CONSTANT FLUX INFILTRATION AND DRAINAGE IN UNSATURATED HETEROGENEOUS SOILS

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ABSTRACT

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Infiltration and drainage are important natural processes in ecology, agriculture and water-resources management. The goal of this study was to further our understanding of the movement of water during infiltration and drainage through heterogeneous field soils. Specific objectives included developing a new analytical solution of Richards' equation for soil water flow, new field measurement techniques, and inverse procedures for estimating soil hydraulic parameters. A series of constant flux infiltration and subsequent drainage experiments were conducted on a heterogeneous sandy soil. Two hundred Multipurpose Time Domain Reflectometry probes were installed along a 7.5 m transect at 4 depths. The probes measured soil water storage, W(t), as a function of time and pressure head during both transient and steady state conditions. The local water flux at each location was determined using the measured water storage during constant infiltration. Measurements at steady state were used to obtain the effective hydraulic conductivity and retention curves for the site. The uniqueness and stability of the inverse problem for estimating the local hydraulic properties from measured water storage during transient infiltration were analyzed. With two pressure head measurements, one at initial condition and the other at steady-state, a single transient W(t) provided unique and stable estimates of saturated hydraulic conductivity, Ks, inverse capillary length scale, α, another shape parameter and saturated water content, θ_s. The estimated parameters and a proposed Haines Jump model of hysteresis accurately predicted the soil water storage during drainage for different initial conditions. A method of a priori estimation of the Haines Jump was proposed and tested. To account for the spatial variability of hydraulic parameters in the horizontal direction, a unified stochastic analytical solution for infiltration and drainage was developed using a small perturbation method. The solution had very good agreement with Monte Carlo simulation for two extremes of spatial correlation between α and Ks fields. The average soil water storage to a fixed depth, $\langle W \rangle$, in the heterogeneous soil was essentially identical to that of a homogeneous soil with soil hydraulic properties equal to the mean hydraulic properties of the heterogeneous soil. The variance of soil water storage to a fixed depth, however, depended on $\langle W \rangle$, the variances of soil hydraulic properties, water flux density, and cross-correlation of the soil hydraulic properties. The new unified stochastic solution can also be used for inverse determination of the mean, variance, and correlation length scale of hydraulic parameters.

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and my loving parents.

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General Introduction

1.1. Background

In efforts to better monitor and manage the migration of chemicals in the soil and subsurface, scientists and engineers over the past several decades have developed analytical and numerical models describing how water and chemicals move into and through the unsaturated zone. These models have become indispensable tools in research for qualifying and integrating the most pertinent physical and chemical processes operative in the unsaturated zone of soils (van Genuchten and Leij, 1992). Since many contaminants are transported as dissolved components in the water phase, water flow is the most important process for modeling.

For water flow in field conditions, the flux boundary condition is most pertinent to rainfall and sprinkler irrigation. Numerous analytical and numerical solutions have been proposed to describe infiltration under flux boundary conditions and subsequent drainage. Though numerical solution is more general in terms of soil hydraulic properties and flexible to accommodate variable initial and boundary conditions, analytical solutions have its irreplaceable advantages (Lindstrom et al., 1989); (1) analytical methods are probably the most efficient alternative when the data necessary for identification of the system are sparse and uncertain; (2) where applicable, these methods are the most economical approach; (3)

analytical solutions provide physical insight into the problem; (4) analytical solutions provide a benchmark for numerical solution; (5) experienced modelers and complex numerical codes are not required; (6), analytical solutions can be used to test the uniqueness of an inverse problem. For these reasons, analytical solutions are continued to be sought and help in our understanding of the physics of water flow and chemical transport through soil.

The reliable application of models to field-scale flow and chemical transport problems implies a commensurate effort in quantifying the model parameters, especially the unsaturated hydraulic properties. The properties are those which define the relationship between hydraulic conductivity (K), volumetric soil water content (θ), and soil water pressure head (ψ). For field soils, these relationships are nonlinear and vary considerably in space (Nielsen, et al., 1973). To characterizing the hydraulic properties of a field, one usually needs to sample the field in dense grids. The sampling intervals must be small enough to capture relevant features of the field soil. The interval varies from soil to soil and range between 0.1 to a few meters (Russo et al., 1992). Thus, adequate characterization requires measuring a large number of samples in a small area. Methods of rapidly and accurately measuring field hydraulic properties are required.

Scientists in the past 30 years have proposed numerous methods to measure and estimate the soil water characteristic functions, $\psi(\theta)$, and hydraulic conductivity functions, $K(\theta)$, both in laboratory and in in-situ fields. These methods can be classified as direct methods, indirect methods, and prediction methods. Indirect methods are those relating statistically the soil hydraulic properties to soil texture and other soil properties, including bulk density, organic matter content and / or cation exchange capacity, clay mineralogy and soil structure by empirical procedures (van Genuchten et al., 1992) or by semi-empirical procedures through analytical expressions derived under highly idealized assumptions(e.g., Arya and Paris, 1981; Haverkamp and Parlange, 1986). Direct methods are those measuring directly soil hydraulic properties or estimating them from measured dependent variables under steady or transient conditions. There are also extensive investigations on prediction methods, that is to predict the hydraulic conductivity from pore-size distribution models, where the water retention curve of a porous medium is interpreted as statistical measure of its equivalent pore-size distribution. In this approach, the conductivity is estimated by applying the concept of viscous fluid flow through capillaries and by using a conceptual model to describe pore interactions and pore connectivity (Mualem, 1976).

