EPA/600/R-98/046

PARAMETER ESTIMATION OF TWO-FLUID CAPILLARY PRESSURE-SATURATION AND PERMEABILITY FUNCTIONS

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Cooperative Agreement
CR822204

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U.S. Environmental Protection Agency
Cincinnati, OH 45268

NOTICE

The U.S. Environmental Protection Agency through its Office of Research and Development partially funded and collaborated in the research described here under Cooperative Agreement No. CR-822204 to the University of California, Davis. It has been subjected to the Agency's peer and administrative review and has been approved for publication as an EPA document. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

All research projects making conclusions or recommendations based on environmentally related measurements and funded by the Environmental Protection Agency are required to participate in the Agency Quality Assurance Program. This project was conducted under an approved Quality Assurance Project Plan. The procedures specified in this plan were used without exception. Information on the plan and documentation of the quality assurance activities and results are available from the Principal Investigator.

FOREWORD

The U.S. Environmental Protection Agency is charged by Congress with protecting the Nation's land, air and water resources. Under a mandate of national environmental laws, the Agency strives to formulate and implement actions leading to a compatible balance between human activities and the ability of natural systems to support and nurture life. To meet these mandates, EPA's research program is providing data and technical support for solving environmental problems today and building a science knowledge base necessary to manage our ecological resources wisely, understand how pollutants affect our health, and prevent or reduce environmental risks in the future.

The National Risk Management Research laboratory is the Agency's center for investigations of technological and management approaches for reducing risks from threats to human health and the environment. The focus of the Laboratory's research program is on methods for the prevention and control of pollution to air, land, water, and subsurface resources; protection of water quality in public water systems; remediation of contaminated sites and ground water, and prevention and control of indoor air pollution. The goal of this research effort is to catalyze development and implementation of innovative, cost-effective environmental technologies; develop scientific and engineering information needed by EPA to support regulatory and policy decisions; and provide technical support and information transfer to ensure effective implementation of environmental regulations and strategies.

Earlier work by the principal investigators has shown that parameter optimization by inverse modeling can be used to estimate the soil water retention and unsaturated hydraulic conductivity functions of soils containing air and water only. The research presented in this report focuses on the application of this method to determine capillary pressure and permeability functions in multi-fluid soil systems (air-water, air-oil and oil-water) using data from the multi-step outflow method. The term multi-fluid is used here to indicate what is traditionally defined as multiphase. Whereas soil water retention and unsaturated hydraulic conductivity are generally used in the soils literature for air-water systems only, the definition of these relationships in general multi-fluid soil systems requires use of the capillary pressure and permeability terminology instead. The authors conclude that the applied inverse model is well posed for the investigated multi-fluid soil systems, and that the parameter optimization yields accurate capillary pressure-saturation and permeability functions.

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ABSTRACT

Capillary pressure and permeability functions are crucial to the quantitative description of subsurface flow and transport. Earlier work has demonstrated the feasibility of using the inverse parameter estimation approach in determining these functions if both capillary pressure and cumulative drainage are measured during a transient flow experiment. However, to date this method has been applied to air-water systems only, while ignoring the air phase, thereby assuming that the air phase has a negligible influence on water flow. In this study, we expanded the inverse parameter estimation method combined with multi-step outflow data, using a modified Tempe cell for air-water, oil (Soltrol)-water, and air-oil fluid pairs in a Columbia fine sandy loam and a Lincoln sand. The commonly applied van Genuchten (VG) - Mualem (M) model of capillary pressure and permeability functions was used in this study. Wetting fluid and oil non-wetting fluid pressures were measured in the center of a soil sample simultaneously with cumulative outflow of the wetting fluid as the initially near-saturated soil core is drained by increasing the non-wetting fluid pressure in a sequence of pressure increments. Results from the multi-step measurements are used to directly estimate capillary pressure and wetting fluid permeability functions. Uniqueness and stability analysis indicated that the inverse model is well posed, and that the multi-step transient outflow experiment provides sufficient information to successfully apply the parameter estimation approach.

This report was submitted in fulfillment of CR-822204 by the University of California, Davis under the partial sponsorship of the U.S. environmental Protection Agency. This report covers a period from October 1993 to September 1996, and work was completed as of September 1996.

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ACKNOWLEDGEMENTS

We are especially grateful to Dr. John Nieber at the University of Minnesota, for supplying us with his transient one-dimensional two-phase flow model that we used to develop a specific two-fluid flow simulator for the inverse parameter estimation. We are also indebted to Dr. N.L. Abbott of the Chemical Engineering Department of the University of California, Davis, for making his laboratory available for the interfacial tension measurements.

Chapter 1
Introduction

Successful environmental protection and remediation strategies associated with hydrocarbon contamination of soil and ground water requires modeling of multi-fluid flow and transport in subsurface soil systems. However, the implementation of such models is often hampered by lack of sufficient information regarding the capillary pressure-saturation and permeability functions for the different soil materials. Multiphase fluid flow in soils has been studied across disciplines in soil science, ground water hydrology and petroleum engineering for decades. Petroleum scientists have focused predominately on brine-oil-natural gas in mostly coarse-textured soils, whereas hydrologists study mostly water flow in a broad range of unsaturated soils.

Flow and transport in porous media is controlled by interfacial processes between fluid-fluid and fluid-solid phases, thereby producing an extremely complex flow field that is dominated by microscopic heterogeneities and discontinuities. Consequently, the macroscopic capillary pressure - saturation (energy-mass) and permeability functions, which together characterize fluid storage and flow properties in unsaturated subsurface soils, are highly nonlinear.

Subsurface properties and flows are discontinuously distributed when viewed at the microscopic scale. Macroscopic continuity is based on the representative element volume (REV) concept and is derived by volume-averaging, which led to the classical flow concepts and quantitative analyses used today. In unsaturated flow, Richards (1931) equation was developed by combining the empirically obtained closed-form Darcy equation with the mass conservation equation. However, in doing so, all uncertainties of the microscopic processes were embedded in the macroscopic constitutive functions; e.g., the capillary pressure and permeability relationships. For decades, scientists who worked in related areas have been working on prediction or estimation of these constitutive relationships from microscopic processes or macroscopic observations. Despite considerable progress by Burdine (1953), Brooks and Corey (1964), Mualem (1976), van Genuchten (1980), and others, the intricate complexity of pore geometry and microscopic processes augmented by the severe limitation of observation techniques make prediction of these relationships difficult. At the same time, the increased efforts in environmental investigations and numerical simulations demand efficient and accurate methods for determination of soil hydraulic characteristics. For immiscible multi-fluid flow systems, such information is often lacking.

Many laboratory and field methods exist to determine soil capillary pressure and permeability functions, which can be categorized as measurement and prediction methods. Direct measurements, including equilibrium and steady-state experimental methods, are often highly restricted by constrained initial and boundary conditions, and are time-consuming, or otherwise inconvenient. This is especially so for the permeability measurements. Moreover, both functions are measured separately, which can cause inconsistent results. With respect to the prediction methods, they are mostly based on a simplified conceptual soil pore model, such as by Burdine (1953) and Mualem (1976) for predicting permeability by using pore-size distribution information obtained from capillary pressure - saturation data. Alternatively, one applies the similarity assumption to predict unknown capillary pressure functions or permeability by using known values of easy-to-measure soil or fluid properties (Leverett, 1941; Miller and Miller, 1956). In contrast with these traditional methods, the inverse modeling approach for estimating the constitutive properties is based on the concept of system analysis and is receiving increased attention. Through the measurement of the system's response of a transient experiment and the simulation of the experimental system, the inverse modeling approach consistently estimates or calibrates the system's constitutive properties. Transient experimental methods are inherently faster and more flexible, and as more powerful computers and simulation models become available, the estimation of the constitutive functions using the inverse method has become more attractive.

The study of inverse parameter estimation for determination of retention and permeability functions started in the 1980's, and was further developed in the 1980's and 1990's (Zachmann et al., 1981, 1982; Hornung, 1983; Kool and Parker, 1988; Russo et al., 1991; Toorman et al., 1992; Eching et al., 1993, 1994). Inverse parameter estimation is a "gray-box" technique, when contrasted with a forward problem (white-box) and inverse problem (black-box). As shown in Figure 1-1, the grayness is used to describe the exposure degree of the constitutive function knowledge, and is defined as transparent, opaque, and translucent, for the forward, inverse, and parameter estimation problems, respectively. The fundamental assumption of parameter estimation is that the constitutive functions can be described by a parametric model for which the unknown parameters can be estimated by minimization of deviations between observed and predicted state variables such as flux or

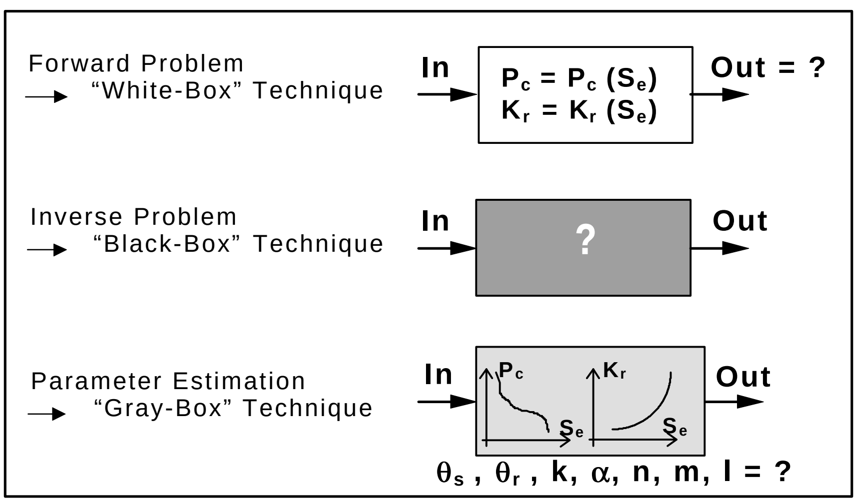

Figure 1-1. Methodology of inverse parameter estimation approach.

capillary pressure. To determine whether the inverse problem is at all solvable, it must be "correctly posed" (Carrera and Neuman, 1986b). Ill-posedness of the inverse problem may result in no solution, nonuniqueness (more than one solution), or instability (solution is sensitive to small changes in input data). Uniqueness requires an identifiable parameter set with a solution, which is sensitive to small changes in the parameters. More detailed discussions on parameter estimation theory can be found in the papers of Carrera and Neuman (1986a), Kool and Parker (1988), and Russo et al. (1991). In contrast to linear optimization, there is usually a high uncertainty in nonlinear parameter estimation (Brooke et al., 1992). Therefore, nonlinear parameter estimation is often recognized as being "ill-posed." In general, there are three concerns related to the uncertainty: (i) it may be difficult to find a solution; (ii) if a solution is found, it may not be unique; and (iii) the solution may be instable or excessively sensitive to experimental data, or insensitive to one or more parameters. Even though theoretically these are unsolved topics, the particular problem to be solved may become "well-posed" as appropriate and sufficient experimental information is obtained.

Previous studies have shown that the experimental method plays an important role in determining whether the parameter estimation problem is well posed, and indicated that a minimum amount of data must be collected to characterize the simulated flow process. For example, Gardner's (1956) one-step transient outflow method may be an ill-posed parameter estimation problem, yielding a non-unique set of parameters for the constitutive relationships. Van Dam et al. (1994) suggested that cumulative outflow be measured during multiple outflow steps, so as to yield sufficient information for determination of a unique parameter set using the inverse method. Including capillary pressure measurements during the outflow experiment further resulted in improved parameter sensitivity (Toorman et al., 1992). Eching and Hopmans (1993) concluded that the measurement of capillary pressure in addition to the multiple outflow measurements provided adequate information for unique solutions of the inverse parameter estimation problem.

Although the limitations with respect to the experiment or modeling are few, the inverse approach relies on the availability of a universally applicable nonlinear optimization algorithm. Problems with the parameter optimization technique generally are associated with the difficulty of defining an objective function, which will yield unique and convergent solutions.

The inverse parameter estimation of soil capillary pressure and permeability functions includes three functional parts: (1) a controlled transient flow experiment for which the boundary conditions and additional flow variables such as capillary pressure and cumulative outflow are accurately measured; (2) a numerical flow model simulating the transient flow regime of the experiment and which includes the parametric models that describe the constitutive relationships; (3) and an optimization algorithm, which estimates the unknown parameters through minimization of the difference between observed and simulated flow variables in the objective function (Figure 1.2). The quality of the final solution of the parameter estimation problem is dependent on the quality of each of these three components as well as that of their internal relationships. Moreover, it is tacitly assumed that the formulated constitutive relationships describe the physical behavior of the soil in question.

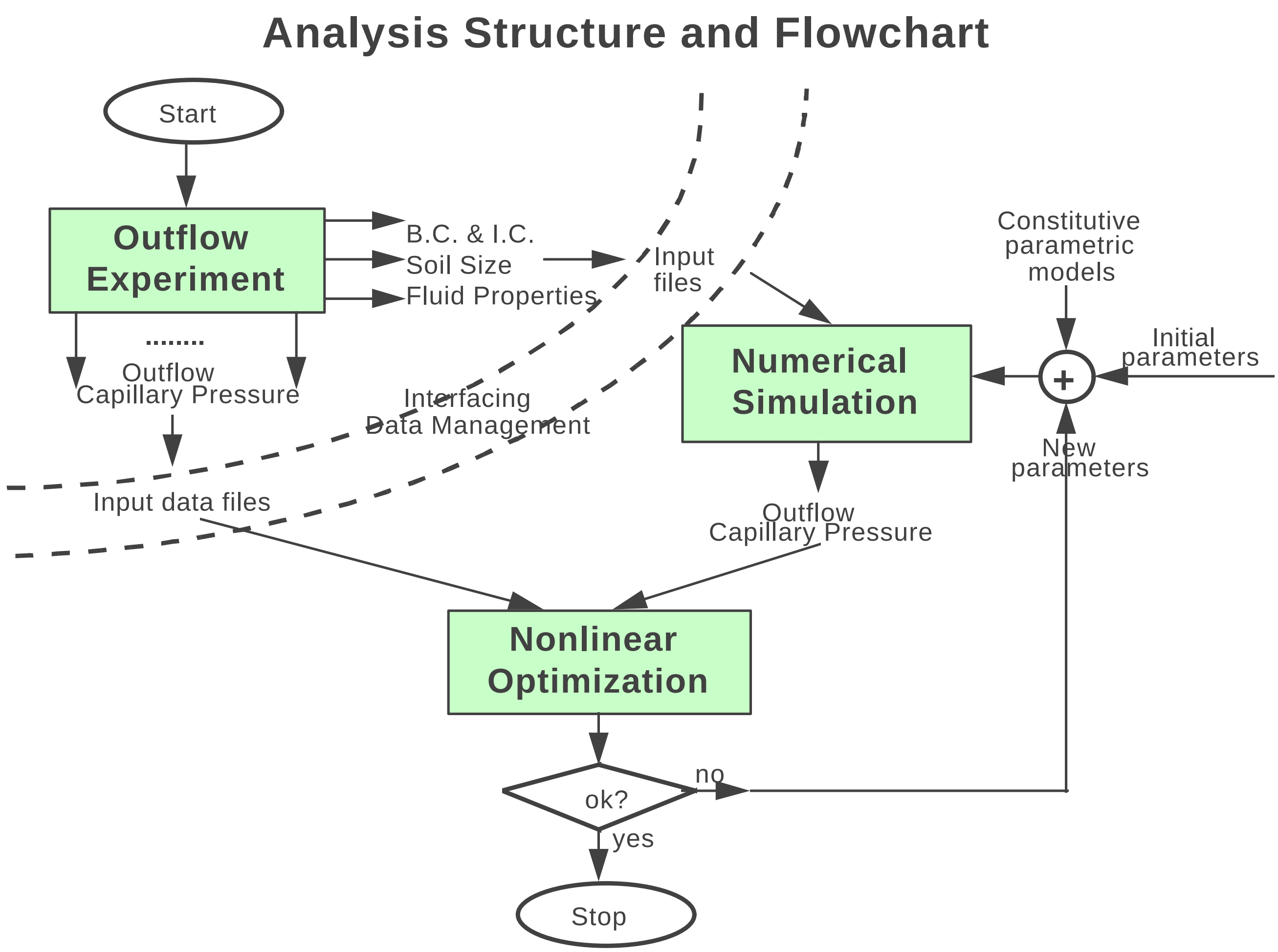

Figure 1-2. Flowchart of parameter optimization approach

Although the inverse parameter estimation approach including experimental and analytical methods has been developed and increasingly applied in recent years, it has been limited to air-water systems only. Under the traditional Richards' assumption that the air-phase has a negligible influence on water flow, air-water systems were treated as one-phase (water) systems. In this study, the inverse parameter estimation method was expanded to two-fluid flow systems including air-water, air-oil, and oil-water.

It was the objective of this study to expand the multi-step outflow method to two-fluid flow systems, and to evaluate how the additional complications and constraints would influence the well-posedness of the inversion problem. We present results of multi-step outflow experiments for three two-fluid systems: air-water, oil (Soltrol)-water, and air-oil in two soils. These systems are typical in immiscible organic contaminant research and important to subsurface flow and transport studies. In this study we also show how capillary pressure- and permeability-saturation relationships can be estimated directly from the capillary pressure and drainage data obtained from a multi-step outflow experiment. Moreover, the scaling concept was tested through scaling of the individual capillary pressure functions from interfacial tension values, and by normalization of the effective permeability using the fluid-independent intrinsic permeability value of the investigated soils. The results are expected to be informative for scientists studying inverse parameter estimation approaches and multi-fluid flow in the subsurface

Chapter 2
Materials and Methods

Experiments

Multi-step outflow experiments were conducted in a constant temperature (20^{o}C) laboratory using a modified Tempe cell (Figure 2-1). The cell contained a 7.6-cm high brass soil core with an outside diameter of 6.4 cm and total soil volume of 216 cm^3. Colombia fine sandy loam collected along the Sacramento river near West Sacramento, California, and Lincoln sand obtained from the EPA R.S. Kerr Environmental Research Laboratory in Ada, Oklahoma, were used for the experiments (Table 2-1). Soil was air-dried, sieved through a 2-mm screen, and uniformly packed. Soil texture and bulk densities for both soils are presented in Table 2-1. For each separate outflow experiment a freshly air-dried soil was packed to the bulk density values listed in Table 2-1. One-dimensional transient experiments of a draining wetting fluid replaced by an invading non-wetting fluid were carried out in three two-fluid systems: (1) air-water, (2) air-oil (Soltrol 130 for Columbia soil and Soltrol 220 for Lincoln soil), and (3) oil-water. Air is considered the non-wetting fluid in the air-water and air-oil systems, with oil being the non-wetting fluid in the oil-water system. Soltrol[1] is a mixture of isoalkanes (C_{10} - C_{13} for Soltrol 130 and C_{13} -C_{17} for Soltrol 220) and has negligible solubility in water. The relevant physical properties of the three fluids are presented in Table 2-2. Different types of Soltrol were used to compare results with earlier measurements. We followed the principles of multi-step outflow for an air-water system described by Gardner (1956) in which an initially water-saturated soil sample placed on a fully water-saturated ceramic plate was subjected to a series of step increases in air pressure, resulting in a cumulative volume of water drainage after each incremental increase of air pressure. In the multi-step experiments, the rate of cumulative drainage and capillary pressure as a function of time were measured (Table 2-3).

Table 2-1. Physical Properties of Experiment Soils

Soil type	Sand	Silt	Clay	Bulk density	$K_{s,water}$ [1]
		%		g/cm^3	cm/hr
Columbia	63.2	27.5	9.3	1.42	4.2
Lincoln	88.6	9.4	2.0	1.69	23.0

1. Saturated hydraulic conductivity, with water as wetting fluid.

[1] Phillips Petroleum Company, Bartlesville, OK

Table 2-2. Physical Properties of Fluids at 20°C.

	Air-Oil[1]	Oil[1]-Water	Air-Water
Interfacial Tension (N/m)			0.0681
[1]Soltrol 130	0.0239	0.0259	
[2]Soltrol 220	0.0259	0.0364	

	Oil	Air	Water
Viscosity (Ns/m^2)		0.0000181	0.00100
[1]Soltrol 130	0.00144		
[2]Soltrol 220	0.00392		
Density (kg/m^3)		1.28	1000
[1]Soltrol 130	762		
[2]Soltrol 220	803		

1. Columbia soil
2. Lincoln soil

Table 2-3. Capillary Pressure Head (h_c) and Cumulative Outflow (Q) Data at the End of Each Applied Pressure Step.

	Applied Pressure (cm)			Q (ml)			Measured h_c (cm)		
	aw	ao	ow	aw	ao	Ow	aw	ao	ow
Columbia	60	20	40	10.0	7.1	19.0	64.4	24.2	43.6
	80	27	53	16.0	14.0	29.4	83.8	30.2	54.4
	120	40	80	35.5	25.3	48.4	120	41.2	76.6
	200	67	133	52.4	59.0	55.6	198	62.4	116
	400	133	266	60.2	68.0	63.2	320	109	218
	700	233	466	66.1	69.1	67.5	682	163	345
Lincoln	40	10	20	13.5	9.0	8.8	43.3	13.1	23.7
	60	15	32	31.0	16.0	27.5	60.6	15.8	32.3
	80	20	42	38.5	26.5	40.8	79.8	20.1	40.1
	100	27	50	45.0	43.5	45.2	99.3	25.3	47.1
	150	33	73	52.5	51.5	53.0	148	29.0	66.5
	200	67	100	54.5	57.5	55.0	194	38.8	80.0
	400		199	57.5		57.0	261		90.7

1.Non-wetting fluid entry pressure with air as non-wetting fluid
2.Non-wetting fluid entry pressure with Soltrol as non-wetting fluid

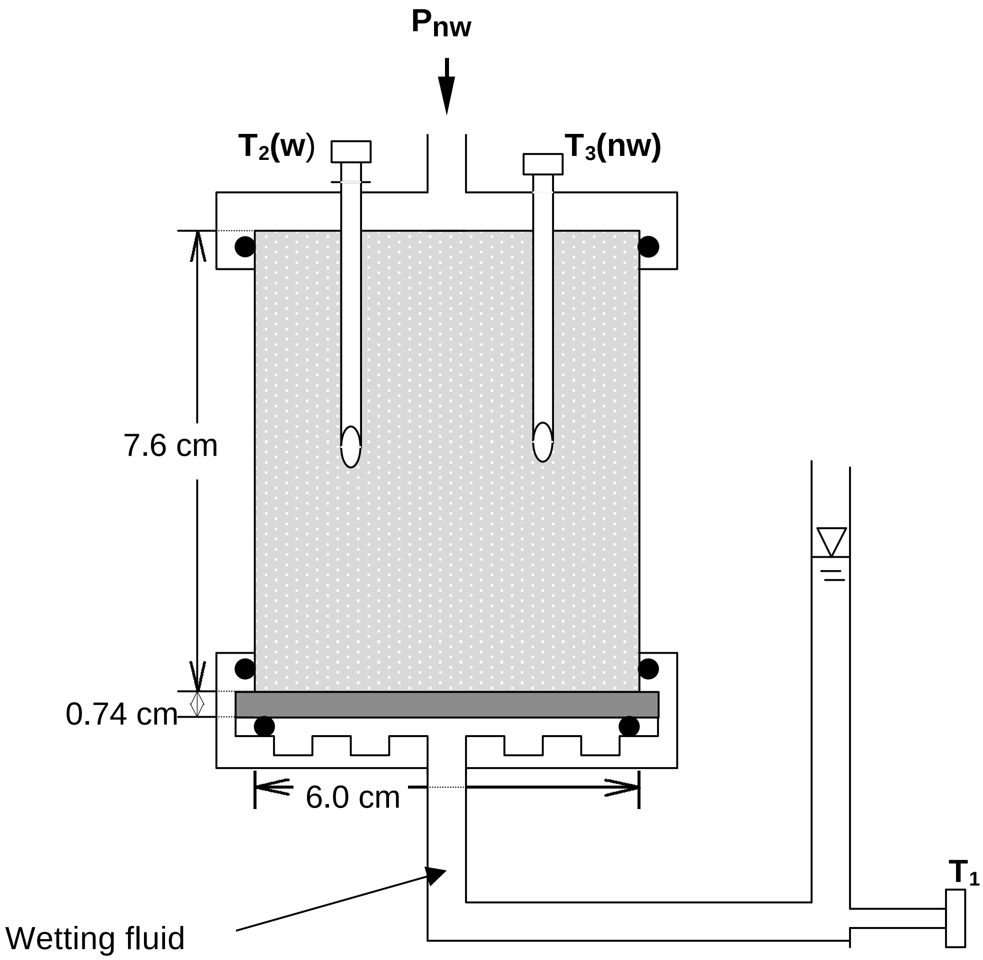

Figure 2-1. Experimental setup for multi-step outflow experiments with water as wetting and Soltrol as non-wetting fluid. T denotes a pressure transducer, and T1 and T2 are the tensiometers for the wetting and non-wetting fluid, respectively.

Using a noninvasive x-ray computed tomography technique, Hopmans et al. (1992) confirmed previous studies indicating that fluid flow can be properly described only if both wetting and non-wetting fluids are continuous. To obtain continuous wetting and non-wetting fluids at the onset of the experiment, the soil core was placed on a high flow rate, 1-bar ceramic plate, and saturated by the wetting fluid from the bottom upwards. The ceramic plate was 0.74 cm thick with a water-saturated hydraulic conductivity of 0.048 cm/h. The ceramic plate accepted Soltrol as a wetting fluid in air-oil systems, just as easy as it absorbs water in air-water systems. Therefore, the ceramic plate could be used for both water and Soltrol as the wetting fluid, without the need for additional treatment. The soil sample, saturated with the wetting fluid, was subsequently drained by applying a suction to the ceramic plate, slightly higher than the non-wetting fluid entry pressure of the investigated soil for that particular fluid pair. The resulting initial condition was hydraulic equilibrium for both fluids, after a static capillary pressure profile was achieved and both fluids were continuous. As positive pressure increments of the non-wetting fluid were applied at the surface of the soil, cumulative outflow of wetting fluid collected in a burette was monitored as a function of time by measurement of the fluid pressure, using a 1-psi pressure transducer[2] connected to the bottom of the burette (Figure 2-1). When air was the non-wetting fluid, air pressure was applied directly through a hole at the top of the Tempe cell. However, when oil was the non-wetting fluid, constant oil pressure for a given pressure increment was maintained using a Marriotte siphon controlled bottle filled with oil connected to pressurized air at one side with the other tube connected to the top of the flow cell and completely filled with oil. By stepwise adjustment of the air pressure, a stepwise constant oil pressure at the upper boundary of the flow cell was attained.

Ceramic tensiometers, connected to transducers, were installed vertically with the tip of the tensiometer placed at the 3.8-cm depth below the soil surface to measure pressure changes of the wetting and non-wetting fluids during drainage of the wetting fluid. Only one tensiometer was needed for the measurement of the wetting fluid pressure in the air-water and air-oil system, since the air pressure is equal to the applied air pressure across the sample at all times. If oil was the non-wetting fluid, both a hydrophilic and a hydrophobic tensiometer were used to monitor pressure changes of the water and oil fluid, respectively. Hydrophobic tensiometers were obtained using the treatment methods described by Lenhard and Parker (1987) and Busby et al. (1995). Since Soltrol is corrosive to the transducer membrane, oil pressures were measured by filling the transducers with water, after which they were connected to the Soltrol-filled Teflon tubing. All transducers were multiplexed and connected to a datalogger for automatic data acquisition of pressures and cumulative outflow during transient drainage at a measurement frequency of 12 readings per minute. Tensiometers were rigid and they were completely filled with either the wetting (water) or non-wetting (Soltrol) fluid, thereby allowing their use as a fast-response tensiometer. The immediate response of the transducer to changing fluid pressures was independently determined, and a response time of less than 10 seconds was adequate for the transient type of experiments described here.

Applied air pressures in the air-water system were 60, 80, 120, 200, 400, and 700 cm above atmospheric pressure for the Columbia soil. These pressure steps were chosen based on previous work by Eching et al. (1994). Selected air pressure steps for the Lincoln soil were 40, 60, 80, 100, 150, 200 and 400 cm above atmospheric pressure. These steps were smaller than that for Columbia soil because of the Lincoln soil's coarser texture. The pressure steps for the other fluid pairs (Table 2-3) were determined using these pressures and the scaled relationships of the interfacial tension between the tested fluid pair and air-water (Table 2-2) in an effort to apply pressure steps that yielded approximately equal drainage volumes for each wetting fluid within each pressure step for an investigated soil. A pressure increment lasted from 5 to 36 hours, and varied according to the pressure of the wetting fluid. After the wetting fluid pressure head (defined by $h_w = P_w/\rho_{H2O}g$, where P_w is the wetting fluid pressure, and ρ_{H2O} and g are the water density and gravitational acceleration constant, respectively) remained approximately constant (i.e., variations of less than 1 cm), the non-wetting fluid pressure was incrementally increased for the next drainage step. Final wetting fluid saturation was determined by oven-drying the soil

[2] MICRO SWITCH, Freeport, IL 61032.

following the last pressure step for the air-water and air-oil systems. Since the oven-drying method can not be used for determination of the final wetting fluid saturation for an oil-water system, the final wetting fluid saturation value for oil-water systems was determined from the average value of the air-water and air-oil systems. The saturated wetting fluid content and initial saturation were calculated based on the final degree of saturation and cumulative outflow. Detailed information on procedures for the multi-step experiment as applied to air-water systems can be found in Eching and Hopmans (1993).

The original outflow experiments for an air-water system assumed a constant air pressure in the draining soil, since air is continuous and its viscosity and density values are relatively low as compared to water. As such, a positive air pressure in the soil sample is assumed to be equivalent to a negative water pressure applied at the lower soil boundary, with the air pressure in the soil at atmospheric pressure (Kool et al. 1985a). This allows use of a single-fluid Richards' equation model for simulation of the draining soil core. If the non-wetting fluid is oil, however, the assumption of a constant non-wetting fluid pressure is not necessarily valid, since the viscosity and density of the oil fluid are similar to that of water (Table 2-2). Thus, a hydrophobic tensiometer was used to monitor the oil pressure during water drainage of the oil-water system.

Values of the interfacial tension between air and water are documented in handbooks and textbooks. But reported interfacial tension values of air-Soltrol and Soltrol-water vary widely. Moreover, since different types of Soltrol (Soltrol 130, Soltrol 170, and Soltrol 220) have been presented for flow and transport investigations in porous media, it was difficult to find exact values from the literature. Therefore, we independently measured the interfacial tensions of air-water and air-oil (Soltrol 130 and Soltrol 220) using the plate method (Adamson, 1990), while the interfacial tension between oil (Soltrol 130) and water was measured by the ring method (Adamson, 1990). The drained pore water at the completion of the air-water experiments was used for measurement of air-water surface tension, thereby including possible interactions of the soil material with the draining fluid. The interfacial tension between Soltrol 220 and water was taken from the work of Schroth et al. (1995), who concluded that the interfacial tension for an oil-water interface is time-dependent due to oil contamination of water at oil-water interfaces.

