should be quantified so that the flow field can be adequately defined.

Determination of saturated hydraulic conductivity (K_{sat}) in the laboratory has been performed for decades. Many papers and texts have been written to describe procedures for determining conductivity, though many concentrate on theory rather than step-by-step descriptions. This chapter will concentrate on field methods which involve the installation of permeameters and infiltrometers. These are considered near surface tests. Methods such as slug and pump tests, which are conducted below the water table but still involve unconsolidated material, will not be covered in this document. The following methods will be discussed in this chapter: air entry permeameters, bore hole infiltrometers (Guelph Permeameters), disc permeameters, and ring infiltrometers.

Amoozegar and Warrick (1986) provide an in-depth discussion on different methods for determining field K_{sat}, as well a large reference section. Hendrickx (1990) also discusses several methods for determining K_{sat}. The reader should consult these references before deciding on a particular method. Unsaturated hydraulic conductivity is discussed in detail in chapter entitled Unsaturated Hydraulic Conductivity. Laboratory experiments for determining saturated hydraulic conductivity are discussed in Appendix A, Section 4.4.

3.2 Principles

The value of saturated hydraulic conductivity measured through experimentation implies that all the pores within the soil core are filled with water and contributing to the overall flow in the experiment. If suction is applied to the soil sample and water is removed, the largest pores will drain first and only the smaller pores will be available for transporting fluids. Because of this phenomenon, the saturated cross-sectional area of the sample will decrease very rapidly at first, then, depending on the pore size distribution, the rate of decrease will change. Change in cross-sectional area affects flow according to Poiseuille's Law, which states that the flow rate through a capillary tube is proportional to radius to the power four. So it can be seen that very small changes in the cross-sectional area leads to large changes in flow. The driving force behind water flow is the hydraulic gradient, and water will always flow down gradient, from high energy status to a lower energy status. Determining the hydraulic gradient between at least two points is critical in the calculation of hydraulic conductivity.

The principles behind the field procedures discussed in this chapter are the same. The experimenter is attempting to measure the flux of water from a reservoir, and if possible, the pressure head. Flux is measured by noting the change in water level and multiplying by the cross-sectional area of the reservoir. The change can be measured manually with a tape measure or hook gage, but more accurately with a pressure transducer.

Each of the methods to be discussed normally assumes that the soil is saturated after the flux rate stabilizes. In reality, this is probably not accurate. Tensiometers can be installed and monitored to check on the degree of saturation. When the pressure head approaches zero, the soil is assumed to be saturated. It would also be possible to determine vertical hydraulic gradients if tensiometers were installed to different depths and the wetting front had passed the upper tensiometer.

3.3 Methods

3.3.1 Air-Entry Permeameter

The air-entry permeameter is a relatively fast method of determining K_{sat} which does not require large amounts of water. Bouwer (1966) developed this method and Topp and Binns (1976) modified it by including a fine tensiometer probe to detect the position of the wetting front. This method is rapid because of the high gradient and head imposed on the soil surface. The test is conducted on the soil surface, though excavation was needed in the original method, after the test, to determine the depth of the wetting front. Proper placement of tensiometers beneath the test area should obviate the need for excavation, thus decreasing the time required for each test.

Aldabagh and Beer (1971) evaluated the method and listed the low manpower, low-water requirement and fast response time as advantages. The listing of the method in the previously listed references makes it unnecessary to include it here. The interested reader should the above references.

3.3.2 Bore Hole Infiltrometer (Guelph Permeameter)

The bore hole infiltrometer is commonly known as the Guelph Permeameter (GP), given its' most current development by Reynolds and Elrick at the University of Guelph, Ontario, Canada. The GP method uses a Mariotte tube principle to set a desired hydraulic head, which can then be used to measure the saturated hydraulic conductivity. The sorptivity and, given empirical equations, the conductivity-pressure head curve relationship may also be calculated. It is, essentially a in-hole Mariotte bottle. The paper by Reynolds and Elrick (1986) includes an in-depth and specific set of instructions for use of this device in low- and high-conductivity material. They also include a substantial list of references on the theory and development of the GP method. Thus, only a cursory discussion will be included here to give the reader enough information to determine if this method is suitable for a given study site.

The GP method requires that a bore hole be excavated or drilled to the depth desired for the test. Experimental logistics make this test a near surface test, probably on the order of one meter or less in depth. Once the bore hole is prepared, the permeameter is entered into the hole, and stabilized with a tripod assembly. The GP is essentially a 3-inch diameter tube with several smaller tubes inside, closed off at both ends except for a bubble tube at the top, and an outlet port at the bottom. The bubble tube is movable so that the hydraulic head can be set. Figure B.3 provides a brief schematic of the GP.

3.3.3 Disc Permeameters

Disc permeameters are similar to the Guelph Permeameter, yet are installed on the soil surface, similar to the air-entry permeameter. The disc permeameter is described by Clothier and White (1981) and was refined by Ankeny et al. (1988). It operates with a screen coarse enough to offer no resistance to flow, yet fine enough to have a bubbling pressure of around 10 cm water. This bubbling pressure allows the reservoir to be filled, and the unit to installed without the water flowing from the permeameter.

The disc permeameter is installed onto a 15 cm diameter ring, which is sealed to the soil surface with bentonite. The soil surface is prepared only to remove larger rocks, or vegetation which could puncture the screen at the bottom of the reservoir. Once the valve on the top of the reservoir is released, water floods the soil surface and begins to infiltrate. The reservoir supplies water to the soil ring at the infiltration rate. The level in the reservoir is recorded until either the water is used up or the system reaches steady state.

Pressure transducers can be used to automate the data collection. It has been shown that using two transducers, one at the top to record the hanging water column and the second at the bottom to measure the water head, significantly reduces error due to the bubbling from the Mariotte tube (Ankeny et al., 1988).

The disc permeameter has the advantage of being able to record very near surface infiltration rates without disturbing the soil surface. The test is rapid, requires only a relatively small amount of water, and is not labor intensive.

