Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media

Part 1

Proceedings of the International Workshop on

Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media

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Edited by

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Preface

These Proceedings document presentations given at the International Workshop "Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media," held in Riverside, California, October 22-24, 1997. The workshop was organized to review various aspects of water flow and solute transport in unsaturated porous media, particularly with respect to the characterization and measurement of the unsaturated hydraulic properties (water retention, hydraulic conductivity). Knowledge of the hydraulic properties is indispensable for addressing many soil, hydrological, environmental, ecological and agricultural problems. They are needed in nearly all basic and applied aspects of soil, water, nutrient, and salinity management research (including precision agriculture), and serve as integrated indices for soil quality. They are also needed in models for heat and mass transport near the soil surface to simulate the extent and effects of regional and global climate change, and to interpret or improve the utility of remotely sensed soil moisture data at a variety of spatial scales.

About 220 scientists and engineers from some 20 countries participated in the Workshop; they included soil physicists, hydrologists, chemical and petroleum engineers, geologists, and agricultural engineers. Topics presented at the Workshop ranged from theoretical to application-oriented research, and from modeling to laboratory and field experimentation. The multidisciplinary nature of the Workshop provided unique opportunities for the participants to interact with each other, to appreciate issues and opportunities in porous media modeling and characterization, and to discover commonalities and differences between the various disciplines.

It is a pleasure and honor to acknowledge all those who contributed to the Workshop and these Proceedings. First and foremost, the Workshop had the fortune of being sponsored by a large number of governmental, professional and private organizations (see next page); their support directly reflects the importance of the Workshop. Success of the Workshop would have been impossible without the input from a large number of colleagues and friends, both here in Riverside and elsewhere. I thank all those who served on the Workshop Advisory Committee (see next page). In Riverside, the help by Donna Cooney, Debbie Noordman and Carol Hansen of the Department of Environmental Sciences of the University of California, Riverside, proved to be indispensable. Donna Cooney's insight and resourcefulness was especially critical. Roberta Cook provided similar support from the U.S. Salinity Laboratory. Special thanks are due to all those involved in the typing, editing and processing of the Workshop Abstracts and these Proceedings. They include Walter Russell, Janice Neal, Louise DeHayes and, especially, Sharon Conditt, whose expertise, commitment and enthusiasm up until her untimely passing in October 1998 inspired us all. Dallas Johnson and Kathy Chapman of Printing and Reprographics at UC-Riverside deserve much credit for their superb job of printing these Proceedings.

I also must thank the many people of the U.S. Salinity Laboratory for their tireless help before, during and after the workshop. These individuals include Bill Alves, Richard Austin, Fred Ernst, Joan Fargerlund, Jack Jobes, Sondra Luther, Binayak Mohanty, Walter Russell, Marcel Schaap, Pete Shouse, Jirka Simunek, Todd Skaggs, and Dong Wang, and of course co-editors Feike Leij and Laosheng Wu. Finally, many thanks to the participants who found it worthwhile to travel to Riverside from around the world, and who prepared first-rate contributions to these Proceedings; it was their input and dedication that made the Workshop such a successful event.

Martinus Th. van Genuchten
Workshop Coordinator

Riverside, California
July, 1999

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FLOW AND TRANSPORT

Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media

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Abstract. Quantifying and elucidating fluid flow in partially saturated porous media remains an important challenge, with many scientific and management applications. This paper contains a synopsis of theoretical and experimental methods to study and estimate the hydraulic properties of unsaturated media. Our main purpose is to provide a framework for the Proceedings of the workshop "Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media." We first discuss some of the problems related to the characterization and modeling of fluid flow in unsaturated media, as well as recent progress in this area. Subsequently we will peruse contributions to the workshop along five broad themes: (i) pore-scale phenomena, including those for multifluid systems, (ii) direct measurement methods, (iii) inverse modeling, (iv) indirect methods, and (v) other contributions pertaining to recent flow and transport research. We conclude by listing a number of topics in need for further investigation; this following a similar list compiled after the previous workshop [*van Genuchten and Leij*, 1992].

INTRODUCTION

The degree of fluid saturation has a profound impact on the transport of substances through porous media. A large part of these proceedings is devoted to the ability of porous media to retain and transmit water. This ability is characterized by the relationships between water content (θ), pressure head (h), and hydraulic conductivity (K). The movement of water and chemicals in the vadose zone and the exchange of heat and mass across the soil-atmosphere boundary, are all influenced by soil hydraulic properties. However, transport processes in many other porous media are also very much of interest [*Dullien*, 1992]. These proceedings reflect the broad array of scientific disciplines that study flow in unsaturated media, viz. soil science, petroleum engineering, civil and environmental engineering, hydrology, geology, building engineering, remote sensing, soil mechanics, and applied mathematics. Because of the many disciplined involved, it should be no surprise that different terminologies are being used for the constitutive relations in the unsaturated flow equation. In this paper we will largely adhere to soil physics terminology.