Numerical modeling of two-fluid phase flow

Governing Equation

Under the assumption that both fluids and the porous medium are incompressible, the most general form of the two-fluid flow equations without source-sink terms is described by the two-fluid volume-averaged momentum and continuity equations (Whitaker, 1986):

$$\phi\frac{\partial S_w}{\partial t} + \nabla \cdot \mathbf{q}_w = 0 \qquad \text{(2-1a)}$$

$$\mathbf{q}_w = -\frac{\mathbf{k}_w}{\mu_w}[\nabla P_w + \rho_w g] + \mathbf{k}_{w,nw} \cdot \mathbf{q}_{nw} \qquad \text{(2-1b)}$$

$$\mathbf{q}_{nw} = -\frac{\mathbf{k}_{nw}}{\mu_{nw}}[\nabla P_{nw} + \rho_{nw} g] + \mathbf{k}_{nw,w} \cdot \mathbf{q}_w \qquad (2\text{-}1c)$$

$$\phi \frac{\partial S_{nw}}{\partial t} + \nabla \cdot \mathbf{q}_{nw} = 0 \qquad (2\text{-}1d)$$

In Eqs. (2-1), the subscripts w and nw denote the wetting and non-wetting fluids, respectively; P_i (i = w, nw) denotes pressure (N/m^2); S_i (i = w, nw) is the degree of fluid saturation relative to the porosity ϕ; $\mathbf{q}_i$ is flux density vector (m/s); μ_i (i = w, nw) denotes fluid dynamic viscosity (Ns/m^2); $\mathbf{k}_i$ (i = w, nw) is the effective permeability tensor (m^2) = k_{ri} $\mathbf{k}$, where $\mathbf{k}$ is the intrinsic permeability (m^2) and $k_{ri} = k_{ri}(S_i)$ is the relative permeability. In Eq. (2-1), the cross term $\mathbf{k}_{ij}$ denotes the viscous drag tensor (Whitaker, 1994) representing the influence of the viscous drag that exists between the flowing wetting and non-wetting fluids. The cross term describes the coupling between the nw- and w- fluids, which appears to be highly dependent on the viscosity ratio of both fluids (Whitaker, 1986 and 1994), and the magnitude of the interfacial areas between the two fluids. Since these cross terms are either undetectable or unimportant or both for flow in complex soil systems, the current practice is that they are of secondary importance. Moreover, as stated by Whitaker (1986), in flow systems with air as the non-wetting fluid, its viscosity is small relative to that of the wetting fluid, thereby justifying the insignificance of the coupling parameters. Also, Bentsen (1994) presented experimental evidence that removing these terms introduced little error. Eqs. [2-1] also hold if air is the non-wetting fluid as in multi-step outflow experiments, if it is assumed that incremental changes in applied air pressure occur instantaneously across the soil sample, and that variations in soil air pressure between pressure increments have a negligible influence on the air density. Otherwise, the continuity equation of the air phase should include a pressure-dependent air density (Celia and Binning, 1992). Consequently, for one-dimensional vertical flow systems with z denoting vertical position, Eq. (2-1) is simplified to:

$$\phi \frac{\partial S_w}{\partial t} + \frac{\partial \mathbf{q}_w}{\partial z} = 0 \qquad (2\text{-}2a)$$

$$\mathbf{q}_w = -\frac{k_w}{\mu_w}\left(\frac{\partial P_w}{\partial z} + \rho_w g\right) \qquad (2\text{-}2b)$$

$$\mathbf{q}_{nw} = -\frac{k_{nw}}{\mu_{nw}}\left(\frac{\partial P_{nw}}{\partial z} + \rho_{nw} g\right) \qquad (2\text{-}2c)$$

$$\phi \frac{\partial S_{nw}}{\partial t} + \frac{\partial \mathbf{q}_{nw}}{\partial z} = 0 \qquad (2\text{-}2d)$$

For an incompressible porous medium, Eq. (2-2) is supplemented by:

$$S_w + S_{nw} = 1 \qquad (2\text{-}3)$$

Substituting (2-3) into (2-2a), and using the definitions of capillary pressure ($P_c = P_{nw} - P_w$) and fluid capacity ($C = -\phi dS_w/dP_c$), one obtains the following governing equations,

$$C\frac{\partial(P_{nw} - P_w)}{\partial t} = \frac{\partial}{\partial z}\left[\frac{k_w}{\mu_w}\left(\frac{\partial P_w}{\partial z} + \rho_w g\right)\right] \qquad (2\text{-}4)$$

$$-C\frac{\partial(P_{nw} - P_w)}{\partial t} = \frac{\partial}{\partial z}\left[\frac{k_{nw}}{\mu_{nw}}\left(\frac{\partial P_{nw}}{\partial z} + \rho_{nw} g\right)\right] \qquad (2\text{-}5)$$

which can be solved simultaneously for the unknown pressures P_w and P_{nw}, and thus for P_c.

In addition, since only non-wetting fluid enters the soil core at the top, and only wetting fluid leaves the core through the bottom, volume balance considerations across the cell at any time (t) requires that:

$$\mathbf{q}_w\big|_{OUT} = \mathbf{q}_{nw}\big|_{IN} = (\mathbf{q}_w + \mathbf{q}_{nw})\big|_z \qquad (2\text{-}6)$$

Boundary and Initial Conditions

The boundary conditions (BC's) and initial conditions (IC's) are determined by the experimental conditions of the transient multi-step outflow experiment during which the wetting fluid is drained from an initially slightly-unsaturated soil core. Figure 2.2 shows an overview of all IC's and BC's. At the upper boundary of soil core, the wetting fluid density flux is zero, and the non-wetting fluid pressure is prescribed by the imposed series of multi-step pressures, described by the stepwise function $P_j(T_j)$:

$$\mathbf{q}_w(z_{top}, t) = 0 \qquad (2\text{-}7a)$$

$$P_{nw}(z_{top}, t) = P_{nw}(T_j), \quad j = 1, 2, ..., M \qquad (2\text{-}7b)$$

In Eq. (2-7b), M is the total number of pressure steps used in the multi-step experiment, and $P_{nw}(T_j)$ is the pressure value applied to the non-wetting fluid at z_{top} during the time period T_j. Using this notation, T_1 is the time period when pressure step one is applied, T_2 is the time period when the pressure step two is applied, and so on. At the lower boundary of the flow system, the flux of the non-wetting fluid is zero, since the entry value of the ceramic plate for the non-wetting fluid is higher than any of the imposed pressures. The wetting fluid pressure at z_{bottom} is the prescribed pressure condition determined by the height of the wetting fluid in the burette, which is a function of time, as the wetting fluid drains into the burette:

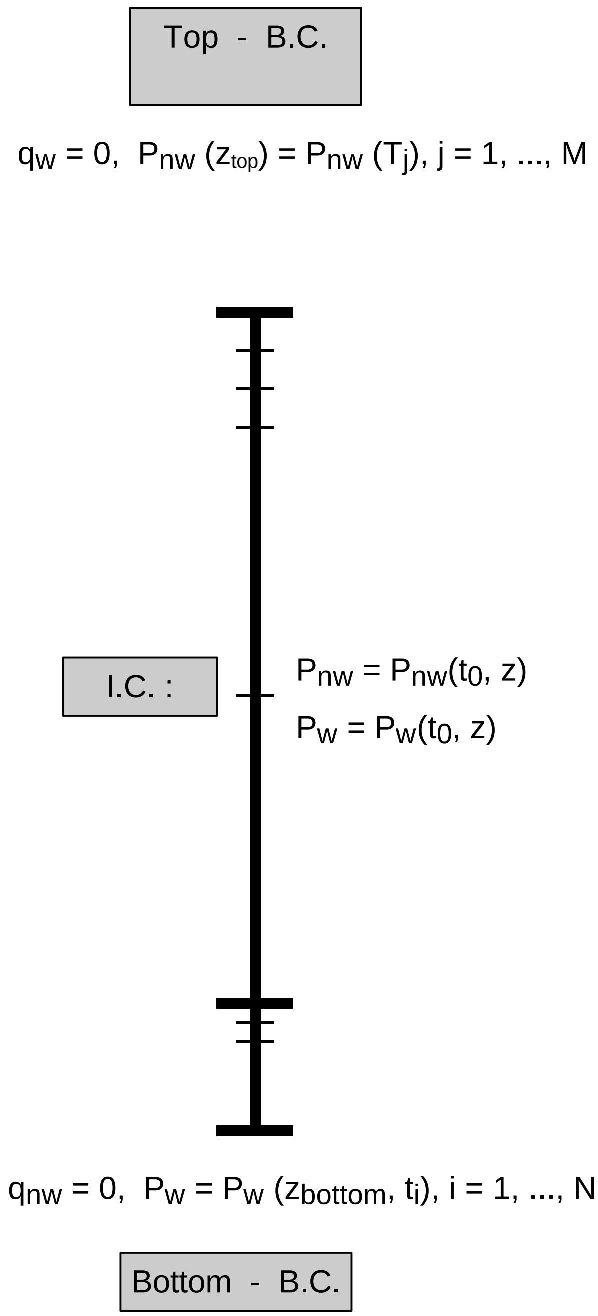

Figure 2.2 Schematic representation of boundary and initial conditions.

$$\mathbf{q}_{nw}(z_{bottom}, t) = 0 \tag{2-8a}$$

$$P_w(z_{bottom}, t) = \rho_w g h_{w|outflow}(t) \tag{2-8b}$$

In Eq. (2-8b), ρ_w is the density of the wetting fluid and $h_{w|outflow}$ (t) is the height of the wetting fluid in the receiving burette above the bottom of the ceramic plate (Figure 2.1). Because limited observations in time were used in the numerical modeling, the lower boundary-pressure measurements are a discrete function of time t_i, i = 1, 2, ..., N.

At time zero, both fluids are in static equilibrium. Because the soil is slightly unsaturated with respect to the wetting fluid, the initial conditions are described by the hydrostatic pressure of each fluid:

$$P_w(z, t_0) = P_w(z_{bottom}, t_0) - \rho_w g z \tag{2-9a}$$

$$P_{nw}(z, t_0) = P_{nw}(z_{top}, t_0) + \rho_{nw} g (z_{top} - z) \tag{2-9b}$$

where z is assumed positive upwards and z = 0 at the bottom of the ceramic plate. $P_w(z_{bottom}, t_0)$ and $P_{nw}(z_{top}, t_0)$ denote the boundary pressure values at the start of the transient outflow experiment.

Constitutive Relationships

The governing Eqs. (2-4) and (2-5) require apriori knowledge of the capillary pressure function $h_c(S_w)$ and permeability function $k_i(S_w)$ with i = w, nw, which are defined by functional parametric models:

$$S_w = S_w(h_c, \mathbf{b}) \tag{2-10a}$$

$$k_w = k_w(S_w, \mathbf{b}) \tag{2-10b}$$

$$k_{nw} = k_{nw}(S_w, \mathbf{b}) \tag{2-10c}$$

where **b** denotes the vector containing the parameters of the assumed functions. In this study, we used the van Genuchten model (1980) to characterize the capillary pressure function, which is used with Mualem's model (Mualem, 1976, Parker et al., 1987; Luckner et al., 1989) to describe the permeability functions:

$$S_{ew} = [1 + (ah_c)^n]^{-m} \qquad (2\text{-}11a)$$

$$k_{r,w} = \frac{k_w}{k} = S_{ew}{}^l [1 - (1 - S_{ew}{}^{\frac{1}{m}})^m]^2 \qquad (2\text{-}11b)$$

$$k_{r,nw} = \frac{k_{nw}}{k} = (1 - S_{ew})^l [1 - S_{ew}{}^{\frac{1}{m}}]^{2m} \qquad (2\text{-}11c)$$

where, k_r is the relative permeability and k denotes the intrinsic permeability (L^2); S_{ew} is the effective saturation of the wetting fluid with $S_{ew} = (S_w\text{-}S_{w,r})/(1\text{-}S_{w,r})$, where $S_w = \theta_w/\phi$ is the saturation of wetting fluid, and $S_{w,r}$ is the residual saturation of the wetting fluid; α and n are unknown parameters which are inversely proportional to the non-wetting fluid entry value and the width of pore-size distribution, respectively, and m was assumed to equal to m = 1-1/n (van Genuchten, 1980); the parameter l is related to the tortuosity of the soil and is here assumed equal to 0.5 for both the wetting and non-wetting fluid.

Numerical Solution

The governing Eqs. (2-4) and (2-5), the boundary and initial conditions (2-7, 2-8, and 2-9), and the constitutive relationships in Eq.(2-11) combined make up the mathematical model of the experimental system. The mathematical model has no analytical solution available because of the nonlinearity of the constitutive functions. Therefore, a numerical model was adapted to simulate the two-fluid flow regime.

The adapted two-phase numerical model in this study was developed from a two-phase model of Dr. John Nieber at the University of Minnesota (personal communication). We used the same numerical scheme, which includes a modified Picard linearization algorithm of the mixed-form governing equation and a lumped finite element approximation (Celia et al., 1990 and 1992). Celia et al. (1990) showed that the numerical solution based on the mixed form equation was inherently mass conservative and that the lumped finite element approximation eliminated oscillations.

Briefly, by using total head **H** instead of pressure ($\mathbf{H}_w$ and $\mathbf{H}_{nw}$ for wetting and non-wetting phases: $\mathbf{H}_{i=w,nw} = \frac{P_i}{\rho_{H_2O}\, g} + \frac{\rho_i}{\rho_{H_2O}} z$), the numerical approximation of governing Eqs. (2-4) and (2-5) becomes:

$$C \frac{D(H_{nw} - H_w)}{Dt} = \frac{D(\frac{\mathbf{k}_w}{\mu_w} \frac{DH_w}{Dz})}{Dz} \qquad (2\text{-}12)$$

and $$-C\frac{(H_{nw}-H_{w})}{D t} = \frac{D(\frac{\mathbf{k}_{nw}}{\mu_{nw}}\frac{D H_{nw}}{D z})}{D z} \qquad (2\text{-}13)$$

Applying the modified Picard and lumped finite element approximation, the finite element matrix equation can be written as

$$(D t \cdot \mathbf{G} + \mathbf{D})\mathbf{H}^{t+D} = D\mathbf{q} - \mathbf{D}\mathbf{H}^{t} \qquad (2\text{-}14)$$

where, **G** is conductance matrix derived from a combination of individual permeability terms, **D** is the storage matrix with elements accounting for the capacity term C, and $\Delta\boldsymbol{\theta}$ is a vector describing fluid-content changes for a time increase Δt. Figure 2.3 demonstrates the makeup of **G** and **D,** from elemental matrices (sub-matrices E1, E2, and E3) and nodes (N1, N2, N3, and N4). Figure 2.3 also demonstrates that each node has

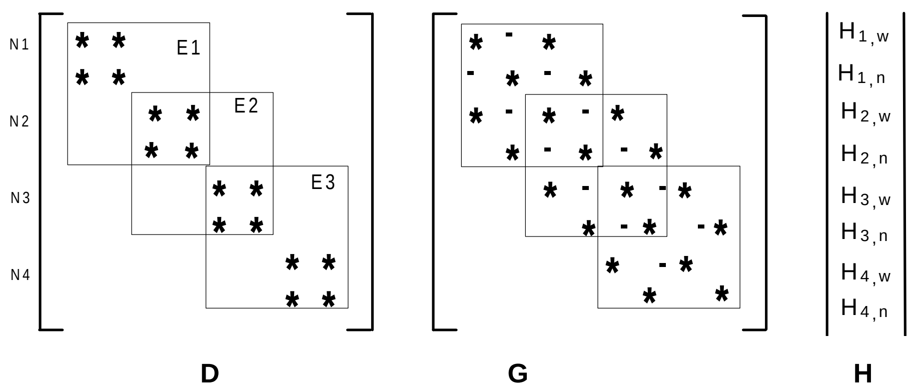

***Figure 2.3** Makeup of conductance G and storage D matrices, and H-vector for 4 nodes. N = node, E = element. Dashes indicate zero-value entries.*

both wetting and non-wetting fluid contributions in all arrays and vectors of Eqs. (2-12) and (2-13). The first subscript of total head **H** vector represents the index of the finite element nodes. The entries out of the diagonal line in Matrix **D** represent the coupling between the two-fluid pressures of each node. From the makeup of matrices in Figure 2.3, it is clear that the left-hand side of Eq.(2-14) consists of a matrix with a total bandwidth of five. The quintic-diagonal algorithm (Vemuri and Korplus, 1981) was used to solve Eq.(2-14). The air-water flow option of this two-fluid flow model was tested by comparing simulations with the model used by Eching and Hopmans (1993).

Optimization

The inverse parameter estimation is cast as a nonlinear optimization problem; i.e., a vector **b** containing the unknown parameters of the constitutive relationships in Eq.(2-11) is estimated by minimizing an objective function O(**b**), containing deviations between observed and predicted system response variables. In general, an optimization procedure includes a formulation of the objective function, a solution algorithm, and an analysis of convergence and uncertainty. Theoretically, the objective function can be formulated from a maximum likelihood (ML) consideration (Carrera and Neuman, 1986a; Kool and Parker, 1988). For a given predictive model, which is assumed to be true with no error, ML yields parameter estimates with non zero values of the objective function being attributed to measurement errors.

Using the notation **v** which is the vector containing the elements of measured flow variables (capillary pressure, outflow) with the subscript m and s denoting measured and simulated values, respectively, the observation error is equal to $\mathbf{e} = \mathbf{v}_m - \mathbf{v}_s$, with the assumption that model errors are zero. When observation errors (n is the total number of observations) are assumed to describe multivariable normal distribution with zero-mean and covariance matrix $\mathbf{V} = E(\mathbf{v}_m - \mathbf{v}_s)(\mathbf{v}_m - \mathbf{v}_s)^T$, the maximum likelihood estimation (Bard, 1974) formulates the objective function O(**b**) as:

$$O(\mathbf{b}) = \frac{n}{2}\ln 2\pi + \frac{1}{2}\ln(\det \mathbf{V}) + \frac{1}{2}\mathbf{e}^T \mathbf{V}^{-1}\mathbf{e} \qquad (2\text{-}15)$$

and leads to the least squares (LS) problem:

$$O(\mathbf{b}) = \mathbf{e}^T \mathbf{V}^{-1}\mathbf{e} \qquad (2\text{-}16)$$

Thus, for a general covariance matrix **V**, Eq. (2-16) is a general least-squares problem (GLS), where the inverse of the error covariance matrix denotes the weighting matrix, and includes measurement accuracies and their correlations. If these errors are independent, but the variance varies among observation type, **V** is a diagonal matrix leading to a weighted least squares problem (WLS). For the case that measurement errors are assumed independent with constant variances, **V** is an identity matrix of size $n \times n$, and Eq. (2-16) reduces to an ordinary least squares problem (OLS). In this study, the assumption is made that the errors **e** are independent and that their variances are proportional to the magnitudes of the mean values of particular measurements (Kool and Parker, 1988). Weighting factors are chosen to be inversely proportional to their mean measured values of cumulative drainage (Q), capillary pressure head (h_c) and initial water content $\theta(h_c, t_0)$, yielding a WLS problem of the form:

$$O(\mathbf{b}) = W_Q \sum_{i=1}^{N} \{w_i [Q_m(t_i) - Q_s(t_i, \mathbf{b})]\}^2$$
$$+W_{h_c} \sum_{j=1}^{M} \{w_j [h_{c,m}(t_j) - h_{c,s}(t_j, \mathbf{b})]\}^2 \qquad (2\text{-}17)$$
$$+W_q \sum_{k=1}^{L} \{w_k [q_m(h_{c,k}, t_k) - q_s(h_{c,k}, t_k, \mathbf{b})]\}^2$$

or using $W = V^{-1}$,

$$\mathrm{O}(\mathbf{b}) = [\mathbf{v}_{\mathrm{m}} - \mathbf{v}_{\mathrm{s}}(\mathbf{b})]^{\mathrm{T}} \mathbf{W} [\mathbf{v}_{\mathrm{m}} - \mathbf{v}_{\mathrm{s}}(\mathbf{b})] = \mathbf{e}^{\mathrm{T}} \mathbf{W} \mathbf{e} \qquad (2\text{-}18)$$

In Eq. (2-17), N, M, and L denote the number of observations of Q, P_c, and θ, respectively and O(**b**) is normalized by the weighting factors:

$$\mathrm{W_Q} = 1 \qquad (2\text{-}19a)$$

$$W_{h_c} = \left(\frac{\frac{1}{N} \sum_{i=1}^{N} Q_m(t_i)}{\frac{1}{M} \sum_{j=1}^{M} h_{c,m}(t_j)} \right)^2 \qquad (2\text{-}19b)$$

$$W_q = \left(\frac{\frac{1}{N} \sum_{i=1}^{N} Q_m(t_i)}{\frac{1}{L} \sum_{k=0}^{L} q_m(h_{c,k}, t_k)} \right)^2 \qquad (2\text{-}19c)$$

where L = 1 with $\theta_m(h_{c,0}, t_0)$ corresponding to the initial volumetric water content value after exceeding the non-wetting fluid entry value. In addition, ω_i, ω_j and ω_k are weighting factors allowing weighting of individual measurements.

The objective of the optimization procedure is to estimate the parameter vector **b**, for which Eq.(2-18) is minimized, thereby yielding a best fit between model-predicted and measured data. The objective function O(**b**) is a nonlinear function of **b**, so that the minimization must be carried out iteratively until pre-defined convergence criteria are satisfied. A commonly applied criterion is based on the RMSSR (Root of Mean Sum Squared Residuals) value:

$$\mathrm{RMSSR} = \sqrt{\frac{\mathrm{O}(\mathbf{b})}{\mathrm{M + N + L}}} \qquad (2\text{-}20)$$

We applied the Levenberg-Marquardt optimization algorithm (More, 1977) to minimize (2-20). The details of Levenberg-Marquardt method and the convergence and uncertainty analysis are included in the Appendix. In this study, an existing optimization program (Eching and Hopmans, 1993) originally developed by Kool et al. (1985a) was modified to interface with the two-fluid flow model.

Scaling Method

The traditional method of estimating the capillary pressure function for one fluid pair from another is based on the scaling method as first introduced by Leverett (1941). The theoretical basis stems from the similarity theory, when identical soils with different fluid-pairs are considered to be similar systems. The basic assumptions include that the solid matrix is rigid with negligible solid-fluid interactions, fluids are held in the porous matrix by capillary forces only, and air-water and oil-water interfaces act independently. Capillary pressure as a function of fluid saturation is determined by interfacial properties such as interfacial tension, contact angle and interfacial curvature. Whereas the interfacial tension and contact angle are dependent on the particular solid and fluid materials, the interfacial curvature is dependent on the pore geometry of the soil matrix. Consequently, Leverett (1941) introduced the dimensionless Leverett's function $J(S_{ew})$ to describe the similarity relationship between soil systems 1 and 2 by,

$$J(S_{ew}) = \frac{P_{c,1}}{\sigma_1}\left(\frac{k_1}{\phi_1}\right)^{\frac{1}{2}} = \frac{P_{c,2}}{\sigma_2}\left(\frac{k_2}{\phi_2}\right)^{\frac{1}{2}} \qquad (2\text{-}21)$$

where σ and k denote interfacial tension and intrinsic permeability, respectively. In Eq. (2-21), $(k/\phi)^{-1/2}$ (length unit, L) denotes the microscopic length for which the size depends on the pore geometry of soil medium only. Thus, for the same soil matrix but different fluid pairs 1 and 2, Eq. (2-21) reduces to:

$$J(S_{ew}) = \frac{P_{c,1}}{\sigma_1} = \frac{P_{c,2}}{\sigma_2} \qquad (2\text{-}22)$$

or,

$$h_{c,2}(S_{ew}) = \left(\frac{s_2}{s_1}\right)h_{c,1}(S_{ew}) \qquad (2\text{-}23)$$

Eq. (2-23) states that from a known soil's capillary pressure head-saturation relationship for a particular fluid-pair (e.g., air-water), the soil's capillary pressure function for another fluid-pair can be predicted according to the corresponding interfacial tension values. Additional assumptions for proper application of Eq. (2-23) are: (i) the soil is completely water-wet; (ii) the oil fluid is present between water and air, and (iii) no fluid trapping occurs. Also, it is assumed that the contact angle is independent of fluid type, which may not be correct (Demond and Roberts, 1991). The optimized capillary pressure $P_c(S_w)$ function from the proposed inverse parameter estimation of the air-water, air-oil, and oil-water systems are scaled to compare the scaling relationships, and to provide a means to test the optimized solutions.

Chapter 3
Results and Discussion

Experimental data

Measured values of capillary pressure and cumulative outflow at the end of each pressure step, together with the applied non-wetting fluid pressure are listed in Table 2-3. Figures 3-1, 3-2, and 3-3 present all the collected cumulative outflow and capillary pressure data as a function of time for air-water, air-oil, and oil-water, respectively, for both soils. Table 3-1 summarizes experimental observations of saturated wetting fluid content, initial and final capillary pressures, and cumulative outflow for the two soils.

Table 3-1. Experimental Wetting Fluid Content (q), Capillary Pressure Head (h_c) and Cumulative Outflow (Q) Data for Each Fluid Pair of Investigated Soils.

	Columbia Soil			Lincoln Soil		
	Air-Water	Air-Oil	Oil-Water	Air-Water	Air-Oil	Oil-Water
θ_s[1] (m^3/m^3)	0.45	0.43	0.44[4]	0.32	0.33	0.33[4]
Initial h_c[2] (cm)	23.0	10.0	18.0	16.0	7.2	10.0
θ_f[3] (m^3/m^3)	0.14	0.11	0.13	0.066	0.059	0.059
Final h_c (cm)	682	163	345	261	39	91
Total Q (ml)	66.1	69.4	67.5	56.7	57.5	57.0

[1] Saturated wetting fluid content
[2] Under suction
[3] Final wetting fluid content
[4] Estimated value

As shown by Hopmans et al. (1992) for air-water systems, the initial capillary pressure head (h_c) must exceed the non-wetting fluid entry pressure, so as to achieve non-wetting fluid continuity at the onset of the transient drainage experiment. The corresponding wetting fluid saturation is estimated from the saturated (θ_s) and cumulative wetting fluid drainage at static equilibrium when the initial capillary pressure head value has been attained, thereby yielding the first point of the capillary pressure curve. The final wetting fluid content (θ_f) was determined from oven-drying upon completion of each experiment. The saturated wetting fluid content (θ_s) was calculated from total cumulative drainage (total Q) and the final wetting fluid content.

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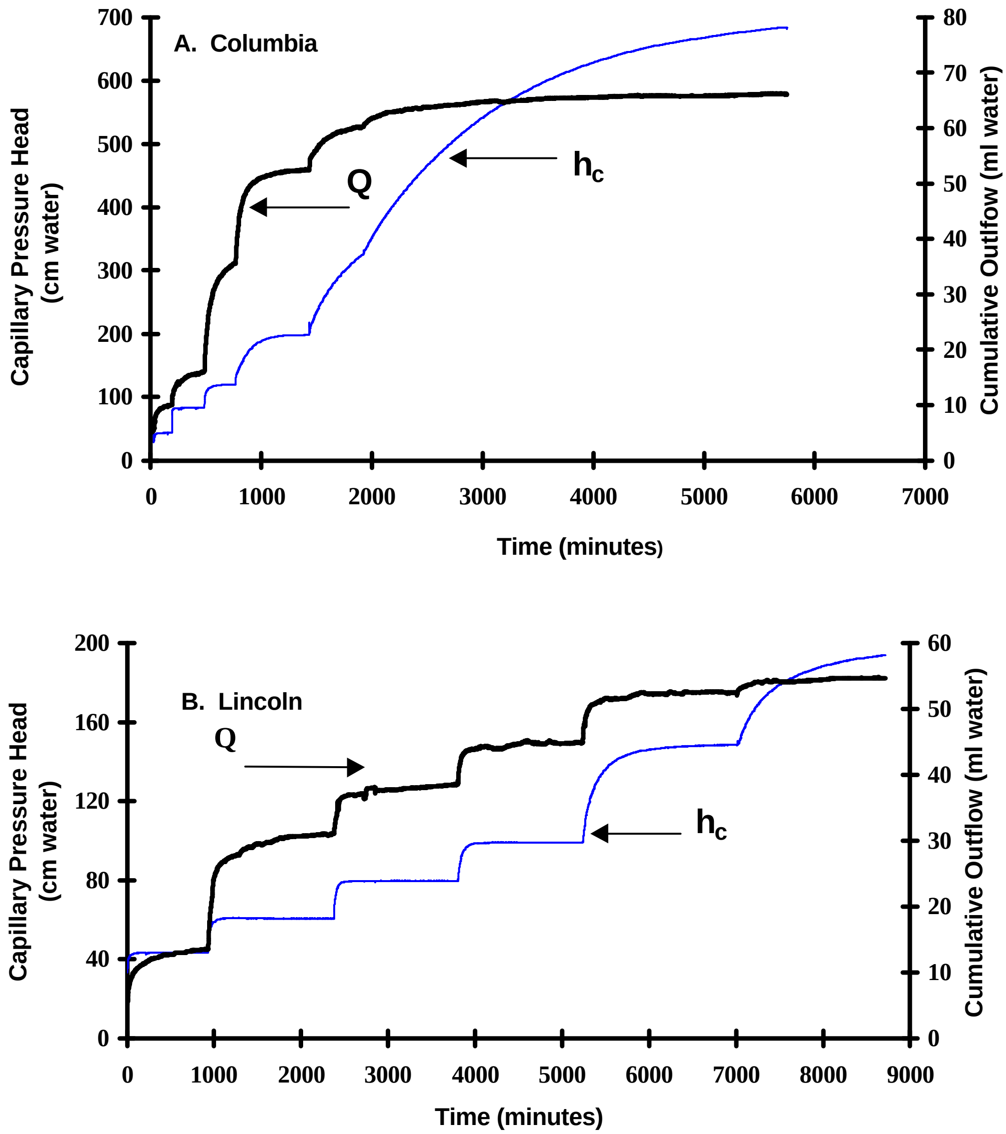

Fig. 3-1. Capillary pressure head (h_c) and cumulative outflow (Q) as a function with time for air-water system of (A) Columbia and (B) Lincoln soil.