3.3.4 Ring Infiltrometers

The ring infiltrometer, which ostensibly measures infiltration rate, can be used to estimate field K_{sat} as well. Amoozegar and Warrick (1986) and Bouwer (1986) describe a method, very similar to the ring infiltrometer, as the cylindrical permeameter method. The method can use one ring (called the single-ring infiltrometer) or two rings (called a double-ring infiltrometer). In this method, one or two rings are driven into the soil surface to a depth of about 15 cm (not critical), using care not to disturb the soil surface. If two rings are used, the second ring of significantly smaller diameter is driven to a slightly shallower depth, concentric to the outer ring. The outer ring is used to reduce the effect of lateral flow on the infiltration results. The major difference between methods described by Amoozegar and Warrick (1986), and Bouwer (1986), is that the

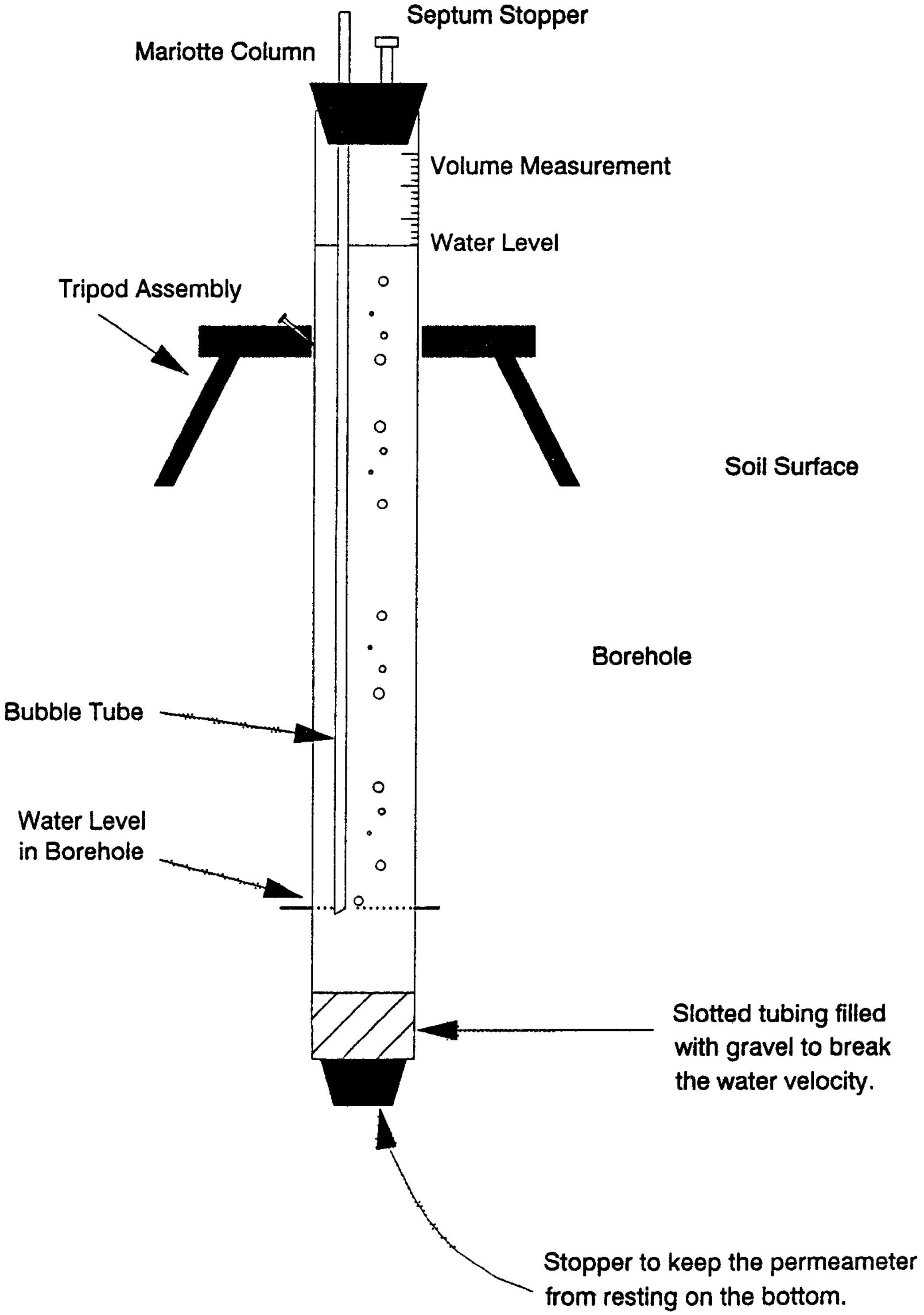


Figure B.3 Diagram of Guelph Permeameter

former method states that the ring can be installed at the bottom of an excavated area, whereas the latter method describes installation of the ring on the soil surface.

The test can be run one of two ways. In the falling head method, a known amount of water is added to the ring, and the water level inside the ring is recorded. By knowing the cross-sectional area of the ring, the volume of water which has infiltrated the soil through time is calculated. If two rings are used, water is added to both rings to the same level. Water level is then recorded in the inner ring only, and the volume calculated accordingly. In the constant head method, water is added to the ring(s) during the test to maintain a constant water level. Water can be added frequently in small amounts, or continuously using a Mariotte system or adjustable pump. Water must be added to both the inner and outer rings simultaneously, if the double-ring test is being conducted; otherwise, lateral hydraulic gradients will develop and non-vertical flow will occur. The amount of water added to the rings through time is recorded, and the infiltration rate is then determined.

When the system approaches steady-state, the infiltration rate will become steady. This final rate, expressed in terms of L/T, approximately equals the field K_{sat}. The value is approximate because the soil may not be completely saturated, and small amounts of entrapped air will have a large effect on the field K_{sat}. It may be necessary to install several tensiometers outside of the inner ring and inside the outer ring, and monitor the tension in the soil. The test should be run until tension drops to near zero. Bouwer (1986) describes the experimental set-up and potential problems which can arise when conducting the test. Also, the American Society of Testing and Materials (ASTM, 1989a) describes the use of the double-ring infiltrometer for measuring intake rate of soils.

3.4 Quality Assurance/Quality Control

The field K_{sat} values obtained using the above methods are strongly dependent on the type and temperature of the fluid used. It is important, therefore that the test fluid be approximately equal in quality to the soil solution (Bouwer, 1986). Incompatible salt concentrations in the fluid can lead to drastically reduced conductivity results, especially if swelling clay is present (Dane and Klute, 1977). It may be necessary to collect a soil sample prior to conducting the conductivity test, and analyze an extract sample for dissolved solids. The test fluid can then be mixed to the same dissolved salt concentrations. Bouwer (1986) also mentions that the solution temperature should be the same as the soil temperature so that soil air does not dissolve into the infiltrating water, thus reducing the conductivity.

Another source of error which spans the tests listed above is the condition of the soil surface or borehole being used for the test. It is critical that the soil surface not be compacted or otherwise disturbed prior to setting the air-entry permeameter, disc permeameter, or ring infiltrometer onto the soil surface. This can create a low conductivity crust on the soil surface which will have a deleterious effect on the conductivity results. The borehole used for the Guelph Permeameter should be treated with a spiked wheel or other means to remove smear layers (Reynolds and Elrick, 1986).