Flow in unsaturated porous media has traditionally been described with the Richards equation, which is based on the Buckingham-Darcy flux equation. In this approach, one-dimensional vertical flow in a homogeneous medium as a result of soil water pressure and gravitational gradients is described by the equation [*Richards*, 1931]

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(h)(\frac{\partial h}{\partial z} + 1)\right] \quad (1)$$

where h is the soil water pressure head [L], θ is the volumetric water content [$L^3\ L^{-3}$], K is the hydraulic conductivity [$L\ T^{-1}$], t is time [T], and z is vertical distance [L] taken positive upward. For unsaturated conditions h is negative (usually expressed in m or cm), although sometimes it is found more convenient to use positive values for h (i.e., suction heads). Alternative variables used to characterize the driving force for flow are pressure (often expressed in kPa) and potential

(J kg^{-1}). Equation (1) may not accurately describe water flow when additional driving forces are present, or when complications exists due to macropore or preferential flow, air flow, and/or the presence of nonuniform soil properties. Other formulations of the Richards equation arise when K is written as a function of θ, or when the soil water diffusivity is used.

Although much progress has been made in the development of improved methods and techniques for measuring the unsaturated hydraulic properties, many of the problems identified at the previous workshop remain [*van Genuchten and Leij*, 1992]. Current technology to determine the soil water retention curve, $\theta(h)$, and, especially, the unsaturated hydraulic conductivity function, $K(h)$ or $K(\theta)$, is still cumbersome, time consuming and inaccurate for many potential applications in view of financial and time constraints. Contributions on indirect methods (including pedotransfer functions), which were featured prominently in the previous Proceedings [*van Genuchten et al.*, 1992], continue therefore to be of interest as a relatively effective way to quantify the hydraulic properties.

The extreme nonlinear behavior of the hydraulic properties as a function of fluid saturation, and the highly irregular nature of the pore geometry of most media, poses substantial challenges for experimental and theoretical investigations of fluid flow and chemical transport in unsaturated porous media. Investigations have been greatly aided by recent advances in computer hardware and software. Computers facilitate fundamental research on flow phenomena at the pore-scale using pore network models, while natural pore systems can now be digitized to enable the development of more realistic pore-size distribution models for the hydraulic properties. The effect of hysteresis, wettability, temperature, chemical composition, and other variables, may be conveniently incorporated in such models. Experimental efforts have also progressed greatly. Techniques such as Nuclear Magnetic Resonance (NMR), High-resolution Computed Microtomography (CMT) and Time Domain Reflectometry (TDR) are now available to explore porous media, while routine and laborious determinations can be conducted more efficiently with automation software packages. Computer codes are essential to describe and analyze experimental results. If direct measurement of hydraulic properties is not feasible, computers offer the possibility to generate indirect estimates using regression or neural network algorithms. Databases are now being compiled and searched for pertinent information on the unsaturated hydraulic properties. User-friendly software packages and the internet are similarly improving the dissemination of results beyond a relatively small circle of experts on unsaturated flow. Last but not least, simulation models and geographic information systems (GIS) have become indispensable tools for quantifying and integrating the most pertinent physical, chemical and biological processes operative in the unsaturated (vadose) zone of soils and fractured rocks. The research community, as well as planning, action, and extension agencies, and the private industry, are increasingly relying on computer models, both in research and for practical field applications.

Still, the tremendous advances in computational power have highlighted deficiencies in the study of unsaturated media. Much fundamental research remains to be done to elucidate the behavior of fluids in porous media. Some areas of interest are: (i) flow and transport in heterogeneous subsurface systems, (ii) pore-scale modeling using more realistic pore geometries, (iii) multi-fluid flow and scaling for different fluid combinations, (iv) the relative contribution of capillary and adsorptive forces to water retention, and (v) the effects of hysteresis, wettability, temperature, and chemical composition on fluid flow. Experimental determination of the hydraulic properties is often a decidedly nonroutine process, and the availability of powerful software and computers is no panacea for the judgment of skilled practitioners. Sampling and sample handling are the first nontrivial steps for many experiments. This also because hydraulic properties of heterogeneous subsurface systems can vary greatly in space and time. Selecting the most appropriate method of measurement is usually not trivial; an inordinate array of experimental procedures exist, all with their own unique advantages and limitations. Moreover, the development and application of indirect methods is still severely hindered by a lack of data for model calibration and independent testing. And while numerical models and GIS are increasingly used for simulating flow and transport in unsaturated media, these tools are of practical value only if reliable methods or data exists for quantifying the hydraulic properties.

The aim of this chapter is to provide a perspective on unsaturated hydraulic property characterization and measurement by reviewing work contained in these Proceedings and by listing topics for further investigation. The review will proceed in a similar sequence as the Proceedings by addressing: (i) pore scale phenomena, including multi-fluid systems; (ii) direct laboratory and field methods, (iii) inverse procedures, (iv) indirect methods using empirical and quasi-empirical models to quantify the hydraulic properties, and (v) other analyses involving flow or transport processes such as variability and scale issues or the transport of other substances. The relatively broad scope of the workshop dictates a fairly general overview; readers should consult the individual contributions, several of them review papers, for more detailed analyses.

PORE-SCALE PHENOMENA

Conventional pore-size distribution models predict the hydraulic conductivity by assuming that water flow through cylindrical pores can be described with Poiseuille's law. An expression for the hydraulic conductivity function of the porous medium is obtained using Darcy's law and one or several calibration parameters to account for the connectivity and tortuosity of pores. The pore-size distribution is usually inferred from water retention data using the well-know equation of Young and Laplace for the pressure drop across a curved interface:

$$P_c = \sigma\left(\frac{1}{r_1} + \frac{1}{r_2}\right) \tag{1}$$

where σ is the interfacial tension, r_1 and r_2 are principle radii of curvature, and P_c is the capillary pressure, which for an air-water system is given by

$$P_c = P_a - P_w \approx \rho g h \tag{2}$$

in which P_a and P_w are the pressures of air and water at the interface. Usually atmospheric air pressure is assumed. As shown by Eq. (2), the capillary pressure is frequently expressed in terms of the pressure head h by making use of the density of water, ρ, and the gravitational constant g.