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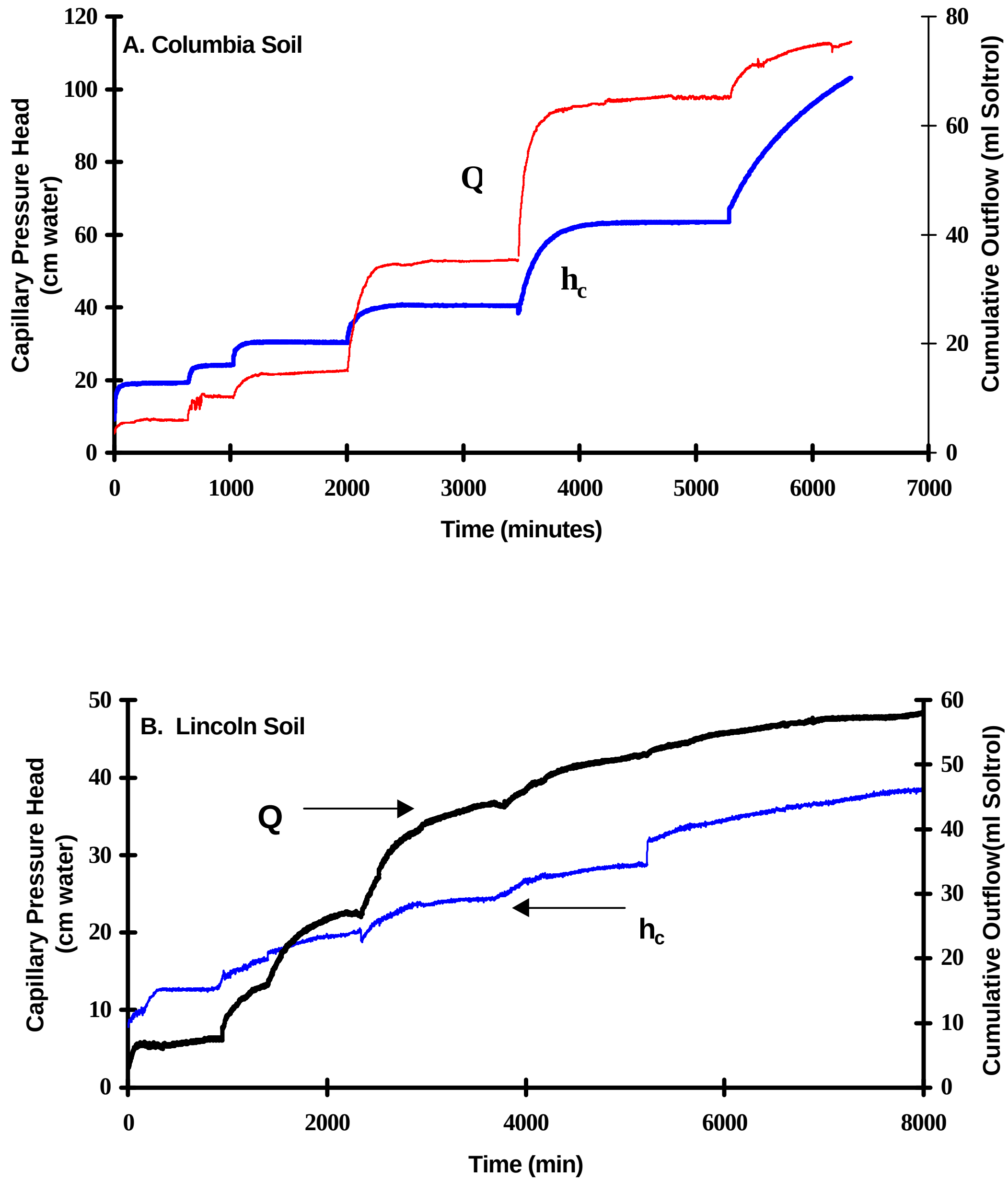

Fig. 3-2. Capillary pressure head (h_c) and cumulative outflow (Q) as a function with time for air-oil system of (A) Columbia and (B) Lincoln soil.

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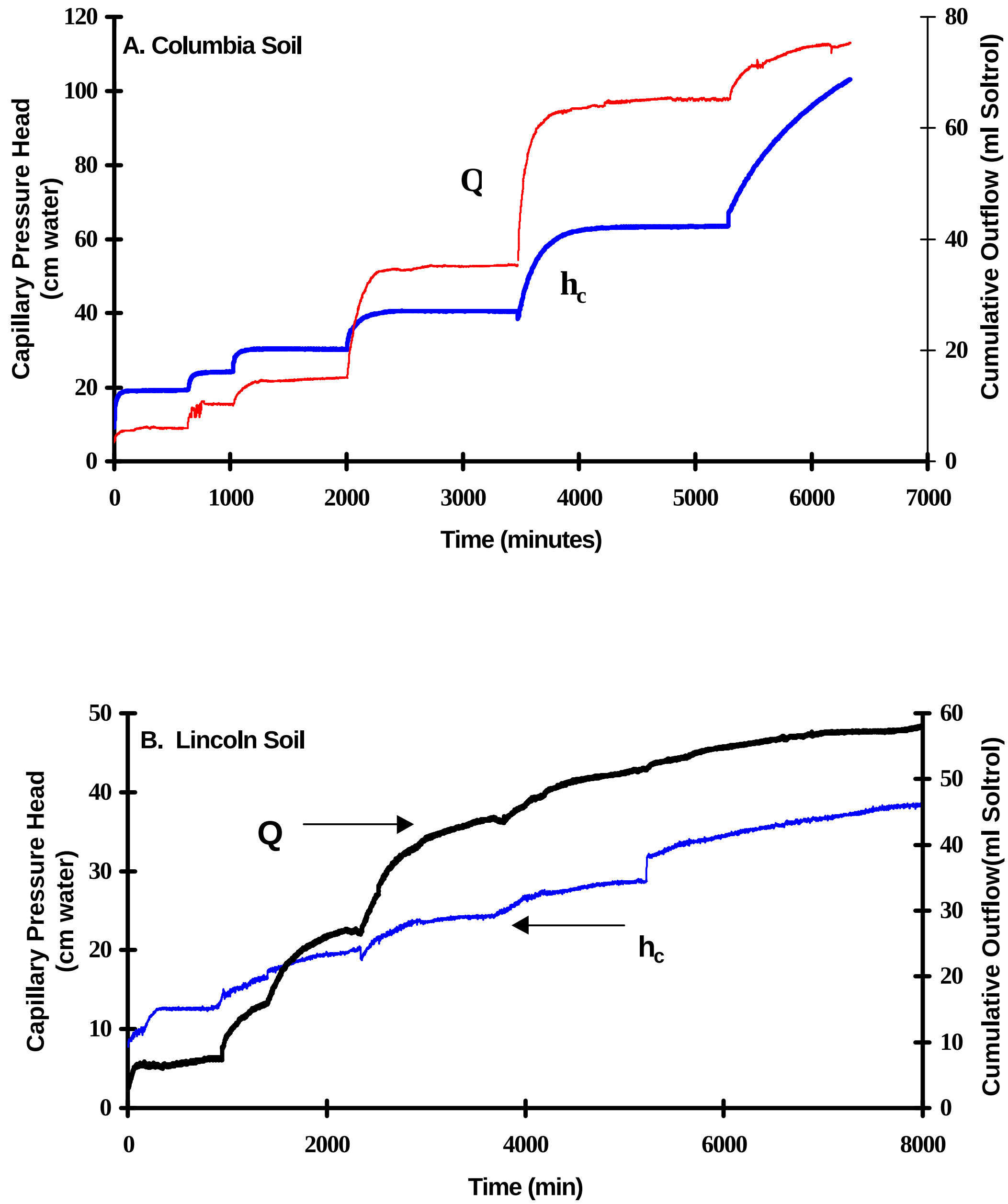


Fig. 3-3. Capillary pressure head (h_c) and cumulative outflow (Q) as a function with time for oil-water system of (A) Columbia and (B) Lincoln soil.

However, for the oil-water system, the θ_s-value was assumed to be the average of measured θ_s-values for the air-water and air-oil systems for each soil.

Since the Lincoln soil is coarser than the Columbia soil (Table 2-1), the Lincoln soil has smaller initial capillary pressure head values than the Columbia soil. Due to the scaling of the non-wetting fluid pressure at the top boundary of the soil sample, total outflow values are approximately equal for the three fluid pairs for each soil.

Air-water system

The measured cumulative outflow and capillary pressure head of the wetting fluid as a function of time for the Columbia and Lincoln soils are presented in Figures 3-1a and 3-1b, respectively. The capillary pressure is computed from the difference between the non-wetting and wetting fluid pressures, and is expressed in capillary pressure head, h_c (cm of water). For the air-water systems, the soil air pressure was assumed to be equal to the applied air pressure everywhere within the sample, whereas the water pressure was measured by the hydrophilic tensiometer at the center of the soil core. Outflow rates are relatively high at the beginning of each pressure increment and decrease toward zero, as the cumulative outflow (Q) approaches a constant value. After the drainage rate is reduced to near zero, the non-wetting fluid pressure was incrementally increased for the next drainage step. The initial high flow rates are the result of the larger capillary pressure gradients when air pressure is increased, and the relatively high effective permeability. As time passes, the capillary pressure head gradient is reduced and the outflow rate decreases toward zero during each pressure step. The capillary pressure head changes rapidly along with the cumulative outflow data for the first few pressure increments at relatively high wetting fluid saturations. However, as the capillary pressure is further increased, drainage rates decrease because of decreasing wetting fluid permeability as the soil desaturates, thereby increasing the time period required to achieve hydraulic equilibrium. As is usually done for estimation of capillary pressure-saturation functions under equilibrium flow conditions, we used simultaneously measured capillary pressure and drainage volume data towards the end of each pressure increment to estimate this function. The data in Table 2-3 also clearly demonstrates that as the applied pressure increases the difference between the applied pressure head and measured capillary pressure head at the end of each pressure increment becomes larger. Note that at true hydraulic equilibrium the measured capillary pressure in the center of the soil core should be equal to the applied air pressure. This tendency of not reaching equilibrium within a reasonable measurement time period had been determined earlier by Eching and Hopmans (1993) for the Oso Flaco sand, and is caused by the low wetting fluid permeability at low saturations, especially for coarse-textured soils. We should also point out that the estimation of the soil’s capillary pressure and permeability data does not require equilibrium soil-water conditions, but assumes a constant capillary pressure gradient in the soil sample. This assumption is satisfied if the soil samples approach hydraulic equilibrium.

Air-oil system

As in the air-water system, air pressure across the vertical profile of the sample is equal to the applied air pressure for each pressure step in the air-oil system. This system differs from the air-water system only by the physical properties of the wetting fluid. Based on the scaling theory of Leverett (1941), the capillary pressure-saturation curve for an air-oil system can be determined from that for an air-water system using the scaling relationship (see also Eq. 2-23):

$$h_{c(ao)} = \left(\frac{\sigma_{ao}}{\sigma_{aw}}\right) h_{c(aw)} \qquad (3\text{-}1)$$

where h_c denotes the capillary pressure head (cm of water), σ is the interfacial tension (N/m), and the subscripts ao and aw indicate air-oil and air-water systems, respectively. Using this relation, the range of measured capillary pressure heads in the air-oil system is approximately one third of the air-water systems (Table 2-2) for the same range in degree of wetting fluid saturation.

Though pressure increments for the air-oil system experiments were adjusted with respect to the ratio of interfacial tensions, the drainage curve differs from that of the air-water system, because times at which the applied air pressure was changed were different for the two systems. However, the measured capillary pressure and cumulative oil outflow versus time data in the air-oil systems for the Columbia and Lincoln soils as shown in Figures 3-2a and 3-2b, respectively, are similar to those for the air-water systems in Figures 3-1a and 3-1b, with the exception of less distinct plateau values for a few pressure steps in the Lincoln soil.

Oil-water system

Shown in Figures 3-3a and 3-3b are the outflow and capillary pressure head changes with time for the oil-water system in the Columbia and Lincoln soils, respectively. Again, the shapes of the curves in Figures 4a and 4b are similar to those of Figures 3-1a and 3-1b, while the range of capillary pressure heads for the oil-water system is between those of air-water and air-oil systems as determined by the adjusted applied air pressures.

Although we assumed a constant non-wetting fluid pressure profile for the air-water and air-oil systems, such a profile was not expected to be the case for oil-water systems, since the viscosity and density values of the non-wetting fluid (Soltrol) are similar to that of water (Table 2-2). As an example, Figure 3-4 shows the pressure head changes of the non-wetting ($h_{oil} = P_{oil}/\rho_{H2O}g$) and wetting fluids ($h_{water} = P_{water}/\rho_{H2O}g$) with time for the Lincoln soil. As expected, the soil-water pressure first increases in response to the increased oil pressure and subsequently decreases with time as the soil water drains, approaching near zero (wetting fluid pressure below ceramic plate) as hydraulic equilibrium is established. However, as the soil desaturates with respect to the wetting fluid (water) at the higher applied oil pressures, the wetting fluid permeability becomes limiting and equilibrium is not achieved within the measured time period. With an increase of the oil pressure at the upper boundary of the soil core, the oil pressure in the center of the sample increases immediately to a value equal to the incremented pressure and thereafter remains constant with time. We postulate that the constant oil pressure in the soil sample is a consequence of the imposed boundary conditions. In our experiments, the oil pressure is equal to the applied oil pressure corrected for static oil pressure at any time for both soils, thereby simplifying the physical description of wetting fluid drainage in the oil-water system.

Simplification to single fluid flow modeling

The one-dimensional Darcy flow equation combined with the continuity equation is used to describe single-fluid transient flow processes in soils. For a homogeneous soil, the flow and continuity equations for the wetting fluid (as indicated by the subscript w) are (see also Eqs. 2-2a and 2-2b):

$$q_w = -\frac{k_w}{\mu_w}\left(\frac{\partial P_w}{\partial z} + \rho_w g\right) \qquad (3\text{-}2)$$

$$\phi \frac{\partial S_w}{\partial t} = -\frac{\partial q_w}{\partial z} \qquad (3\text{-}3)$$

where q_w is Darcy's flux (L/T), k_w is the effective permeability (L^2) of the wetting fluid, P_w is the wetting fluid pressure ($M/L\,T^2$) , ρ_w is the density of the wetting fluid (M/L^3), μ_w is viscosity of the wetting fluid (M/T L) , g is the gravitational acceleration constant (L/T^2), ϕ is porosity, $S_w = \theta/\theta_s$ (-) is degree of saturation of the wetting fluid, t is time (T), and z is the vertical coordinate (L, positive upwards). The effective permeability is defined as:

$$k_w = k k_r \qquad (3\text{-}4)$$

where k is the intrinsic permeability (L^2) and k_r is the relative permeability of the wetting fluid, which is a function of degree of saturation and is related to the unsaturated hydraulic conductivity $K(S_w)$ by

$$K(S_w) = \frac{k_w \rho_{H2O}\, g}{\mu_w} \qquad (3\text{-}5)$$

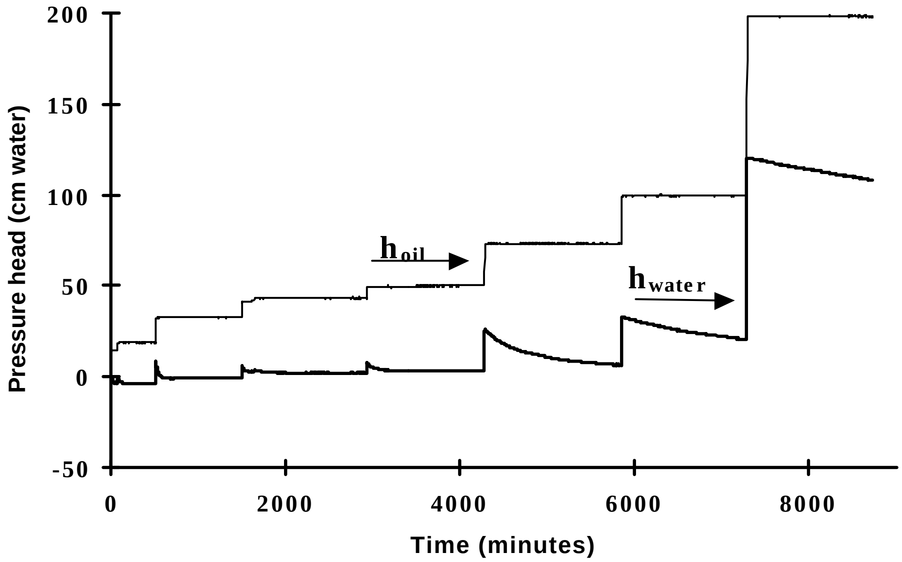


Figure 3-4. Change of oil and water pressure head as a function of time for oil-water system of Lincoln soil.

where μ_w is the viscosity of the wetting fluid. Combining Eqs. (3-2) and (3-3) yields:

$$\phi \frac{\partial S_w}{\partial P_c}\frac{\partial (P_c)}{\partial t} = \frac{\partial}{\partial z}\left[\frac{k_w}{\mu_w}\left(\frac{\partial P_w}{\partial z} + \rho_w g\right)\right] \qquad (3\text{-}6)$$

where $P_c=P_{nw}-P_w$ is the capillary pressure. While Eq. (3-6) has two unknowns, P_{nw} and P_w, we already noted that changes of the non-wetting fluid pressure with time were negligible in our experiments, hence Eq. (3-6) can be rewritten as:

$$C\frac{\partial P_w}{\partial t} = \frac{\partial}{\partial z}\left[\frac{k_w}{\mu_w}\left(\frac{\partial P_w}{\partial z} + \rho_w g\right)\right] \qquad (3\text{-}7)$$

where $C = \phi(\partial S_w/\partial P_c)$ is the slope of the capillary pressure-saturation curve. Hence, it seems to be adequate to apply a single-liquid flow model to simulate pressure changes of the wetting fluid in an oil-water system, much the same as in predicting water pressure changes in an air-water system (Kool et al., 1985b). Thus, the assumption of the time-independent non-wetting fluid pressure, equal to the applied non-wetting fluid pressure and augmented with the hydrostatic oil pressure in the soil core, simplifies the wetting-fluid phase flow to the original Richards equation.

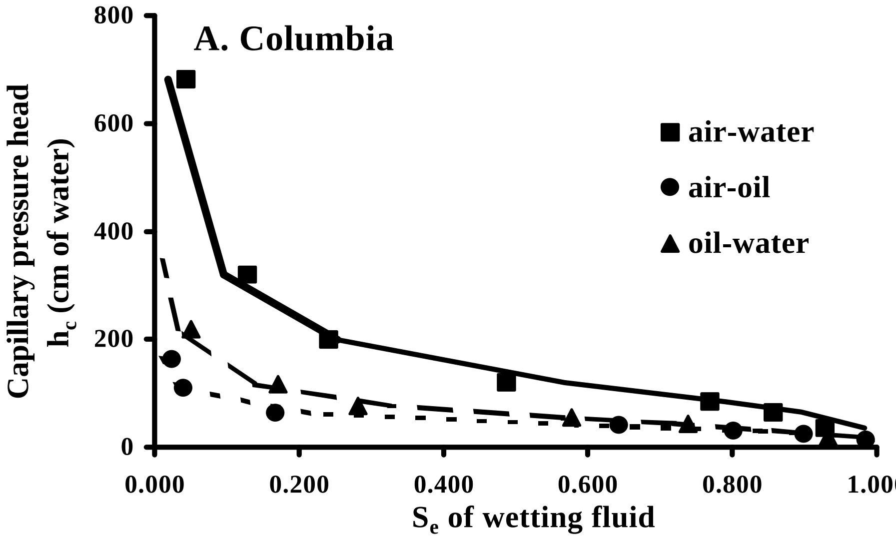
Estimation of capillary pressure function

The outflow and capillary pressure data in Figures 3-1, 3-2, and 3-3 show that both measured capillary pressure and cumulative outflow change rapidly at the beginning of each pressure step. In most experiments, drainage flow rate approaches zero at the end of each pressure step when the capillary pressure head in the center of the soil core reaches a constant value. At the end of each pressure increment then, the capillary pressure profile can be assumed to vary linearly with vertical position in the 7.6-cm tall soil core (Eching et al. 1994). Therefore, the measured outflow and capillary pressure data at the end of each pressure step can be used to estimate the capillary pressure-saturation function. The volumetric wetting fluid content (θ) is an average value of the soil core, just prior to increasing the non-wetting fluid pressure, calculated from cumulative outflow and initial wetting fluid content. The capillary pressure measured simultaneously in the center of the soil sample is thus assumed to correspond to the sample-average capillary pressure.

The capillary pressure-saturation function in Eq. (2-11a) of van Genuchten equation (1980) was fit to the experimental data shown in Fig. 3-5. Through curve fitting, using nonlinear least squares optimization, provided in the spreadsheet program EXCEL® (Wraith and Or, 1997), the parameters of the van Genuchten capillary pressure functions (Table 3-2) were obtained for each fluid pair. Figure 3-5 shows the measured (data points) and fitted capillary pressure-saturation functions (lines) for the three fluid pairs and both soils.

Table 3-2. Parameters of Individual Capillary Pressure-Saturation Functions (q_s, q_r, a, and n) and of the Combined Van Genuchten-Mualem Model, Fitting the Scaled Capillary Pressure and Permeability Data (q_s, q_r, a, n, and k).

	Columbia				Lincoln			
	Air-Water	Air-Oil	Oil-Water	Van Genuchten-Mualem model	Air-Water	Air-Oil	Oil-Water	Van Genuchten-Mualem model
θ_s	0.44	0.44	0.43	0.44	0.32	0.31	0.32	0.32
θ_r	0.120	0.112	0.132	0.112	0.06	0.001	0.056	0.062
α (cm^{-1})	0.009	0.024	0.02	0.009	0.019	0.051	0.033	0.019
n	3.197	4.423	3.352	2.873	3.686	4.180	4.633	5.712
k (cm^2)				2.0×10^{-9}				7.0×10^{-9}



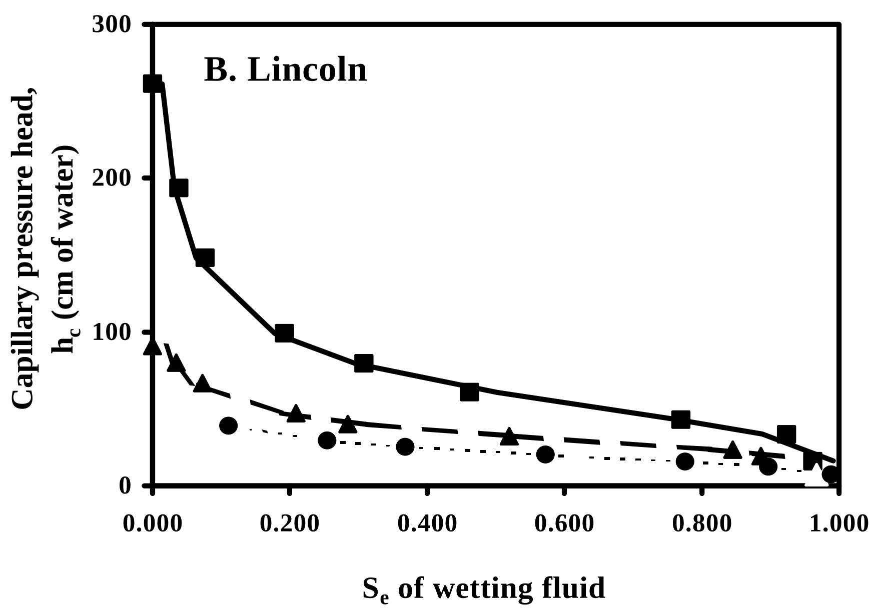


Figure 3-5. Measured capillary pressure head (h_c) and wetting fluid saturation (S_e) data for (A) Columbia and (B) Lincoln soil.

The θ_r-values reported in Table 3-2 are obtained from fitting capillary pressure data to the van Genuchten Eq. [3-8], and were not independently measured as done by Demond and Roberts (1991).

Using the interfacial tension ratios, the estimated capillary pressure-saturation data of air-oil and oil-water systems for each soil were scaled relative to the air-water capillary pressure data, and these are plotted versus effective saturation in Fig. 3-6. Demond and Roberts (1991) demonstrated that the coalescing of capillary pressure data using the interfacial tension-scaling concept was more successful if the capillary pressure is plotted against effective saturation of the wetting fluid, rather than simple saturation. Although not presented, we found little difference in scaling results when h_c was plotted against wetting fluid saturation. Nevertheless, the presented scaling results in Fig. 3-6 demonstrate excellent agreement between scaled and measured relationships for both soils, with spreading between scaled and measured capillary pressure data increasing at lower values of effective saturation. Similar findings were reported by Demond and Roberts (1991), who attributed discrepancies to the uncertainty of residual saturation values and the possible need to include the contact angle in the original Leverett scaling relationship. The fitted curve in Figure 3-6 was obtained by the combined fitting of all scaled capillary pressure and permeability data to the van Genuchten-Mualem relationship, which will be discussed later. Also the θ_r-values used in the presentation of the scaled capillary pressure data in Fig. 3-6 were estimated from the fitting of the combined van Genuchten-Mualem model.

Estimation of permeability functions

Measured outflow and capillary pressure data were used to estimate relative permeability functions of the wetting fluid for the different soil and fluid pair systems. Since changes in outflow are relatively high at the beginning of each pressure step, only data from the time periods immediately following an increase in non-wetting fluid pressure were used to estimate permeability functions. The principle of permeability estimation is the same as the direct K(θ)-method as discussed by Eching et al. (1994) from calculation of $P_{w,top}$ at the soil-plate interface. However, since the reported experiments include wetting fluids other than water, the Darcy flux equation, Eq. [3-2], was rearranged to yield

$$P_{w,top} = P_{w,bottom} - d\left[\frac{m_w q_w}{k_w} + r_w g\right] \qquad [3-8]$$

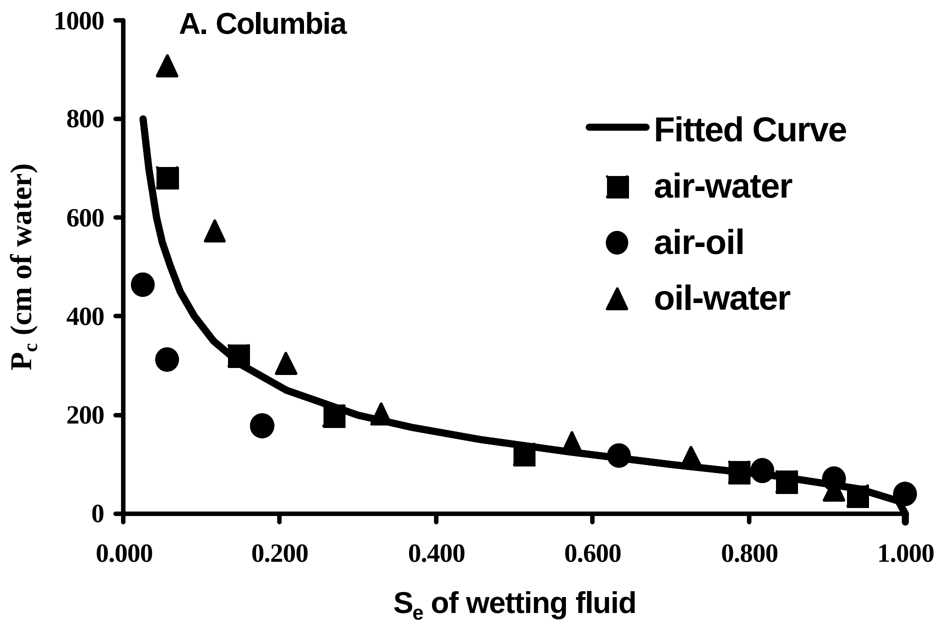
Thus, the wetting fluid pressure at the soil-plate interface was estimated from the effective permeability (k_w) and thickness (d) of the saturated porous plate in combination with known measured values of the wetting fluid pressure at the bottom of the plate ($P_{w,bottom}$) and the measured drainage rate (q_w), after a pressure increment was applied. Although q_w is decreasing with time within one pressure step, we assumed a constant average flux for the small time interval used at the beginning of each pressure step. The effective permeability of the soil was subsequently estimated using Eq. [3-2] by solving for $k_w(S_e)$, after substituting the average drainage rate and the assumed P_w-gradient in the soil core using the measured wetting fluid pressures in the center of the core and $P_{w,top}$. The estimation of the average wetting fluid pressure gradient in the soil sample is based on a linear distribution of wetting fluid pressure in the bottom half of the soil core. While this assumption appears to hold for the finer-textured Columbia soil (Eching et al., 1994), it may not be satisfactory for the larger applied non-wetting fluid pressures in the coarser-textured Lincoln soil. Possible errors caused by the constant gradient assumption can be largely reduced by placing the wetting-fluid tensiometer nearer to the outflow end of the soil sample, thereby providing a more accurate wetting-fluid pressure gradient representative for the measured drainage rate. Moreover, the need for a separate calculation of the wetting-fluid pressure at the soil-plate interface is eliminated if the thick porous ceramic plate is replaced by a thin nylon porous membrane with a non-wetting fluid entry pressure large enough for the intended capillary pressure range. The low resistance nylon membrane[3] (Table 3-2) causes only minor differences in wetting fluid pressure across the membrane, and is now routinely used in outflow experiments.

Finally, the intrinsic permeability was estimated using the pore-size distribution model of Mualem (1976) to predict the permeability-saturation function (Eq. 2-11b). The scaled capillary pressure (Fig. 3-6) and estimated permeability data were fitted to the combined van Genuchten-Mualem model using the same Excel spreadsheet program used for fitting capillary pressure-saturation data. As in the estimation of the capillary pressure-saturation curve, average saturation was obtained from cumulative outflow and initial saturation data. The fitting parameter values of θ_r, α, n, and k (Table 3-2) together describe the capillary pressure and permeability functions for all three fluid pairs, and characterize the pore structure and pore-size distribution of both soils. The fitted curves in Figures 3-6 (scaled capillary pressure-saturation) and Figure 3-7 (permeability functions) were obtained using an l-value of 0.5 and m-values of m=1-1/n. The plotted relative permeability data for the three fluid pairs were computed using the fitted intrinsic permeability values. As is shown in Figure 3-7, the $k_r(S_e)$ estimates for the three fluid-pair combinations for both soils are well described by a single relationship, thereby indicating that the relative permeability is independent of the fluids present being a function of the porous medium properties only.