Indirect methods and prediction methods, using available information or easily measured soil properties, are accurate for unstructured, repacked coarse material. However, for estimation of hydraulic properties of field soils, the most accurate methods are direct measurements on undisturbed sample in the laboratory or field measurements. While laboratory experiments are more controlled and generally more convenient than in-situ field experiments, the utility of soil properties determined on typical small core samples is limited . This can cause problems for predicting in situ behavior. This thesis concentrates on in situ direct field methods.

Field soil hydraulic properties have considerable spatial variability, even in apparently homogeneous soils (Nielsen et al., 1973). Therefore, the spatial structures of hydraulic properties need to be identified. This requires small sampling intervals and a large number of samples.

One approach is to take point or local scale measurements when boundary condition are set and repeated for many locations. This includes method using one-dimensional analysis such as single or twin-ring infiltration and three-dimensional analysis such as the Guelph Permeameter (Reynolds and Elrick, 1985; Elrick et al., 1992), and disk tension infiltrometer(Perroux et al., 1988; Reynolds and Elrick, 1991; Zhang, 1997). These methods are fast and cost-effective for determination of soil hydraulic properties for a single point in a field. However, when the purpose is to determine the spatial structure of soil hydraulic properties of a field, which is usually required for stochastic analysis of soil water flow and chemicals transport, these methods can be tedious and time-consuming. Since these methods are either destructive (e.g., ring methods and bore hole methods) or measurement scale is too large (all the three dimensional methods), which do not allow small sampling intervals.

Another approach is to apply water over a large area and take many simultaneous measurements (Parkin et al., 1992). This approach is facilitated by the recent measurement technique-time domain reflectometry (TDR), which allows rapid, nondestructive, and automated measurement of water storage from many locations. Measurements made by TDR with a vertical probe are direct measurements of water storage, the measurement volume is defined and does not change with water content.

When a non-point source water application is adopted, the water flow can be simplified as one dimensional and vertical (Hopmans et al., 1988; Prospapas and Bras, 1991). The flux boundary condition is easy to control and most pertinent to rainfall, sprinkler irrigation and gravity drainage. Focus of this thesis is on determination of hydraulic properties and modeling water flow for a constant flux boundary. In the following we give a review of the literature relevant to: (1) analytical solutions of one-dimensional infiltration and gravity drainage; (2) methods for determining soil hydraulic properties based on 1-d infiltration and gravity drainage; (3) stochastic models for transient infiltration and drainage. At end of this chapter, the objectives of this thesis are outlined.

1.2. Analytical solutions for constant flux boundary condition

For one-dimensional vertical flow, a combination of the equation of continuity for conservation of water mass, together with the Buckingham-Darcy law for unsaturated flow, leads to the familiar Richards conservation equation for water content for rigid and uniform soils.

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}[D(\theta)\frac{\partial \theta}{\partial z}] - \frac{dK(\theta)}{d\theta}\frac{\partial \theta}{\partial z} \qquad (1\text{-}1)$$

Where t (s) is time, z (m) is depth, θ(m^3 m^{-3}) is soil water content, D(m^2 s^{-1}) is soil water diffusivity and K(m s^{-1}) is the unsaturated hydraulic conductivity. Eq. [1-1] is a highly nonlinear second order partial differential equation. To solve it, appropriate initial and boundary conditions must be provided. For this thesis, the constant flux boundary conditions are used which include infiltration and drainage.

1.2.1 Analytical solutions for constant flux infiltration

1.2.1.1 Approximate solutions.

Parlange (1972) described an approximate integral procedure for the solution of infiltration by exploiting the rapid change in diffusivity with water content. The shortcomings of this solution are discussed in detail by Knight and Philip (1974). Parlange (1972) does not give a clear or consistent account of the physical meaning either of his initial approximation or of the subsequent steps in his method. Furthermore, Parlange (1972) has nothing in the procedure to ensure convergence (Knight and Philip, 1974). In addition, Philip and Knight(1974) showed how Parlange's method could be improved to any desired accuracy through use of a concept called the flux-concentration relation F (Philip, 1973). The use of the flux-concentration relation, in principle, permits quasi-analytical solution of the highly nonlinear flow equation to be found for a wide range of flow phenomena in soils. In general, F is a function not only of soil water content, but also of initial and surface water content, and time. Moreover, F is, in most cases, unknown a priori. To use F to predict the important aspects of flow in porous media, either the iterative procedures of Philip and Knight (1974) must be followed, or a sufficiently accurate estimated for F must be made. For flow problems subject to general flux boundary conditions, iterative procedures are not available and approximations to F must be used.

Subsequent work by White et al.(1979) used simple time-independent approximations for F. These approximations, which greatly simplify computation, were chosen to be consistent with the known behavior of F found by Philip (1973) for the linear soil and Green& Ampt soil and with Philip's hypotheses on the general regime of F for the relevant boundary conditions. The choice of an approximate F, however, can only be justified empirically.