Two of the most popular pore-size distribution models for the hydraulic conductivity are those by *Burdine* [1953]:

$$K(S_e) = K_s S_e^{\ell}\left[\int_0^{S_e} h^{-2}(x)\,dx \Big/ \int_0^1 h^{-2}(x)\,dx\right] \tag{3}$$

and *Mualem* [1976]:

$$K(S_e) = K_s S_e^{\ell}\left[\int_0^{S_e} h^{-1}(x)\,dx \Big/ \int_0^1 h^{-1}(x)\,dx\right]^2 \tag{4}$$

where K_s is the saturated hydraulic conductivity, ℓ is a pore-connectivity (or tortuosity) parameter, $S_e = (\theta - \theta_r)/(\theta_s - \theta_r)$ is effective saturation such that $0 \le S_e \le 1$, θ_r and θ_s are the residual and saturated water contents, respectively, and x is a dummy variable for integration of the water retention curve. Effective saturation, S_e (often referred to also as the reduced water content), is usually represented by closed-form expressions such as those of *Brooks and Corey* [1964]:

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \begin{cases} (\alpha h)^{-\lambda} & (\alpha h > 1) \\ 1 & (\alpha h \le 1) \end{cases} \tag{5}$$

or *van Genuchten* [1980]:

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} = [1 + (\alpha h)^n]^{-m} \tag{6}$$

in which α is a parameter inversely related to the air entry value, and λ, m, and n are parameters that affect the slope or, together with α, the location of the inflection point on the retention curve.

An example of inserting a retention function into a conductivity model is given by *Corey and Brooks* [1999]. *Kosugi* [1999] uses a lognormal pore-size distribution in an attempt to provide a more physical basis for the retention and conductivity functions. *Hoffmann-Riem et al.* [1999] report that popular pore-size distribution models for the hydraulic conductivity lack a solid physical basis judging from the erratic values of the hydraulic parameters in those models (especially the pore-connectivity parameter ℓ). The widely invoked conceptualization of the pore space as a bundle of cylindrical pores, usually either completely filled with water or empty, is an obvious simplification that requires calibration with empirical tortuosity or connectivity factors and at least one matching point (too often only K_s is used for this purpose). In an effort to develop a more realistic conductivity model, *Ruan and Illangasekare* [1999] consider water flow in a film of variable thickness and the curvature of the air-water interface.

Percolation or pore-scale network models assume that the pore space can be represented by a series of well-defined pore bodies connected by pore throats. The flow and equilibrium fluid distributions in the network are obtained numerically using models based on the Young-Laplace and Poiseuille equations, while additional refinements can be included to account for viscous and capillary flow, entrapment, wettability, hysteresis, and degree of connectivity. Network models are used by *Mani and Mohanty* [1999] to modify Darcy's law for oil flow in an air-oil-water system, by *Fischer et al.* [1999] to establish the dependency of the gas permeability on a continuous air distribution (rather than on the total amount), by *Bartelds and Bruining* [1999] to study permeabilities in the presence of polymers that are excluded from part of the pore space, by *Dijkstra et al.* [1999] to study flow and liquid retention in an oil-water medium with different mechanisms for fluid entrapment, by *Ferrand* [1999] to investigate the effects of temperature and freezing on soil water retention, and by *Reeves and Celia* [1999] to compute interfacial areas. An imaging method to determine interfacial areas experimentally is presented by *Montemagno and Ma* [1999]. The geometry of pore bodies and throats in network models is for this purpose varied according to the natural medium that is being mimicked. *Rösslerová-Kodešová and Kodeš* [1999] use electron microscopy to quantify the pore space of soil samples for input to a network model based on either a unimodal or bimodal pore-size distribution. *Perrier et al.* [1999] assume a fractal-type pore-size distribution that is directly related to retention data, while *Vogel and Roth* [1999] include morphological data in their network model.

Pore-scale phenomena are also important for understanding multi-liquid systems. *Morrow and Xie* [1999] treat wetting and drainage of triangular tubes, which are considered physically more realistic for the pore space than circular tubes since a fraction of the wetting phase will remain in the corners after drainage. These authors derive expressions for the work involved in draining and imbibing a perfectly wetted triangle. Most porous media do not exhibit perfect wettability. *Bradford et al.* [1999] show how the conductivity of two- and three-fluid media with fractional wettability can be predicted from retention data. *Lenhard and Oostrom* [1999] similarly propose a model for the hydraulic properties of mixed-wet media that captivate the saturation-path history. The model is successfully used to describe the imbibition of oil containing asphaltenes (which make the solids more oil wet) into an initially water-saturated sand pack. Measurements of the hydraulic properties of multi-phase flow systems are more complicated than those of traditional air-water systems having a stagnant air phase. *Watson and Nortvedt* [1999] discuss a generalized procedure to estimate constitutive relations for two- and three-phase flow using transient experiments. *Dane et al.* [1999] describe steady-state procedures to more accurately determine the retention and conductivity functions for media containing non-aqueous phase liquids and water or air. *Kemmesies et al.* [1999] employ a multistep procedure for oil-air-water systems using fluid displacement. They show a discrepancy between the results for two- and three-fluid systems. The chemistry of the porous system is known to affect its wettability and interfacial tensions, and hence its hydraulic properties. *Demond et al.* [1999] report on the effect of pH on the retention of air - water and o-xylene - water systems.