Table 3-3. Thickness (d), Saturated Hydraulic Conductivity (Ks), Plate Resistance (Rp), and Air Entry Pressure for Various Porous Materials.

	t (cm)	$K_{s,water}$ (cm/hr)	R_p (hr)	Air-entry pressure
Ceramic	0.74	0.0498	14.86	1000
Plastic	0.05	0.0166	3.01	400
Stainless Steel	0.1	0.0265	3.77	250
Nylon	0.01	0.025	0.4	1700

3 MSI Inc, P.O. Box 1046, Westborough, MA 01581-6046



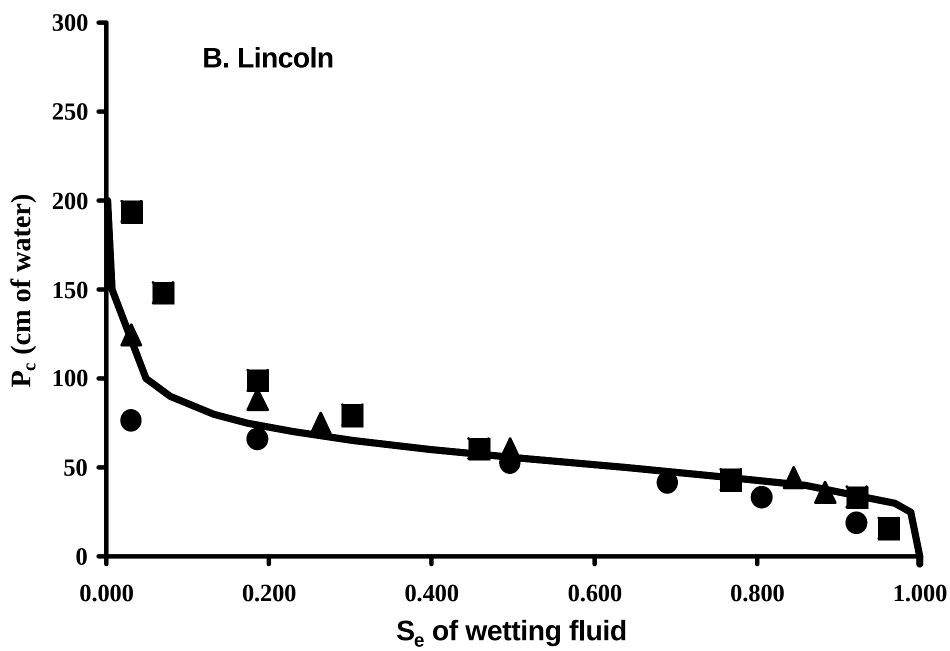
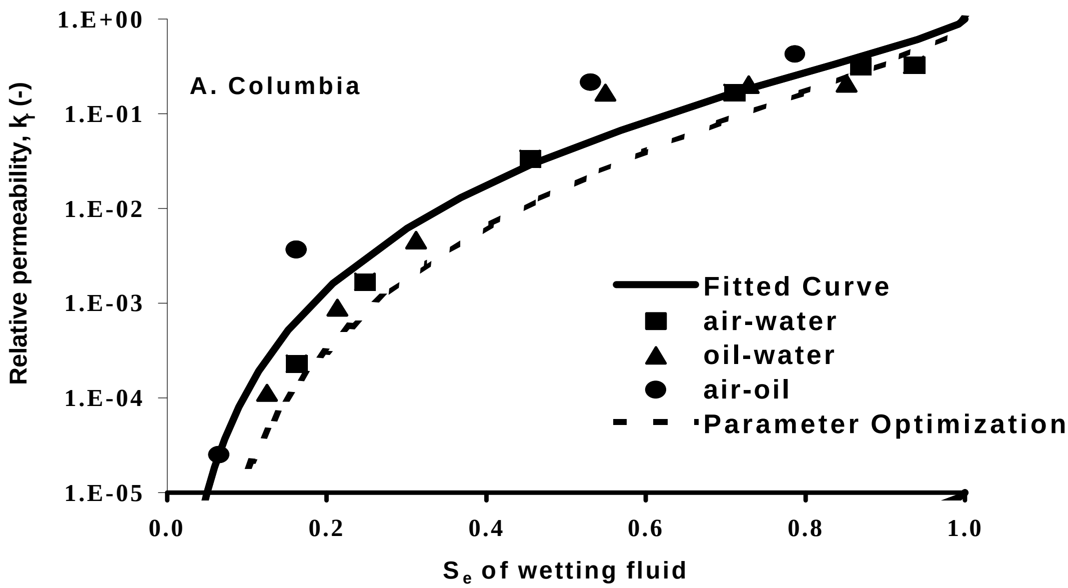


Figure 3-6. Scaled and fitted capillary pressure head versus effective saturation of wetting fluid for (A) Columbia and (B) Lincoln soil.



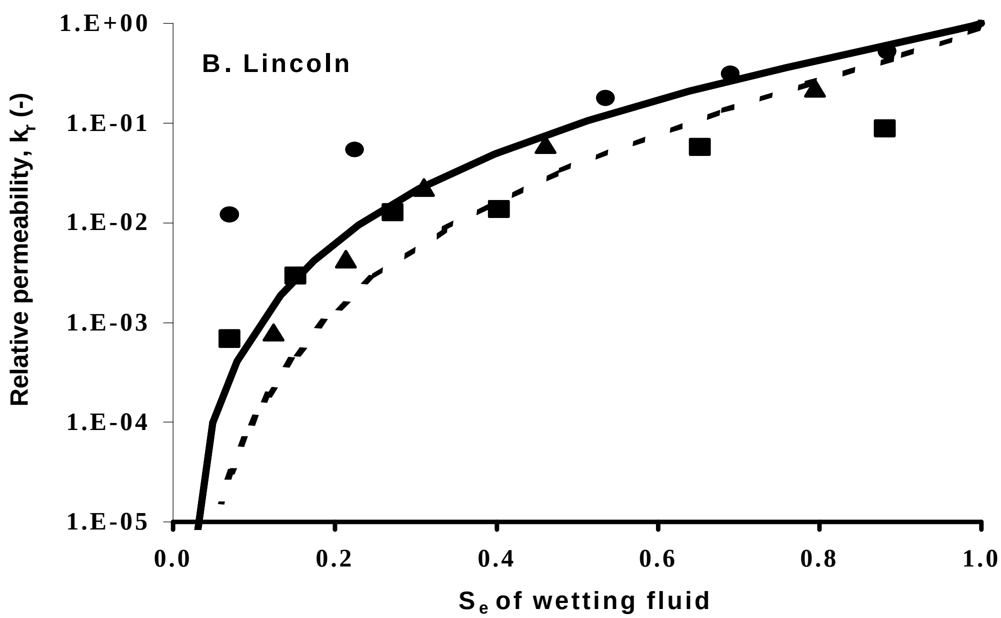


Figure 3-7. Measured relative permeability (symbols) with predicted (solid) and fitted (dashed) curves using parameters in Table 3-2.

Permeability functions were also estimated using a parameter optimization procedure (Eching et al., 1994) for the air-water systems of soil cores having identical bulk densities. In this approach, the capillary pressure and permeability functions were estimated indirectly by numerical solution of the water flow equation (Eq. [3-7] with water as the wetting fluid) for the imposed experimental boundary and initial conditions. Parameters for the capillary pressure and permeability functions (van Genuchten-Mualem model for air-water system) were optimized by minimization of an objective function containing the sum of squared deviations between the measured and simulated flow variables (capillary pressure and cumulative outflow). The resulting optimized relative permeability functions are included in Fig. 3-7. For both soils, the estimated permeability data for the air-water system matched the independently-estimated permeability functions using the parameter optimization approach quite well.

Parameter optimization

Using the described methodology, the inverse parameter estimation procedure was carried out for all 3 two-fluid (air-water, air-oil, and oil-water) flow systems of the Lincoln and Columbia soil. Figures 3-8 and 3-9 compare the measured (circles) and optimized (line) cumulative outflow Q(cm^3) and capillary pressure head ($h_c = P_c / \rho_{H2O} g$ cm equivalent head of water), for the air-water (aw), air-oil (as), and oil-water (ow) systems of the Lincoln (Figure 3-8) and Columbia (Figure 3-9) soils. Overall, the optimized simulations show an excellent match with the corresponding measurements, indicating that the optimized parameters captured the main features of the measured flow procedure.

The RMSSR values (Eq. 2-20), the optimization iteration numbers, with respect to the different initial parameter (IP) values, are listed in Tables 3-4 and 3-5 for each two-fluid flow system for the Lincoln and Columbia soil, respectively. The initial parameters were chosen to cover a relatively broad range of soils, especially for the most sensitive parameters α and n. The choice of the final selected parameters was based on two considerations: (1) selection of the parameter set with minimum RMSSR value, or (2) selection of the mean parameter set if there are several parameter sets with identical RMSSR values. The obtained capillary pressure - saturation and permeability - saturation curves, based on the optimized parameters are summarized in Table 3-6, and are shown in Figure 3-10 and Figure 3-11 for the Lincoln and Columbia soil, respectively. As described in Eq. 2-11a, the capillary pressure function is dependent on and n only, where is inversely proportional to the non-wetting-fluid entry value, and thus varies among fluids and as their corresponding interfacial tension values. The n-parameter is inversely proportional to the soil's pore-size distribution and determines the slope of the capillary pressure curve. Relative permeability functions (Eqs. 2-11b and 2-11c) are only dependent on n, if l is fixed to a value of 0.5.

Several important concerns are involved in the above results: the choice of the adjustable or optimizing parameters, the well-posedness of the relevant inverse problem, and the scaling relationship of the resulting inverse parameter estimation. In total, the parametric models of

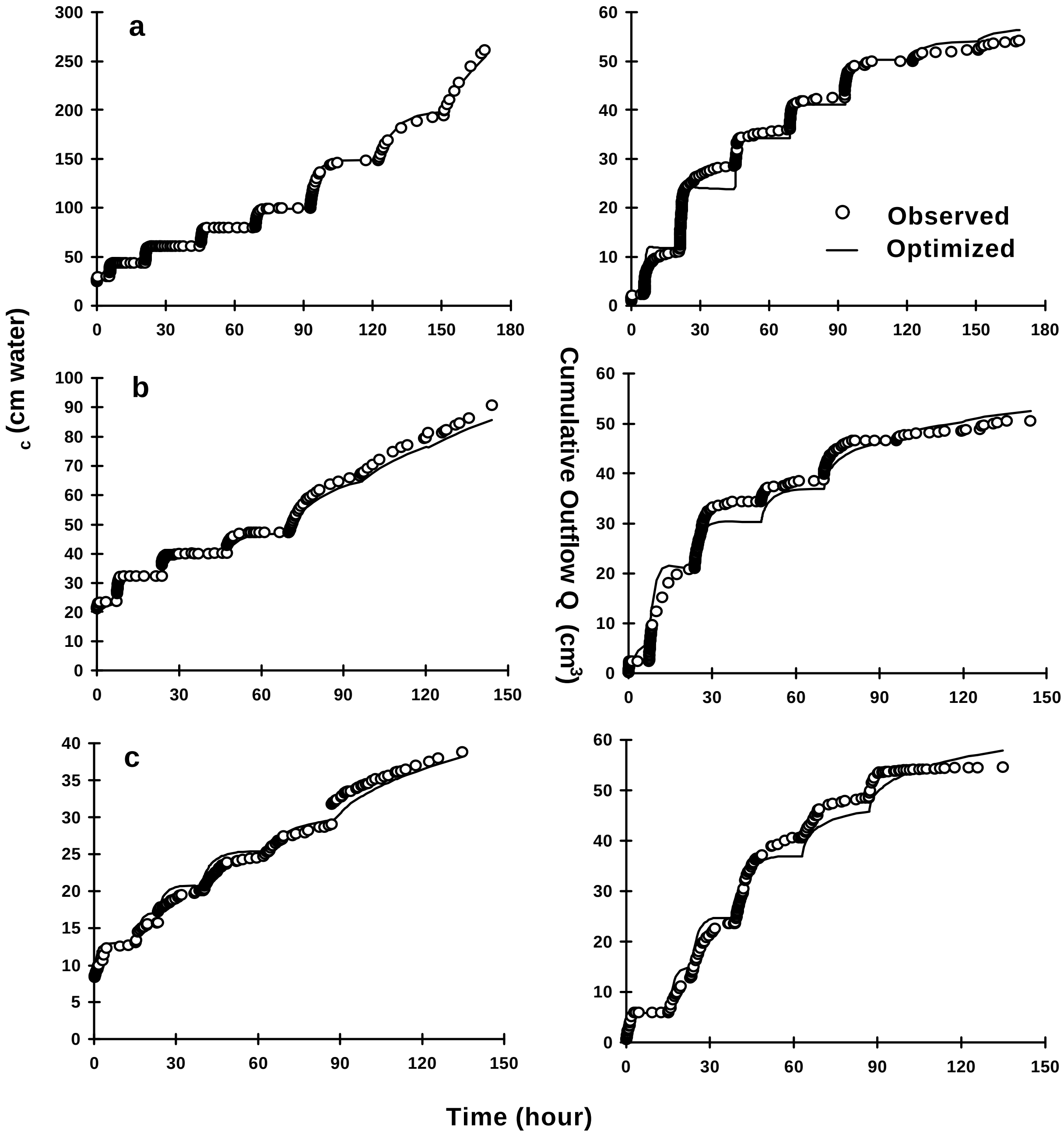


Figure 3-8. Comparison of the measured and optimized h_c and Q - values of Lincoln soil: (a) air-water system, (b) oil-water system, (c) air-oil system.

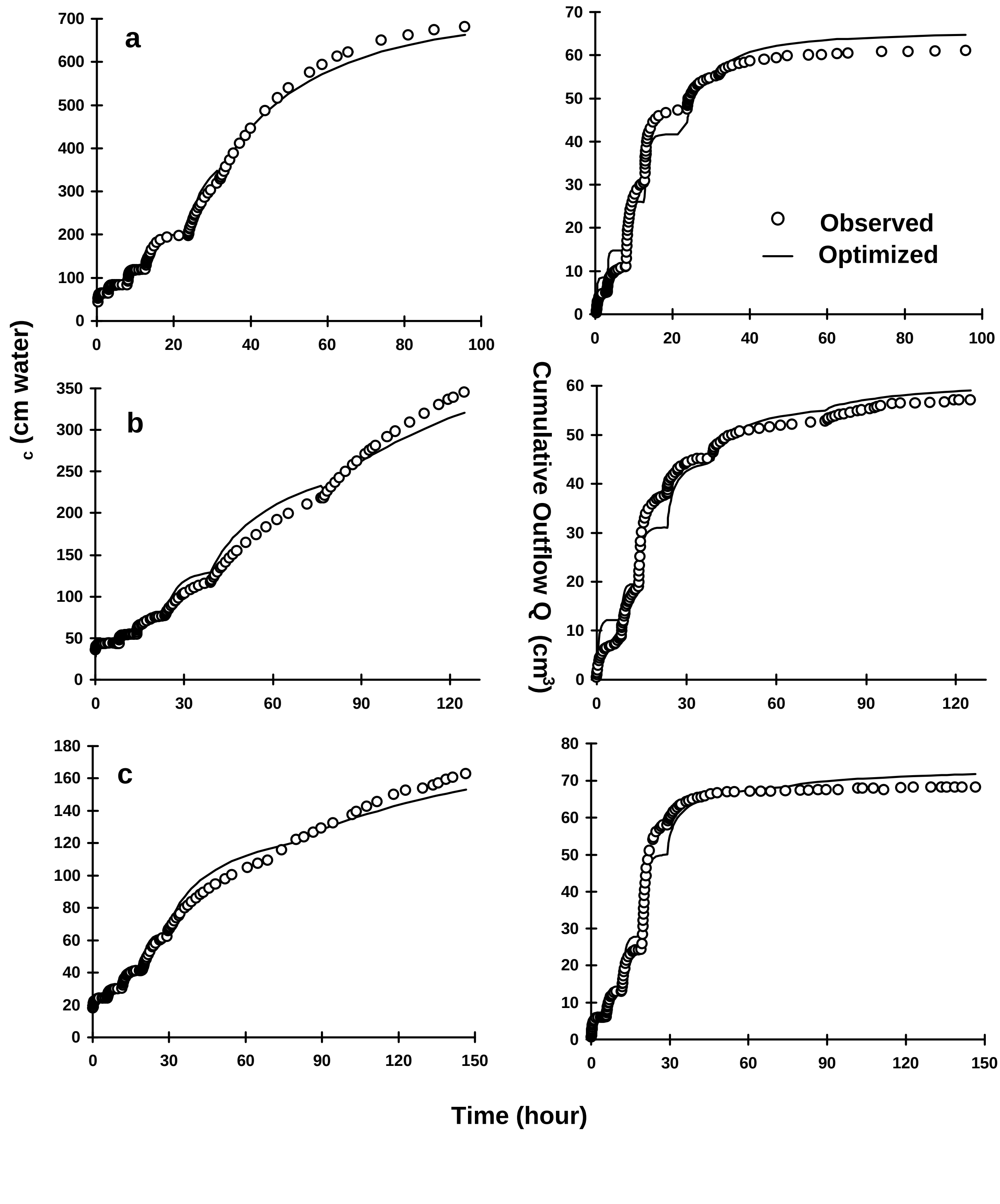


Figure 3-9. Comparison of the measured and optimized h_c and Q - values of Columbia soil: (a) air-water system, (b) oil-water system, (c) air-oil system.

Table 3-4. Optimized VG-Mualem Parameters of Lincoln Soil for Different Initial Estimates.

System	Set	Parameter	IP[1]	Iterations	RMSSR[2]	FP[3]	S_i[4]	CV_i[5](%)
Air-Water	1	θ_r(cm^3/cm^3)	0.11	8	1.656	0.0212	0.003	14.151
		k (10^{-9} cm^2)	5.08			24.8	0.708	7.9266
		α (cm^{-1})	0.04			0.0189	0.000	0.0000
		n (-)	2.00			2.8124	0.040	1.4223
	2	θ_r	0.05	7	1.656	0.0211	0.003	14.218
		k	2.00			24.7	0.706	7.9236
		α	0.02			0.0189	0.000	0.0000
		n	3 .00			2.8120	0.040	1.4225
	3	θ_r	0.05	12	1.656	0.0210	0.003	14.286
		k	8.00			24.7	0.704	7.9048
		α	0.05			0.0189	0.000	0.0000
		n	4 .00			2.8098	0.040	1.4236
Oil-Water	1	θ_r	0.11	10	2.663	1.11e-5	0.008	-*
		k	5.08			9.4	0.445	13.404
		α	0.04			0.0366	0.001	2.7322
		n	2.00			2.9472	0.079	2.6805
	2	θ_r	0.05	9	2.640	1.5E-7	0.008	-
		k	2.00			9.3	0.361	9.9730
		α	0.03			0.0365	0.001	2.7397
		n	1.80			2.9660	0.097	3.2704
	3	θ_r	0.10	7	2.640	0.0143	0.008	-
		k	4.00			9.0	0.488	16.267
		α	0.05			0.0350	0.001	2.8571
		n	4 .00			3.3070	0.082	2.4796
Air-Oil	1	θ_r	0.11	10	3.760	2.02e-5	0.011	-
		k	6.11			10.9	0.170	17.375
		α	0.04			0.0519	0.001	1.9268
		n	2.00			3.0590	0.080	2.6152
	2	θ_r	0.05	8	3.830	1.85e-5	0.011	-
		k	2.00			8.4	0.128	16.929
		α	0.02			0.0525	0.001	1.9048
		n	3 .00			3.0360	0.008	0.2635
	3	θ_r	0.01	12	3.760	3.2e-6	0.010	-
		k	10.00			11.3	0.211	17.653
		α	0.06			0.0538	0.001	1.8587
		n	4 .00			2.9450	0.071	2.4109

Fixed parameters: θ_s = 0.33 (cm^3/cm^3), m = 1-1/n, l = 0.5

[1] IP : Initial Parameter

[2] RMSSR : Root of Mean Sum Square Residual

[3] FP : Final Parameter obtained from the inverse parameter estimation

[4] S_i : Standard deviation of parameter b_i

[5] CV_i : Coefficient Variance of parameter b_i as defined by $CV_i = (S_i / FP_i)\cdot 100$

Table 3-5 Optimized VG-Mualem Parameters of Columbia Soil for Different Initial Estimates.

System	Set	Parameter	IP[1]	Iterations	RMSSR[2]	FP[3]	S_i[4]	CV_i[5](%)
	1	$\theta_r(cm^3/cm^3)$	0.11	12	2.919	0.0917	0.008	8.7241
		k (10^{-9} cm^2)	5.08			5.3	0.186	9.7546
		α (cm^{-1})	0.04			0.0099	0.000	0.0000
		n (-)	2.00			2.1474	0.049	2.2818
Air-Water	2	θ_r	0.05	8	2.919	0.0914	0.008	8.7527
		k	2.00			5.3	0.184	9.6689
		α	0.02			0.0099	0.000	0.0000
		n	3 .00			2.1447	0.049	2.2847
	3	θ_r	0.05	10	2.919	0.0912	0.008	8.7719
		k	4.00			5.2	0.184	9.6832
		α	0.05			0.0100	0.000	0.0000
		n	4 .00			2.1433	0.049	2.2862
	1	θ_r	0.11	6	3.155	0.0724	0.006	8.2873
		k	5.08			8.0	0.306	10.5765
		α	0.04			0.0239	0.000	0.0000
		n	2.00			2.0372	0.031	1.5217
Oil-Water	2	θ_r	0.10	5	3.155	0.0723	0.006	8.2988
		k	4.00			8.0	0.307	10.6243
		α	0.02			0.0239	0.000	0.0000
		n	1.20			2.0367	0.031	1.5221
	3	θ_r	0.01	8	3.155	0.0723	0.006	8.2988
		k	8.08			8.0	0.306	10.5996
		α	0.05			0.0239	0.000	0.0000
		n	4 .00			2.0368	0.031	1.5220
	1	θ_r	0.11	7	3.854	0.0612	0.006	9.8039
		k	5.08			6.2	0.172	10.4299
		α	0.04			0.0253	0.000	0.0000
		n	2.00			2.6939	0.048	1.7818
Air-Oil	2	θ_r	0.05	7	3.854	0.0613	0.006	9.7879
		k	2.00			6.2	0.172	10.4198
		α	0.02			0.0253	0.000	0.0000
		n	3 .00			2.6945	0.048	1.7814
	3	θ_r	0.05	5	3.949	0.0485	0.004	8.2474
		k	7.00			5.6	0.037	2.9152
		α	0.05			0.0248	0.000	0.0000
		n	4 .00			2.6175	0.038	1.4518

Fixed parameters: θ_s = 0.45 (cm^3/cm^3), m = 1-1/n, l = 0.5

[1] IP : Initial Parameter

[2] RMSSR : Root of Mean Sum Square Residual

[3] FP : Final Parameter obtained from the inverse parameter estimation

[4] S_i : Standard deviation of parameter b_i

[5] CV_i : Coefficient Variance of parameter b_i as defined by $CV_i = (S_i / FP_i)\cdot 100$

Table 3-6. Optimized VG-Mualem Parameters of Lincoln and Columbia Soil.

Soil \ Term	Parameter	Air-Water	Oil-Water	Air-Oil
Lincoln	θ_r (cm^3/cm^3) k (10^{-9} cm^2) α (cm^{-1}) n (-)	0.0210 24.8 0.0189 2.8111	0.0072 9.4 0.0358 3.1365	0.00001 10.9 0.0529 3.002
Columbia	θ_r k α n	0.0913 5.3 0.0100 2.1451	0.0723 8.0 0.0239 2.0369	0.0613 6.2 0.0253 2.6942

Eq. (2-11) requires seven parameters (θ_s, θ_r, k, α, n, m, l). The choice of how many and which parameters to optimize was based on a number of considerations. First, it must be recognized that as the number of optimized parameters increases, the parameter estimation procedure will generally lead to better matching of optimized with measured flow variables. However, this occurs at the expense of the uniqueness of the optimized solution and a corresponding increase in the uncertainty of the parameter estimates. Thus, it is preferred to minimize the total number of free parameters. If any of the parameters can be measured independently with relatively high accuracy, it should be fixed rather than optimized. This is certainly the case for the saturated wetting-fluid content (θ_s), which was obtained experimentally for each soil core from cumulative outflow, initial fluid saturation and oven drying of the soil core. Also, the intrinsic permeability (k) can be used as a fixed parameter in the parameter optimization procedure. However, fixing its value appears to overly constrain the permeability relationship, allowing it to be a function of n (or) m only. Moreover, differences in pore geometry between the larger pores (defining soil structure) and soil matrix pores (defined by soil texture) preclude the use of relationships (2-11b and c) across the whole saturation range, using a physically-based intrinsic permeability value as measured from a saturated soil (Demond and Roberts, 1993). Thus, the largest soil pores (macropores) are not viewed as being predictive of the hydraulic properties of the bulk soil matrix. Following Mualem (1976), we also reduced the number of optimized parameters by setting $l = 0.5$ in the permeability function (2-11b and c) for both the wetting and non-wetting fluids. Finally, we used the relationship between n and m to reduce the number of optimized parameters further. As determined by Toorman et al. (1992), this final set of four free parameters is sensitive to the experimental conditions of the multi-step outflow experiment, when cumulative outflow measurements are supplemented with capillary pressure measurements. Also

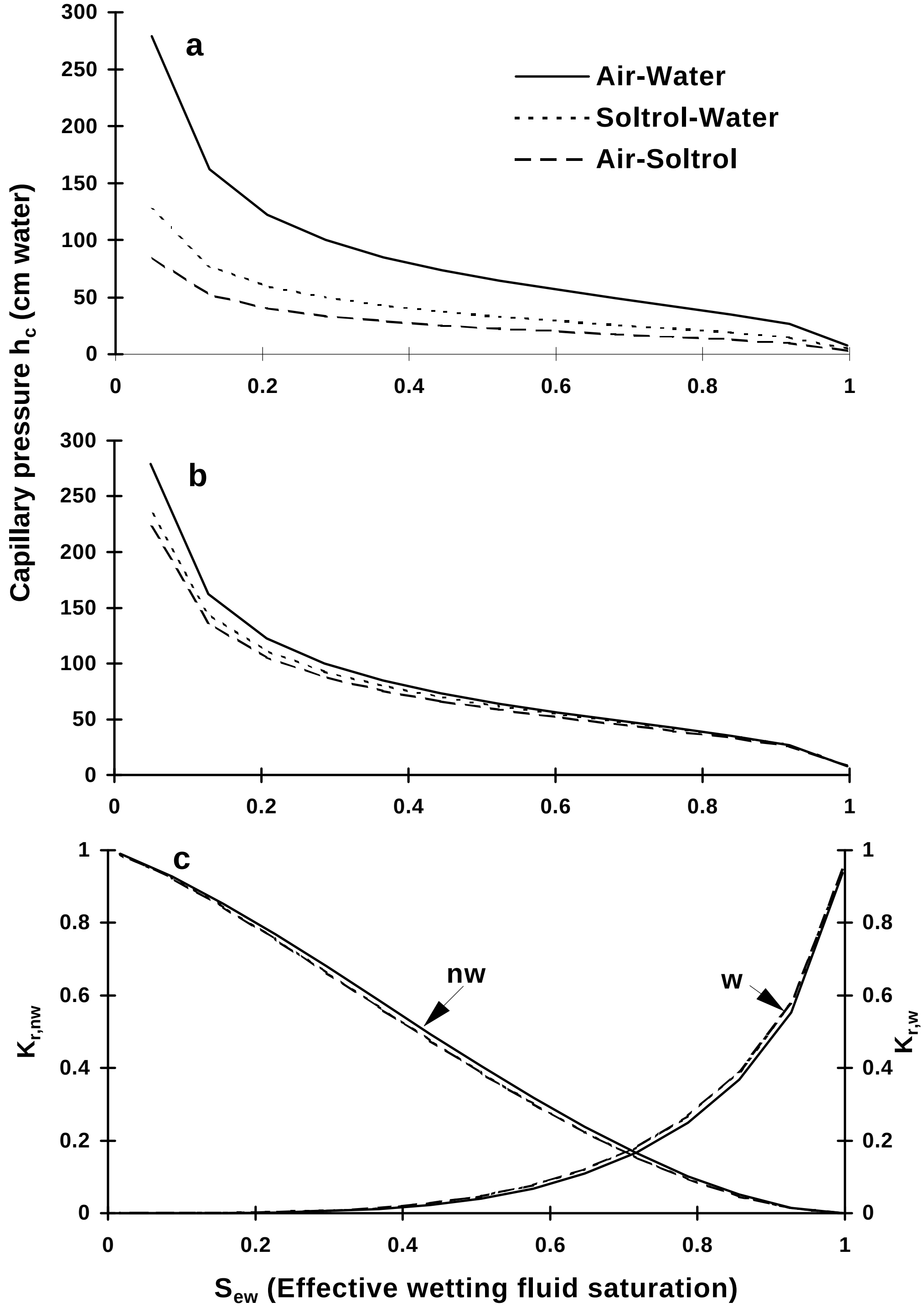


Figure 3-10. Optimized constitutive functions of Lincoln soil corresponding to the parameter listed in Table 2.2: (a) Individual capillary pressure functions, (b) Scaled capillary pressure functions, (c) Relative permeability functions.

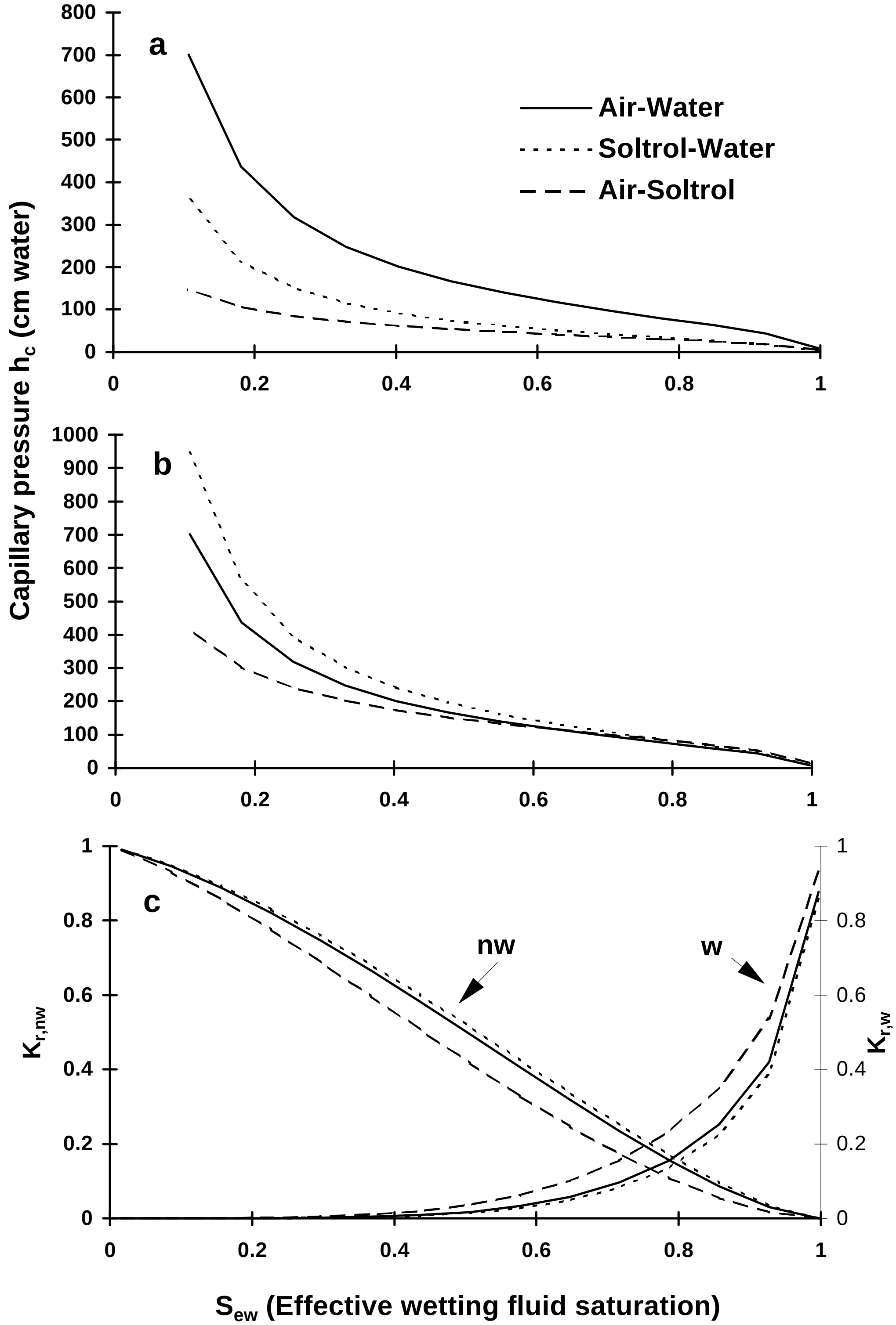


Figure 3-11. Optimized constitutive functions of Columbia soil corresponding to the parameter listed in Table 2.2: (a) Individual capillary pressure functions, (b) Scaled capillary pressure functions, (c) Relative permeability functions.