White at al. (1979) analyzed constant flux adsorption using an approximate flux-concentration relation. Experiments using a fine sand confirmed the approach and showed both the surface water content and the water content profile could be predicted accurately for the horizontal adsorption of water supplied to the sand at a wide range of constant flux rates. They found that the time dependence of $F(\Theta,t)$ for constant flux adsorption into Bugendore fine sand was negligible and the measured $F(\Theta,t)$ was only slightly above the line $F(\Theta,t)=\Theta$. After examining a number of approximations for $F(\Theta,t)$, they concluded that predictions of surface water content and water content profile were more sensitive to the errors encountered in determining $D(\theta)$ than they were to errors arising from the use of approximate flux-concentration relations.

Perroux et al. (1981) extended the solution to constant flux infiltration and concluded sufficiently accurate predictions of moisture profile development can be made by using the simpler adsorption analysis of White et al. (1979). Boulier et al. (1984) confirmed the ability and the versatility of the flux-concentration relation-based approach to predict water infiltration into soils and expanded the solution to nonuniform initial conditions.

1.2.1.2 Exactly-solvable solutions.

For one dimensional flow, there exists useful integrable nonlinear parabolic equations closely related to the Richards equation. These equation may be characterized by the existence of Lie-Bäklund symmetries, or by certain infinite dimensional symmetry groups. Through certain transform, the integrable second-order partial differential equations are classified by Broadbridge et al (1996) in one of four classes.

(1). The linear class, with canonical form

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + g(x)u \qquad (g\ arbitrary) \tag{1-2}$$

including the linear model for Richards equation

$$\frac{\partial \theta}{\partial t} = D\frac{\partial^2 \theta}{\partial z^2} - \frac{K_s}{\theta_s - \theta_n}\frac{\partial \theta}{\partial z} \tag{1-3}$$

with D, K_s, θ_s, and θ_n constant;

Braester (1973), linearized Eq. [1-1] to Eq. [1-3], and derived expressions for both the variation of surface moisture content and movement of the wetting front during constant flux infiltration. His approach assumed constant soil water diffusivity (independent of soil water content), but also required the hydraulic conductivity at the initial soil water content to equal zero and the hydraulic conductivity to be exponentially related to the pressure potential. Such linearized solutions can only be expected to predict, approximately, the integral properties of soil-water system. Parlange (1976) has pointed out that the disparity between surface moisture contents calculated from this linearized solution and those calculated numerically are unacceptable. In addition, the linear convection term does not permit the development of a traveling wave solution at large infiltration times.

(2) The Burgers' class, with canonical form

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + 2u\frac{\partial u}{\partial x} + g(x)u \qquad (g\ arbitrary) \tag{1-4}$$

including the weakly nonlinear Burgers' model for the Richards equation

$$\frac{\partial \theta}{\partial t} = D\frac{\partial^2 \theta}{\partial z^2} - 2K_s\frac{\theta - \theta_n}{\theta_s - \theta_n}\frac{\partial \theta}{\partial z} \tag{1-5}$$

Burgers' equation retains important characteristics of the soil-water flow equation of real soil by preserving nonlinearity. Therefore, the solution to Burgers' equation satisfactorily described rainfall infiltration in an undisturbed field soil (Clothier et al., 1981). However, like the linear soil, Burgers' solution treats diffusivity as constant, even though many materials exhibit soil water diffusivity that vary over several orders of magnitude across the water content range of interest. There are analytical solutions for Burger's equation over a wide range of boundary conditions, such as constant flux (Clothier et al., 1981), and monotonically increasing flux with time (Broadbridge et al., 1987).

(3) The Fijita class with canonical form

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}[u^{-2}\frac{\partial u}{\partial x}] \tag{1-6}$$

including the strongly nonlinear form of the Richards equations

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}[\frac{a}{(b-\theta)^2}\frac{\partial \theta}{\partial z}] - [\frac{\lambda}{2(b-\theta)^2} - \gamma]\frac{\partial \theta}{\partial z} \tag{1-7}$$

The Richards equation based on Fujita form have solutions for constant flux boundary conditions for finite and semi-infinite systems (Hills and Warrick, 1993; Broadbridge and White, 1988; Sander et al., 1990). For variable-flux boundary conditions, Barry and Sander(1991) generalized the work by Sander et al.(1988), and obtained a quasi-analytical solution, containing a function that is specified by a Volterra integral equation, which must be evaluated numerically. Warrick et al. (1991) presented an analytical solution for any initial condition as well as arbitrary surface infiltration rates as a series of step inputs. The solution is approximate since numerical integration is needed. Different from those of Barry and Sander (1991) and Warrick et al. (1991), Broadbridge et al. (1996) presented another closed form solutions for specific flux boundary conditions using a quite different sequence of inverse transformations, including the hodograph transformation. This method is that it does not require numerical solution of an integral equation, but does require specific soil hydraulic properties and specific boundary conditions, restricting their application.

Parkin et al. (1992) derived an analytical solution for water storage to a fixed depth based on the analytical solution of Broabridge and White (1988) and Sander et al.(1988). The model result can be used directly to interpret the measurement from vertically installed TDR probes. However, like the solutions of Broabridge and White (1988) and Sander et al.(1988), solutions of Parkin et al. require specific forms of diffusivity and hydraulic conductivity dependence of water content.