DIRECT METHODS

Reliable and efficient experimental procedures are critical to improve the understanding of flow and transport processes in variably-saturated media, regardless of advances in the formulation of indirect methods, or the development of more sophisticated physical and mathematical analyses. While considerable progress has been made in the development of experimental procedure, as these Proceedings attest to, major impediments remain. An overview of recent innovations in the measurement of retention and conductivity is given by *Gee and Ward* [1999]. The review is geared toward soils, with the merits and disadvantages of many laboratory and field procedures being discussed with an eye to the future. The many contributions on experimental procedures in these Proceedings are grouped according to three categories: (i) laboratory methods, (ii) case studies, and (iii) field procedures.

Laboratory Methods

Measurement of the hydraulic conductivity, which poses the greatest obstacle, is treated by *Dirksen* [1999] with an emphasis on benchmark, laboratory procedures. *Faybishenko* [1999] illustrates the problem of obtaining consistent results for the quasi-saturated conductivity, which may vary two or more orders of magnitude among different field and laboratory methods. Frequently, both direct and indirect methods are available. *Flint et al.* [1999] compare conductivity results measured directly with a centrifuge method and estimated from retention data, while *Santos et al.* [1999] present a two-step method that is compared with the hot-air and crust methods to determine the conductivity over a wide range of saturation values.

The automation of many experiments and, as discussed earlier, the availability of simulation and optimization software, has alleviated the problems of measuring hydraulic properties. A popular example is the evaporation method by Wind [*Wind*, 1968]. *Gabele and Hoch* [1999] investigate the use of a flexible evaporation rate, while *Bertuzzi et al.* [1999] provide an error analysis for the method. *Van den Elsen et al.* [1999] describe the automation of several unsaturated hydraulic measurements. Increasingly, user-friendly software packages and the internet are available to also permit laypersons to tackle traditional soil physical problems [*Mizoguchi*, 1999; *Perrier et al.*, 1999].

The introduction of Time Domain Reflectometry (TDR) has greatly helped the in-situ measurement of liquid saturations and concentrations. *Si et al.* [1999] use a multi-purpose TDR probe to measure water content and soil water pressure head in the field. *Nguyen et al.* [1999] describe a Frequency Domain Reflectometry (FDR) method to determine water saturation profiles in laboratory cores. New analytical solutions are presented by *Zhang et al.* [1999] to determine hydraulic properties with TDR for constant water flow from a line source. An alternative approach for in-situ measurements is reported by *Song et al.* [1999] who describe a dual-probe heat pulse technique for high-resolution water content measurements. A review of measurement errors of selected soil water sensors is given by *Bilskie* [1999]. Magnetic Resonance Imaging (MRI) offers great promise to observe *in situ* flow events. *Císlerová et al.* [1999] show how MRI can be used to study preferential flow. Nuclear Magnetic Resonance (NMR) detects different relaxation times of water in different pores and can be used to explore pore-size distributions [*Hinedi and Chang*, 1999].

Case Studies

Improvements and refinements in experimental or simulation methods are now permitting more detailed studies of fingered flow [*Cho and de Rooij*, 1999; *di Carlo et al.*, 1999] and flow in swelling soils [*Garnier and Rieu*, 1999; *Baumgartl and Horn*, 1999; *Angulo-Jaramillo et al.*, 1999]. Using a root zone substrate in greenhouse horticulture as the porous medium, *Heinen and Raats* [1999] and *Otten et al.* [1999] characterize hysteresis and present hydraulic parameters for different substrates, respectively. *Roth et al.* [1999] show how measured retention and conductivity data can be used to elucidate the spatial impact of tillage and field traffic during water balance modeling. The effect of temperature on hydraulic conductivity is being reported by *Stoffregen et al.* [1999]. While the experimentally determined effect on the conductivity was twice as strong as would be expected based upon changes in surface tension and viscosity, no dependency was found for the soil water pressure. *Toride* [1999] and *Moutier et al.* [1999] discuss the effects of solution composition, caused by dispersion and swelling, on the hydraulic properties.

Field Procedures

Several somewhat related techniques have recently been proposed to determine the unsaturated hydraulic properties in the field. *Kodešová et al.* [1999] use a cone penetrometer that includes a screen through which water is applied, as well as two tensiometers to monitor soil water pressure. Unsaturated hydraulic properties are obtained by optimizing cumulative inflow and pressure head readings. *Evett et al.* [1999] apply tension infiltrometry and laboratory retention data to determine the effect of tillage on the unsaturated hydraulic properties. Ring infiltrometer experiments can be made more useful by using a falling head analysis augmented with TDR to determine soil water contents, as shown by *Parkin et al.* [1999]. The influence of infiltrometer disk size is investigated by *Wang et al.* [1999]. Other experiments using tension disk infiltrometry are reported by *Auzet et al.* [1999] for coarse-textured soils, *Logsdon* [1999] for estimating the hydraulic properties near saturation, and *Moreno et al.* [1999] for studying the effect of alternative irrigation and tillage practices on different soils in Spain.