Finsterle and Pruess (1995) showed that k, α, and n are the most sensitive parameters in two-fluid flow modeling. In Tables 3-4 and 3-5, the terms S_i and CV_i are the standard deviation and coefficient variance of the parameter b_i, which were used to measure the estimation accuracy as well as the sensitivity of parameter b_i in the inverse parameter estimation. Of the four adjustable VG-M parameters (θ_r, k, α and n), α and n are the most sensitive and accurate parameters.

The optimization results were obtained by imposing constraints on the allowable ranges of the adjustable parameters. These ranges were set to allow the maximum possible flexibility of the parameter values, yet limit them so that their values remain to have physical meaning. The limitation on determining a global feasible region stems from the intrinsic limitation of global nonlinear optimization theory. The determination of the feasible range for each optimized parameter is done a priori by a trial-error procedure.

The well-posedness analysis of the inverse parameter estimations was performed by carrying out the optimizations for different initial parameter estimations for each of the two-fluid flow systems. According to Russo et al. (1991), the evaluation of the well-posedness of an inverse problem can be obtained by solving the problem several times with different initial parameter estimates. The restriction on a priori evaluation of the posedness of an inversion problem stems from the fact that it is generally impossible to examine whether the converged solution corresponds to global minimum of the objective function. The final parameters in Tables 3-5 and 3-6, obtained from the optimizations started at different initial parameter estimates, to test the uniqueness of the solution. The choice of the initial parameter estimations was based on the consideration to cover the largest feasible range of the adjustable parameters, especially for the most sensitive parameters (α and n) of the constitutive function models. The tests show that the feasible initial parameter estimates were more limited for the single-fluid case, indicating a higher constraint on the two-fluid flow constitutive relationships than for single fluid flow. The low estimation errors (RMSSR values) also indicated an acceptable fit of the data, considering that the minimum value of the RMSSR is 1.0, if the objective function is a WLS problem. Consequently, we conclude that the presented two-fluid flow inverse parameter estimation of a transient multi-step outflow experiment is well-posed.

For the Leverett assumption to apply to each of the two-fluid flow systems, the n-value for the three fluid pairs should be identical for each soil, since it is determined by soil pore geometry only. The permeability functions in Figures 3-10c and 3-11c, which are dependent only on the n-values, show indeed that they are similar for the three two-fluid flow systems. Furthermore, scaling requires that the α-values be inversely proportional to the interfacial tension values. Indeed, we found that the ratios of interfacial tension values (Table 2-2) were quite similar to the α-ratios from scaling (Table 3-7).

Table 3.7 Comparison of α Ratio and Interfacial-Tension Ratio.

Lincoln Soil Systems		**Columbia Soil Systems**	
σ-Ratio	**α-Ratio**	**σ-Ratio**	**α-Ratio**
$\sigma_{ao}/\sigma_{aw} = 0.380$	$\alpha_{aw}/\alpha_{ao} = 0.373$	$\sigma_{ao}/\sigma_{aw} = 0.351$	$\alpha_{aw}/\alpha_{ao} = 0.400$
$\sigma_{ow}/\sigma_{aw} = 0.534$	$\alpha_{aw}/\alpha_{ow} = 0.514$	$\sigma_{ow}/\sigma_{aw} = 0.380$	$\alpha_{aw}/\alpha_{ow} = 0.417$

To further examine the scaling relationships between the two-fluid flow systems of the same soil, we included the scaled capillary pressure functions in Figure 3-10b (Lincoln) and 3-11b (Columbia), using the capillary pressure curve of the air-water system as a reference. The scaling factor was simply determined from the corresponded interfacial tensions by using the dimensionless Leverett's function (2-23):

$$\hat{h}_{c,aw}(S_{ew})|_1 = \left(\frac{\sigma_{aw}}{\sigma_{aw}}\right) \cdot h_{c,aw}(S_{ew}) = h_{c,aw}(S_{ew}) \qquad \text{(3-9a)}$$

$$\hat{h}_{c,aw}(S_{ew})|_2 = \left(\frac{\sigma_{aw}}{\sigma_{ao}}\right) \cdot h_{c,ao}(S_{ew}) \qquad \text{(3-9b)}$$

$$\hat{h}_{c,aw}(S_{ew})|_3 = \left(\frac{\sigma_{aw}}{\sigma_{ow}}\right) \cdot h_{c,ow}(S_{ew}) \qquad \text{(3-9c)}$$

The subscripts i = 1, 2, and 3 denote the scaled air-water curves $\hat{h}_{c,aw}(S_{ew})|_i$, obtained from the optimized air-water, air-oil and oil-water curves, respectively. The scaled curves coalesce well in the high saturation range. The deviations in the low saturation ranges coincide with the findings of Demond and Roberts (1991), who indicated that deviations might be caused by limitations of the traditional Leverett's (1941) scaling function. Demond and Roberts (1991) included other measurements such as intrinsic contact angle and roughness to correct the scaling factor, thereby improving the match at the low saturation range. Nevertheless, the close agreement between our scaling ratios with the interfacial tension ratios attests to the accuracy of the parameter optimization method.

Chapter 4
Conclusions

Multi-step outflow experiments have been successfully used for indirect estimation of capillary pressure and permeability functions for air-water systems. Here, we extend the application of the multi-step method to two-fluid phase systems in general, and present results for air-water, air-Soltrol and Soltrol-water systems in a Columbia fine sandy loam and Lincoln sandy loam for direct estimation. Subsequently, the experimental data were used in a parameter optimization algorithm using an inverse technique, thereby providing an indirect method for estimating capillary pressure and permeability functions. Because of the transient nature of the multi-step outflow experiments, capillary pressure and permeability functions can be obtained much faster than by conventional equilibrium methods. This aspect is especially useful when several capillary pressure and permeability functions are needed to characterize heterogeneous contaminated sites with large soil spatial variability.

When the experimental capillary pressure-drainage data for the three two-fluid systems are compared, the interfacial tension of each fluid pair is important because the capillary pressure value at a given degree of saturation decreases with decreasing interfacial tension. Therefore, non-wetting fluid pressure increments for each fluid pair were based on the ratio of the interfacial tension relative to that of air-water, so as to obtain approximately equal amounts of wetting fluid drainage for each fluid pair combination. The oil-water experiments showed that the oil pressure remained constant within a pressure increment and was equal to the applied oil pressure, adjusted for its hydrostatic pressure in the soil core. We therefore conclude from the presented data that a single-fluid flow model is sufficient for the description of water flow in multi-step outflow experiments with oil present as a non-wetting fluid.

Using the multi-step outflow method, capillary pressure-saturation and permeability functions are directly estimated from the experimental data; i.e, from capillary pressure measured in the draining soil core and from cumulative drainage of the wetting fluid. The accuracy of the directly measured capillary pressure functions was determined from the success by which interfacial tension ratio values coalesced individual capillary pressure-saturation curves to a single curve. Assuming that the scaling factor is only dependent on the interfacial tension of each fluid pair, scaled capillary pressure-saturation curves were in good agreement with the modified Leverett's scaling relationship, especially at high saturation values, though some discrepancies occurred at low wetting-fluid saturations. The combined relative permeability data of both soils coalesced to a single van Genuchten-Mualem permeability function, thus confirming their independence of the fluids present in the porous medium. It appears that the employed assumptions with regard to the wetting-fluid pressure gradient in the draining soil core could be largely removed by inserting the wetting-fluid tensiometer nearer to the outflow end of the soil core and by replacing the ceramic porous plate with a thin, nylon porous membrane.

This study also demonstrated the feasibility of using the inverse parameter estimation for two-fluid flow systems. Using the proposed indirect approach the governing flow equations for both the wetting and non-wetting fluid are solved, so that no assumptions are needed with regard to the influence of the non-wetting fluid on outflow or wetting fluid pressure gradients. Even though it is impossible to remove the inherent uncertainty that stems from the high nonlinearity and complexity of soil systems, the posteriori analysis of the presented inversion problem indicates that the inverse parameter estimation of the constitutive functions from transient multi-step outflow experiments of a two-fluid soil system is a well-posed problem. Of the four adjustable VG-M parameters θ_r, k, α and n, the parameters α and n are the most sensitive for the inverse parameter estimation approach. The selection of proper initial parameter estimate has been shown to be important for successful optimization. The comparison of the results with those from using the Leverett scaling method provided a means to test the presented solutions. The advantage of the proposed method is (1) that the measurements are simple and accurate, (2) simultaneous estimation of capillary pressure and permeability functions are obtained from a single sample, and (3) parameter estimation using a flow simulator is consistent with computer modeling flow simulations.

Appendix A.
Optimization Algorithm

Levenberg-Marquardt Method

Generally, a solution algorithm searches the solution for the objective function:

$$\mathrm{O}(\mathbf{b}) = \mathbf{e}^{\mathrm{T}}\mathbf{V}^{-1}\mathbf{e} = \mathbf{e}^{\mathrm{T}}\mathbf{W}\mathbf{e} \qquad \text{(A-1)}$$

where, $\mathrm{O}(\mathbf{b})$ denotes the objective function, $\mathbf{e} = \mathbf{v}_m - \mathbf{v}_s$ is the observation error vector with $\mathbf{v}_m$ and $\mathbf{v}_s$ denoting the measured and simulated variables, and $\mathbf{W} = \mathbf{V}^{-1}$ is the weighting matrix, with $\mathbf{V}$ the covariance matrix of the error $\mathbf{e}$ defined by $\mathbf{V} = \mathrm{E}(\mathbf{v}_m - \mathbf{v}_s)(\mathbf{v}_m - \mathbf{v}_s)^{\mathrm{T}}$. The Levenberg-Marquardt (LM) method has become a standard solution algorithm for nonlinear least-squares problems. Basically, the LM method is a Newton-type minimization method in which the objective function is locally approximated to a quadratic form (Press et al., 1992):

$$\mathrm{O}(\mathbf{b}) = \mathrm{O}(\mathbf{b_i}) + (\mathbf{b} - \mathbf{b_i}) \cdot \nabla\mathrm{O}(\mathbf{b_i}) + \frac{1}{2}(\mathbf{b} - \mathbf{b_i}) \cdot \mathbf{H} \cdot (\mathbf{b} - \mathbf{b_i}) \qquad \text{(A-2)}$$

or

$$\nabla\mathrm{O}(\mathbf{b}) = \nabla\mathrm{O}(\mathbf{b_i}) + \mathbf{H} \cdot (\mathbf{b} - \mathbf{b_i}) \qquad \text{(A-3)}$$

where, $\mathbf{H}$ is the Hessian matrix, the second derivative of objective function $\mathrm{O}(\mathbf{b})$, with $\mathbf{H}_{ij} = \dfrac{\partial^2 \mathrm{O}}{\partial \mathbf{b_i} \partial \mathbf{b_j}}$. In Newton's method, we set the left-hand side of (A-3) equal to zero in order to determine the next iteration point, or:

$$\mathbf{H} \cdot D\mathbf{b} = -\nabla\mathrm{O}(\mathbf{b}_i) \qquad \text{(A-4)}$$

with

$$\mathbf{b}^{i+1} = \mathbf{b}^{i} + D\mathbf{b} \qquad \text{(A-5)}$$

Substitution of (A-1) into (A-4) and defining $\nabla\mathbf{e} = \mathbf{J}$ (Jacobian or sensitivity matrix), with $J_{ij} = \partial e_i / \partial b_j$, one obtains:

$$\mathbf{H} \cdot D\mathbf{b} = -\mathbf{J}^{\mathrm{T}}\mathbf{W}\mathbf{e} \qquad \text{(A-6)}$$

Since the Hessian matrix is difficult to calculate, one uses a Hessian approximation $\mathbf{H} = \mathbf{J}^{T}\mathbf{W}\mathbf{J}$ (Kool and Parker, 1988) in (A-6) to yield the Gauss-Newton algorithm:

$$\mathbf{J}^{\mathrm{T}}\mathbf{W}\mathbf{J} \cdot D\mathbf{b} = -\mathbf{J}^{\mathrm{T}}\mathbf{W}\mathbf{e} \qquad \text{(A-7)}$$

By inspection of (A4), for the optimization to proceed in a descending direction, **H** or its approximation $\mathbf{J}^T\mathbf{WJ}$ must be positive-definite. This is ensured in the Levenberg-Marquardt algorithm by adding a positive quantity to $\mathbf{J}^T\mathbf{WJ}$**:**

$$(\mathbf{J}^T\mathbf{WJ} + \lambda\mathbf{D}^T\mathbf{D})D\mathbf{b} = -\mathbf{J}^T\mathbf{We} \qquad \text{(A-8)}$$

where λ is a positive scalar or Levenberg parameter, and D is a diagonal scaling matrix with elements equal to the norms of the corresponding columns of J (More,1977). Marquardt (1963) developed an effective strategy to update λ. When far from the minimum, λ is given a large value, yielding a step in the steepest descent direction, whereas, when approaching the optimum, λ is given a small value, so that (A-8) converges to a Gauss-Newton step.

The parameter optimization problem formulated by the objective function (A-1) and solved by the iteration solution (A-8) is referred to as unconstrained optimization. Usually, there are physical and mathematics constraints for the estimated parameters. With the added parameter bounds, the corresponding optimization is therefore referred to as bounded optimization. When the parameters are outside the constrains, they will be forced back to the bounded region. Kool and Parker (1988) reported on a bounded iteration strategy.

Convergence and Reliability

The iteration solution of optimization (A-8) is terminated by convergence criteria. The commonly used stopping criteria include two types of tests. The first one is based on the magnitude of the RMSSR as defined by:

$$\text{RMSSR} = \sqrt{\frac{\text{O}(\mathbf{b})}{\text{M}+\text{N}+\text{L}}} \qquad \text{(A-9)}$$

$$D\text{RMSSR} \le \tau_1 \quad \text{or} \quad \frac{D\text{RMSSR}}{\text{RMSSR}+\varepsilon_a} \le \tau_1' \qquad \text{(A-10)}$$

whereas the second criterion was the relative change in parameter values:

$$D\mathbf{b}^i \le \tau_2 \quad \text{or} \quad \frac{D\text{b}_i}{|\mathbf{b}_i| + \varepsilon_b} \le \tau_2 \qquad \text{(A-11)}$$

where ε_a and ε_b are small values ensuring that the denominators are not equal to zero, τ_1, τ_1' and τ_2 are convergence accuracy tolerances. Usually, the second criterion (A-11) is tested after the first criterion (A-10) is satisfied. Only using the second criterion (A-11) or meeting a small step $\Delta\mathbf{b}$ does not guarantee that the solution is at a minimum, since a large value for λ will also produce a very small step $\Delta\mathbf{b}$. The accuracy tolerance τ_1' is equal to 0 in order for the RMSSR to change toward to the decrease direction. The accuracy tolerance τ_2 is often problem dependent and is a compromise between estimation accuracy and computational expense. For example, when the level of uncertainty in input data is increased, objective function has flat minimum, the parameters will tend to wander around near the minimum. In that case, the smaller convergence criterion has little effect on estimation accuracy, but leads to additional iterations, thereby significantly increasing computational expense. An accuracy tolerance $\tau_2 = 0.01$ is chosen in our study.

The uncertainty measurement of the estimated parameters is expressed by their confidence region, which is derived from linear regression analysis under the assumption of normality and linearity. The normality assumption is that the distribution of a sum of random variables always tends towards normal if the sample size is sufficiently large. The implication is that the measurement errors are dependent on a linear combination of a large number of small random factors. The linearity assumption is that nonlinear functions of parameters **b** can be approximated by a linearization within the confidence region. For a maximum likelihood estimator, the parameter covariance matrix is asymptotically given by :

$$\hat{\mathbf{C}} = s_o^{\ 2}\mathbf{H}(\hat{\mathbf{b}})^{-1} \qquad \text{(A-12)}$$

or under Hessian approximation of $\mathbf{H} = \mathbf{J}^T\mathbf{W}\mathbf{J}$, get:

$$\hat{\mathbf{C}} = s_o^{\ 2}(\mathbf{J}^{\mathrm{T}}\mathbf{W}\mathbf{J})^{-1} \qquad \text{(A-13)}$$

with

$$s_o^{\ 2} = \frac{\mathbf{e}^{\mathrm{T}}\mathbf{W}\mathbf{e}}{n-m} \qquad \text{(A-14)}$$

where, the circumflex indicates a posterior value, n is the total number of observations, m is the number of parameters to be estimated, and s_o^2 is the estimated residual variance at the optimum. Consequently, the standard deviation s_i of the parameter b_i and the confidence region can be described by (Kool and Parker, 1988):

$$s_i = \sqrt{C_{ii}} \qquad \text{(A-15)}$$

$$\Pr(\hat{\mathbf{b}}_i - tC_{ii}^{\frac{1}{2}} \le \mathbf{b}_i \le \hat{\mathbf{b}}_i + tC_{ii}^{\frac{1}{2}}) = 1-\alpha \qquad \text{(A-16)}$$

where, α is the probability that hypothesis is rejected even though it is true, C_{ii} is the parameter variance, $t = t_{v,1\text{-}0.5\alpha}$ is the value of Student's t-distribution for confident level 1-α and v-degrees of freedom. For example, with a 95% confidence level, the boundaries of the confidence region are:

$$b_{i,min} = b_{i,opt} - t_{v,0.975}\, s_i \qquad \text{(A-17)}$$

$$b_{i,max} = b_{i,opt} + t_{v,0.975}\, s_i \qquad \text{(A-18)}$$

where $b_{i,opt}$ is the optimized value of the parameter b_i.

Appendix B
Description of Two-fluid Flow Model (TF-OPT)

Introduction

What is TF-OPT and *when* is it useful?

TF-OPT is a software specifically developed for estimation of the constitutive functions (capillary pressure and permeability) of two-fluid flow in a soil core from multi-step outflow experiments. TF-OPT consists of two parts: a one-dimensional two-fluid flow model with a finite element scheme and an optimization algorithm using Levenberg-Marquardt (LM) method.

Which steps are needed for using TF-OPT?

- Install TF-OPT: TF-OPT is written in FORTRAN and has been run on PC-compatibles and UNIX environments. The software can be downloaded via anonymous FTP from **theis.ucdavis.edu** (128.120.37.3) by using the user's E-mail address as password. It is located in the directory /pub/out/tf-opt. The files in tf-opt/ are:

README	Explanation file
example.in	Example input file
example.out	Example output file
TF-OPT.for	TF-OPT FORTRAN code file
tfcombk.dat	Include file of TF-OPT

- Prepare input file:

The efforts have been made to make the input file user-friendly and self-explainable. However, the setup of the system conditions (IC and BC and choice of finite element nodes), appropriate selection of the parametric model of capillary pressure and permeability functions, choice of initial parameter estimates and parameter limits are determined by user.

- Search for successful optimization solution:

"*As well been known, it is generally more difficult to find solutions to nonlinear optimization problems than to linear ones.* ***For difficult nonlinear problems, users usually have to pay much more attention to apparently inconsequential details than they would like****."*

— GAMS Release 2.25

It has been demonstrated that the inverse parameter estimation of the multi-step outflow experiment of soil column is a `well-posed' problem. After preparing the input file, changes might be needed. For example, you may need to change the parameter-limits, or initial parameter estimates, or adjust the data-type weighting factors. A proper choice of the parametric model for the capillary pressure and permeability function is also needed to obtain a successful solution.

Example

A-2-1 Input file

```
--------   INPUT FILE  --------
--------   PART I:   MODELING DATA
--- Total-Nodes Plate-nodes Obs-node Soil-L Plate-L Core-Dia. (L in cm)
--- (Plate-node and Plate-L is set as 0 if a thickless membrane is used)
       60          6         33      7.64       0.74     6.
--- Ceramic-Plate Hydraulic-Property (any value for a thickless membrane)
--- Theta-s         Ks
      0.506    0.0477
--- Fluid Property:
--- RhoW RhoNW MuW MuNW (Rho:density in g/cm3; Mu:viscosity in dyn.s/cm2)
    1.   0.       1.E-2    1.81E-4
--- Tmax(hr)   DTmax   IDT(=1,CONST.DT)   INIDT    Err
     170.      5.         1            0.1     0.1
--- IEQ (1-VGM, 2-VGB, 3-BCM, 4-BCB, 5-BRB, 6-GDM, 7-LNM)
     1
--- MODE (1:TF_Simu., 2:TF_opti.; -1:ESF_Simu., -2:ESF_Opti.):
--- (TF-two_fluid flow; ESF-Equivalent single_fluid flow)
 2
--- hnw0 (Initial NW total head at top), HB0 (Initial outflow height)
20.6      0.
--- Step number of Multi-step pressure: ITIM
 8
--- B.C. :  time(hr),applied pressure (pb(i),i=1,itim,in cm water)
  0.0     25.5
  5.67    40.8
  21.25   61.2
  45.3    81.6
  69.05    102.
  92.97    153.
  122.6    204.
  150.9    408.
--------- PART II:  OPTIMIZATION DATA
--- MAXTRY   MIT
     15    15
--- NTOB(Time Points), IPAR (Parameter Number),ITYP (Data-Type Number)
    229   8        3
--- Data-type weighting factor
--- IWHC   IWQ  IWTHETA
    1     1      30
--- PARAMETER NAMES
 THETAS(cm3/cm3)
 THETAR(cm3/cm3)
 INTRIK(cm2)
 ALPHA(-)
 N(-)
 M(-)
 L(-)
 NONE
--- PVALI(I),PMINI(I),PMAXI(I),IOPT(I),I=1,IPAR
--- (Initial estimate, Limits(MIN, MAX), Fixed:0/Free:1)
   0.32               0.25                  0.362          0
   0.11               0.000                 0.3            1
   0.000000014399     0.00000000141723      0.000000141723 1
   0.04               0.001                 0.5            1
   2.0                1.1                          10.     1
   1.                 1.                           1.      0
```

```
  0.5               1.                            1.     0
--- Observation data points:
--- Time(hr),  hc(cm), Q(cm3), HB(cm)
  1.                1.                            1.     0
      .0167    24.2000      .8300      .1500
      .0334    25.4400     1.1500      .2100
      .0500    26.1500     1.3400      .2400
      .0667    26.6000     1.5200      .2700
      .0834    27.0000     1.6600      .3000
      .1167    27.4900     1.8000      .3200
      .2667    28.4200     1.9800      .3600
      .5334    28.9600     2.0700      .3700
     4.1667    29.6200     2.2100      .4000
     5.4334    29.6200     2.3000      .4100
     5.6834    33.4500     2.5300      .4600
     5.7000    34.2500     2.6800      .4800
     5.7167    35.1800     2.9200      .5200
     5.7334    35.7600     3.1500      .5700
     5.7500    36.3800     3.3000      .5900
     5.7667    36.8700     3.4500      .6200
     5.7834    37.3600     3.6100      .6500
     5.8000    37.7600     3.8400      .6900
     5.8167    38.1600     3.9900      .7200
     5.8500    38.8300     4.2200      .7600
     5.8834    39.3200     4.5300      .8100
     5.9167    39.7600     4.6800      .8400
     5.9500    39.7600     4.9100      .8800
     5.9834    40.1600     5.1500      .9300
     6.0167    40.4800     5.3700      .9700
     6.0667    40.8300     5.6000     1.0100
     6.1500    41.3700     5.8300     1.0500
     6.2334    41.8100     6.0600     1.0900
     6.3000    41.9000     6.3000     1.1300
     6.3834    42.2100     6.5200     1.1700
     6.4834    42.4300     6.7500     1.2200
     6.6334    42.4800     6.9900     1.2600
     6.7500    42.7400     7.2200     1.3000
     6.9000    42.8800     7.4500     1.3400
     7.1167    42.9700     7.6000     1.3700
     7.3667    43.0600     7.9100     1.4200
     7.6500    43.2300     8.1400     1.4600
     7.9500    43.3200     8.3700     1.5100
     8.3334    43.3200     8.6000     1.5500
     8.7500    43.3200     8.8300     1.5900
     9.2667    43.3200     8.9900     1.6200
     9.6167    43.3200     9.2900     1.6700
    10.2500    43.3200     9.5200     1.7100
    11.3167    43.3200     9.7500     1.7500
    12.2667    43.3200     9.9000     1.7800
    12.7334    43.3200    10.2100     1.8400
    14.7167    43.3200    10.3600     1.8700
    16.2334    43.3200    10.5200     1.8900
    19.4167    43.3200    10.9000     1.9600
    20.6167    43.3200    10.9800     1.9800
    21.2667    43.3200    11.5000     2.0700
    21.2834    46.2000    11.8300     2.1300
    21.3000    47.4000    12.3300     2.2200
    21.3167    48.4200    12.6600     2.2800
    21.3334    49.2200    12.9900     2.3400
    21.3500    49.9800    13.3100     2.4000
    21.3667    50.1500    13.6400     2.4500
    21.3834    51.0900    13.9700     2.5100
    21.4000    51.6200    14.2200     2.5600
    21.4167    52.0700    14.4600     2.6000
    21.4334    52.5100    14.7100     2.6500

               ---------------------

    93.6334   112.7300    46.4900     8.3700
    93.7334   114.0700    46.7400     8.4100
    93.8500   115.6200    47.0800     8.4700
    93.9667   117.0000    47.2400     8.5000
```

94.3000	120.3400	47.7400	8.5900
94.6000	122.9600	47.9900	8.6400
95.0000	125.9900	48.2400	8.6800
94.1000	118.3400	47.4900	8.5500
95.6167	129.5900	48.4900	8.7300
96.7334	134.2600	48.8200	8.7900
97.2000	135.7700	48.9900	8.8200
101.5167	143.3800	49.1600	8.8500
102.3667	144.1300	49.4900	8.9100
102.7500	144.4900	49.6600	8.9400
104.7334	145.7400	50.0000	9.0000
117.1167	148.0000	50.0000	9.0000
122.5167	148.4000	50.0000	9.0000
122.6667	148.6100	50.2000	9.0400
122.8000	149.0600	50.3900	9.0700
123.0834	151.2800	50.5900	9.1100
123.4834	154.3000	50.7800	9.1400
124.2667	159.1500	51.0400	9.1900
124.7000	161.4200	51.1600	9.2100
125.4500	164.8900	51.2900	9.2300
126.4167	168.5800	51.5500	9.2800
132.5500	181.6100	51.6800	9.3000
139.2334	188.4200	51.9300	9.3500
146.0834	192.2000	52.2000	9.4000
150.9000	193.8900	52.2000	9.4000
151.1000	198.9500	52.4300	9.4400
151.2500	199.3800	52.5200	9.4500
152.6000	205.6400	52.8300	9.5100
153.5500	210.0800	53.0800	9.5500
155.5500	219.0700	53.3200	9.6000
157.7834	227.7900	53.5500	9.6400
162.8834	244.7900	53.8000	9.6800
167.5500	257.6900	53.9500	9.7100
168.9167	261.2000	54.2000	9.7600
16.0000	.3080		

Input file variable Description

Line	Variable	Description
5	NNP	Total finite element nodes
	IFNODE	Interfacial node between the soil core and ceramic plate (= 0 if a nylon membrane is used instead of a ceramic plate)
	IOBSNODE	Observation node
	SLENTH	Soil core length
	PLTLENTH	Ceramic plate thickness (= 0 for nylon membrane case)
	DIAM	Soil core diameter
8	PLTPROP	PLTPROP(1) = K_s and PLTPROP(2) = θ_s of ceramic plate
11	RHOW	Wetting fluid density (g/cm^3)
	RHONW	Non-wetting fluid density (g/cm^3)
	CMUW	Wetting fluid viscosity (dyne sec/cm2)
	CMUNW	Non-wetting fluid viscosity (dyne sec/cm^2)
13	TMAX	Maximum simulation time (user defined unit)
	DTMAX	Maximum time step for used in the numerical scheme
	IDT	Index of time step, equal to 1 for the constant time step case
	INIDT	Initial time step
	ERR	Numerical solution accuracy
15	IEQ	Index of the constitutive functions (h_c-S_e and k_r-S_e) model: 1: van Genuchten - Mualem model (VGM) 2: van Genuchten - Burtine model (VGB) 3: Brooks-Corey -Mualem model (BCM) 4: Brooks-Corey-Burdine model (BCB) 5: Brutseart-Burdine model (BRB) 6: Gardner-Mualem model (GDM) 7: Lognormal-Mualem model (LNM)
18	MODE	Index of calculation type: 1: Two-fluid flow forward simulation 2: Two-fluid flow inverse parameter estimation
20	hnw0	Initial non-wetting fluid total head at top
	HB0	Initial outflow height
22	ITIM	Total number of multi-step pressure step
24 - 31	TIM(I), PB(I), I = 1, ..., ITIM,	time moment and value of each pressure step
34	MAXTRY	Maximum running number in each optimization iteration
	MIT	Maximum iteration number
36	NTOB	Total observation time points
	IPAR	Total parameter number (maximum is 8)
	ITYP	Total number of data type
39	IWHC	Weighting factor for capillary pressure h_c data
	IWQ	Weighting factor for cumulative outflow Q_w data
	IWTHETA	Weighting factor for the $\theta_w(h_c)$ data
41-43	THETAS, THETAR, INTRIK:	Fixed names for parameter 1, 2 and 3
44-48	ALPHA, N, M, L, NONE:	User defined name for parameter 4, 5, 6, 7, and 8
51-58	PVALI(I), PMIN(I), PMAX(I), IOPT(I), I = 1,..., IPAR,	initial estimates, minimum, maximum, and adjustable index (1: free, 0: fixed) of parameters
61-End	Time(I), h_c(I), Q(I), HB(I), I = 1, ..., NTOB,	Observation data
End-line:		Initial h_c and θ_w data when soil core is in equilibrium state

Output file

INITIAL OBS-CAL FITTING:

TIME	OBS-HC	CAL-HC	DFHC	OBS-Q	CAL-Q	DFQ	
0.017	24.200	25.039	0.839	0.830	0.075	0.755	
0.033	25.440	25.192	0.248	1.150	0.168	0.982	
0.050	26.150	25.338	0.812	1.340	0.257	1.083	
0.067	26.600	25.479	1.121	1.520	0.343	1.177	
0.083	27.000	25.615	1.385	1.660	0.427	1.233	
0.117	27.490	25.870	1.620	1.800	0.583	1.217	
0.267	28.420	26.793	1.627	1.980	1.140	0.840	
0.533	28.960	27.903	1.057	2.070	1.791	0.279	
4.167	29.620	29.672	0.052	2.210	2.789	0.579	
5.433	29.620	29.657	0.037	2.300	2.780	0.480	
5.683	33.450	29.747	3.703	2.530	3.066	0.536	
5.700	34.250	30.039	4.211	2.680	3.372	0.692	
5.717	35.180	30.410	4.770	2.920	3.645	0.725	
5.733	35.760	30.830	4.930	3.150	3.892	0.742	
5.750	36.380	31.236	5.144	3.300	4.118	0.818	
5.767	36.870	31.627	5.243	3.450	4.328	0.878	
5.783	37.360	31.999	5.361	3.610	4.524	0.914	
5.800	37.760	32.351	5.409	3.840	4.705	0.865	
5.817	38.160	32.689	5.471	3.990	4.877	0.887	
5.850	38.830	33.318	5.512	4.220	5.186	0.966	
5.883	39.320	33.897	5.423	4.530	5.467	0.937	
5.917	39.760	34.433	5.327	4.680	5.723	1.043	
5.950	39.760	34.932	4.828	4.910	5.957	1.047	
5.983	40.160	35.401	4.759	5.150	6.173	1.023	
6.017	40.480	35.839	4.641	5.370	6.372	1.002	
6.067	40.830	36.441	4.389	5.600	6.640	1.040	
6.150	41.370	37.298	4.072	5.830	7.016	1.186	
6.233	41.810	38.051	3.759	6.060	7.335	1.275	
6.300	41.900	38.599	3.301	6.300	7.561	1.261	
6.383	42.210	39.200	3.010	6.520	7.806	1.286	
6.483	42.430	39.813	2.617	6.750	8.052	1.302	
6.633	42.480	40.588	1.892	6.990	8.355	1.365	
6.750	42.740	41.081	1.659	7.220	8.544	1.324	
6.900	42.880	41.607	1.273	7.450	8.743	1.293	
7.117	42.970	42.190	0.780	7.600	8.960	1.360	
7.367	43.060	42.675	0.385	7.910	9.138	1.228	
7.650	43.230	43.050	0.180	8.140	9.273	1.133	
7.950	43.320	43.308	0.012	8.370	9.365	0.995	
8.333	43.320	43.506	0.186	8.600	9.435	0.835	
8.750	43.320	43.620	0.300	8.830	9.474	0.644	
9.267	43.320	43.683	0.363	8.990	9.496	0.506	
9.617	43.320	43.694	0.374	9.290	9.498	0.208	
10.250	43.320	43.680	0.360	9.520	9.492	0.028	
11.317	43.320	43.643	0.323	9.750	9.477	0.273	
12.267	43.320	43.609	0.289	9.900	9.464	0.436	
12.733	43.320	43.582	0.262	10.210	9.453	0.757	
14.717	43.320	43.511	0.191	10.360	9.426	0.934	
16.233	43.320	43.484	0.164	10.520	9.416	1.104	
19.417	43.320	43.436	0.116	10.900	9.397	1.503	
20.617	43.320	43.400	0.080	10.980	9.382	1.598	
21.267	43.320	43.416	0.096	11.500	9.709	1.791	
21.283	46.200	43.566	2.634	11.830	9.948	1.882	
21.300	47.400	43.795	3.605	12.330	10.139	2.191	
21.317	48.420	44.098	4.322	12.660	10.305	2.355	
21.333	49.220	44.431	4.789	12.990	10.451	2.539	
21.350	49.980	44.770	5.210	13.310	10.581	2.729	
21.367	50.150	45.107	5.043	13.640	10.700	2.940	
21.383	51.090	45.435	5.655	13.970	10.809	3.161	
21.400	51.620	45.749	5.871	14.220	10.909	3.311	
21.417	52.070	46.053	6.017	14.460	11.004	3.456	
21.433	52.510	46.344	6.166	14.710	11.093	3.617	
21.450	52.870	46.622	6.248	14.960	11.177	3.783	

21.483	53.670	47.148	6.522	15.370	11.333	4.037
21.500	54.030	47.395	6.635	15.530	11.406	4.124
21.533	54.510	47.866	6.644	15.860	11.544	4.316
21.550	54.780	48.089	6.691	16.110	11.609	4.501
21.567	55.000	48.307	6.693	16.270	11.673	4.597
21.600	55.490	48.723	6.767	16.600	11.792	4.808
21.633	55.940	49.118	6.822	16.850	11.905	4.945
21.650	56.120	49.308	6.812	17.000	11.960	5.040
21.683	56.430	49.675	6.755	17.330	12.063	5.267
21.700	56.610	49.853	6.757	17.420	12.113	5.307
21.750	57.050	50.359	6.691	17.830	12.254	5.576
21.783	57.230	50.683	6.547	17.990	12.344	5.646
21.817	57.490	50.993	6.497	18.320	12.429	5.891
21.850	57.670	51.293	6.377	18.480	12.510	5.970
21.883	57.940	51.582	6.358	18.730	12.589	6.141
21.933	58.160	51.994	6.166	18.970	12.699	6.271
21.983	58.610	52.385	6.225	19.300	12.802	6.498
22.033	58.740	52.758	5.982	19.470	12.900	6.570
22.067	58.740	52.998	5.742	19.630	12.963	6.667
22.083	58.740	53.116	5.624	19.880	12.993	6.887
22.100	58.740	53.232	5.508	20.130	13.023	7.107
22.117	58.740	53.346	5.394	20.370	13.051	7.319
22.133	58.740	53.459	5.281	20.710	13.079	7.631
22.150	58.740	53.568	5.172	20.950	13.106	7.844
22.167	58.740	53.676	5.064	21.110	13.133	7.977
22.183	58.740	53.783	4.957	21.190	13.159	8.031
22.217	58.740	53.987	4.753	21.450	13.210	8.240
22.283	58.740	54.369	4.371	21.690	13.305	8.385
22.350	58.740	54.728	4.012	21.930	13.394	8.536
22.417	58.830	55.067	3.763	22.100	13.478	8.622
22.533	59.360	55.610	3.750	22.510	13.611	8.899
22.650	59.540	56.102	3.438	22.670	13.730	8.940
22.767	59.720	56.550	3.170	22.920	13.837	9.083
22.900	59.900	57.012	2.888	23.160	13.946	9.214
23.050	60.160	57.475	2.685	23.410	14.054	9.356
23.233	60.250	57.967	2.283	23.660	14.168	9.492
23.467	60.340	58.498	1.842	23.910	14.289	9.621
23.750	60.520	59.023	1.497	24.150	14.407	9.743
24.117	60.520	59.552	0.968	24.400	14.525	9.875
24.650	60.520	60.100	0.420	24.640	14.646	9.994
25.600	60.520	60.667	0.147	24.970	14.770	10.200
26.167	60.520	60.853	0.333	25.130	14.809	10.321
27.150	60.520	61.027	0.507	25.380	14.846	10.534
27.433	60.520	61.050	0.530	25.700	14.849	10.851
27.600	60.520	61.056	0.536	25.870	14.849	11.021
27.900	60.520	61.057	0.537	26.110	14.849	11.261
28.483	60.520	61.047	0.527	26.360	14.846	11.514
29.567	60.610	61.017	0.407	26.610	14.839	11.771
30.717	60.610	60.979	0.369	26.850	14.829	12.021
32.017	60.610	60.934	0.324	27.100	14.818	12.282
33.033	60.610	60.895	0.285	27.350	14.809	12.541
34.117	60.610	60.851	0.241	27.590	14.798	12.792
36.067	60.610	60.783	0.173	27.930	14.782	13.148
37.650	60.610	60.736	0.126	28.090	14.771	13.319
41.150	60.610	60.685	0.075	28.340	14.758	13.582
44.633	60.610	60.648	0.038	28.500	14.750	13.750
45.317	64.370	60.641	3.729	28.680	14.944	13.736
45.333	65.220	60.667	4.553	28.940	15.060	13.880
45.367	66.640	60.830	5.810	29.180	15.217	13.963
45.383	67.310	60.944	6.366	29.370	15.286	14.084
45.400	67.840	61.083	6.757	29.490	15.346	14.144
45.417	68.370	61.243	7.127	29.670	15.402	14.268
45.450	69.260	61.610	7.650	29.800	15.498	14.302
45.483	70.110	61.992	8.118	30.040	15.584	14.456
45.517	70.780	62.370	8.410	30.280	15.661	14.619

45.533	71.130	62.555	8.575	30.410	15.698	14.712
45.567	71.760	62.916	8.844	30.530	15.765	14.765
45.617	72.560	63.431	9.129	30.780	15.858	14.922
45.667	73.400	63.910	9.490	30.960	15.944	15.016
45.717	73.980	64.358	9.622	31.140	16.023	15.117
45.767	74.470	64.777	9.693	31.270	16.097	15.173
45.817	74.960	65.173	9.787	31.510	16.166	15.344
45.867	75.400	65.547	9.853	31.640	16.232	15.408
45.900	75.630	65.787	9.843	31.700	16.274	15.426
45.950	75.940	66.131	9.809	31.820	16.334	15.486
45.967	75.940	66.244	9.696	32.990	16.354	16.636
46.000	76.340	66.462	9.878	33.300	16.390	16.910
46.183	77.230	67.543	9.687	33.480	16.576	16.904
46.417	78.120	68.742	9.378	33.660	16.784	16.876
46.667	78.700	69.869	8.831	33.910	16.975	16.935
46.900	78.870	70.800	8.070	34.090	17.129	16.961
47.233	79.230	71.965	7.265	34.210	17.319	16.891
47.983	79.410	74.032	5.378	34.390	17.644	16.746
50.867	79.630	77.988	1.642	34.580	18.231	16.349
53.150	79.630	79.096	0.534	34.700	18.387	16.313
53.367	79.670	79.157	0.513	35.010	18.395	16.615
55.117	79.670	79.483	0.187	35.130	18.440	16.690
57.533	79.720	79.680	0.040	35.320	18.467	16.853
61.233	79.720	79.753	0.033	35.560	18.476	17.084
64.100	79.720	79.750	0.030	35.690	18.476	17.214
67.883	79.720	79.723	0.003	35.940	18.471	17.469
69.033	79.810	79.708	0.102	36.000	18.469	17.531
69.067	80.060	79.714	0.346	36.270	18.577	17.693
69.083	80.590	79.716	0.874	36.620	18.634	17.986
69.117	81.610	79.746	1.864	37.070	18.709	18.361
69.150	82.680	79.812	2.868	37.430	18.769	18.661
69.183	83.610	79.922	3.688	37.780	18.819	18.961
69.217	84.460	80.068	4.392	38.050	18.864	19.186
69.233	84.900	80.149	4.751	38.230	18.884	19.346
69.267	85.620	80.335	5.285	38.500	18.922	19.578
69.317	86.640	80.648	5.992	38.760	18.972	19.788
69.400	88.060	81.197	6.863	39.120	19.045	20.075
69.483	89.310	81.732	7.578	39.390	19.110	20.280
69.533	90.020	82.041	7.979	39.660	19.146	20.514
69.617	91.000	82.531	8.469	39.920	19.201	20.719
69.700	91.800	82.991	8.809	40.090	19.252	20.838
69.833	92.870	83.668	9.202	40.370	19.327	21.043
69.983	93.850	84.356	9.494	40.640	19.402	21.238
70.217	95.180	85.304	9.876	40.910	19.508	21.402
70.933	97.140	87.639	9.501	41.250	19.771	21.479
71.983	98.290	90.201	8.089	41.430	20.053	21.377
74.050	98.870	93.575	5.295	41.790	20.409	21.381
74.850	99.050	94.484	4.566	41.790	20.501	21.289
79.367	99.270	97.366	1.904	41.960	20.786	21.174
80.500	99.270	97.722	1.548	42.220	20.820	21.400
87.633	99.270	98.679	0.591	42.490	20.910	21.580
92.967	99.270	98.837	0.433	42.500	20.925	21.575
93.000	99.430	98.834	0.596	42.990	21.078	21.912
93.017	100.100	98.836	1.264	43.750	21.122	22.628
93.033	100.500	98.839	1.661	43.990	21.158	22.832
93.067	101.390	98.858	2.532	44.330	21.215	23.115
93.100	102.330	98.897	3.433	44.570	21.264	23.306
93.133	103.210	98.962	4.248	44.830	21.307	23.523
93.167	104.020	99.053	4.967	44.990	21.345	23.645
93.233	105.620	99.337	6.283	45.320	21.412	23.908
93.317	107.440	99.797	7.643	45.490	21.484	24.006
93.383	108.730	100.204	8.526	45.820	21.536	24.284
93.467	110.200	100.747	9.453	45.990	21.595	24.395
93.550	111.530	101.301	10.229	46.240	21.648	24.592
93.633	112.730	101.853	10.877	46.490	21.698	24.792

93.733	114.070	102.505	11.565	46.740	21.753	24.987
93.850	115.620	103.239	12.381	47.080	21.813	25.267
93.967	117.000	103.942	13.058	47.240	21.869	25.371
94.100	118.340	104.708	13.632	47.490	21.928	25.562
94.300	120.340	105.790	14.550	47.740	22.011	25.729
94.600	122.960	107.280	15.680	47.990	22.123	25.867
95.000	125.990	109.072	16.918	48.240	22.257	25.983
95.617	129.590	111.533	18.057	48.490	22.437	26.053
96.733	134.260	115.383	18.877	48.820	22.708	26.112
97.200	135.770	116.825	18.945	48.990	22.806	26.184
101.517	143.380	127.143	16.237	49.160	23.450	25.710
102.367	144.130	128.691	15.439	49.490	23.538	25.952
102.750	144.490	129.348	15.142	49.660	23.574	26.086
104.733	145.740	132.377	13.363	50.000	23.739	26.261
117.117	148.000	142.770	5.230	50.000	24.260	25.740
122.517	148.400	144.812	3.588	50.000	24.355	25.645
122.667	148.610	144.855	3.755	50.200	24.431	25.769
122.800	149.060	144.908	4.152	50.390	24.494	25.896
123.083	151.280	145.174	6.106	50.590	24.578	26.012
123.483	154.300	146.018	8.282	50.780	24.661	26.119
124.267	159.150	148.348	10.802	51.040	24.780	26.260
124.700	161.420	149.659	11.761	51.160	24.833	26.327
125.450	164.890	151.769	13.121	51.290	24.914	26.376
126.417	168.580	154.178	14.402	51.550	25.004	26.546
132.550	181.610	165.220	16.390	51.680	25.405	26.275
139.233	188.420	173.547	14.873	51.930	25.682	26.248
146.083	192.200	179.793	12.407	52.200	25.875	26.325
150.900	193.890	183.191	10.699	52.200	25.974	26.226
151.100	198.950	183.140	15.810	52.430	26.090	26.340
151.250	199.380	183.242	16.138	52.520	26.134	26.386
152.600	205.640	185.435	20.205	52.830	26.334	26.496
153.550	210.080	187.972	22.108	53.080	26.427	26.653
155.550	219.070	193.455	25.615	53.320	26.583	26.737
157.783	227.790	198.991	28.799	53.550	26.724	26.826
162.883	244.790	209.850	34.940	53.800	26.980	26.820
167.550	257.690	218.553	39.137	53.950	27.169	26.781
168.917	261.200	220.952	40.248	54.200	27.218	26.982
16.000	0.308	0.287	0.021			

ITERATION	SSQ	THETAR(cm3/cm3)	INTRIK(cm2)	ALPHA(-)	N(-)
0	0.1159E+02	0.1100	0.0000000144	0.0400	2.0000
1	0.6138E+01	0.0068	0.0000000149	0.0155	2.2677
2	0.1968E+01	0.0146	0.0000000230	0.0203	2.5337
3	0.1675E+01	0.0115	0.0000000211	0.0192	2.6716
4	0.1659E+01	0.0172	0.0000000233	0.0191	2.7513
5	0.1657E+01	0.0197	0.0000000245	0.0190	2.7906
6	0.1656E+01	0.0209	0.0000000252	0.0190	2.8079
7	0.1656E+01	0.0212	0.0000000253	0.0189	2.8124

MEET MAXIMUM NET, NO FURTHER REDUCTION IN SSQ.
CONVERGENCE.
RSQ= 0.998517455981560
ssq= 1.65646876697055
Correlation Matrix:

	1	2	3	4
1	1.000			
2	0.777	1.000		
3	-0.166	0.018	1.000	
4	0.892	0.699	-0.483	1.000

NON-LINEAR LEAST-SQUARES ANALYSIS: FINAL RESULTS
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VARIABLE	VALUE	S.E.COEFF.	95% CONFIDENCE LIMITS LOWER	UPPER

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 THETAR(cm3/          0.021          0.003          0.015          0.028
 INTRIK(cm2)          0.000          0.000          0.000          0.000
 ALPHA(-)             0.019          0.000          0.019          0.019
 N(-)                 2.812          0.040          2.734          2.891
 THETAS(cm3/cm3)=  0.320000000000000
 THETAR(cm3/cm3)=  2.115814578887867E-002
 INTRIK(cm2)    =  2.531770278228916E-008
 ALPHA(-)       =  1.893833661150859E-002
 N(-)           =   2.81236060923382
 M(-)           =  0.644426821824804
 L(-)           =  0.500000000000000
 NONE           =   1.00000000000000
Ksw(cm/hr)=   8.93208554159162
Ksnw(cm/hr)=   493.485389038211