4 Field Unsaturated Hydraulic Conductivity

4.1 Introduction

The rate, direction and volumes of water which migrate through the soil are dependent in large part on the hydraulic conductivity, which in turn is dependent on the water content of the soil. Computer models that predict migration rates in unsaturated material require a knowledge of the relationship between hydraulic conductivity and water content ($K(\theta)$) and water tension ($K(h)$). To determine these relationships, samples often are collected from the field and taken to the laboratory for analysis. The data are then used directly in the models, with the assumption that the laboratory-derived data will represent conditions observed in the field.

Extensive testing of this assumption was performed at the Las Cruces Trench site, where 594 undisturbed soil cores were collected from 9 soil horizons and taken to the laboratory for determination of the water retention function and the saturated conductivity (Wierenga et al., 1989). The van Genuchten (1980) equation was fit to the data and numerical determinations of the $K(\theta)$ function were made. In addition, 450 field saturated hydraulic conductivity tests were conducted at sites immediately adjacent to locations where the undisturbed cores were sampled. The results showed considerable differences between laboratory and field conductivity values, though the overall pattern of variability was similar (Wierenga et al., 1991). Experiments currently underway are designed to improve the modeling results (Hills and Wierenga, 1991). We note here that these tests for saturated conductivity do not apply directly to discussions concerning unsaturated conductivity, but rather they are mentioned to illustrate that laboratory test results may not accurately define field conditions. Thus, field tests to obtain in-situ hydraulic conductivity values should be considered when characterizing sites for LLW disposal.

This section discusses two methods of determining in-situ unsaturated hydraulic conductivity: tension infiltrometer for "point" measurements, and the internal drainage method. Other tests may be available, such as the double-ring infiltrometer test. However, here we are only considering those tests which are both accurate and reasonably easy to set-up. The tension infiltrometer is acceptable on both of these points. The internal drainage method is very useful in determining an average unsaturated conductivity value for larger volumes of soil, though more difficult in the actual performance.

Two references are worth noting here, as they will be referenced several time herein. Green et al. (1986), and Hillel (1980) discuss several methods of determining in-situ conductivity with the internal drainage method, as well as theory behind in-situ tests. Discussions about tension infiltrometers referenced in more recent reports.

4.2 Principles

4.2.1 Tension Infiltrometry

The tension infiltrometer provides a measure of the steady-state unsaturated conductivity at tensions ranging from zero to about 25 cm. The principle equation behind it's use was first proposed by Wooding (1968). The equation he developed relates the unsaturated conductivity at the supply potential and a macropore capillary length parameter, later found to be a function of the sorptivity and conductivity (White and Sully 1987). Wooding's equation is as follows:

$$q_\infty = \pi r^2 K_o + 4rK_o\lambda_c \qquad (28)$$

where q_∞ = steady-state flux rate (L^3/T)
r = radius of the disc in the infiltrometer (L)
λ_c = macropore capillary length (L)
K_o = unsaturated hydraulic conductivity (L/T)

The first term on the right of equation (28) represents the contribution of gravity to the total flow from the surface disc and the second term presents capillarity (Hussen 1991).

The macropore capillary length parameter is described as the "mean" height of capillary rise above a water table (White and Sully, 1987), and is determined by

$$\lambda_c = [K(h_o) - K(h_n)]^{-1} \int_{h_n}^{h_o} K(h)dh \qquad (29)$$

After substituting in the relationship of λ_c into equation (28), and solving for K_o, we are left with the following equation

$$K_o = q_\infty/\pi r^2 - 2.25\, S_o^2/[\pi r(\theta_o - \theta_n)] \qquad (30)$$

where S_o = slope of the calculated cumulative infiltration versus square root of time, ($L/T^{1/2}$)
θ_o = volumetric water content at supply potential (L^3/L^3)
θ_n = initial volumetric water content (L^3/L^3)

The conductivity value determined from equation (30) is related to the tension applied from the infiltrometer. Thus, a number of tests need to be run at different tensions allowing the system to reach steady-state before calculating the final flux rate. A potential problem with using equation (30), however, is the possibility of obtaining negative conductivity values; an incorrectly high value of sorptivity will cause this. Therefore, a modification of this equation, proposed by Wooding (1968), is:

$$\frac{q_\infty}{\pi r^2} = K_o(1 + 4\lambda_c/\pi r) \qquad (31)$$

By determining the conductivities (K_o) for different flux rates, it is possible to solve the system of equations for λ_c, which is then plugged back into equation (31) and solved for K_o.

The original tension infiltrometer was designed by Clothier and White (1981), which consisted of a vertical tower filled with water, attached to a bottom porous plate. A hypodermic needle was installed 4 cm above the porous plate, where atmospheric pressure was maintained. The porous plate was placed on a layer of sand,