Characterizing the hydraulic properties of relatively large areas of land poses additional challenges. *Cuenca and Kelly* [1999] report on efforts to quantify the soil hydraulic properties (from particle-size data, tension infiltrometry, and water retention measurements) and the energy balance of a boreal forest. *Famiglietti et al.* [1999] and *Houser* [1999] give preliminary results on the characterization of surface soil water content to be used in conjunction with remote sensing. Chemical and unsaturated hydraulic data generally permit better predictions or interpretations when considered in tandem. In an effort to assess the potential of nitrate leaching, *Harter et al.* [1999] investigate the transport of nitrogen components in a deep vadose zone using core sampling up to a depth of 15 m. *Izbicki et al.* [1999] show how chloride and tritium measurements can be used to estimate the travel time for water through a 130-m thick vadose zone in the Mojave Desert.

INVERSE METHODS

Increasingly, soil hydraulic properties are estimated by matching observations and simulation results for a particular unsaturated flow event using a parameter optimization code. The procedure generally leads to estimates of the hydraulic parameters in specific expressions of the constitutive relationships. Iterative solutions of inverse problems are offering tremendous opportunities. Hydraulic parameters can now be estimated from transient flow experiments in which ease and speed of the experiment have become the primary criteria, while mathematical complexity is increasingly becoming less of a concern because of the availability of more advanced numerical techniques and computer hardware. *Hopmans and Šimůnek* [1999] review some of the merits and pitfalls of the inverse estimation of hydraulic properties. *Durner et al.* [1999] provide specific recommendations for estimating hydraulic properties from inflow/outflow experiments on laboratory soil columns. *Romano* [1999] evaluates inverse procedures by comparing retention and conductivity data for two soils with data from an instantaneous profile method. He shows that inverse methods yield reliable results with less experimental effort. Of course, the utility of inverse methods relies on the accuracy with which hydraulic functions can be parameterized. The suitability of various closed-form expressions for the constitutive relationships was previously investigated by *Leij et al.* [1997], among others. *Vogel et al.* [1999] in these Proceedings discuss the parameterization near saturation.

The optimization procedure – usually a minimization of the sum of the squared deviations between observed and simulated water contents, pressure heads, water flow rates, and/or other attributes characterizing unsaturated flow – continues to be a topic of investigation because the invoked objective function and/or optimization algorithm can greatly affect the final results. *Abbaspour et al.* [1999] present an inverse program where the estimation of hydraulic parameters is conditioned. *Takeshita and Kohno* [1999] advocate the use of genetic algorithms, while *Pan and Wu* [1999] use simulated annealing and the downhill simplex method. Inverse procedures are especially attractive for analyzing more complicated flow experiments in both the laboratory and the field. *Šimůnek et al.* [1999] illustrate this by determining the hydraulic parameters from laboratory evaporation experiments, while *Inoue et al.* [1999] optimize field hydraulic parameters from vacuum extraction and tensiometer data. Laboratory data can in many cases effectively augment field observations as additional input in inverse modeling. *De Vos et al.* [1999] quantify the hydraulic properties from drainage discharge and groundwater level data, while *Bohne et al.* [1999] analyze ponded infiltration results. Tension infiltration experiments are now also routinely analyzed using inverse estimation procedures [*Wendroth and Šimůnek*, 1999; *Jacques et al.*, 1999].

Inverse methods have made it much easier to study the hydraulic properties of porous media exhibiting more complex hydraulic behavior caused by the presence of multiple pore domains and associated nonequilibrium phenomena. Soils having multimodal pore-size distributions require corresponding changes in the mathematical functions describing the retention and conductivity curves. *Durner et al.* [1999] sum the retention and conductivity functions of each subcurve to obtain apparent (lumped) hydraulic properties. In a related study, *Mohanty* [1999] analyzes hydraulic conductivity data by discerning a noncapillary component for macropore flow and a series of capillary domains for flow in the matrix (the micropores). Instead of lumping the contributions of different pore domains in one retention and one conductivity function, separate hydraulic functions and flow equations (typically two) may also be used for the different subdomains. *Jarvis et al.* [1999] use this dual-permeability concept to investigate the hydraulic conductivity near saturation where a small drop in soil water pressure can cause a large reduction in flow. A third approach to tackle complications caused by the presence of different hydraulic and flow domains is to use an equilibration time constant that reflects the time required for the actual water content to approach a final or equilibrium value [*Ross and Smettem*, 1999]. This approach obviates the need for partitioning the porous medium into subdomains, or the addition of subdomain retention and conductivity functions. Some of the discrepancies between "static" and actual hydraulic functions may also be attributed to air flow [*Schultze et al.*, 1999], which is not considered in classical analyses of unsaturated flow using the Richards equation.

Several experimental studies deal with hydraulic observations involving fractured media and/or possible nonequilibrium effects. *Sisson and Hubbel* [1999] present water potential readings for fractured basalt and sedimentary interbeds for depths up to 30 m. Tensiometry for fractured rock is further scrutinized by *Finsterle and Faybishenko* [1999] using laboratory experiments and numerical simulations. *Wildenschild and Hopmans* [1999] report an increase in retention and a decrease in the hydraulic conductivity at increased flow rates during one- and multi-step outflow experiments on coarse soil samples. *Plagge et al.* [1999], on the other hand, observe an increase in the conductivity with flow rate. Finally, *Hollenbeck and Jensen* [1999] show that the one- and multi-step methods yield results that are poorly reproducible.