(4) The Freeman-Satsuma class, with canonical form

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}[u^{-2}\frac{\partial u}{\partial x}] - 2 \tag{1-8}$$

including the Richards equation with plant root absorption term,

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}[\frac{a}{(b-\theta)^2}\frac{\partial \theta}{\partial z}] - v\frac{a}{(b-\theta)^2}\frac{\partial \theta}{\partial z} - Re^{-vz} \tag{1-9}$$

Other exact solutions include those presented by Ross and Parlange (1994), which are analytical solutions valid for the boundary condition where the flux on the surface is proportional to the surface water content during infiltration and drainage. This unusual boundary condition leaves the application of the solution for largely assessing the numerical solutions.

1.2.2 Analytical solution for redistribution and drainage.

The redistribution of soil water is an important natural process in ecology, agriculture and water-resources management. In addition, controlled redistribution has been used by Nielson et al. (1973), Jones and Wagnet (1984) and many others (Rose, 1965; Watson (1966); Chong et al., 1981; Libardi et al., 1980; Sisson et al., 1980) to measure soil hydraulic properties.

1.2.2.1. Exact solutions to Richards equation

Raats (1983), assuming exponential dependence of hydraulic conductivity upon pressure head and water content, obtained analytical solutions for drainage for specific initial condition, which allows separation of space and time variables. An analytical solution for drainage can be obtained by assuming constant diffusivity and linear dependence of hydraulic conductivity upon water content. This solution exaggerates the effect of gravity, resulting in a faster depletion of water storage than reality. Broadbridge and Rogers (1990) and Warrick et al. (1995) independently solved the Burgers' equation for gravity drainage. The solution expresses soil water content as a direct function of time and depth, which is convenient for application. Broadbridge and Rogers (1990) and Warrick et al. (1990) solved the Richards' equation for drainage for semi-infinite system and Sander et al. (1993) for finite system with realistic hydraulic properties. Ross and Parlange (1993) developed analytical solution for drainage for general soil hydraulic properties, but for restricted boundary condition.

1.2.2.2 Unit-gradient solutions

Chong et al. (1981), derived an analytical expression for the K(θ) dependence on the depth averaged water content, based on two assumptions: unit gradient and a power law dependence of depth average water content with time. Libardi et al. (1980) adopted three assumptions: unit gradient, linear water content-storage relationship, and an exponential K(θ) relationship. They produced the relationship between θ and time t either by the flux method or solving Richards equation directly.

Sisson et al. (1980), assuming unit gradient in vertical direction, solved the Richards equation which takes the form of well-known convection equation, using the Lax solution. However, in this solution, surface water content drops immediately to the background level,

θ_n. In fact, at z=0, the zero-flux boundary of the redistribution problem requires that the downward gravitational component of flux should be balanced by upward (including diffusive) components so that the unite gradient approximation cannot be valid near the surface. Under this circumstance, it would seem unlikely for the weaker condition of negligible capillary-flux gradient to hold and we share, along with the previous users of convection equation, a distrust of its predictions near z=0. Parlange (1982) modified the fundamental solution of Sisson et al. (1980) by adjusting the profile upwards and time to conserve mass. This modification was quite successful in term of agreement with the fully numerical solutions. However, the modification, though physically sound, is approximate. Broadbridge and Rogers (1990), provided an improved solution of Sisson et al. (1980) , and obtained a better prediction of surface water content. They also compared their exact solution, to Burgers' equation and the Lax solution, and concluded that the unite gradient solution is worse than the solution of Burgers' equation when compared with the exact nonlinear solution. The advantage of the unite gradient solution is that it allows general hydraulic properties and analytical inversion of hydraulic parameters. The drawback is the solution generally applies only to deep soils.

1.2.3 Connection between infiltration and drainage

Richards equation has exact solutions for both constant flux infiltration and gravity drainage based on Eq. [1-1], which is the diffusion form of Richards equation. There are unified solutions able to predict drainage from infiltration or predict infiltration from drainage in the absence of hysteresis (Warrick et al., 1990). When hysteresis exists, Eq. [1.1] becomes invalid because $D(\theta)$ is no longer single-valued. The solutions for infiltration and drainage will have different sets of hydraulic parameters, making the two continuous processes unpredictable from one another. Progress has been made in describing numerous scanning curves of a soil using simple models (Muelem, 1984a, 1984b; Parlange, 1976). The hysteresis models of Parlange (1976) and Mualem (1984) only need one branch of a scanning loop to predict all the scanning curves. However, the models of Parlange(1976) and Mualem(1984) do not have exact analytical solutions for infiltration or drainage.

1.3. Determination of hydraulic parameters using inverse procedures

Forward problem and identifiability

Given a parametric model of the physical system and values of the model parameters, the prediction of the system output (response) to any input is referred as the forward problem. In some cases, different sets of parameters may lead to different output, that is, the parameters are identifiable. In other cases, different sets of parameters lead to the same output. That is, the parameters are unidentifiable. The un-identifiability may stem from their over-parametrization, or from a lack of sufficient information to distinguish alternative parameter sets. An example of un-identifiability is the constant flux or concentration adsorption with governing equation

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x}[D(\theta)\frac{\partial \theta}{\partial x}]$$

where θ is water content, t is time, x is spatial coordinate, $D(\theta)=K_s\, C(C-1)\,/[\alpha\, \Delta\theta(C-\Theta)^2\,]$ for the Broadbridge &White (1988) form. The saturated hydraulic conductivity Ks and the inverse capillary length scale α are not identifiable simultaneously, since different Ks and α result in the same output if the ratio of the two remains the same. In this simple example, the unidentifiable parameters can be easily found. However, it is usually very difficult to determine a priori whether parameters can be identified or not.