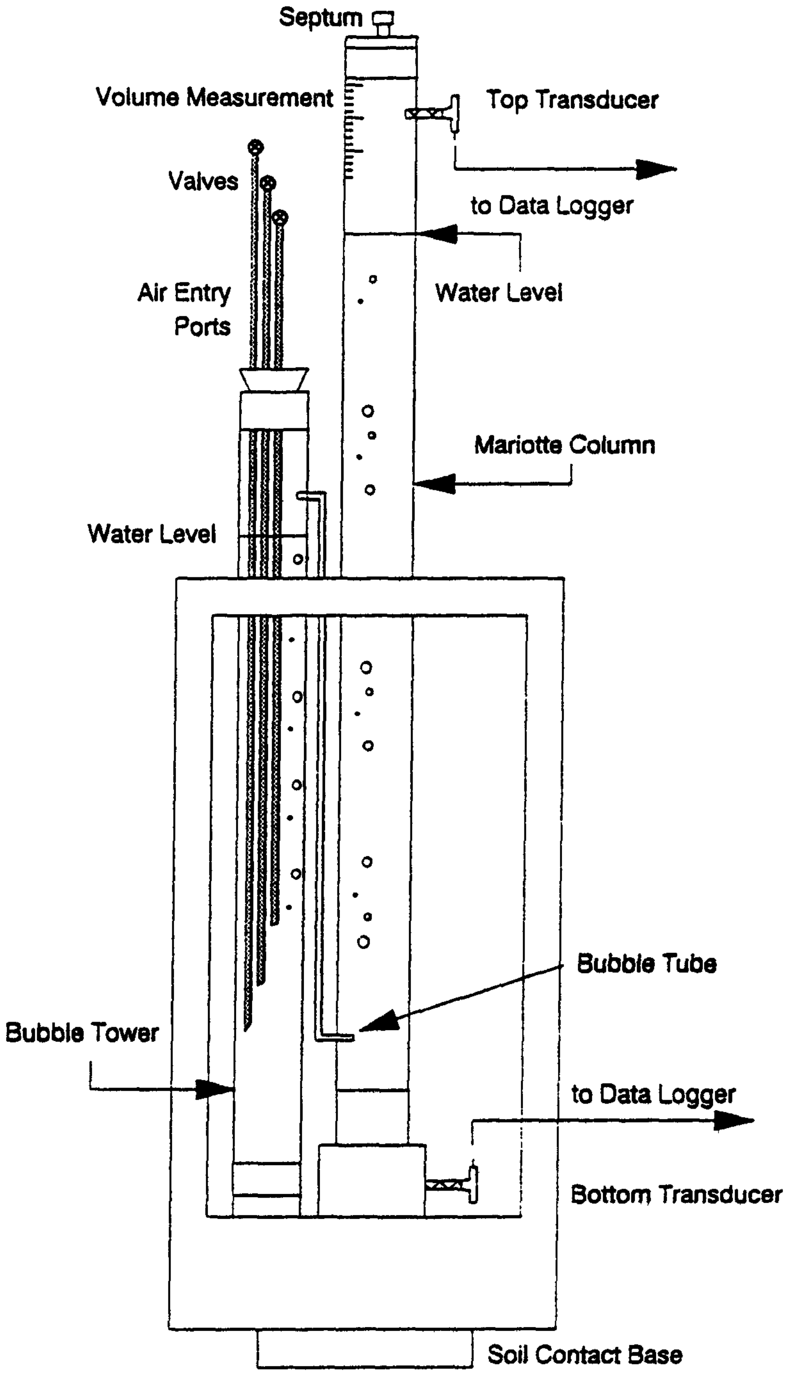


Figure B.4 Diagram of tension infiltrometer

thereby providing a hydraulic contact between it and the soil profile. This design was modified by Watson and Luxmore (1986) in which they added a second water column for pressure control (Figure B.4). Using the two tower design, they were able to determine conductivity at different tensions, depending on the difference between the bottom of the air entry port and the water level. The design has been further modified by Soil Measurement Systems (Tucson, Arizona) in which the bubble tower is connected to the Mariotte column with flexible tubing. This reduces problems associated with instability of the two tower system during high wind or rearrangement of transducer wires. The maximum tension which can be used on the tension infiltrometer, regardless of the design, depends on the height of the bubble tower and the air entry value of the porous membrane.

4.2.2 Internal Drainage Method

The internal drainage method, also known as the unsteady drainage method or the instantaneous profile method, is a transient field method which can provide the unsaturated conductivity for soil profiles larger than the tension infiltrometer. Experimental set-up is much more extensive, though, requiring neutron probe access tubes, and a series of tensiometers. A simplified experimental set-up is described by Green et al. (1986).

The experiment is carried out by ponding a known amount of water on the soil surface, covering the soil surface to inhibit evaporation, and measuring the location of the wetting front, and the water content and water tension above the wetting front. Measurements are taken during redistribution of water.

Richards equation for one-dimensional, isothermal, nonhysteretic unsaturated flow is used to analyze the data

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(K(\theta)\frac{\partial H(z,t)}{\partial z}\right) \tag{32}$$

where θ = volumetric water content (L^3/L^3)

If the changes in water content and water tension with time are known, we can integrate equation (32) to obtain the average conductivity of a soil profile. The equation is as follows:

$$\frac{\partial}{\partial t}\int_{0}^{z} \theta(z,t) = K(\theta)\frac{\partial H(z,t)}{\partial z}\bigg|_{z} \tag{33}$$

Diffusivity can be determined from the results of this experiment by calculating the ratio of the hydraulic conductivity to the water holding capacity of the soil. Sorptivity is also determined from the results of the experiment. Hillel (1980) provides a discussion of the theory behind the internal drainage method.

A number of configurations can be designed for measuring the change in water content and water tension with depth during an experiment. Neutron probe access tubes can be installed in the center of the test plot (see Figure B.5) for accurate determinations in the changes in water content. The total change in the mass of the water in the profile can be calculated discretely by using the trapezoidal rule for estimating continuous functions (Green et al., 1986). Tensiometers should also be installed at different depths and spatial locations so that the vertical gradient can be calculated. Rapid determinations of water tension can be obtained by using

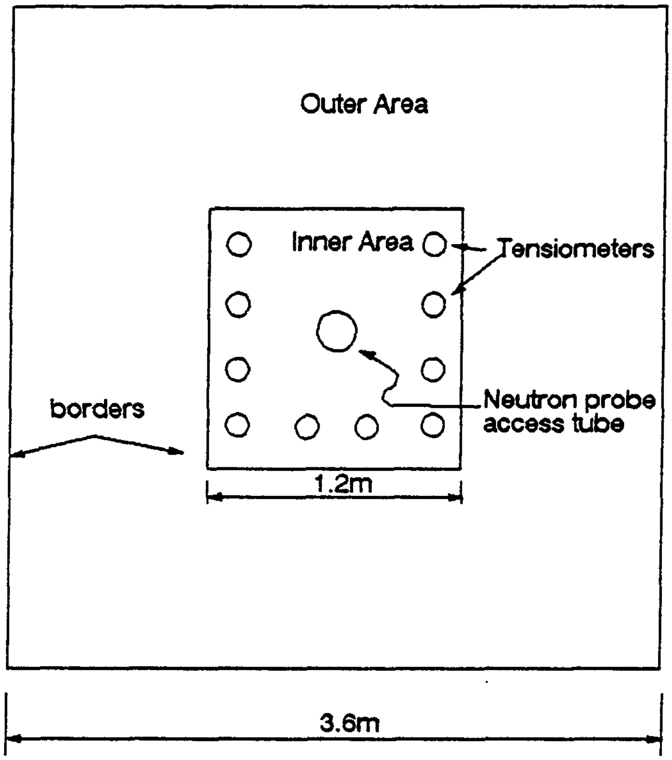


Figure B.5 Map view of set-up for determining field unsaturated hydraulic conductivity using internal drainage method (after Green et al., 1986)

pressure transducers and a data acquisition system. By automating the collection of data, both the water content and water tension can be recorded simultaneously and the conductivity calculated as a function of water content.

A simplified internal drainage method is described by Green et al. (1986). Data is collected periodically, and conductivity is determined as a power function, not directly from the measurements. An assumption during redistribution for the simplified method is that the hydraulic gradient is unity, and that only gravitational flow is occurring, and lateral flow is negligible. Unless the plot is large (more than 2 m on a side) significant lateral flow may occur during these tests.

4.3 Procedures

4.3.1 Tension Infiltrometry

Although the technique of tension infiltrometry is not standardized by the American Society for Testing and Materials, or described in the Methods of Soil Analysis (Klute, 1986), a number of references are available that describe how to set up the experiments. Clothier and White (1981), Watson and Luxmore (1986), Ankeny et al. (1988), and Hussen (1991) are just a few of several references which describe the tension infiltrometer and experimental set-up. White and Sully (1987) describe the importance of λ_c and how to obtain this information directly from the experimental results. A very recent publication which describes the step by step set-up and operation of these experiments is Hussen (1991). Hussen also provides a very up-to-date list of references.