FINAL OBS-CAL FITTING:
TIME   OBS-HC   CAL-HC  DFHC  OBS-Q  CAL-Q  DFQ
    0.017    24.200    24.819     0.619     0.830    -0.116     0.946
    0.033    25.440    25.115     0.325     1.150     0.023     1.127
    0.050    26.150    25.386     0.764     1.340     0.151     1.189
    0.067    26.600    25.638     0.962     1.520     0.273     1.247
    0.083    27.000    25.871     1.129     1.660     0.386     1.274
    0.117    27.490    26.276     1.214     1.800     0.587     1.213
    0.267    28.420    27.514     0.906     1.980     1.224     0.756
    0.533    28.960    28.663     0.297     2.070     1.846     0.224
    4.167    29.620    29.675     0.055     2.210     2.417     0.207
    5.433    29.620    29.656     0.036     2.300     2.406     0.106
    5.683    33.450    30.185     3.265     2.530     2.746     0.216
    5.700    34.250    30.871     3.379     2.680     3.154     0.474
    5.717    35.180    31.514     3.666     2.920     3.543     0.623
    5.733    35.760    32.113     3.647     3.150     3.913     0.763
    5.750    36.380    32.671     3.709     3.300     4.263     0.963
    5.767    36.870    33.198     3.672     3.450     4.598     1.148
    5.783    37.360    33.694     3.666     3.610     4.917     1.307
    5.800    37.760    34.158     3.602     3.840     5.220     1.380
    5.817    38.160    34.600     3.560     3.990     5.510     1.520
    5.850    38.830    35.398     3.432     4.220     6.042     1.822
    5.883    39.320    36.120     3.200     4.530     6.529     1.999
    5.917    39.760    36.770     2.990     4.680     6.974     2.294
    5.950    39.760    37.361     2.399     4.910     7.382     2.472
    5.983    40.160    37.899     2.261     5.150     7.757     2.607
    6.017    40.480    38.388     2.092     5.370     8.099     2.729
    6.067    40.830    39.030     1.800     5.600     8.552     2.952
    6.150    41.370    39.906     1.464     5.830     9.174     3.344
    6.233    41.810    40.626     1.184     6.060     9.689     3.629
    6.300    41.900    41.114     0.786     6.300    10.040     3.740
    6.383    42.210    41.618     0.592     6.520    10.403     3.883
    6.483    42.430    42.097     0.333     6.750    10.749     3.999
    6.633    42.480    42.646     0.166     6.990    11.146     4.156
    6.750    42.740    42.957     0.217     7.220    11.372     4.152
    6.900    42.880    43.250     0.370     7.450    11.584     4.134
    7.117    42.970    43.524     0.554     7.600    11.783     4.183
    7.367    43.060    43.703     0.643     7.910    11.913     4.003
    7.650    43.230    43.799     0.569     8.140    11.982     3.842
    7.950    43.320    43.834     0.514     8.370    12.007     3.637
    8.333    43.320    43.832     0.512     8.600    12.006     3.406
    8.750    43.320    43.808     0.488     8.830    11.988     3.158
    9.267    43.320    43.773     0.453     8.990    11.962     2.972
    9.617    43.320    43.743     0.423     9.290    11.940     2.650
   10.250    43.320    43.690     0.370     9.520    11.901     2.381
   11.317    43.320    43.637     0.317     9.750    11.862     2.112
   12.267    43.320    43.601     0.281     9.900    11.836     1.936
   12.733    43.320    43.569     0.249    10.210    11.813     1.603
   14.717    43.320    43.506     0.186    10.360    11.767     1.407
   16.233    43.320    43.481     0.161    10.520    11.748     1.228
```

19.417	43.320	43.435	0.115	10.900	11.715	0.815
20.617	43.320	43.394	0.074	10.980	11.685	0.705
21.267	43.320	43.961	0.641	11.500	12.217	0.717
21.283	46.200	44.666	1.534	11.830	12.747	0.917
21.300	47.400	45.345	2.055	12.330	13.247	0.917
21.317	48.420	45.997	2.423	12.660	13.727	1.067
21.333	49.220	46.622	2.598	12.990	14.186	1.196
21.350	49.980	47.217	2.763	13.310	14.622	1.312
21.367	50.150	47.791	2.359	13.640	15.041	1.401
21.383	51.090	48.342	2.748	13.970	15.443	1.473
21.400	51.620	48.867	2.753	14.220	15.824	1.604
21.417	52.070	49.374	2.696	14.460	16.192	1.732
21.433	52.510	49.862	2.648	14.710	16.544	1.834
21.450	52.870	50.327	2.543	14.960	16.879	1.919
21.483	53.670	51.198	2.472	15.370	17.500	2.130
21.500	54.030	51.610	2.420	15.530	17.795	2.265
21.533	54.510	52.386	2.124	15.860	18.341	2.481
21.550	54.780	52.753	2.027	16.110	18.601	2.491
21.567	55.000	53.110	1.890	16.270	18.851	2.581
21.600	55.490	53.772	1.718	16.600	19.311	2.711
21.633	55.940	54.386	1.554	16.850	19.735	2.885
21.650	56.120	54.678	1.442	17.000	19.936	2.936
21.683	56.430	55.226	1.204	17.330	20.310	2.980
21.700	56.610	55.486	1.124	17.420	20.487	3.067
21.750	57.050	56.192	0.858	17.830	20.962	3.132
21.783	57.230	56.627	0.603	17.990	21.253	3.263
21.817	57.490	57.028	0.462	18.320	21.520	3.200
21.850	57.670	57.400	0.270	18.480	21.765	3.285
21.883	57.940	57.744	0.196	18.730	21.991	3.261
21.933	58.160	58.205	0.045	18.970	22.292	3.322
21.983	58.610	58.615	0.005	19.300	22.557	3.257
22.033	58.740	58.980	0.240	19.470	22.792	3.322
22.067	58.740	59.205	0.465	19.630	22.936	3.306
22.083	58.740	59.312	0.572	19.880	23.005	3.125
22.100	58.740	59.414	0.674	20.130	23.069	2.939
22.117	58.740	59.511	0.771	20.370	23.131	2.761
22.133	58.740	59.603	0.863	20.710	23.188	2.478
22.150	58.740	59.690	0.950	20.950	23.242	2.292
22.167	58.740	59.772	1.032	21.110	23.294	2.184
22.183	58.740	59.850	1.110	21.190	23.343	2.153
22.217	58.740	59.994	1.254	21.450	23.433	1.983
22.283	58.740	60.238	1.498	21.690	23.586	1.896
22.350	58.740	60.444	1.704	21.930	23.715	1.785
22.417	58.830	60.619	1.789	22.100	23.824	1.724
22.533	59.360	60.858	1.498	22.510	23.972	1.462
22.650	59.540	61.035	1.495	22.670	24.082	1.412
22.767	59.720	61.167	1.447	22.920	24.163	1.243
22.900	59.900	61.273	1.373	23.160	24.228	1.068
23.050	60.160	61.352	1.192	23.410	24.276	0.866
23.233	60.250	61.406	1.156	23.660	24.308	0.648
23.467	60.340	61.435	1.095	23.910	24.325	0.415
23.750	60.520	61.435	0.915	24.150	24.325	0.175
24.117	60.520	61.412	0.892	24.400	24.309	0.091
24.650	60.520	61.368	0.848	24.640	24.282	0.358
25.600	60.520	61.306	0.786	24.970	24.243	0.727
26.167	60.520	61.271	0.751	25.130	24.221	0.909
27.150	60.520	61.223	0.703	25.380	24.190	1.190
27.433	60.520	61.196	0.676	25.700	24.172	1.528
27.600	60.520	61.173	0.653	25.870	24.158	1.712
27.900	60.520	61.131	0.611	26.110	24.131	1.979
28.483	60.520	61.068	0.548	26.360	24.091	2.269
29.567	60.610	61.003	0.393	26.610	24.050	2.560
30.717	60.610	60.955	0.345	26.850	24.020	2.830
32.017	60.610	60.909	0.299	27.100	23.990	3.110
33.033	60.610	60.866	0.256	27.350	23.963	3.387

34.117	60.610	60.821	0.211	27.590	23.934	3.656
36.067	60.610	60.761	0.151	27.930	23.896	4.034
37.650	60.610	60.717	0.107	28.090	23.868	4.222
41.150	60.610	60.680	0.070	28.340	23.844	4.496
44.633	60.610	60.645	0.035	28.500	23.822	4.678
45.317	64.370	61.016	3.354	28.680	24.326	4.354
45.333	65.220	61.651	3.569	28.940	24.793	4.147
45.367	66.640	62.950	3.690	29.180	25.609	3.571
45.383	67.310	63.557	3.753	29.370	25.992	3.378
45.400	67.840	64.144	3.696	29.490	26.351	3.139
45.417	68.370	64.715	3.655	29.670	26.692	2.978
45.450	69.260	65.782	3.478	29.800	27.308	2.492
45.483	70.110	66.769	3.341	30.040	27.870	2.170
45.517	70.780	67.681	3.099	30.280	28.379	1.901
45.533	71.130	68.117	3.013	30.410	28.621	1.789
45.567	71.760	68.936	2.824	30.530	29.063	1.467
45.617	72.560	70.044	2.516	30.780	29.646	1.134
45.667	73.400	71.038	2.362	30.960	30.159	0.801
45.717	73.980	71.931	2.049	31.140	30.611	0.529
45.767	74.470	72.735	1.735	31.270	31.010	0.260
45.817	74.960	73.460	1.500	31.510	31.362	0.148
45.867	75.400	74.112	1.288	31.640	31.674	0.034
45.900	75.630	74.515	1.115	31.700	31.865	0.165
45.950	75.940	75.064	0.876	31.820	32.121	0.301
45.967	75.940	75.238	0.702	32.990	32.200	0.790
46.000	76.340	75.556	0.784	33.300	32.343	0.957
46.183	77.230	76.880	0.350	33.480	32.938	0.542
46.417	78.120	78.012	0.108	33.660	33.435	0.225
46.667	78.700	78.773	0.073	33.910	33.761	0.149
46.900	78.870	79.213	0.343	34.090	33.947	0.143
47.233	79.230	79.576	0.346	34.210	34.098	0.112
47.983	79.410	79.879	0.469	34.390	34.224	0.166
50.867	79.630	79.955	0.325	34.580	34.255	0.325
53.150	79.630	79.925	0.295	34.700	34.242	0.458
53.367	79.670	79.913	0.243	35.010	34.235	0.775
55.117	79.670	79.853	0.183	35.130	34.210	0.920
57.533	79.720	79.820	0.100	35.320	34.195	1.125
61.233	79.720	79.780	0.060	35.560	34.178	1.382
64.100	79.720	79.750	0.030	35.690	34.164	1.526
67.883	79.720	79.715	0.005	35.940	34.149	1.791
69.033	79.810	79.689	0.121	36.000	34.137	1.863
69.067	80.060	79.874	0.186	36.270	34.556	1.714
69.083	80.590	80.264	0.326	36.620	34.890	1.730
69.117	81.610	81.274	0.336	37.070	35.405	1.665
69.150	82.680	82.360	0.320	37.430	35.839	1.591
69.183	83.610	83.335	0.275	37.780	36.213	1.567
69.217	84.460	84.212	0.248	38.050	36.541	1.509
69.233	84.900	84.623	0.277	38.230	36.694	1.536
69.267	85.620	85.392	0.228	38.500	36.971	1.529
69.317	86.640	86.430	0.210	38.760	37.335	1.425
69.400	88.060	87.914	0.146	39.120	37.843	1.277
69.483	89.310	89.196	0.114	39.390	38.270	1.120
69.533	90.020	89.898	0.122	39.660	38.499	1.161
69.617	91.000	90.925	0.075	39.920	38.825	1.095
69.700	91.800	91.826	0.026	40.090	39.106	0.984
69.833	92.870	93.053	0.183	40.370	39.480	0.890
69.983	93.850	94.173	0.323	40.640	39.811	0.829
70.217	95.180	95.493	0.313	40.910	40.192	0.718
70.933	97.140	97.681	0.541	41.250	40.800	0.450
71.983	98.290	98.725	0.435	41.430	41.081	0.349
74.050	98.870	99.043	0.173	41.790	41.165	0.625
74.850	99.050	99.040	0.010	41.790	41.164	0.626
79.367	99.270	99.025	0.245	41.960	41.159	0.801
80.500	99.270	98.994	0.276	42.220	41.150	1.070
87.633	99.270	98.935	0.335	42.490	41.133	1.357

92.967	99.270	98.910	0.360	42.500	41.126	1.374
93.000	99.430	99.259	0.171	42.990	41.911	1.079
93.017	100.100	99.586	0.514	43.750	42.199	1.551
93.033	100.500	100.065	0.435	43.990	42.439	1.551
93.067	101.390	101.093	0.297	44.330	42.789	1.541
93.100	102.330	102.268	0.062	44.570	43.092	1.478
93.133	103.210	103.367	0.157	44.830	43.356	1.474
93.167	104.020	104.379	0.359	44.990	43.589	1.401
93.233	105.620	106.219	0.599	45.320	43.990	1.330
93.317	107.440	108.221	0.781	45.490	44.416	1.074
93.383	108.730	109.659	0.929	45.820	44.718	1.102
93.467	110.200	111.314	1.114	45.990	45.051	0.939
93.550	111.530	112.843	1.313	46.240	45.351	0.889
93.633	112.730	114.273	1.543	46.490	45.622	0.868
93.733	114.070	115.871	1.801	46.740	45.914	0.826
93.850	115.620	117.601	1.981	47.080	46.222	0.858
93.967	117.000	119.209	2.209	47.240	46.498	0.742
94.100	118.340	120.914	2.574	47.490	46.780	0.710
94.300	120.340	123.233	2.893	47.740	47.146	0.594
94.600	122.960	126.273	3.313	47.990	47.603	0.387
95.000	125.990	129.672	3.682	48.240	48.081	0.159
95.617	129.590	133.805	4.215	48.490	48.622	0.132
96.733	134.260	138.965	4.705	48.820	49.242	0.422
97.200	135.770	140.510	4.740	48.990	49.416	0.426
101.517	143.380	146.930	3.550	49.160	50.099	0.939
102.367	144.130	147.372	3.242	49.490	50.143	0.653
102.750	144.490	147.527	3.037	49.660	50.158	0.498
104.733	145.740	148.046	2.306	50.000	50.210	0.210
117.117	148.000	148.552	0.552	50.000	50.260	0.260
122.517	148.400	148.559	0.159	50.000	50.260	0.260
122.667	148.610	148.658	0.048	50.200	50.541	0.341
122.800	149.060	149.368	0.308	50.390	50.789	0.399
123.083	151.280	152.075	0.795	50.590	51.110	0.520
123.483	154.300	155.718	1.418	50.780	51.419	0.639
124.267	159.150	161.105	1.955	51.040	51.844	0.804
124.700	161.420	163.549	2.129	51.160	52.029	0.869
125.450	164.890	167.254	2.364	51.290	52.298	1.008
126.417	168.580	171.322	2.742	51.550	52.576	1.026
132.550	181.610	186.739	5.129	51.680	53.490	1.810
139.233	188.420	193.726	5.306	51.930	53.844	1.914
146.083	192.200	196.766	4.566	52.200	53.989	1.789
150.900	193.890	197.799	3.909	52.200	54.037	1.837
151.100	198.950	197.441	1.509	52.430	54.290	1.860
151.250	199.380	197.777	1.603	52.520	54.385	1.865
152.600	205.640	204.953	0.687	52.830	54.802	1.972
153.550	210.080	209.578	0.502	53.080	54.987	1.907
155.550	219.070	217.566	1.504	53.320	55.287	1.967
157.783	227.790	225.113	2.677	53.550	55.548	1.998
162.883	244.790	239.653	5.137	53.800	55.988	2.188
167.550	257.690	250.848	6.842	53.950	56.280	2.330
168.917	261.200	253.840	7.360	54.200	56.351	2.151
16.000	0.308	0.313	0.005			

Listing of TF-OPT

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C.............................................................................
C.    PROGRAM           : TF-OPT.FOR
C.    PURPOSE           : INVERSE PARAMETER ESTIMATION OF TWO-PHASE FLOW
C.                        CAPILLARY PRESSURE AND PERMEABILITY FUNCTION IN
C.                        MULTI-STEP OUTFLOW EXPERIMENT OF SOIL COLUMN
C.    DEVELOPED BY      : JIAYU CHEN (HYDROLOGIC SCIENCE, LAWR, UCD)
C.    BASED ON          : - TPH1D FROM DR.JOHN NIEBER (UNIV. MINNESOTA)
C.                          FOR TWO-PHASE UNSATURATED FLOW MODEL
C.                        - MLSTPM (LAWR PAPER NO.100021 OF UNIVERSITY
C.                          OF CALIFORNIA AT DAVIS) FOR LEVENBERG-MARQUARDT
C.                          OPTIMIZATION
C.                      : OCT., 1997
C.............................................................................

      PARAMETER (MNOB=500,MPAR=8,MTYP=5,NDIM=100)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION FC(MNOB),FC1(MNOB),FC2(MNOB),R(MNOB)
      DIMENSION FREEPAR(MPAR),X1(MPAR),X2(MPAR)
      DIMENSION DD(MPAR,MPAR),A(MPAR,MPAR),AS(MPAR,MPAR)
      DIMENSION E(MPAR),EWJAC(MPAR),C(MPAR),CHI(MPAR)
      CHARACTER*60 INFILE,OUTFILE
      INCLUDE 'tfcombk.dat'
      DATA ZERO/0./

C...  initiation
      WRITE(*,*) 'Enter the input file name:'
      READ(*,'(A60)') INFILE
      OPEN(UNIT=11,FILE=INFILE,STATUS='OLD')
      WRITE(*,*) 'Enter the output file name:'
      READ(*,'(A60)') OUTFILE
      OPEN(UNIT=12,FILE=OUTFILE,STATUS='UNKNOWN')
      CALL INPUT(FREEPAR)
      DO 4 I=1,NPAR
       X1(I)=FREEPAR(I)
       X2(I)=X1(I)
4     CONTINUE

C...  first model call
      NIT = 0
      WRITE(*,*) 'NIT=',NIT
      CALL MODEL(FC)
      IF (ABS(MODE) .eq. 1) THEN
       CALL SIMULATION_REPORT(FC)
       GO TO 8888
      ENDIF
      CALL OPTIMIZATION_INITIAL_REPORT(FC)

C..   check data fitness
      SSQ=0.
      DO 10 I = 1,NOB
       R(I) = WGHT(I)*(FO(I)-FC(I))
       SSQ = SSQ+R(I)*R(I)
10    CONTINUE
      sssq=SQRT(SSQ/NOB)
      IF (NPAR .NE. 0) THEN
```

```
       WRITE(12,1040) (PNAMA(I),I = 1,NPAR)
       WRITE(*,1040)  (PNAMA(I),I = 1,NPAR)
       WRITE(12,1042) NIT,sssq,(X1(I),I = 1,NPAR)
       WRITE(*,1042)  NIT,sssq,(X1(I),I = 1,NPAR)
      ELSE
       WRITE(12,1040)
       WRITE(12,1042) NIT,sssq
      ENDIF
      IF (MIT .EQ. 0 .OR. NPAR .EQ. 0) GO TO 8000
1040  FORMAT(/T2,'ITERATION',3X,'SSQ',2X,A16,1X,7(A12,1X))
1042  FORMAT(4X,I3,2X,E12.4,3X,F8.4,1X,F12.10,6(F8.4,1X))

C...  optimization loop ..........................................
      GA = 0.02
      STOPCR = 0.01
      DO 18 I = 1,NPAR
18    E(I) = 0.
20    NIT = NIT+1
      NET = 0
      GA = 0.1*GA

C...  evaluate weighted jacobian j(i,j) = dr(i)/dx1(j) and ewjac(j)
      WRITE(*,*) 'NIT=',NIT
      DO 38 J = 1,NPAR
       PVALA(TRFPAR(J)) = 1.01*X1(J)
       IF (X1(J) .EQ. 0.) STOP 'X1(J)=0, DEVIDED BY ZERO ERROR.'
       EWJAC(J) = 0.
       CALL MODEL(FC1)
       DO 36 I = 1,NOB
          QJAC(I,J) = WGHT(I)*(FC1(I)-FC(I))
          EWJAC(J) = EWJAC(J)+QJAC(I,J)*R(I)
36       CONTINUE
       EWJAC(J) = 100.*EWJAC(J)/X1(J)
       PVALA(TRFPAR(J)) = X1(J)
38    CONTINUE

      DO 44 I = 1,NPAR
       DO 42 J = 1,I
          SUM = ZERO
          DO 40 K = 1,NOB
             SUM = SUM+QJAC(K,I)*QJAC(K,J)
40          CONTINUE
          DD(I,J) = 10000.*SUM/(X1(I)*X1(J))
          DD(J,I) = DD(I,J)
42       CONTINUE
       SCAL=DD(I,I)
       IF (SCAL .LT. 1.0E-30) SCAL=1.0E-30
       SCAL=DSQRT(SCAL)
       IF (E(I) .LT. SCAL) E(I)=SCAL
44    CONTINUE

50    DO 53 I = 1,NPAR
       DO 52 J = 1,NPAR
          A(I,J) = DD(I,J)/(E(I)*E(J))
52       CONTINUE
53    CONTINUE
      DO 54 I = 1,NPAR
       C(I) = EWJAC(I)/E(I)
```

```
       CHI(I) = C(I)
       A(I,I) = A(I,I)+GA
54    CONTINUE

      CALL QRSOLV(A,NPAR,C)

      STEP = 1.
56    NET = NET+1
      IF ( NET .GE. MAXTRY ) THEN
       WRITE(*,*) 'MEET MAXIMUM NET, NO FURTHER REDUCTION IN SSQ.'
       WRITE(12,*) 'MEET MAXIMUM NET, NO FURTHER REDUCTION IN SSQ.'
       GO TO 96
      ENDIF
      DO 58 I = 1,NPAR
       X2(I) = C(I)*STEP/E(I)+X1(I)
       IF (X2(I) .LT. PMINA(I)) X2(I)=PMINA(I)
       IF (X2(I) .GT. PMAXA(I)) X2(I)=PMAXA(I)
       C(I) = (X2(I)-X1(I))*E(I)/STEP
       PVALA(TRFPAR(I)) = X2(I)
58    CONTINUE

      SUM1 = ZERO
      SUM2 = ZERO
      SUM3 = ZERO
      DO 62 I = 1,NPAR
       SUM1 = SUM1+C(I)*CHI(I)
       SUM2=SUM2+C(I)*C(I)
       SUM3=SUM3+CHI(I)*CHI(I)
62    CONTINUE
      DUM=SUM2*SUM3
      IF (DUM .EQ. 0.) DUM=0.000000001
      ARG=SUM1/DSQRT(SUM2*SUM3)
      ANGLE=57.29578*DATAN2(DSQRT(1.-ARG*ARG),ARG)

      DO 64 I=1,NPAR
       IF ( X1(I)*X2(I) .LE. 0.) GO TO 70
64    CONTINUE
      SUMB = ZERO
      CALL MODEL(FC2)
      DO 66 I = 1,NOB
       R(I) = WGHT(I)*(FO(I)-FC2(I))
66    SUMB = SUMB+R(I)*R(I)
C      SUMB=SQRT(SUMB/NOB)
      IF (NET .GE. MAXTRY) THEN
       WRITE(*,*) 'NO FURTHER REDUCTION IN SSQ.'
       WRITE(12,*) 'NO FURTHER REDUCTION IN SSQ.'
       GO TO 96
      ENDIF
      IF ( SUMB/SSQ-1. GT. 0.) GO TO 70
      IF ( SUMB/SSQ-1. LE. 0.) GO TO 80

70    DO 75 I = 1,NPAR
       PVALA(TRFPAR(I)) = X1(I)
75    CONTINUE
      IF ( ANGLE-30.0 .GT. 0.) THEN
       GA=10.*GA
       IF (GA .GT. 100.) GA=100.
       GO TO 50
```

```
      ELSE
       STEP = 0.5*STEP
       GO TO 56
      ENDIF

80    ssum=sqrt(sumb/nob)
      WRITE(*,1042) NIT,ssum,(X2(J),J=1,NPAR)
      WRITE(12,1042) NIT,ssum,(X2(J),J=1,NPAR)
      DO 90 I = 1,NPAR
       DUM = ABS(C(I)*STEP/E(I))/(1.0E-20+ABS(X2(I)))-STOPCR
       IF (DUM .GT. 0.) THEN
          DO 82 J = 1,NPAR
82          X1(J) = X2(J)
          DO 83 J = 1,NOB
83          FC(J) = FC2(J)
          SSQ=SUMB
          IF (NIT .LT. MIT) THEN
            GO TO 20
          ELSE
             WRITE(*,*) 'MEET MAXIMUM NIT, NO FURTHER REDUCE IN SSQ.'
             GO TO 96
          ENDIF
       ENDIF
90    CONTINUE

C     ----- END OF ITERATION LOOP -----
96    CONTINUE
      WRITE(*,*) 'CONVERGENCE.'
      WRITE(12,*) 'CONVERGENCE.'
      CALL MATINV(DD,NPAR)

C     ----- WRITE RSQUARE, CORRELATION MATRIX -----
      SUMS=SUMB
      ssum=sqrt(SUMB/NOB)
        SUMS1=0.0
      SUMS2=0.0
      DO 98 I=1,NOB
       FOS=FO(I)
       SUMS1=SUMS1+FOS
       SUMS2=SUMS2+FOS*FOS
98    CONTINUE
      RSQ= 1.-SUMS/(SUMS2-SUMS1*SUMS1/NOB)
      WRITE(*,*) 'RSQ=',RSQ
      WRITE(12,*) 'RSQ=',RSQ
      write(*,*) 'ssq=',ssum
      write(12,*) 'ssq=',ssum
      DO 100 I=1,NPAR
       E(I)=DD(I,I)
       IF (E(I) .LT. 1.0E-30) E(I)=1.0E-30
       E(I)=DSQRT(E(I))
100   CONTINUE
      WRITE(*,*) 'Correlation Matrix:'
      WRITE(12,*) 'Correlation Matrix:'
      WRITE(*,*) (I,I=1,NPAR)
      WRITE(12,*) (I,I=1,NPAR)
      DO 104 I=1,NPAR
       DO 102 J=1,I
          AS(J,I)=DD(J,I)/(E(I)*E(J))
```

```
102      CONTINUE
       WRITE(*,105) I,(AS(J,I),J=1,I)
       WRITE(12,105) I,(AS(J,I),J=1,I)
104   CONTINUE
105   FORMAT(1X,I6,1X,4(F14.3,1X))

C     ----- CALCULATE 95% CONFIDENCE INTERVAL -----
106   ZZ = 1./FLOAT(NOB-NPAR)
      SDEV = DSQRT(ZZ*SUMS)
      WRITE(*,1052)
      WRITE(12,1052)
1052  FORMAT(//11X,'NON-LINEAR LEAST-SQUARES ANALYSIS: FINAL RESULTS'/
     111X,48(1H=)/53X,'95% CONFIDENCE LIMITS'/11X,'VARIABLE',8X,'VALUE',
     27X,'S.E.COEFF.',4X,'LOWER',8X,'UPPER')
      TVAR=1.96+ZZ*(2.3779+ZZ*(2.7135+ZZ*(3.187936+2.466666*ZZ**2)))
      DO 108 I=1,NPAR
       SECOEF=SNGL(E(I))*SDEV
       TSEC=TVAR*SECOEF
       TMCOE=X2(I)-TSEC
       TPCOE=X2(I)+TSEC
       WRITE(*,109) PNAMA(I),X2(I),SECOEF,TMCOE,TPCOE
       WRITE(12,109) PNAMA(I),X2(I),SECOEF,TMCOE,TPCOE
108   CONTINUE
109   FORMAT(1X,A12,1X,4(F14.3,1X))

      CALL OPTIMIZATION_FINAL_REPORT(FC2)

8000  CLOSE(UNIT=11)
      CLOSE(UNIT=12)
8888  STOP 'OKAY'
      END
C-----------------------------------------------------------------------
      SUBROUTINE OPTIMIZATION_INITIAL_REPORT(FC)
C
C     PURPOSE: TO REPORT THE MATCH OF OBSERVATION AND INITIAL-GUESS
C              CALCULATION
C
      PARAMETER (MNOB=500,MPAR=8,MTYP=5,NDIM=100)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION FC(MNOB)
      INCLUDE 'tfcombk.dat'

      WRITE(12,*) 'INITIAL OBS-CAL FITTING:'
      WRITE(12,*) 'TIME   OBS-HC   CAL-HC  DFHC  OBS-Q  CAL-Q  DFQ'
      DO 6 I=1,NTOB
       NH=2*I-1
       NQ=2*I
       DFHC=abs(FO(NH)-FC(NH))
       DFQ=abs(FO(NQ)-FC(NQ))
       WRITE(12,7) FTIME(I),FO(NH),FC(NH),DFHC,FO(NQ),FC(NQ),DFQ
6     CONTINUE
      I=NTOB+1
      NTH=2*I-1
      DFTH=ABS(FO(NTH)-FC(NTH))
      WRITE(12,8) FTIME(I),FO(NTH),FC(NTH),DFTH
7     FORMAT(1X,7(F9.3,1X))
8     FORMAT(1X,4(F9.3,1X))
      WRITE(12,*)
```

```
      RETURN
      END
C----------------------------------------------------------------------
      SUBROUTINE OPTIMIZATION_FINAL_REPORT(FC)
C
C     PURPOSE: TO REPORT THE OPTIMIZATION RESULTS
C
      PARAMETER (MNOB=500,MPAR=8,MTYP=5,NDIM=100)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION FC(MNOB)
      INCLUDE 'tfcombk.dat'

C     ----- PREPARE FINAL OUTPUT -----
      IF (IEQ .EQ. 1) PVALA(6) = 1-1/PVALA(5)
      DO 2 I=1,MPAR
       WRITE(*,*) PNAMI(I),'=',PVALA(I)
       WRITE(12,*) PNAMI(I),'=',PVALA(I)
2     CONTINUE
      CKSW=(3600*980)*PVALA(3)/CMUW
      CKSNW=CKSW*RATIOK

      WRITE(12,*) 'Ksw (cm/hr) =',CKSW
      WRITE(12,*) 'Ksnw (cm/hr)=',CKSNW
      WRITE(12,*)
      WRITE(12,*) 'FINAL OBS-CAL FITTING:'
      WRITE(12,*) 'TIME   OBS-HC   CAL-HC  DFHC  OBS-Q  CAL-Q  DFQ'
      DO 6 I=1,NTOB
       NH=2*I-1
       NQ=2*I
       DFHC=abs(FO(NH)-FC(NH))
       DFQ=abs(FO(NQ)-FC(NQ))
       WRITE(12,7) FTIME(I),FO(NH),FC(NH),DFHC,FO(NQ),FC(NQ),DFQ
6     CONTINUE
      I=NTOB+1
      NTH=2*I-1
      DFTH=ABS(FO(NTH)-FC(NTH))
      WRITE(12,8) FTIME(I),FO(NTH),FC(NTH),DFTH
7     FORMAT(1X,7(F9.3,1X))
8     FORMAT(1X,4(F9.3,1X))

      RETURN
      END
C----------------------------------------------------------------------
      SUBROUTINE SIMULATION_REPORT(FC)
C
C     PURPOSE: TO REPORT THE SIMULATION RESULTS
C
      PARAMETER (MNOB=500,MPAR=8,MTYP=5,NDIM=100)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION FC(MNOB)
      INCLUDE 'tfcombk.dat'

      WRITE(12,*) 'Observation depth Z=',Z(iobsnode)
      WRITE(12,*) '  Time   hc   ohc    Qw    OQw     Sw    Snw'
      WRITE(*,*) 'Observation depth Z=',Z(iobsnode)
      WRITE(*,*) '  Time   hc   ohc    Qw    OQw     Sw    Snw'
      DO 5 I=1,NTOB
       NH=2*I-1
```

```
        NQ=2*I
        HA=FC(NH)
        HW=0.
        CALL COEFT(HW,HA,CKW,CKA,CWW,CAA,CWA,SW,SA)
        WRITE(12,7) FTIME(I),FC(NH),FO(NH),FC(NQ),FO(NQ),SW,SA
        WRITE(*,7) FTIME(I),FC(NH),FO(NH),FC(NQ),FO(NQ),SW,SA
5      CONTINUE
7      FORMAT(1X,7(F9.3,1X))

       RETURN
       END
C----------------------------------------------------------------------
       SUBROUTINE QRSOLV(A,NP,B)
C
C      PURPOSE: TO SOLVE LINEAR SYSTEM A*X=B BY QR-DECOMPOSITION
C               WHERE A IS J'*J , B IS J'*R, AND ' DENOTES TRANSPOSE.
C               THE SOLUTION X IS THE PARAMETER CORRECTION
C
       PARAMETER (MNOB=500,MPAR=8,MTYP=5,NDIM=100)
       IMPLICIT REAL*8 (A-H,O-Z)
       DIMENSION A(MPAR,MPAR),B(MPAR),A1(MPAR),A2(MPAR)
C
C      REDUCE A TO UPPER TRIANGULAR FORM BY HOUSEHOLDER TRANSFORMATIONS
C      ----------
       IF(NP.EQ.1) THEN
       B(NP)=B(NP)/A(NP,NP)
       GO TO 300
       ENDIF
       NR=NP-1
       DO 200 K=1,NR
        IF (A(K,K) .EQ. 0.) THEN
           A1(K) = 0.
           GO TO 200
        ENDIF
        SS = 0.
        DO 20 I = K,NP
           A(I,K) = A(I,K)
           SS = SS+A(I,K)*A(I,K)
20       CONTINUE
        SIGM = DSQRT(SS)
        IF (A(K,K) .LT. 0.) SIGM = -SIGM
        A(K,K) = A(K,K)+SIGM
        TERM = SIGM*A(K,K)
        A1(K) = TERM
        A2(K) = -SIGM
        DO 100 J = K+1,NP
           SS = 0.0
           DO 80 I = K,NP
              SS = SS+A(I,K)*A(I,J)
80            CONTINUE
           SS = SS/TERM
           DO 90 I = K,NP
              A(I,J) = A(I,J)-SS*A(I,K)
90            CONTINUE
100      CONTINUE
200    CONTINUE
       A2(NP) = A(NP,NP)
C
```

```
C     ------ APPLY TRANSFORMATIONS TO B ------
      DO 230 J = 1,NR
       SS = 0.
       DO 210 I = J,NP
          SS = SS+A(I,J)*B(I)
210       CONTINUE
       SS = SS/A1(J)
       DO 220 I = J,NP
         B(I) = B(I)-SS*A(I,J)
220      CONTINUE
230   CONTINUE

C     ------ SOLVE TRIANGULAR SYSTEM -----
      B(NP) = B(NP)/A2(NP)
      DO 260 I = NR,1,-1
       SS = 0.
       DO 250 J=I+1,NP
          SS = SS+A(I,J)*B(J)
250      CONTINUE
       B(I) = (B(I)-SS)/A2(I)
260   CONTINUE

C     ----- DONE, SOLUTION IS RETURNED IN B -----
300   RETURN
      END
C----------------------------------------------------------------------
      SUBROUTINE MATINV(A,NP)
C
C     PURPOSE : TO INVERT J'*J
C     ----------