INDIRECT METHODS

As an alternative to direct measurement, indirect methods encompass a wide array of procedures to the estimate hydraulic properties from data that are more easily measured or more widely available (usually soil survey type data). Indirect methods have been applied mostly to soils but, as far as we know, rarely to other porous media such as rock samples. The basic premise of indirect methods is to deduce hydraulic properties from the surrogate soil data using some empirical or quasi-empirical functional relationship or algorithm between selected input and output variables. Possible input variables include soil textural class, particle-size distribution, bulk density, organic matter content and/or porosity, whereas the output variables involve specific soil hydraulic data and/or parameters in closed-form expressions of the unsaturated soil hydraulic properties. The algorithms, typically determined using regression analysis, are known in the parlance of soil science as pedotransfer functions (PTFs) [*Wösten and Bouma*, 1992]. In the following we will cover contributions addressing quasi-empirical methods, empirical methods involving different hydraulic functions, developments in the formulation and evaluation of PTFs, applications of PTFs, and soil hydraulic databases.

Nimmo [1999] shows how to improve conventional texture-based predictions of retention and conductivity by including a structural component derived from the aggregate-size distribution. The importance of soil structure is also emphasized by *Lin et al.* [1999] who develop PTFs from a soil morphological quantification system. *Arya et al.* [1999] incorporate the textural-dependency of the scaling parameter α in the well-known water retention model of *Arya and Paris* [1981]. *Bouraoui et al.* [1999] explore the shape similarity between the cumulative particle-size distribution and water retention curves to predict retention parameters from knowledge of the clay and silt fractions. The cumulative particle-size distribution is also used by *Kravchenko and Zhang* [1999] to determine a fractal dimension. The latter parameter serves as exponent in a retention model, which subsequently is used to predict the unsaturated conductivity. Examples of PTFs for predicting water retention are given by *Bastet et al.* [1999], *Mayr et al.* [1999], *Rajkai et al.* [1999], *Shein* [1999], and *Williams et al.* [1999]. The saturated conductivity, K_s, is primarily governed by larger pores, which are more closely related to soil structure rather than texture. *Giménez et al.* [1999] present several approaches of characterizing soil structure for predicting K_s according to the Kozeny-Carman equation. This same equation is also used by *Timlin et al.* [1999] to predict K_s from porosity data. Pore-size distribution models have been widely used for predicting the unsaturated hydraulic conductivity from retention data. Several modifications of this approach, as well as alternative formulations, have been investigated. *Renger et al.* [1999] present an empirical autoregressive procedure that implicitly incorporates the effect of soil structure. *Eckhardt and Wagenet* [1999] and *Jauhiainen and Karvonen* [1999] evaluate the suitability of different functions and parameter combinations to describe the hydraulic conductivity, whereas *McVay and Radcliffe* [1999] compare experimental results with indirect estimates for the conductivity using different retention functions.

An important consideration is the reliability of flow and/or transport predictions when direct or indirect methods are used to estimate the unsaturated hydraulic properties. Functional analyses of this type [*Wösten et al.*, 1990] are becoming increasingly popular. *Vereecken and Kaiser* [1999] use results from multi-step outflow experiments and PTFs to predict water flow and solute transport in a lysimeter, while *Bristow et al.* [1999] employ bulk density and clay and silt contents as input to PTFs for subsequent use in water balance models of tropical soils. *Priesack et al.* [1999] similarly develop PTFs from three-dimensional texture, bulk density, and organic matter data to simulate water flow at a research farm. The use of the Brooks-Corey and van Genuchten functions, as well as three different methods to convert parameters between the Brooks-Corey and van Genuchten functions, to describe water retention in the Root Zone Water Quality Model (RZWQM) is discussed by *Ma et al.* [1999]. The functional analysis approach is also followed by *Creswell et al.* [1999] to more effectively quantify – within an Australian context – hydraulic properties from direct and indirect methods. *Bond et al.* [1999] evaluate the ability of six different procedures for directly and indirectly estimating hydraulic properties to model field bromide transport and water balances during periods of rainfall excess and deficit. In another study, *Conca et al.* [1999] characterize the hydraulic properties using a relatively advanced unsaturated flow apparatus (based on the centrifuge method) as well as measured retention and predicted conductivity data, and use the results to estimate recharge in arid regions. *Gonçalves et al.* [1999]

report fairly successful predictions of the hydraulic parameters in the van Genuchten-Mualem model for some 70 soils in Portugal.

The particular algorithm used for a PTF continues to be of interest. In addition to using basic soil taxonomic data as input to the PTF, *Tietje* [1999] also considers the interdependency of hydraulic output data. Artificial neural network analyses have recently gained popularity for deriving PTFs. An advantage of neural network approaches is that they partly circumvent the problem of having to a priori commit to particular input parameters and, more important, to an explicit mathematical relationship. *Krenn* [1999] obtains more accurate predictions of water retention with a newly trained neural network based PTF than with two independent PTFs taken from the literature. *Schaap et al.* [1999] show how neural network analyses can be combined with bootstrapping to provide probability distributions of the output parameters. *Tamari and Wösten* [1999] report that neural networks do not materially improve the accuracy of PTFs as compared to multilinear regression. We expect this last conclusion to change when qualitatively and quantitatively better hydraulic databases become available.