Tension infiltrometers have been obtained by the authors from Soil Measurement Systems (Tucson, Arizona). An attachment to the Borehole (Guelph) Infiltrometer for measuring the conductivity at tensions up to 25 cm has also been obtained from the Soilmoisture Equipment Corporation (Santa Barbara, California).

The listing of procedures in the aforementioned references obviates the need to repeat them here. It is recommended that the user consult these references and manufacturers when preparing to conduct this experiment.

4.3.2 Internal Drainage Method

Step by step procedures for performing internal drainage experiments, and equipment needs, are described by Green et al. (1986). Green et al. (1986) also include a sample table for recording data, and suggested methods of data analysis.

4.4 Quality Assurance/Quality Control

Many of the QA/QC issues involve choosing the proper locations for setting up and performing the experiments. With regard to the tension infiltrometer, it is important that the sites chosen are as undisturbed as possible. Even disturbance due to footsteps, for example, were found to alter conductivity values more than tillage, because flow is transmitted through the surface horizon (Hussen, 1991). Thus, once sites are chosen, they should be cordoned off and avoided until the experiment is completed. The locations should be as level as possible, and free of large stones or sharp objects. Sites which are sloped increase the probability that the reservoir tower will not be stable, leading to a loss of contact with the sand layer unless the reservoir tower and disc are connected by a flexible tube. This may be especially important if pressure transducers are used to measure the water levels; wires leading to a data recorder can be accidentally pulled or hooked, causing the water tower to fall over. Therefore, it may be necessary to level the site very carefully. Objects, such as large stones can also decrease the contact with the sand. Twigs, cactus spines, or other sharp objects can puncture the thin porous membrane, damaging the infiltrometer. The references above should be consulted for more information.

Quality control items with respect to the experimental setup, operation, and data analysis, are described by Green et al. (1986) under the "Comments" section. The reader should consult this reference before beginning this experiment.

5 Field Water Content

5.1 Introduction

Field determinations of water content are based on the same principles as laboratory determinations. Field water contents can be important indicators of possible failures of a containment system, and long-term deep recharge into disposal units or surrounding soil. In most cases, water contents will change before the detection of contaminants, even when retardation is negligible (Elabd et al., 1988). Accurate detection of changes in water content can provide additional time for the implementation of remedial actions before the contaminant reaches the point of compliance. Unfortunately, accurate measurement of water content in the field is not easy. Further, it should be understood that water content change alone does not determine flow. A steady downward drainage of several cm of water per day can occur under conditions of constant water content simply because of gravity drainage. Water content changes can denote transient pulses of water that may or may not be drainage related (evaporation or transportation may also be acting).

Both indirect and direct methods are available for determining field water content, but given the experimental control in the laboratory, indirect measurements are more common. Of the indirect methods available, tensiometry, electrical conductivity and capacitance, and neutron thermalization are most common, so they will be discussed here. A thorough review of the theory and importance of water content, methods for calculating water content, and determinations of error associated with these methods are included in Gardner (1986).

5.2 Principles

As mentioned above, obtaining direct measurements of water content in the field is difficult, especially during experiments. Experimental control of the soil volume, a priori knowledge of the water content before the experiment begins, and sampling of the soil all contribute to the difficulties of measuring in-situ water content directly. In most cases, direct measurements require that a soil sample be collected and transported to the laboratory where it is weighed, placed in an oven for drying, then weighed again. Initial conditions may change within the time necessary for the weighing and drying process.

Indirect methods involve the measurement of a physical or chemical property that is affected by water content. These usually involve the measurement of (1) the energy status of the water in the soil matrix using e.g., a tensiometer, (2) the electrical properties, using e.g., a Time Domain Reflectometer, or (3) the neutron scattering method using a neutron probe. Indirect methods have the advantage over direct methods in that they allow the use of automated data collection systems for non-destructive determinations of in-situ water content. A disadvantage of indirect methods is the need, in most cases, for calibration. This requirement can be very challenging when using some instruments (e.g., neutron probe) that measure larger volumes of soil, and the need to control precisely the amount of water present in the soil volume. Also, instrument response is often affected by the wetting history of the soil. This phenomenon, known as hysteresis, can cause significant errors in the calibration curves which are difficult to quantify. Hysteresis may, for example, require the user to generate one calibration curve for drying soil, and one for wetting soil.

5.3 Methods

5.3.1 Soil Water Tension

Measuring soil water tension for determining water content is commonly practiced in the field and laboratory. However, a complete discussion on this method can be found in Appendix A, so it will not be repeated herein.

5.3.2 Electrical Conductivity and Capacitance

The ability to measure the electrical conductivity and capacitance of soil, and apply these measurements to water content, allows for remote and non-destructive sampling procedures which can be automated. This automation increases the utility of these methods, especially for Time Domain Reflectometry (TDR), which can be used to measure water content of soils in the field, with data downloaded directly to computer (Figure B.6). Additional information on these methods is found in Appendix A, Section 4.1.

5.3.3 Neutron Thermalization

Neutron thermalization as a tool for determining water content is based on the slowing down of high-energy neutrons from a radioactive source (e.g., americium-beryllium) by hydrogen nuclei contained in the soil. This method has utility in that the major source of hydrogens in the soil is water. As high-energy ("fast") neutrons are emitted from the source, they collide with hydrogen atoms and form what are known as thermal neutrons. These collisions form a thermal cloud of neutrons, whose size is constant, but whose density is dependent on the water content. Higher water content leads to increased thermalization and denser thermal clouds. The density of the thermal cloud is measured by a detector installed adjacent to the source. This detector is sensitive only to transformed neutrons called "slow" neutrons. The number of slow neutrons counted is based on the statistical probability of a collision occurring between fast neutrons and hydrogen, and on the degree of energy transfer causing the transformation to slow neutrons. Therefore, the number of counts from the detector is directly related to the water content. Greacen (1981) provides an excellent discussion on neutron thermalization. The interested reader should consult this reference.