      PARAMETER (MNOB=500,MPAR=8,MTYP=5,NDIM=100)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION A(MPAR,MPAR),TINDX(6,2)

      DO 2 J=1,6
    2 TINDX(J,1)=0
      I=0
    4 AMAX=-1.0D0
      DO 12 J=1,NP
      IF(TINDX(J,1).NE.0.0) GO TO 12
    6 DO 10 K=1,NP
      IF(TINDX(K,1).NE.0.0) GO TO 10
    8 P=DABS(A(J,K))
      IF(P.LE.AMAX) GO TO 10
      IR=J
      IC=K
      AMAX=P
   10 CONTINUE
   12 CONTINUE
      IF(AMAX) 30,30,14
   14 TINDX(IC,1)=IR
      IF(IR.EQ.IC) GO TO 18
      DO 16 L=1,NP
      P=A(IR,L)
      A(IR,L)=A(IC,L)
   16 A(IC,L)=P
      I=I+1
      TINDX(I,2)=IC
```

```
   18 P=1./A(IC,IC)
      A(IC,IC)=1.
      DO 20 L=1,NP
   20 A(IC,L)=A(IC,L)*P
      DO 24 K=1,NP
      IF(K.EQ.IC) GO TO 24
      P=A(K,IC)
      A(K,IC)=0.0
      DO 22 L=1,NP
   22 A(K,L)=A(K,L)-A(IC,L)*P
   24 CONTINUE
      GO TO 4
   26 IC=TINDX(I,2)
      IR=TINDX(IC,1)
      DO 28 K=1,NP
      P=A(K,IR)
      A(K,IR)=A(K,IC)
   28 A(K,IC)=P
      I=I-1
   30 IF(I) 26,32,26
   32 RETURN
      END
C-----------------------------------------------------------------------
      SUBROUTINE INPUT(FREEPAR)
      PARAMETER (MNOB=500,MPAR=8,MTYP=5,NDIM=100)
      IMPLICIT REAL*8 (A-H,O-Z)
      INCLUDE 'tfcombk.dat'
      DIMENSION FREEPAR(MPAR),NOBS(MNOB),SUMFO(MNOB),AVFO(MTYP)
      DIMENSION SETWT(MTYP)

      READ(11,*)
C..   PART I:  MODELLING DATA
      READ(11,*)
      READ(11,*)
      READ(11,*)
      READ(11,*) NNP,IFNODE,IOBSNODE,SLENTH,PLTLENTH,DIAM
      READ(11,*)
      READ(11,*)
      READ(11,*) (PLTPROP(I),I=1,2)
      READ(11,*)
      READ(11,*)
      READ(11,*) RHOW,RHONW,CMUW,CMUNW
      READ(11,*)
      READ(11,*) TMAX,DTMAX,IDT,DT1,ERR
      READ(11,*)
      READ(11,*) IEQ
      READ(11,*)
      READ(11,*)
      READ(11,*) MODE
      READ(11,*)
      READ(11,*) hnw0,HB0
      READ(11,*)
      READ(11,*) ITIM
      READ(11,*)
      DO 2 I=1,ITIM
       READ(11,*) TIM(I),PB(I)
2     CONTINUE
      RATIOK=CMUW/CMUNW
```

```
      AREA=3.14156*DIAM**2/4
      n1=IFNODE-1
      n2=NNP-1
      dz1=PLTLENTH/n1
      dz2=SLENTH/(NNP-IFNODE)
      do 10 i=1,n1
10    z(i)=(i-1)*dz1
      do 20 i=n1,n2
20    z(i+1)=PLTLENTH+(i-IFNODE+1)*dz2

C..   PART II:  OPTIMIZATION DATA
      READ(11,*)
      READ(11,*)
      READ(11,*) MAXTRY,MIT
      READ(11,*)
      READ(11,*) NTOB,IPAR,ITYP
      NOB=2*NTOB+1
      NOA=NOB-1
      READ(11,*)
      READ(11,*)
      READ(11,*) (SETWT(I),I=1,ITYP)
      READ(11,*)
      DO 29 I=1,IPAR
       READ(11,'(A16)') PNAMI(I)
29    CONTINUE
      READ(11,*)
      READ(11,*)
      DO 30 I=1,IPAR
       READ(11,*) PVALI(I),PMINI(I),PMAXI(I),IOPT(I)
30    CONTINUE

      READ(11,*)
      READ(11,*)
      DO 40 I=1,NTOB
       READ(11,*) DUMTIME,HC,QW,HB(I)
       FTIME(I)=DUMTIME
       FO(2*I-1)=HC
       FO(2*I)=QW
       IDATTYP(2*I-1)=1
       WGHT(2*I-1)=SETWT(1)
       IDATTYP(2*I)=2
       WGHT(2*I)=SETWT(2)
   40 CONTINUE
      READ(11,*) FTIME(NTOB+1),FO(NTOB*2+1)
      IDATTYP(NTOB*2+1)=3
      WGHT(NTOB*2+1)=SETWT(3)

C...  wls : adjustment weights according to IDATTYP -----
      DO 50 I = 1,ITYP
       SUMFO(I) = 0.
       NOBS(I) = 0
50    CONTINUE
      DO 60 I = 1,NOB
       SUMFO(IDATTYP(I)) = SUMFO(IDATTYP(I))+FO(I)
       NOBS(IDATTYP(I)) = NOBS(IDATTYP(I))+1
60    CONTINUE
      DO 70 I = 1,ITYP
       IF (NOBS(I) .GT. 0)  AVFO(I) = SUMFO(I)/REAL(NOBS(I))
```

```
70    CONTINUE
      DO 72 I = 1,ITYP
       SETWT(I) = SETWT(I) * DABS( DBLE(AVFO(2) / AVFO(I)) )
72    CONTINUE
      DO 80 I = 1,NOB
       WGHT(I) = WGHT(I) * DABS(DBLE(AVFO(2) /AVFO(IDATTYP(I))))
80    CONTINUE

C...  rearrange parameter array
      NPAR = 0
      DO 90 I = 1,IPAR
       PVALA(I) = PVALI(I)
       IF (IOPT(I) .EQ. 1) THEN
          NPAR = NPAR+1
          PNAMA(NPAR) = PNAMI(I)
          FREEPAR(NPAR) = PVALI(I)
          PMINA(NPAR) = PMINI(I)
          PMAXA(NPAR) = PMAXI(I)
          TRFPAR(NPAR) = I
        ENDIF
90    CONTINUE

      RETURN
      END
C-----------------------------------------------------------------------
      SUBROUTINE MODEL(FC)
      PARAMETER (MNOB=500,MPAR=8,MTYP=5,NDIM=100)
      IMPLICIT REAL*8 (A-H,O-Z)
      INCLUDE 'tfcombk.dat'
      DIMENSION FC(MNOB)
      DIMENSION A(2*NDIM,2*NDIM),GG(2*NDIM,2*NDIM)
      DIMENSION G(2*NDIM),PHI(2*NDIM),PHINEW(2*NDIM)
      DIMENSION SW(NDIM),SA(NDIM)
      DATA CUMBW,CUMSA,cumq/0.,0.,0./
      DATA IDT,DT1 /1,0.1/

C...  INITIALIZATION
      WRITE(*,*) 'START SIMULATION NOW.'
      CALL INITIATION(PHI,PHINEW)
      IF (MODE .EQ. 1) THEN
       CALL VOLUME(PHI,VSW1,VSA1)
       VW=VSW1*AREA
       WRITE(12,*) 'INI. SOIL WATER VOLUME (POROSITY=',pvala(1),'):',VW
      ENDIF

      CALL VOLUME(PHI,VSW1,VSA1)
      VW=VSW1*AREA
      TIME=0.
      NUM=0
      NTRY=0
      cumq=0.
      NP2=NNP*2

C.... START A TIME STEP ..............................................
50    CONTINUE

C...  SET UP THE GLOBAL MATRIX
      CALL EQ(A,G,GG,PHINEW,PHI)
```

```
C...  DIRECT EQ SOLVER
      CALL BDEQSOL(A,G,NP2)

C...  CHECK CONVERGENCE OF SOLUTION: PICARD ITERATION
      NUM=NUM+1
      CALL CONV(G,PHINEW,DMAXW,DMAXA)
      IF (DMAXW.GT.ERR .OR. DMAXA.GT.ERR) THEN
        IF (NUM.EQ.200) GO TO 63
        IF (NUM.LT.200) GO TO 50
63        DT=0.75*DT
        DT1=DT
        NUM=0
        GO TO 50
      ENDIF

C.... A SUCCESS TIME STEP DT .........................
      TIME=TIME+DT

C...  DETERMINE THE FLUX OF WATER AND AIR AT THE BOTTOM AND TOP BOUNDARIES
      CALL FLUX(G,GG)

C...  CALCULATE SATURATIONS
      NP1=2*NNP-1
      N=0
      DO 100 I=1,NP1,2
       N=N+1
       CPW=G(I)-Z(N)*RHOW
       CPA=G(I+1)-RHONW*Z(N)
       CALL COEFT(CPW,CPA,CKW,CKA,CWW,CAA,CWA,SW(N),SA(N))
100   CONTINUE

C...  STORAGE CHANGE & MASS BALANCE ERROR
      CALL VOLUME(G,VSW,VSA)
      DQW=QBW
      DQA=QSA
      DVW=VSW-VSW1
      DVA=VSA-VSA1
      cumq=cumq-DVW*AREA
      ERRW=ABS(ABS(DQW)-ABS(DVW))
      ERRA=ABS(ABS(DQA)-ABS(DVA))

C...  OUTPUT RESULTS FOR THIS TIME STEP
      CALL OUTPUT(G,FC)

C...  UPDATE FOR NEXT TIME STEP
99    IF (TIME.GE.TMAX) GO TO 1000
      VSW1=VSW
      VSA1=VSA
      DO 156 I=1,NNP
       PHI(2*I)=PHINEW(2*I)
       PHI(2*I-1)=PHINEW(2*I-1)
156   CONTINUE

C...  CONTROLABLE TIME STEP DT
      NUM=0
      DTOLD=DT
      CALL NEWDT
```

```
      IF (DT.EQ.0.0) THEN
       WRITE(*,*) 'TIME STEP IS ZERO'
       GO TO 1000
      ENDIF

      GO TO 50

1000  RETURN
      END
C----------------------------------------------------------------------
      SUBROUTINE INITIATION(PHI,PHINEW)
      PARAMETER (MNOB=500,MPAR=8,MTYP=5,NDIM=100)
      IMPLICIT REAL*8 (A-H,O-Z)
      INCLUDE 'tfcombk.dat'
      DIMENSION PHINEW(2*NDIM),PHI(2*NDIM)

      CUMBW=0.
      CUMSA=0.
      NTIM=1
      NTOUT=1
      TIMOUT=FTIME(NTOUT)
      DT=DT1
      DTC=DT

      HBB=(HB0+HB(1))/2
      IF (MODE .GT. 0) THEN
          DO 5 I=1,NNP
           PHI(2*I-1)=HBB
             PHI(2*I)=hnw0
             HW=PHI(2*I-1)-RHOW*Z(I)
             HA=PHI(2*I)-RHONW*Z(I)
             IF(HA .LE. HW) stop 'Pc<=0 Error --> Check the I.C.!'
5         CONTINUE
      ENDIF
      IF (MODE .LT. 0) THEN
          HW_TOP=hnw0-RHONW*Z(NNP)
            DO 6 I=1,NNP
             PHI(2*I-1)=HBB-HW_TOP
             PHI(2*I)=RHONW*Z(NNP)
             HW=PHI(2*I-1)-RHOW*Z(I)
             HA=PHI(2*I)-RHONW*Z(I)
             IF(HA .LE. HW) stop 'Pc<=o Error --> Check the I.C.!'
6           CONTINUE
      ENDIF
      NP2=NNP*2
      DO 10 I=1,NP2
10    PHINEW(I)=PHI(I)
      RETURN
      END
C----------------------------------------------------------------------
      SUBROUTINE OUTPUT(G,FC)
      PARAMETER (MNOB=500,MPAR=8,MTYP=5,NDIM=100)
      IMPLICIT REAL*8 (A-H,O-Z)
      INCLUDE 'tfcombk.dat'
      DIMENSION G(2*NDIM)
      DIMENSION HW(NDIM),HA(NDIM),HTW(NDIM),HTA(NDIM)
      DIMENSION FC(MNOB)
```

```
      J=0
      NP1=2*NNP-1
      DO 90 I=1,NP1,2
       J=J+1
       HW(J)=G(I)-Z(J)*RHOW
       HTW(J)=G(I)
       HA(J)=G(I+1)-RHONW*Z(J)
       HTA(J)=G(I+1)
90    CONTINUE

      IF (NTOUT .GT. NTOB) GO TO 99
      IF ((TIME-0.0001).LT.TIMOUT.AND.(TIME+0.0001).GT.TIMOUT) THEN
         NH=2*NTOUT-1
         NQ=2*NTOUT
           FC(NH)=HA(IOBSNODE)-HW(IOBSNODE)
         FC(NQ)=cumq
c        DFH=ABS(FC(NH)-abs(FO(NH)))
c              DFQ=ABS(FC(NQ)-abs(FO(NQ)))
c        WRITE(*,95) TIMOUT,FC(NH),abs(FO(NH)),DFH,IDATTYP(NH)
c        WRITE(12,95) TIMOUT,FC(NH),abs(FO(NH)),DFH,IDATTYP(NH)
c        WRITE(*,95) TIMOUT,FC(NQ),abs(FO(NQ)),DFQ,IDATTYP(NQ)
c        WRITE(12,95) TIMOUT,FC(NQ),abs(FO(NQ)),DFQ,IDATTYP(NQ)
         NTOUT=NTOUT+1
         IF (NTOUT .GT. NTOB) THEN
            N=IOBSNODE
            HAA=FTIME(NTOUT)
            HWW=0.
            CALL COEFT(HWW,HAA,CKW,CKA,CWW,CAA,CWA,SWW,SAA)
            NTH=2*NTOUT-1
            FC(NTH) = SWW*PVALA(1)
c           DF=ABS(FC(NTH)-FO(NTH))
c           WRITE(*,95) FTIME(NTH),FC(NTH),FO(NTH),DF,IDATTYP(NTH)
c           WRITE(12,95) FTIME(NTH),FC(NTH),FO(NTH),DF,IDATTYP(NTH)
              TIMOUT = FTIME(NTOUT-1)
              GO TO 99
            ENDIF
          TIMOUT=FTIME(NTOUT)
          HBB=(HB(NTOUT-1)+HB(NTOUT))/2
      ENDIF
95    FORMAT(1X,4(F9.3,1X),I5)
99    RETURN
      END
C-----------------------------------------------------------------------
C...  SUBROUTINE TO BUILD THE TWO-PHASE FLOW COEFFICIE MATRICES
C..
      SUBROUTINE EQ(A,G,GG,PHINEW,PHI)
      PARAMETER (MNOB=500,MPAR=8,MTYP=5,NDIM=100)
      IMPLICIT REAL*8 (A-H,O-Z)
      INCLUDE 'tfcombk.dat'
      DIMENSION GG(2*NDIM,2*NDIM),DD(2*NDIM,2*NDIM),A(2*NDIM,2*NDIM)
      DIMENSION G(2*NDIM),PHINEW(2*NDIM),PHI(2*NDIM)
      DIMENSION COND(4,4),CAP(4,4),DTH(2*NDIM)

C...  DETERMINE HALF-TIME AND ESTIMATED NEW-TIME HYDRAULIC HEAD
      NP2=NNP*2
      DO 291 I=1,NP2
       DO 290 J=1,NP2
          GG(I,J)=0.0
```

```
         DD(I,J)=0.0
290    CONTINUE
291   CONTINUE

      DO 330 I=1,4
      DO 330 J=1,4
       CAP(I,J)=0.0
330   COND(I,J)=0.0

      NELEM=NNP-1
      DO 320 N=1,NELEM
       ZLENTH=Z(N+1)-Z(N)
       HW1=PHINEW(2*N-1)-Z(N)*RHOW
       HA1=PHINEW(2*N)-RHONW*Z(N)
       HW2=PHINEW(2*(N+1)-1)-Z(N+1)*RHOW
       HA2=PHINEW(2*(N+1))-RHONW*Z(N+1)
       CALL COEFT(HW1,HA1,CKW1,CKA1,CWW1,CAA1,CWA1,SW1,SA1)
       CALL COEFT(HW2,HA2,CKW2,CKA2,CWW2,CAA2,CWA2,SW2,SA2)
C...  EVALUATE THE CAPACITANCE INTEGRAL FOR ELEME N
       CAP(1,1)=ZLENTH*CWW1/2.
       CAP(1,2)=ZLENTH*CWA1/2.
       CAP(2,2)=ZLENTH*CAA1/2.
       CAP(3,3)=ZLENTH*CWW2/2.
       CAP(3,4)=ZLENTH*CWA2/2.
       CAP(4,4)=ZLENTH*CAA2/2.
       CAP(2,1)=CAP(1,2)
       CAP(4,3)=CAP(3,4)

C...  EVALUATE THE CONDUCTIVITY INTEGRAL FOR ELEME N
       TKW=0.5*(CKW1+CKW2)/ZLENTH
       TKA=0.5*(CKA1+CKA2)/ZLENTH
       COND(1,1)=TKW
       COND(1,3)=-TKW
       COND(3,1)=-TKW
       COND(3,3)=TKW
       COND(2,2)=TKA
       COND(2,4)=-TKA
       COND(4,2)=-TKA
       COND(4,4)=TKA

C...  CONSTRUCT THE GLOBAL STIFFNESS MATRICES GG AND DD
       DO 360 I=1,4
          NROW=2*N-2+I
          DO 350 J=1,4
             NCOL=2*N-2+J
             GG(NROW,NCOL)=GG(NROW,NCOL)+COND(I,J)
             DD(NROW,NCOL)=DD(NROW,NCOL)+CAP(I,J)
350         CONTINUE
360    CONTINUE

320   CONTINUE

      DO 61 I=1,NP2
       DO 60 J=1,NP2
          A(I,J)=GG(I,J)*DT+DD(I,J)
60     CONTINUE
61    CONTINUE
```

```
      CALL DTHET(PHINEW,PHI,DTH)

      DO 80 I=1,NP2
       G(I)=0.
       DO 70 J=1,NP2
          G(I)=G(I)+DD(I,J)*PHINEW(J)
70       CONTINUE
       G(I)=G(I)-DTH(I)
80    CONTINUE

C...  TOP & BOTTOM B.C.TREATMENT
      DO 90 J=1,NP2
       A(1,J)=0.
       A(NP2,J)=0.
90    CONTINUE
      A(1,1)=1.
      A(NP2,NP2)=1.
      IF (MODE .GT. 0) THEN
          PHINEW(1)=HBB+Z(1)*RHOW
          PHINEW(NP2)=PB(NTIM)+Z(NNP)*RHONW
      ENDIF
      IF (MODE .LT. 0) THEN
          PHINEW(1)=HBB+Z(1)*RHOW-PB(NTIM)
          PHINEW(NP2)=RHONW*Z(NNP)
          DO 95 I=1,NNP
             DO 93 J=1,NP2
                A(2*I,J)=0.
93           CONTINUE
             A(2*I,2*I)=1.
             PHINEW(2*I)=RHONW*Z(NNP)
             G(2*I)=PHINEW(2*I)
95      CONTINUE
      ENDIF
      G(1)=PHINEW(1)
      G(NP2)=PHINEW(NP2)

      RETURN
      END
C----------------------------------------------------------------------
      SUBROUTINE BDEQSOL(AA,BB,NN)
      PARAMETER (MNOB=500,MPAR=8,MTYP=5,NDIM=100)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION AA(2*NDIM,2*NDIM),BB(2*NDIM),X(2*NDIM),Y(2*NDIM)
      DIMENSION ALPHA(2*NDIM),GAMA(2*NDIM),BETA(2*NDIM)

C...  TRANSFOR QUINDIAGONAL MATRIX TO UPPER DIAGONAL MATRIX
      I=1
      ALPHA(I)=AA(I,I)
      IF (ALPHA(I) .EQ. 0.) GO TO 400
      BETA(I)=AA(I,I+1)/ALPHA(I)
      GAMA(I)=AA(I,I+2)/ALPHA(I)
      Y(I)=BB(I)/ALPHA(I)

      I=2
      ALPHA(I)=AA(I,I)-AA(I,I-1)*BETA(I-1)
      IF (ALPHA(I) .EQ. 0.) GO TO 400
      BETA(I)=(AA(I,I+1)-AA(I,I-1)*GAMA(I-1))/ALPHA(I)
      GAMA(I)=AA(I,I+2)/ALPHA(I)
```

```
      Y(I)=(BB(I)-AA(I,I-1)*Y(I-1))/ALPHA(I)
      DO 100 I=3,NN-2
       A=AA(I,I-2)
       B=AA(I,I-1)
       C=AA(I,I)
       D=AA(I,I+1)
       E=AA(I,I+2)
       F=BB(I)
       DUM=B-A*BETA(I-2)
       ALPHA(I)=C-A*GAMA(I-2)-DUM*BETA(I-1)
       IF (ALPHA(I) .EQ. 0.) GO TO 400
       BETA(I)=(D-DUM*GAMA(I-1))/ALPHA(I)
       GAMA(I)=E/ALPHA(I)
       Y(I)=(F-A*Y(I-2)-DUM*Y(I-1))/ALPHA(I)
100   CONTINUE

      I=NN-1
      DUM=AA(I,I-1)-AA(I,I-2)*BETA(I-2)
      ALPHA(I)=AA(I,I)-AA(I,I-2)*GAMA(I-2)-DUM*BETA(I-1)
      IF (ALPHA(I) .EQ. 0.) GO TO 400
      BETA(I)=(AA(I,I+1)-DUM*GAMA(I-1))/ALPHA(I)
      GAMA(I)=0.
      Y(I)=(BB(I)-AA(I,I-2)*Y(I-2)-DUM*Y(I-1))/ALPHA(I)

      I=NN
      DUM=AA(I,I-1)-AA(I,I-2)*BETA(I-2)
      ALPHA(I)=AA(I,I)-AA(I,I-2)*GAMA(I-2)-DUM*BETA(I-1)
      IF (ALPHA(I) .EQ. 0.) GO TO 400
      BETA(I)=0.
      GAMA(I)=0.
      Y(I)=(BB(I)-AA(I,I-2)*Y(I-2)-DUM*Y(I-1))/ALPHA(I)

C...  BACKWARD SUBSTITUTION FROM LAST ROW
      X(NN)=Y(NN)
      X(NN-1)=Y(NN-1)-BETA(NN-1)*X(NN)
      DO 200 J=1,NN-2
       I=NN-1-J
       X(I)=Y(I)-BETA(I)*X(I+1)-GAMA(I)*X(I+2)
200   CONTINUE

      DO 300 I=1,NN
       BB(I)=X(I)
300   CONTINUE
      GO TO 500

400   WRITE(*,*) 'Sigular EQ:  '
      WRITE(*,*) '- In 1st iteration: Check your initial parameter set.'
      WRITE(*,*) '- After some iterations: Check your parameter limits.'
      WRITE(*,*) 'Stop here.'
      STOP
500   RETURN
      END
C-----------------------------------------------------------------------
      SUBROUTINE NEWDT
      PARAMETER (MNOB=500,MPAR=8,MTYP=5,NDIM=100)
      IMPLICIT REAL*8 (A-H,O-Z)
      INCLUDE 'tfcombk.dat'
```

```
      IF (IDT.EQ.0) THEN
       IF (DT.LT.DT1) THEN
          DT=DT1
       ELSE
          IF (NUM.LT.4) DT=1.04*DT
          IF (NUM.GE.12) DT=DT/1.04
          IF (DT.GT.DTMAX) DT=DTMAX
          DT1=DT
       ENDIF
      ELSE
       DT=DTC
      ENDIF

      IF (NTOUT.GT.NTOB) GO TO 101

      IF ((TIME+DT) .GT. TIMOUT) DT=TIMOUT-TIME
101   IF ((TIME+DT) .GT. TMAX) DT=TMAX-TIME
      IF (NTIM .LT. ITIM) THEN
       I=NTIM+1
       IF (TIME+DT .GT. TIM(I)) DT=TIM(I)-TIME
       IF (TIME.GE.(TIM(I)-0.0001).AND.TIME.LE.(TIM(I)+0.0001)) THEN
          NTIM=NTIM+1
          DT=0.001
       ENDIF
      ENDIF

      RETURN
      END
C----------------------------------------------------------------------
      SUBROUTINE CONV(G,PHINEW,DMAXW,DMAXA)
      PARAMETER (MNOB=500,MPAR=8,MTYP=5,NDIM=100)
      IMPLICIT REAL*8(A-H,O-Z)
      INCLUDE 'tfcombk.dat'
      DIMENSION G(2*NDIM),PHINEW(2*NDIM)
      DIMENSION SP(2),WP(2),WPS(2),WP1(2)

      EP1=20.
      EP2=20.
      NP2=2*NNP
      IIT=1

      PMAX1=0.0
      PMAX2=0.0
      DO 90 I=1,NNP
       PMAX1=MAX(PMAX1,ABS(G(2*I-1)))
90    PMAX2=MAX(PMAX2,ABS(G(2*I)))

      DMAXW=0.0
      DMAXA=0.0
      DO 100 I=1,NNP
       p1=g(2*I-1)
       p2=g(2*I)
       if (p1.eq.0.0) p1=1.
       if (p2.eq.0.0) p2=1.
       RERRW=DABS((PHINEW(2*I-1)-G(2*I-1))/p1)
       RERRA=DABS((PHINEW(2*I)-G(2*I))/p2)
       AERRW=DABS(PHINEW(2*I-1)-G(2*I-1))
       AERRA=DABS(PHINEW(2*I)-G(2*I))
```

```
      IF (RERRW.GT.DMAXW.AND.AERRW.GT.0.001) THEN
         DMAXW=RERRW
         DPHIW=G(2*I-1)-PHINEW(2*I-1)
         NODE1=I
      ENDIF

      IF (RERRA.GT.DMAXA.AND.AERRA.GT.0.001) THEN
         DMAXA=RERRA
         DPHIA=G(2*I)-PHINEW(2*I)
         NODE2=I
      ENDIF

100  CONTINUE

     IF (IIT.EQ.0) THEN
      DO 115 I=1,NNP
         PHINEW(2*I-1)=G(2*I-1)
         PHINEW(2*I)=G(2*I)
         HW=G(2*I-1)-Z(I)*RHOW
         HA=G(2*I)-RHONW*Z(I)
         IF ((HA .LE. HW) .AND. (I .GE. IFNODE)) THEN
             PHINEW(2*I-1)=HA+RHOW*Z(I)-0.01
         ENDIF
115   CONTINUE
     ELSE
      IF (NUM.EQ.1) THEN
         SP(1)=0.00
         SP(2)=0.00
      ELSE
         IF (DPHIW0.EQ.0.00) DPHIW0=1.0
         IF (DPHIA0.EQ.0.00) DPHIA0=1.0
         SP(1)=DPHIW/(WP(1)*DPHIW0)
         SP(2)=DPHIA/(WP(2)*DPHIA0)
      ENDIF

      IF (SP(1).GE.-1.00) THEN
         WPS(1)=(3.+SP(1))/(3.+DABS(SP(1)))
      ELSE
         WPS(1)=1/(2.*DABS(SP(1)))
      ENDIF

      IF (SP(2).GE.-1.00) THEN
         WPS(2)=(3.+SP(2))/(3.+DABS(SP(2)))
      ELSE
         WPS(2)=1/(2.*DABS(SP(2)))
      ENDIF

      IF (WPS(1)*DABS(DPHIW).LE.EP1) THEN
         WP1(1)=WPS(1)
      ELSE
         WP1(1)=EP1/DABS(DPHIW)
      ENDIF

      IF (WPS(2)*DABS(DPHIA).LE.EP2) THEN
         WP1(2)=WPS(2)
      ELSE
         WP1(2)=EP2/DABS(DPHIA)
```

```
        ENDIF

          TMP1=G(1)
        TMP2=G(NP2)
        DO 103 I=1,NNP
           G(2*I-1)=WP1(1)*(G(2*I-1)-PHINEW(2*I-1))+PHINEW(2*I-1)
           PHINEW(2*I-1)=G(2*I-1)
           G(2*I)=WP1(2)*(G(2*I)-PHINEW(2*I))+PHINEW(2*I)
           PHINEW(2*I)=G(2*I)
           HW=G(2*I-1)-Z(I)*RHOW
           HA=G(2*I)-RHONW*Z(I)
           IF ((HA .LE. HW) .AND. (I .GE. IFNODE)) THEN
                 PHINEW(2*I-1)=HA+RHOW*Z(I)-0.01
           ENDIF
103       CONTINUE
          G(1)=TMP1
          G(NP2)=TMP2
        PHINEW(1)=G(1)
        PHINEW(NP2)=G(NP2)

        WP(1)=WP1(1)
        WP(2)=WP1(2)
        DPHIW0=DPHIW
        DPHIA0=DPHIA
       ENDIF

       RETURN
       END
C-----------------------------------------------------------------------
       SUBROUTINE COEFT(HW,HA,CKW,CKA,CWW,CAA,CWA,SW,SA)
       PARAMETER (MNOB=500,MPAR=8,MTYP=5,NDIM=100)
       IMPLICIT REAL*8 (A-H,O-Z)
       INCLUDE 'tfcombk.dat'
C..
C...   VAN GENUCHTEN RETENSION FUNCTION
C..
       PA=3.1415927
       TS=PVALA(1)
       TR=PVALA(2)
       SR=TR/TS
       CKSW=(3600*980)*PVALA(3)/CMUW
       CKSA=CKSW*RATIOK
       HAW=HA-HW
       IF (N.LE.NNP .AND. N.GE.IFNODE) THEN
        A=PVALA(4)
        B=PVALA(5)
        C=PVALA(6)
        DDD1=PVALA(7)
          DDD2=PVALA(8)
        IF (HAW .GE. 0.) THEN
C.........VGM_model
           IF (IEQ .EQ. 1) THEN
              AM=(1.-1./B)
              SWE=(1./(1.+(A*HAW)**B))**AM
              SW=(1.-SR)*SWE+SR
              SA=1.0-SW
              CWW=TS*A*(B-1.)*(1.-SR)*(SWE**(1./AM))
              CWW=CWW*(1.-SWE**(1./AM))**AM
```

```
            CAA=CWW
            CWA=-CWW
            CKW=CKSW*(SWE**DDD1)*(1.-(1.-SWE**(1./AM))**AM)**2.
            CKA=CKSA*((1.0-SWE)**DDD1)*(1.-SWE**(1./AM))**(2.*AM)
         ENDIF
C.........VGB_model
         IF (IEQ .EQ. 2) THEN
            AM=(1.-2./B)
            SWE=(1./(1.+(A*HAW)**B))**AM
            SW=(1.-SR)*SWE+SR
            SA=1.0-SW
            CWW=TS*A*(B-1.)*(1.-SR)*(SWE**(1./AM))
            CWW=CWW*(1.-SWE**(1./AM))**AM
            CAA=CWW
            CWA=-CWW
            CKW=CKSW*SWE**(2.)*(1.-(1.-SWE**(1./AM))**AM)
            CKA=CKSA*(1.0-SWE)**(2.)*(1.-SWE**(1./AM))**(AM)
         ENDIF
C.........BCM_model
         IF (IEQ .EQ. 3) THEN
            IF (HAW .LE. A) SWE=1.
            IF (HAW .GT. A) SWE=(A/HAW)**B
            SW=(1.-SR)*SWE+SR
            SA=1.0-SW
            IF (HAW .LE. A) CWW=0
            IF (HAW .GT. A) CWW=(TS-TR)*B*(A**B)/HAW**(B+1)
            CAA=CWW
            CWA=-CWW
            CKW=CKSW*SWE**(C+2+2/B)
            CKA=CKSA*(1.0-SWE)**C*(1.-SWE**(1+1/B))**2
         ENDIF
C.........BCB_model
         IF (IEQ .EQ. 4) THEN
            IF (HAW .LE. A) SWE=1.
            IF (HAW .GT. A) SWE=(A/HAW)**B
            SW=(1.-SR)*SWE+SR
            SA=1.0-SW
            IF (HAW .LE. A) CWW=0
            IF (HAW .GT. A) CWW=(TS-TR)*B*(A**B)/HAW**(B+1)
            CAA=CWW
            CWA=-CWW
            CKW=CKSW*SWE**(3+2/B)
            CKA=CKSA*(1.0-SWE)**(2)*(1.-SWE**(1+2/B))
         ENDIF
C.........BRB_model
           IF (IEQ .EQ. 5) THEN
              SWE=1/(1+A*HAW**B)
              SW=(1.-SR)*SWE+SR
              SA=1.0-SW
              CWW=(TS-TR)*A*B*HAW**(B-1)*SWE**2
              CAA=CWW
              CWA=-CWW
              CKW=CKSW*SWE**2*(1-(1-SWE)**(1-2/B))
              CKA=CKSA*(1-SWE)**(3-2/B)
           ENDIF
C...........GDM_model
           IF (IEQ .EQ. 6) THEN
              DUM=-0.5*A*HAW
```

```
                SWE=EXP(DUM)*(1-DUM)
                SW=(1.-SR)*SWE+SR
                SA=1.0-SW
                CWW=(TS-TR)*1/4*A**2*HAW*EXP(DUM)
                CAA=CWW
                CWA=-CWW
                CKW=CKSW*EXP(-A*HAW)
                CKA=CKSA*(1-EXP(DUM))**2
             ENDIF
C.........LNM_model
           IF (IEQ .EQ. 7) THEN
              DUM=DLOG(HAW/A)/B
              X=DUM/(2**0.5)
              SWE=0.5*ERFCC(X)
              SW=(1.-SR)*SWE+SR
              SA=1.0-SW
              CWW=(TS-TR)/((2*PA)**0.5*B*HAW)
              CWW=CWW*EXP(-(DLOG(HAW/A))**2/(2*B**2))
              CAA=CWW
              CWA=-CWW
              X=(DUM+B)/(2**0.5)
              CKRW=0.5*ERFCC(X)
              CKW=CKSW*SWE**C*CKRW**2
              CKA=CKSA*(1.0-SWE)**C*(1-CKRW)**2
           ENDIF
        ELSE
           WRITE(*,*) 'Error! (Pc<=0) --> Stop!'
           WRITE(12,*) 'Error! (Pc<=0) --> Stop!'
           WRITE(*,*) 'n=',n,'    ha=',ha,'    hw=',hw
           WRITE(*,*)'Check:ini. cond.; ini. para. guess; or para.limits'
           STOP
        ENDIF
       ELSE IF (N.LT.IFNODE.AND.N.GE.1) THEN
        CKW=PLTPROP(2)
        CKA=1.0E-30
        CWW=PLTPROP(3)
        CAA=CWW
        CWA=-CWW
        SWE=1.00
        SAE=0.0
        SW=1.00
        SA=0.00
       ENDIF
200    CONTINUE
       RETURN
       END
C-----------------------------------------------------------------------
       SUBROUTINE DTHET(PHIN,PHIO,DTH)
       PARAMETER (MNOB=500,MPAR=8,MTYP=5,NDIM=100)
       IMPLICIT REAL*8 (A-H,O-Z)
       INCLUDE 'tfcombk.dat'
       DIMENSION PHIN(2*NDIM),PHIO(2*NDIM),DTH(2*NDIM)
       DIMENSION HW2(2),HW1(2),HA2(2),HA1(2),SW2(2),SW1(2),SA2(2),SA1(2)

       NELEM=NNP-1
       NP2=2*NNP
       DO 10 I=1,NP2
        DTH(I)=0.0
```

```
10    CONTINUE

      por=PVALA(1)
      DO 100 N=IFNODE,NELEM
       DO 50 J=1,2
          K=N+J-1
          HW2(J)=PHIN(2*K-1)-Z(K)*RHOW
          HW1(J)=PHIO(2*K-1)-Z(K)*RHOW
          HA2(J)=PHIN(2*K)-RHONW*Z(K)
          HA1(J)=PHIO(2*K)-RHONW*Z(K)
          CALL COEFT(HW2(J),HA2(J),CKW,CKA,CWW,CAA,CWA,SW2(J),SA2(J))
          CALL COEFT(HW1(J),HA1(J),CKW,CKA,CWW,CAA,CWA,SW1(J),SA1(J))
50       CONTINUE
       ZLENTH=Z(N+1)-Z(N)
       J=N
       J1=J+1
       DTH(2*J-1)=DTH(2*J-1)+POR*ZLENTH*(SW2(1)-SW1(1))/2.
       DTH(2*J1-1)=DTH(2*J1-1)+POR*ZLENTH*(SW2(2)-SW1(2))/2.
       DTH(2*J)=DTH(2*J)+POR*ZLENTH*(SA2(1)-SA1(1))/2.
       DTH(2*J1)=DTH(2*J1)+POR*ZLENTH*(SA2(2)-SA1(2))/2.
100   CONTINUE

      DO 200 N=1,IFNODE-1
       DTH(2*N-1)=0.
       DTH(2*N)=0.
200   CONTINUE
      RETURN
      END
C-----------------------------------------------------------------------
      SUBROUTINE FLUX(G,GG)
      PARAMETER (MNOB=500,MPAR=8,MTYP=5,NDIM=100)
      IMPLICIT REAL*8 (A-H,O-Z)
      INCLUDE 'tfcombk.dat'
      DIMENSION G(2*NDIM),GG(2*NDIM,2*NDIM)

      NP2=NNP*2
      QBW=GG(1,1)*(G(1)-G(3))
      QSA=-GG(NP2,NP2)*(G(NP2-2)-G(NP2))

      CUMBW=CUMBW+QBW*DT*AREA
      CUMSA=CUMSA+QSA*DT*AREA

      RETURN
      END
C-----------------------------------------------------------------------
      SUBROUTINE VOLUME(PHI,VSW,VSA)
      PARAMETER (MNOB=500,MPAR=8,MTYP=5,NDIM=100)
      IMPLICIT REAL*8 (A-H,O-Z)
      INCLUDE 'tfcombk.dat'
      DIMENSION PHI(2*NDIM),HW(2),HA(2),SW(2),SA(2)

      POR=PVALA(1)
      VSW=0.0
      VSA=0.0
      NELEM=NNP-1
      DO 200 N=IFNODE,NELEM
       ZLENTH=Z(N+1)-Z(N)
       L=N-1
```

```
        DO 100 I=1,2
           L=L+1
           K=2*L-1
           HW(I)=PHI(K)-Z(L)*RHOW
           HA(I)=PHI(K+1)-RHONW*Z(L)
           CALL COEFT(HW(I),HA(I),CKW,CKA,CWW,CAA,CWA,SW(I),SA(I))
           VSA=VSA+POR*ZLENTH*SA(I)/2.
           VSW=VSW+POR*ZLENTH*SW(I)/2.
100       CONTINUE
200   CONTINUE
      RETURN
      END
C...
C.... COMPLEMENTARY ERROR FUNCTION
      FUNCTION ERFCC(X)
      IMPLICIT REAL*8 (A-H,O-Z)
      Z=ABS(X)
      T = 1./(1+0.5*Z)
      ERFCC = T*EXP(-Z*Z-1.26551223+T*(1.00002368+T*(0.37409196+
     *        T*(.09678418+T*(-.18628806+T*(.27886807+T*(-1.13520398+
     *        T*(1.48851587+T*(-.82215223+T*.17087277)))))))))
      IF (X .LT. 0.) ERFCC = 2.-ERFCC
      RETURN
      END
```

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