The development and evaluation of indirect methods hinges on the availability of reliable retention and conductivity data sets, as well as basic soil properties or other information pertinent to the hydraulic behavior of soils. The willingness of soil scientists and vadose zone hydrologists to disseminate and share experimental findings has allowed the development of several databases of soil hydraulic data. Such databases serve an educational purpose, they also constitute a ready source (some would say too ready for non-expert users) of unsaturated hydraulic property data. Three databases, with different restrictions on availability and the targeted user group, are described in these Proceedings by *Leij et al.* [1999], *Lilly et al.* [1999], and *Fredlund et al.* [1999]. The use of hydraulic databases creates many opportunities, but also poses challenges. *Nemes et al.* [1999] evaluate different procedures to interpolate nonuniform particle-size distributions within the HYPRES database of *Lilly et al.* [1999]. *Grossman and Harms* [1999] illustrate the problem of employing soil survey data when such data are not use-invariant. *Miller* [1999] discusses soil information resources for application in soil-vegetation-atmosphere transfer schemes to quantify transport across the interface between the land surface and the atmosphere. The development of PTFs should always be tailored to the information that is available in a database. *Rawls et al.* [1999] combine information from two databases to develop PTFs that can accommodate widely different available input data. Finally, *Schindler et al.* [1999] present experimental and simulation results for a hydrology catchment area where the simulations use a database of different PTFs.

FLOW AND TRANSPORT

Characterizing the unsaturated hydraulic properties, and applying them to specific flow and transport problems, are inherently error-prone tasks. For example, porous media can be extremely heterogeneous, experimental procedures often involve errors and approximations, while the scales at which hydraulic results are applied differ often radically from those at which they were observed. Real-world applications generally also involve time and money constraints. No simple solution exists for these problems. Still, the experimental and application efforts can be made more successful if the uncertainty is better understood. *Neuman et al.* [1999] follow a deterministic approach to predict unsaturated flow in a heterogeneous soil by using the first and second conditional moments of pressure heads, water contents, and fluxes. They conclude that the concept of an effective hydraulic conductivity is generally not applicable. *Hunt* [1999] uses percolation theory to arrive at a somewhat similar conclusion that changes in hydraulic conductivity with system size are not compatible with Darcy's law. *Ungaro et al.* [1999] apply a Kalman filter method to water content and pressure head data obtained for a drainage experiment in a spatially variable field. The method, which accounts for measurement and system uncertainty, yields improved estimates for the conductivity. *Yeh* [1999] discusses the use of conditional and unconditional effective hydraulic properties for unsaturated flow in an heterogeneous unsaturated medium. *Desbarats* [1999] numerically studies the upscaling of constitutive relationships with a characteristic capillary length, whereas *Rockhold et al.* [1999] report on the conditional simulation of unsaturated water and tracer movement for an experimental field study using upscaling to obtain effective hydraulic properties. *Mohanty and Shouse* [1999] represent disk infiltrometer data with one conductivity curve using the saturated conductivity as a scaling factor. The infiltration process at different scales is described by *Morel-Seytoux* [1999]. The uncertainty associated with indirect estimates for hydraulic parameters is estimated by *Meyer et al.* [1999] using a neural network model for use in infiltration modeling, while *Vaughan and Suarez* [1999] analyze the sensitivity of a numerical transport model to hydraulic input parameters.

Transport phenomena in porous media are closely related to the hydraulic properties. The most obvious example is the transport of dissolved substances, i.e., solute transport can only be simulated reliably if the flow field is known. Conversely, transport data can be used to infer hydraulic properties [*Russo*, 1999]. *Mitchell and Mayer* [1999] demonstrate that hysteresis and horizontal flow can have a substantial impact on solute transport during predominantly vertical flow. *Kasteel et al.* [1999] use two independent hydraulic data sets obtained in the laboratory and the field to simulate solute transport. Unsaturated hydraulic properties may also be deduced from other transport phenomena that are affected in a similar manner by pore geometry. *Jacobsen et al.* [1999] predict the saturated conductivity from gas diffusivity and retention data, and from additional hydraulic parameters obtained with one-step outflow experiments. Unsaturated water flow subject to non-atmospheric air pressure may occur below ponded water. This phenomenon is of considerable importance for paddy field soils [*Chikushi*, 1999]. *Šimůnek and van Genuchten* [1999] describe the HYDRUS software package for application to both forward and inverse problems of water and solute movement in variably-saturated media, while *Wu et al.* [1999] report on the use of inverse procedures to estimate parameters for water, air, and heat flow at the Yucca Mountain site. Temperature gradients pose additional challenges for accurate descriptions of unsaturated flow. *Globus* [1999] treats non-isothermal flow, including soil water freezing, using the classical model of *Philip and de Vries* [1957] as a starting point. Similarly, *Grunewald et al.* [1999] provide a thermodynamic treatment for coupled heat, air, and water flow in porous building materials.

SUMMARY AND OPPORTUNITIES FOR RESEARCH

The contributions to these Proceedings deal with many aspects of flow in unsaturated porous media, reflecting diverse scientific backgrounds of the authors and a wide spectrum of potential applications. Many of the papers already provide suggestions for future research. We summarize below several areas of research that we believe are in need of further investigation; this following a similar list or research needs that we compiled after the first workshop [*van Genuchten and Leij*, 1992].

1. The interdisciplinary nature of studies involving unsaturated flow in porous media was even more evident than during the last workshop. Soil scientists, hydrologists, geologists, and engineers all have contributed uniquely to the current state-of-the-art. It is imperative that such cooperation and communication between the various disciplines continue notwithstanding diverging research priorities, different funding sources, a fragmented scientific literature, and the introduction of increasingly complex experimental and theoretical approaches.