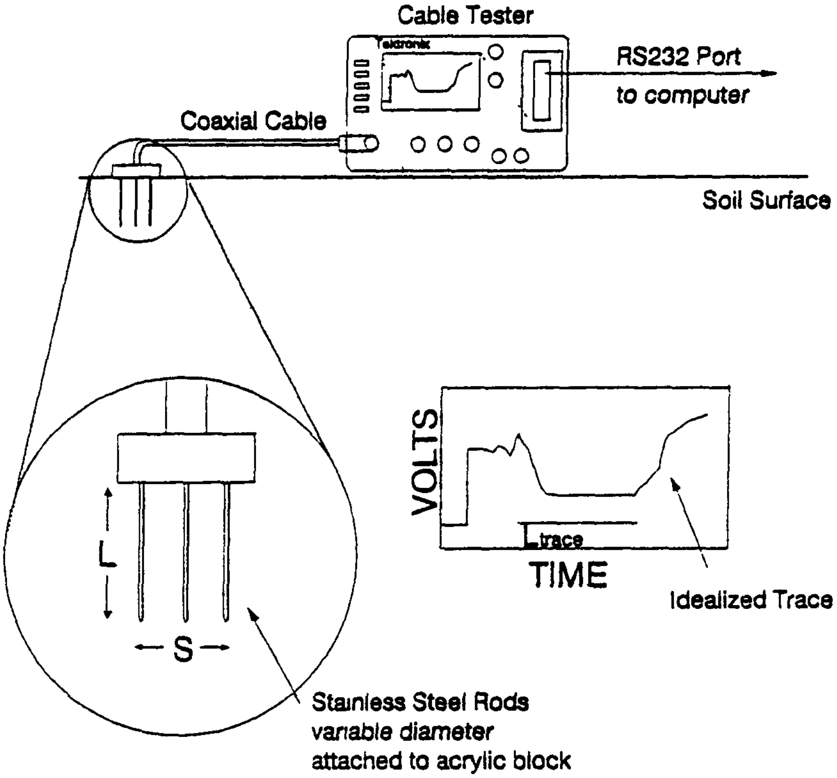


Figure B.6. Diagram of time domain reflectometry for measuring field water content

The neutron probe is very effective for measuring water content at depth. The probe can be lowered into a borehole (often called a neutron probe access tube), and used to measure water content at desired intervals. Highly reproducible results can be achieved over long periods of time (Wierenga et al., 1990). A disadvantage of the neutron probe is difficult calibration. Because the thermal cloud has a certain volume, sampling a block of soil to be used for calibration is challenging. In-situ calibration, with subsequent sampling adjacent to a neutron probe access tube precludes the development of a calibration curve for a wide range of the water contents for the soil sample. Furthermore, organic material rich in hydrogens, or organic liquid contamination in the soil, will affect the calibration. Finally, because the neutron probe contains a radioactive source, NRC permits, and possibly state permits, are required. Additional worker health and safety issues need to be considered.

5.4 Quality Assurance/Quality Control

Possible errors associated with indirect field methods for determining water content can be numerous. This is because calibration curves are used to convert physical, electronic and nuclear responses to water content. In some agricultural applications, these calibration curves need not be as accurate, because the resolution required for the water content is low. However, this is usually not the case in environmental applications, where errors in water contents of less than a percent can affect the hydraulic conductivity by several times. It is especially important that procedures be developed for tracking the performance of particular pressure transducers, neutron probes, and TDR probes. For pressure transducers, each sensor has a specific calibration equation associated with it. The calibration equation may drift somewhat over time, leading to errors in tension readings. The user should track each calibration equation to ensure that the drift is within manufacturers specifications. Often times, recalibration is the only way to detect a problem with the transducer. Thus, recalibration should be an integral part of the use of these sensors.

For neutron thermalization, the calibration curve is associated only for the particular probe, counter and soil. If more than one neutron probe is used for a study, a calibration equation for each probe must be generated. Protocol for tracking when a particular probe is used will ensure that the correct calibration equation is used to calculate the water content. If the probe is changed, a transformation equation relating the new probe to the old probe must be developed. This can be achieved by taking readings with the old and new components of the system, then calculating a regression equation to relate the two systems. The transformation equation is especially needed if, for example, the probe is returned to the manufacturer for source replacement, or probe rewiring. Replacement, or addition, of a counter can also change the readings, thus requiring a transformation equation. It is also prudent to take standard counts each time the probe is used, or at specified time intervals. The results of the standard counts should be very similar, though count ratios will decrease with time due to source decay. Methods of taking standard counts must be standardized.

It will be experienced by many that the majority of time devoted to indirect methods of determining water content will go towards developing calibration curves. However, the rewards for solving these problems will be realized in greatly reduced staff time requirements and increased experimental efficiency. Obviously, the scope of this text falls short of providing methods to generate calibration curves. The user is directed to manufacturers' data sheets for a list of possible errors for their respective instruments, and to the references listed below for additional information.

6 Field Water Tension

This section discusses field measurements of soil water tension, (also called pressure potential or pressure head). Field measurement of tension is used, in the environmental field, to predict where soil water may be flowing. This, of course, becomes very important when demonstrating compliance at disposal facilities, since changes in tension signal water movement. The ability to monitor soil water tension at different depths and laterally across the site requires that monitoring devices be placed in the vicinity of one another, and that data be collected at or about the same time.

Soil water tension varies with water content, being 0 at saturation and as high as 80 bars (8.0 MPa) or more in dry soils. The relationship between tension and water content is called the water retention function and is represented by the water release curve (see Water Retention Function in Appendix A). This curve is determined in the laboratory on a representative number of samples, collected from soil horizons which may be involved in flow processes from the site. Analyses of soil water movement requires that the water retention curve is well defined. Several mathematical expressions have been developed to fit single values of water content and water tension (e.g., Brooks and Corey, 1964; Mualem, 1976; van Genuchten, 1980). The accuracy of these fitted curves is based, in part, on the accuracy of the tension-water content data determined through experimentation.

Model predictions of soil water movement depend, in part, on the ability of the monitoring network to describe the hydraulic behavior of the soil at the disposal site. Though the input data of soil physical properties is frequently generated in the laboratory, verifying that the model is describing the processes observed in the field requires accurate field data. Because of the diversity of physical conditions at different disposal sites, this section will not provide concrete numbers or locations where monitoring devices should be installed. Rather, it will provide a basis for choosing which devices to install, and which methods of measuring water tension are most accurate under field situations.

The two most common methods of determining water tension are tensiometry and thermocouple psychrometry. Their use in the field is the same as the laboratory, thus their descriptions are the same also. In the need to remain brief, we refer the reader to Laboratory Water Tension (Appendix A) for a complete discussion.

Appendix C

Database Example
(Las Cruces Trench Study)

1 Database Example (Las Cruces Trench Study)

The experimental program at the Las Cruces Trench site (Wierenga et al., 1989, 1990) is designed to provide data to test deterministic and stochastic models for water flow and solute transport through the vadose zone. The emphasis is on site conditions typical of low level waste sites located in arid regions. A series of experiments have been performed to characterize the site and to study the movement of water and solutes through spatially variable soils. Water with solute tracers are applied to the surface of the site through carefully controlled irrigation systems and the movement of the water and tracers through the soil profile is monitored using dense grids of neutron probe measurements, tensiometers, and solute samplers. The data from these experiments are organized to provide modelers from various organizations easy access to both raw and processed data. By comparing model predictions to experimental observations, the numerical models used to predict the movement of water and contaminants through unsaturated soils can be tested.