Identifiability depends highly on the model structure. Russo et al. (1992) showed that the two parameters (Ks, and α) in the Gardner & Russo form of hydraulic functions are identifiable for a given infiltration rate (ponded infiltration), since the contours of infiltration rate intersect only at one point in the Ks-α plane. On the other hand, contours of infiltration rates for different infiltration times, merge into a single contour for the two shape parameters of the van Genuchten & Mualem form. Thus, to reduce un-identifiability, fewer parameters are needed or simpler model structure must be adopted.

Inverse problem and ill-posedness.

The estimation of model parameters given the parametric system model and an input-output relationship is known as the inverse problem. An inverse problem is well-posed if (1) the solution exists and (2) is unique and (3) stable, which means small change in the response does not result in large change in the parameters (Carerra and Neuman, 1986). If one of the three requirement is not satisfied, the problem is ill-posed. The first two of these requirements insure that mathematically there is a unique solution. The third requirement insures that the inverse solution is physically meaningful (not overly sensitive to measurement error). In most physical cases, the existence of a solution is guaranteed on physical grounds so that the last two requirements are the main concern of inverse problems.

Tikhonov and Arsenin (1977) indicated how a nonunique and unstable problem with linear forward operator can be transformed into a well-posed problems by appropriate regularization. This has been used in steady state flow problem, such as the recovery of the release history of a groundwater contaminant (Skaggs and Kabala, 1994) and to measure the apparent electrical conductivity of soils by electromagnetic induction (Borchers et al., 1997).

For transient unsaturated flow with a nonlinear forward operator, there are usually two steps to estimate hydraulic parameters. The first step is the parametrization of the hydraulic properties. The second step is to condition the parameters on the measured response through Richards equation or its linearized form. In the first step, the relationship between ψ and θ and between K and θ or ψ are expressed through functions with a few hydraulic parameters. These functions usually have 3 to 5 parameters each. To be parsimonious and to reduce ambiguity in the parameters, closed functional forms of hydraulic properties are adopted in routine applications. Usually, an empirical form of $\psi(\theta)$ or $K(\psi)$ is assumed, and the corresponding $K(\theta)$ or $\psi(\theta)$ relationship is derived through either Mualem or Burdine's capillary bundle theories. Some examples of this are the Brooks & Corey, van Genuchten & Mualem, and Gardner & Russo functions. On some occasions, the $\psi(\theta)$ and $K(\psi)$ are purely empirical to achieve an analytical solution of Richards equation. A typical example is the Broadbridge and White (1988) form. Those functions greatly simplify the representation of hydraulic properties and reduce the dimensionality of the estimation problem.

With parsimonious parametrization of hydraulic properties and high quality response measurements, the inversion of Richards equation in some applications becomes well-posed. However, the well-posedness of such a nonlinear inverse problem is generally not known a priori and has to be analyzed case by case. The task is to find under which situation the inversion become unique and stable, and what information is needed to make an ill-posed problem, well-posed.

Identifiability is different from uniqueness. Identifiability refers to forward problem, while uniqueness refers to inverse problem. The relationship between the two depends on the formulation of the inverse problem. When the inverse problem is expressed as a exact solution of the boundary value problem, the inverse solution is unique if and only if the parameters are identifiable (Carrera and Neuman, 1986b). However, when the inverse problem is not posed in this direct manner or approximations occur in the estimation process, uniqueness and identifiability are no longer equivalent.

Formulation of the inversion problem

In a saturated confined aquifer, the inverse problem is a typical distributed parameter system, where the response of the system is governed by a partial differential equation and the parameters imbedded in the equation are spatially dependent. In the unsaturated zone, the inverse problem can be also formulated as a distributed parameter, but because of the complication of the high nonlinearity of the flow equation, the problem may be very difficult to solve. The strategy is to consider soil properties as discrete in space. The hydraulic parameters are first estimated at individual points. The spatial structure of the soil hydraulic properties is then estimated from the known point-wise values. Thus, the parameter inversion in the unsaturated zone is mainly a lumped parameter system, instead of a distributed parameter system. Numerically, the problem is greatly simplified. However, the information provided by the system is not fully utilized, such as the spatial continuity of the hydraulic parameters. Therefore, the problem is more likely to be nonunique than the distributed system formulation.