2. Considerable progress has been made in the formulation of more realistic pore-scale models by incorporating physically-based pore-size distributions, accounting for capillary and viscous forces, and considering noncircular pores. Further work is needed on well-defined media to further refine pore-scale models using experimental and theoretical advances that quantify interfacial areas, pore geometry, adsorbed and capillary bound water, wettability, multi-fluid displacement, entrapment, hysteresis, and other phenomena. The next challenge is to make such models also useful for natural porous media, and to establish procedures for quantifying model parameters.

3. Several studies during the past few years are addressing the need for improved descriptions and measurements of the soil water retention and hydraulic conductivity functions near saturation. Complications near saturation arise because of air entrapment and/or water flowing through soil macropores or rock fractures. Such efforts should go hand-in-hand with the development and implementation of improved flow models that capture changes in fluid saturation over the entire range of pores and fractures.

4. By comparison, less contributions have addressed the problem of liquid and vapor flow at very low fluid saturations; this despite the importance of this issue when simulating water flow and solute transport in arid and semi-arid areas.

5. A wide range of contributions has been made on the variability of hydraulic properties, and errors in model output using hydraulic properties. Further work is needed to better quantify the uncertainty of hydraulic properties obtained using either direct or indirect methods, and to assess how this uncertainty propagates into flow and transport predictions.

6. Several databases have now been established that contain soil hydraulic properties and other pertinent data. Efforts need to continue to improve the accessibility of this information and to alleviate the relative lack of unsaturated hydraulic conductivity data.

7. There remains a glaring lack of standardized procedures for measuring the unsaturated hydraulic properties. The problem is exacerbated by the involvement of different scientific disciplines – often using different terminology and having a diverging research focus – that study flow in partially saturated media. In soil science, soil physicists seldom report reliable errors for the unsaturated hydraulic properties, nor invoke materials and methods that allow others to readily reproduce their results.

8. Many exciting new experimental procedures and methods are becoming available. TDR and EMI are now increasingly being used, although accurate calibration remains a concern, especially for field applications. Unfortunately, advanced procedures such as NMR and CMT require sophisticated equipment and dedicated personnel. Specialized equipment to measure the unsaturated hydraulic properties is generally expensive because of a relatively small market. Because of this, a disproportionate amount of time and money is still being used to conduct routine experimental work. On the positive side, experimental procedures are now greatly benefitting from the use of flexible inverse procedures, improved numerical models, more powerful computers, and increased automation in data collection efforts.

9. Studies delineating the effects of effects of temperature, swelling and shrinking, hysteresis, and especially solution chemistry, on the hydraulic properties are still progressing only slowly. More advances are needed in these areas of research.

10. The overwhelming heterogeneity of the subsurface, and the associated spatial and temporal variability of hydraulic properties, is another area requiring further studies before variably-

saturated flow and transport models can be reliably applied to field-scale problems. The issues of hydraulic property scaling, upscaling of hydraulic parameters and/or flow processes, and the existence and estimation of effective properties remain largely unresolved. Also requiring attention is the effective combination of pedotransfer functions and soil taxonomic data as a method of upscaling hydrological processes to watershed or even larger scales.

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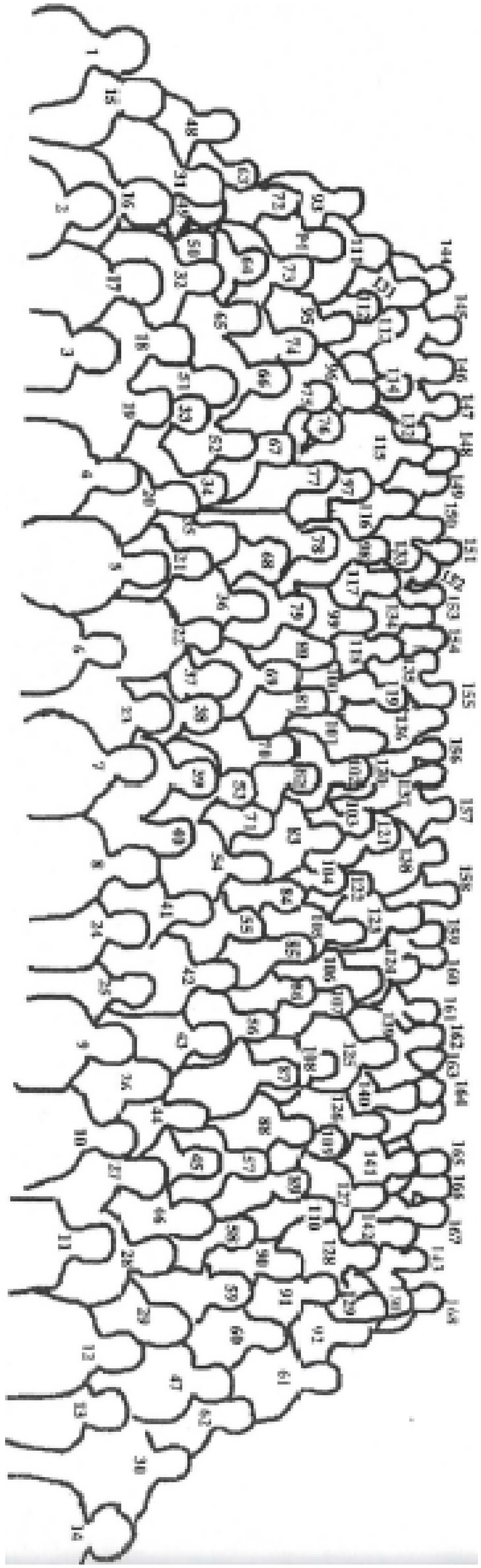

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