1.1 Overview of Database Objectives

The Las Cruces Trench Experiments are unique in that the end users (i.e., the modelers) who access the data are well versed in the programming of both mainframe and personal computers. In addition, the users are mostly interested in the processed data. As a result, the most useful database format from the end user's perspective is simply to organize ASCII text formatted files in a systematic fashion and store the resulting files on a computer accessible through national networks. The use of formal database software would hinder the modelers access to the data since they would have to learn the software.

In contrast, the database needs of the experimentalist are more complicated. For the experimentalist, the database provides a mechanism to store raw data, to process the data, and to check data consistency through computer visualization. These requirements have to be met in a user friendly fashion since the computer literacy of most experimentalists is not as high as for the modelers. As is the case for most experimentalists, the experimentalists at the Las Cruces Trench site are familiar with the use of personal computer spreadsheets.

To meet the needs of both the experimentalists and the modelers, the data input, data processing, and data visualization are done on personal computers using carefully constructed graphical spreadsheets. Macros were written for the spreadsheets to automate the data entry as much as possible, to process the data, to plot the data in a form familiar and useful to the experimentalists, and finally, to put the processed data in ASCII text format for use by the modelers. The ASCII formatted files are then uploaded to a Digital VAX with easy network access, and organized into a structured set of files. While the bulk of the data exists on personal computers, a complete copy of the processed data and some of the raw data are maintained on the VAX for access by the modelers. Details of the data and database procedures are discussed below.

1.2 Data Collected and Database Procedures

Both static and dynamic data were collected at the Las Cruces Trench site. The static data consists of characterization data which can be measured, processed, and distributed to the modelers as a unit. In contrast, the dynamic data is measured continuously and must be processed and released to the modelers in a continuous fashion. The data collected, which are available to the modelers, are summarized in Table C.1.

The characterization data were generated using both laboratory and field techniques (see Table C.1). The experimental procedures were labor intensive and little automation was possible. In addition, the data processing required for the characterization parameters was fairly involved. The estimation of the van Genuchten parameters θ_r, n, and α, for example, required the use of nonlinear estimation procedures which were beyond the capabilities of common personal computer database packages. As a result, the retention data

Table C.1 Parameters measured during the Las Cruces trench experiments

Parameter	Scale	Technique	Reference
		Characterization Variables	
K_{sat}	8 cm	Measured flow through saturated cores	Elrick et al. (1980), Wierenga et al. (1989)
K_{sat}	10 cm	Borehole permeameter	Reynolds el al. (1984), Wierenga et al. (1989)
θ_r, θ_s, n, α	8 cm	Cores and constant pressure apparatus combined with parameter estimation	Wierenga et al. (1989)
Particle size distribution	8 cm	Soil sieves and modified pipet method	Gee and Bauder (1986), Wierenga et al. (1989)
		Dynamic Variables	
θ	50 cm	Neutron Probe	Wierenga et al. (1990)
h	2 cm	Tensiometers	Wierenga et al. (1990)
Concentrations of solutes	2 cm	Solute Samplers	Wierenga et al. (1990)

were uploaded to a Digital VAX, the van Genuchten parameters were evaluated using nonlinear parameter estimation software, and both the retention data and the resulting van Genuchten parameters were transferred into the database. The experimental procedures and all data analysis for the characterization experiments are documented in Wierenga et al. (1989).

While the data processing requirements for the dynamic data were more modest than those required for the static data, the quantity of dynamic data was much larger. The data had to be processed continuously to provide immediate feedback to the experimentalists and to provide the modelers access to the processed data. The following procedures were set-up to expedite data entry and processing.

(1) A computerized spreadsheet software package (WingZ, Informix Software, Inc., 1988) with good graphical and programming capabilities was chosen for use with Macintosh personal computers as the data processing system. Macintosh computers were chosen because they are easy to use, already available to the project participants, and adequate for the data needs of the project. In addition, the database manager and the lead field technician already possess a good working knowledge of their use.

(2) Spreadsheet macros were written to automate the data input as much as possible, to automate data processing, to generate graphics, and to dump the processed data in the appropriate ASCII file format for uploading to the VAX.

(3) The neutron probe used to measure water content has sufficient internal digital storage for one day of readings. The data are stored as neutron counts in the probe, dumped to a floppy disk through an IBM personal computer, digitally transferred into the Macintosh spreadsheet program, and processed. In contrast, the tensiometer readings and solute sample chemical analysis were performed on a sample by sample basis and were entered into the corresponding Macintosh spreadsheets

manually. The experimental procedures used to generate the dynamic data are documented in Wierenga et al. (1990).

(4) Graphical macros were written to automate the plotting of the following processed quantities while in the spreadsheets:

a. Contour plots of the changes in water content between two days chosen by the user can be plotted. The changes are plotted as a function of depth and neutron probe access tube number. Inspection of the resulting contour plots highlight if and where anomalous changes in water content occur. Because each contour plot represents approximately 1000 measurement locations, the contour plots provide an efficient mechanism for the experimentalists to monitor the measurements across the site. In addition, the movement of water as illustrated by the contour plots, helps to define when and where additional neutron probe access tubes should be installed.

b. X-Y plots of water content versus depth for each neutron probe access tube location can be plotted. Two days of data can be plotted simultaneously. Once the user detects an anomalous behavior from the contour plots, the corresponding X-Y plots can be used to study the detail of the anomalous behavior.

c. Tension can be plotted as a function of time for each tensiometer location. This allows the experimentalist to detect if the tensiometer readings displayed unusual behavior such as occurs when a tensiometer loses water or develops small air or water leaks. This also allows the experimentalist to determine when and where to add tensiometers as the water plume moves through the soil profile.

d. Breakthrough curves for each of the solutes analyzed can be plotted. The plotting of breakthrough curves helps define where the solute plumes are, whether additional solute samplers are needed, and if there are systematic problems in the solute sampling and chemical analysis.

Each plot can be initiated by a simple mouse command while in the spreadsheet.

(5) Once the data are read into the spreadsheets and plotted to check for consistency, the data are dumped in appropriate ASCII format for import into the database. Spreadsheet macros were generated to fully automate this process so that the data could be dumped with a single command. The entire process of importing the neutron probe readings for one day (approximately 1000 readings), processing the data, plotting the results to check for consistency, and outputting the processed data in database format requires approximately 5 minutes.