To solve an inverse problem, we need a estimator. Generally speaking, the best estimators are those which minimize the discrepancy between the measurement and predicted response, while best reflecting the hydraulic properties of the medium(McLaughlin et al., 1996). There are many ways to fulfil the task, for examples, the least square and maximum likelihood methods. However, the most general, intuitively appealing and theoretically sound estimator is the maximum a posteriori estimator (MAP), by incorporating additional measurements and prior information into the estimator (Bard, 1974). In this way, the obtained parameters are guaranteed physically meaningful and may convert a degenerate equation into a non-degenerate case (Bard, 1974). The joint probability distribution function of the hydraulic parameters, L(β), depends on the distribution of measurement error e and prior β* through the Bayesian theorem.

$$L(\beta) \propto P(e|\beta)\ P(\beta^{*})$$

Usually, a Gaussian model is adopted for measurement errors and prior information. Since the logarithm is a monotonic increasing function of its argument, the value of β that maximizes L(β) also maximizes log (L(β)). Since log L is frequently a simpler function than L, the maximum likelihood estimates are generally obtained by minimizing the negative log of the a posterior likelihood function

$$\varphi = -2\log(L(\beta)) \propto -\frac{1}{2}[(\hat{y}(\beta)-y)^T G_y (\hat{y}(\beta)-y)] - \frac{1}{2}[(\beta-u)^T G_\beta (\beta-u)] \qquad [1\text{-}10]$$

where y is the response variable vector. indicates the estimated value of y. G_y, and G_β are covariance matrix of the response, prior information, respectively. β is the parameter vector. The vector u represents a prior estimate of β based on data other than y. The matrix G_β represents the accuracy of this prior estimate. In the combined criterion the third term penalizes deviations of model predictions from observations and the last term penalizes deviations of parameters from the prior estimate. The matrix G_β serves to weigh the last term against the third: the larger the G_β , the less important the last term.

The MAP is equivalent to the generalized least square estimator.

$$\varphi = -2\log(L(\beta)) = (\hat{y}(\beta)-y)^T G_y (\hat{y}(\beta)-y) + (\beta-u)^T G_\beta (\beta-u) \qquad [1\text{-}11]$$

By further assuming uniform measurement error(constant variance), then MAP is equivalent to weighted least square estimator:

$$S = \Sigma(\hat{y}(\beta)-y)^2 + W(\beta-u)^2 \qquad [1\text{-}12]$$

where W is the ratio of the variance of measurement error to the variance of prior estimator.

W is seldom known exactly. W can be treated as either an unknown or known parameter in minimizing S. For situations where nonuniqueness is more a problem, W should be treated as constant and an approximation for W should be used.

Justifications for assumptions in the previous description are:

1) The multi-normal distribution of measurement error was assumed in deriving Eq. [1-12].There is strong experimental evidence that experimental error is roughly normally-distributed. Furthermore, under "central limit condition," theory suggests that data distributions should cluster about the normal and not about some other distribution (Box and Tiao, 1973). If many observations are available, the Gaussian assumption is not crucial (Schweppe, 1973, P. 442).

2) It is reasonable to assume independence between response and prior information, because the measurements of different responses are usually taken by different instrumentation and measured at different times. In addition, the prior information is usually a good guess from another source of information, thus the error associated with prior estimator is irrelevant to the measurement error.

3). It is also reasonable to assume that the measurement error has a constant variance (deviation from the true value does not likely increase or decrease with the increase of the true value). For example, measurement errors by TDR do not increase or decrease significantly with the increase in water content (Topp et al., 1980). However, this assumption depends on the measurement technique and must be justified.

4). The assumption of normally distributed prior information is reasonable, since information theory suggests that the entropy is maximal for a Gaussian distribution if no additional information but the mean and variance are available (Bard, 1974). In some situations, only an approximate range is known about a parameter. In this situation, the most possible probability distribution is the exponential distribution (Woodbury et al., 1996). Under these conditions, minimizing Eq. [1-10] is a constrained optimization, which do not help to make the inverse problem well-posed. Therefore, for prior information to be useful, the mean and variance must be provided. It is difficult to have a prior estimator with an accurate mean and variance. A badly chosen u value will detrimentally affect the results. However, not utilizing u means failing to take advantage of information and may result in nonunique solutions to the inverse problem (Katanidis, 1997). In this situation, adding measurements of another response variable may be an obvious alternative.

The concept of "prior" information needs to be discussed in more detail. Prior information can take any form, but the most useful is an estimate (guess) of the average values of the parameters and their variances. The actual values of the parameters obtained from optimization can differ from the estimated average, but the possibility of the parameter being wildly different is constrained by the values of the estimated variance. This may seem like "cheating", but good estimates are available from most field soils. For example, a coarse sandy soil is likely to have a Ks somewhere near 10^{-4} ms^{-1}. Even if the variance is estimated at a standard deviation of 1 order of magnitude, the prior estimates is still useful in the optimization.

With the above assumptions, the Map can be simplified as least squares methods. The methods can be classified as linear or nonlinear least squares methods.

Generalized Linear least square method

Sometimes, Richards equation can be solved analytically for particular hydraulic properties, initial and boundary conditions. In some cases, these solution may be linear in the parameters. There are also situations where these analytical solutions are nonlinear in the parameters. However, certain transforms, $y1(\beta)=v[y(\beta)]$, may result in the new variable $y1$ linear in β. Consequently, the inversion problem becomes a linear least square estimation problem and the parameters can be isolated through matrix inversion. This method was very popular 10 years ago. However, there are a few limitations. First, the method requires specific boundary conditions and hydraulic functions, and thus limited applicability. Secondly, the statistical distribution of the errors on the calculated values of $y1 \equiv v(y(\beta))$ is not the same as that of the errors in y. Therefore, it may be appropriate to apply the least squares criterion to the residuals in y but not in y1 (Bard, 1974, P79). Bard (1974) introduced first-order analysis to correct Gy. The transform $v(Y(\beta))$ also introduces bias; i.e., if the errors in y have zero means, those in y1 do not.

The nonuniqueness of a linear least squares method can be examined through the analysis of rank deficiency of the Jacobian matrix(derivative of SSE with respective to β) (Carrera and Neuman, 1986b) . If the rank of the Jacobian matrix is smaller than the number of parameters, the matrix is singular and its inverse does not exists. To solve the problem a generalized inverse can be employed. However, there are numerous generalized inverse solution to the design matrix. Thus such an inverse problem is nonunique (different solutions result in the same S). The Penrose-Moore inverse is unique (SAS Institute Inc., 1990), however, the resulting parameters must be interpreted with caution. When the Jacobian matrix is singular, the resulting parameters may be highly correlated, thus the inverse solution would be very unstable.

The generalized linear least squares method has wide applications in the unit gradient approaches (Libardi et al., 1980; Chong et al., 1981; Sisson et al., 1980), Guelph Permeameter (Elrick and Reynolds, 1992), and tension disc infiltrometer (Reynolds and Elrick, 1990; Zhang, 1997);

Nonlinear least square methods

When the solution to Richards equation is nonlinear or numerical, the least squares methods becomes nonlinear. The nonlinear least squares method optimizes the hydraulic parameters by successively approximating the nonlinear problem by a linear problem. Thus , the analytical tools for analyzing nonuniqueness of linear least squares do not apply in the nonlinear least square methods. For non-linear problem, a common procedures are to draw the contours of prediction error (SSE) in the parameter spaces. For a well-posed inverse problem, there is only one minimum in the parameter space. In the following situations, the inverse problem is ill-posed:

(1). SSE increases or decreases monotonicly in the direction perpendicular to the contour in the parameter space, indicating no minimum exists (non-concave).

(2). Parameter space contains regions over which SSE remain nearly constant. Sometimes, the contours show a well-defined valley, and sometimes the valley is very narrow, being essentially a line in the parameter space. In this case, any value in the valley may result in the same SSE (flat region)

(3). Parameter space contain multiple points where SSE attains a local minimum (Multiple minimum).

For cases (1) and (2), the inverse problem must be reformulated or additional information must be provided. Problem (3) can sometimes can be solved using a global optimization procedure(i.e., simulate annealing, generic algorithm, etc.). However, like the Penrose-Moore inverse in the linear problem, the physical meaning of the resulting parameters is not guaranteed.

If the SSE contours are concentric circles, the two parameters are equally sensitive and uncorrelated. If the contours are elliptical, the parameter corresponding to the longer axis of the ellipse is less sensitive. A tilted ellipse indicates that the two parameters are correlated.

This contour analysis applies only to the case where there are two unknown parameters. Because of our limitation of understanding in higher dimensions, the uniqueness analysis for problems with three unknowns or more is usually carried out in two-dimension, by fixing one or more of the other parameters. However, the information provided by the contours are nonconclusive regarding the well-posedness, but conclusive regarding the ill-posedness of the inverse problem. To judge if the problem is well-posed, numerical experiments with different initial guesses are needed. If the local minimum or flat region are present, the different estimate runs will likely converge to different sets of parameter estimates. For convex SSE, the algorithm will not converge.

Uncertainty in the parameter estimates can be examined from the statistics provided by the nonlinear estimation. Unacceptable high variances and high correlation between two parameters means possible ill-posedness of the inverse problem. However, the estimated standard error in a parameter is an estimate of the lower bound of covariance matrix based on the Cramer-Rao theorem(Bard, 1974). It gives good approximation to the standard error to the extent that the sum of squares is locally linear in the parameters.

Due to the generality, this approach has had ever-increasing applications in estimating the hydraulic properties in the last two decades (Dane and Hruska, 1983; Zachmann et al., 1982; Kool et al., 1985, 1988; Russo et al., 1992; Simunek et al., 1996).

1.4 Stochastic analysis of unsaturated flow

1.4.1 Limitations of the deterministic models

It has been well recognized that soil hydraulic properties, such as the hydraulic conductivity and water retention curve have strong spatial variability. Thus, in many cases, thousands of samples are needed to get estimates within the 95 % confidence interval. Since all the hydraulic properties are difficult to measure (costly and time-consuming), it is impractical to take the number of samples required. By the time sufficient samples have been collected, the field would be disturbed so much, that the physical characteristics would probably be altered. Therefore, scarcity of measurements of hydraulic properties is a rule for modeling field hydraulic processes.

Measurement errors are unavoidable. Even very accurate soil water measurements using time domain reflectometry(TDR), still has a measurement error of 1-2% under ideal conditions. The presence of gaps around TDR rods and unparallel rod insertion can introduce additional measurement error (Ferré, 1997). The propagation of these errors would result in measurement or estimation error in the estimated hydraulic parameters.

Some of the hydraulic parameters are not directly measurable, for example the inverse macroscopic capillary length scale, α. Usually some kind of assumptions has to be made in order to simplify the calculations. For example, a popular field methods to measure Ks and α, the Guelph Permeameter method, assumes the Glover's approximate solution for an anger hole and the additivity of the effects of gravity and unsaturated flow. This approximations contribute to the uncertainty of the estimated hydraulic parameters.