(6) All spreadsheets are kept in a single directory tree with sub directories used to organize the various types of data.

(7) Copies of the entire directory tree are kept on two separate Macintosh systems located in separate buildings. One is used by the experimentalists to input the data and to check for consistency. The second is used by the database manager to re-check for consistency, to provide backup protection, and to dump the processed data in the appropriate format for uploading to the VAX. Additional backups of the data are kept on Bernoulli disks.

(8) The appropriate data are uploaded to a protected account on a Digital VAX which has easy network access using FTP. The VAX account is protected so that general users can read but not modify or

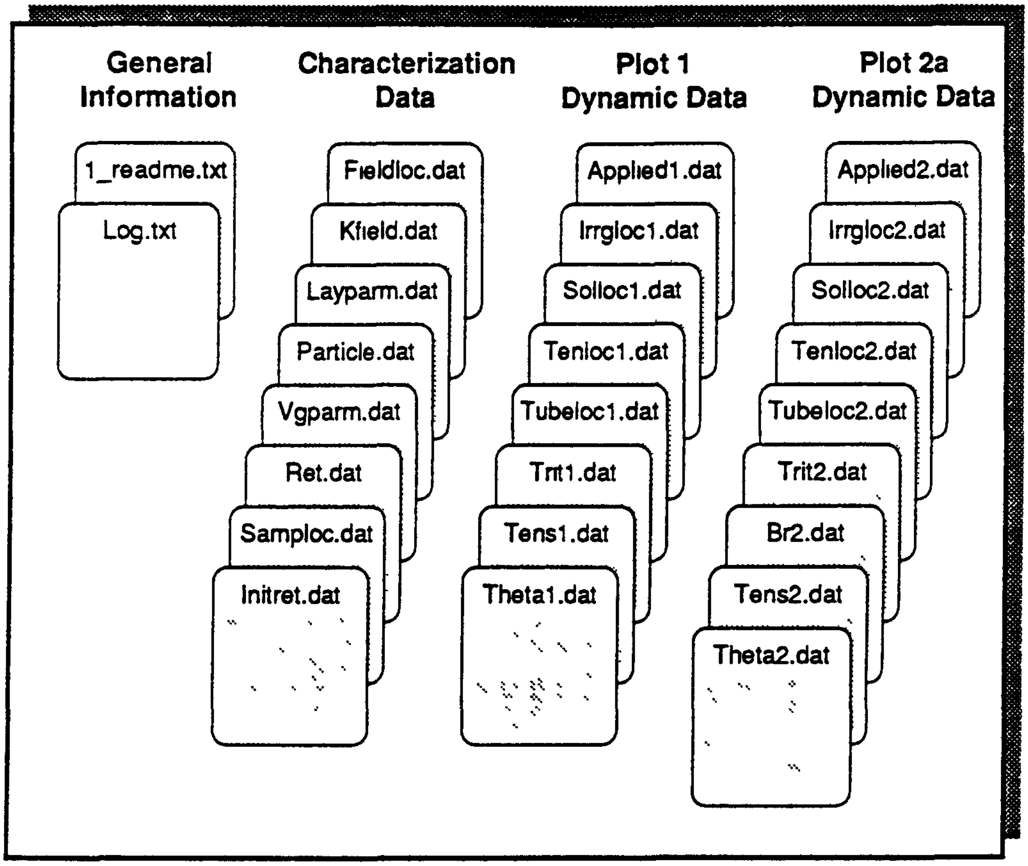


Figure C.1 Illustration of data file organization for Las Cruces Trench data

delete data. The data is organized into a series of ASCII text files as illustrated in Figure C.1 and stored in a single directory. A README.TXT file is provided fully documenting the contents and formats of each of the files. A LOG.TXT file is provided to notify end users of changes and updates made to the files on a continuing basis. The data files are organized in simple column structure, are tab delimited, and use carriage returns to denote end of records. As a result, the data can be easily read using unformatted FORTRAN read statements, or imported directly into most personal computer based spreadsheets, databases, or graphical packages. The structure of the VAX database and the formats of the database files are also documented in Wierenga et al. (1990).

Overall, the procedures used for data acquisition, processing, and storage have proven to work well. There has been no data lost, the data are well protected, and they are easy to access by both the experimentalists and the modelers.

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(See instructions on the reverse)

1 REPORT NUMBER
(Assigned by NRC. Add Vol., Supp., Rev., and Addendum Numbers, If any.)
NUREG/CR-5988
PNL-8480

2 TITLE AND SUBTITLE
Soil Characterization Methods for Unsaturated Low-Level Waste Sites

3 DATE REPORT PUBLISHED

MONTH	YEAR
February	1993

4 FIN OR GRANT NUMBER
L1007

5 AUTHOR(S)
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C. T. Kincaid, T. J. Nicholson[3], R. E. Cady[3]

6 TYPE OF REPORT

7. PERIOD COVERED *(Inclusive Dates)*

8 PERFORMING ORGANIZATION – NAME AND ADDRESS *(If NRC, provide Division, Office or Region, U S Nuclear Regulatory Commission, and mailing address, if contractor, provide name and mailing address.)*
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9 SPONSORING ORGANIZATION – NAME AND ADDRESS *(If NRC, type "Same as above" if contractor, provide NRC Division, Office or Region, U S Nuclear Regulatory Commission, and mailing address.)*
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10. SUPPLEMENTARY NOTES

11. ABSTRACT *(200 words or less)* To support a license application for the disposal of low-level radioactive waste (LLW), applicants must characterize the unsaturated zone. This requires an integrated plan to be developed for sampling and analyzing the soil horizons for physical and hydraulic properties. This document provides a strategy for developing this characterization plan. It describes principles of contaminant flow and transport, site characterization and monitoring strategies, and data management. It also discusses methods and practices that are currently used to monitor properties and conditions in the soil profile, how these properties influence water and waste migration, and why they are important to the license application. The methods part of the document is divided into sections on laboratory and field-based properties, then further subdivided into the description of methods for determining 18 physical, flow, and transport properties. Because of the availability of detailed procedures in many texts and journal articles, the reader is often directed for details to the available literature. References are made to experiments performed at the Las Cruces Trench site, New Mexico, that support LLW site characterization activities. A major contribution from the Las Cruces study is the experience gained in handling data sets for site characterization and the subsequent use of these data sets in modeling studies.

12 KEY WORDS/DESCRIPTORS *(List words or phrases that will assist researchers in locating the report)*
unsaturated waste sites
soil
characterization methods
physical properties
hydraulic properties
database
field methods
laboratory procedures

13 AVAILABILITY STATEMENT
unlimited

14 SECURITY CLASSIFICATION
(This Page)
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(This Report)
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15 NUMBER OF PAGES

16 PRICE