The basic hydraulic laws are the Darcy' law and the conservation mass equation. Their combination results in the Richards' equation for unsaturated flow, which is a second order partial differential equation. Mathematically, this equation has numerous solution (analytical or numerical). To define a solution, initial and boundary conditions need to be defined. These conditions are usually difficult to control in the fields; thus approximate boundary and initial conditions are often provided. These approximations also lead to the uncertainty of the parameters.

For convenience, $\theta(\psi)$ is described in a functional form, such as the Brooks & Corey(1963) or van Genuchten(1980) equations. Furthermore, in order to reduce the number of parameters, ad hoc capillary bundle theory such as those of Burdine or Mualem (van Genuchten, 1980)are used to derive the functional relationship for $K(\theta)$. This greatly reduces the nonuniqueness when inverse approach is adopted. However, because of heterogeneous pore water system in soil, there are no simple universal equations that describe the relationship perfectly. Therefore, approximations are applied in modeling the hydraulic properties.

The uncertainty associated with the spatial variability, paucity of measurements, measurement errors, and modeling errors exist in the hydraulic parameters. This generally exclude the use of deterministic approaches and suggests a statistical approach or stochastic approach, which can take into account those uncertainties.

1.4.2 Statistical representation of heterogeneous soils.

Field experiments (Nielsen et al., 1973; Sudicky, 1986; Unlu et al., 1990; Russo and Bouton, 1992; White and Sully, 1992; Russo et al., 1997) suggest that ln(Ks), and ln(α)are approximately normally distributed in space. The following relationships can be used to convert the arithmetic and geometric means and variances (Dagan, 1989).

$$K_A = \exp(m_Y + \sigma_Y^2) \quad ; \quad \sigma_K^2 = \exp(2m_Y + \sigma_Y^2)[\exp(\sigma_Y^2 - 1] \quad ; \quad K_G = \exp(m_Y)$$

Where, K_A is the arithmetic and K_G is the geometric mean, respectively, and σ^2_Y and m_Y are the variance and mean of the log Ks, respectively. The following assumptions which are in agreement with field experiments are adopted by most stochastic analyses of heterogeneous media.

(1). The log saturated hydraulic conductivity, Y(x)=ln(Ks(x)), is assumed as a multi-normal random function in space (x) that is expressed through its stationary mean <Y> and a spatial covariance with a finite integral scale. Their spatial structure is modeled by the isotropic exponential model(Sydicky, 1986):

$$C_Y(r) = \langle Y'(x)Y'(x+r)\rangle = C_Y(r) = \sigma_Y\, e^{-r/I_Y} \qquad (1\text{-}10)$$

where, C_Y is covariance of Y, σ_Y is the variance of Y and r is lag between two points, and I_Y is the integral scale of Y. Parameter α is also treated as a random spatial function and is assumed statistically homogeneous and isotropic with constant mean, $<\alpha>$, variance σ^2_α and a similar spatial structure as Eq.[1-10].

(2). The α field is assumed to be either perfectly correlated(negative or positive) or uncorrelated with the log saturated hydraulic conductivity field Y(x) (Yeh et al., 1985). No experimental evidence supports negative correlation. Some field experiments suggest a positive correlation (Unlu et al., 1990; White and Sully, 1992; Russo et al., 1997), there are field evidence that $\alpha(x)$ is not correlated with Y(x) (Russo et al., 1992). Thus, perfectly positive correlated flow and uncorrelated flow are usually taken as the two extremes.

(3) The flow domain is much bigger than I_Y or I_α such that the ergodicity assumption can be invoked. Under this assumption, the spatial average and ensemble average are identical.

The flow domain is usually three dimensional and anisotropical. Therefore, representation of a field needs considerable information, which is generally not available. Scientists in the last two decades have proposed a few simplifications to approximate the three dimensional continuum model. So far, reasonable approximations are the scale-invariance model(Sposito, 1995), parallel column model (Dagan and Bresler, 1983) and perfect stratification model(Yeh et al., 1985).

Scale-invariance approach

To solve Richards equation for a spatially variable field, hydraulic functions K(θ) and

$\psi(\theta)$ or $D(\theta)$ as a function of space position(x,y) must be a priori determined. These functions have four to six parameters, each a function of x, and y. A major and considerable simplification can be achieved by assuming scale invariance. Sposito (1995) has presented a comprehensive summarization of the scaling approach.

"One imagines a heterogeneous field to be the union of approximately homogeneous spatial domains, each of which can be associated with a small number of characteristic length scales that are related to the equilibrium properties and movement of water. Heterogeneity is then simplified into the spatial variability of these local length scales, while the generic functional relationships that describe soil water properties remain uniform. These generic functional relationships include not only the dependence of water content and hydraulic conductivity on matric potential but also the partial differential equations of transport and the empirical flux law they contain."

The early study of scale-invariance of soil water flow started from Miller similitude, which assume a soil is geometrically similar, thus its hydraulic properties of all regions of the soil can be calculated from the hydraulic properties of a single reference region if the scaling factor distribution is know(Miller et al., 1956). However, field soil heterogeneity appears to be described poorly by scale magnification. For example, the porosity of a field soil commonly has a CV in the order of 10 %, which violates the assumption of geometric similitude, which requires that the porosity be constant. For this reason, scaling of field hydraulic properties is usually preceded by dividing water content by the local value of porosity, and scaling the properties as a function of relative saturation (Warrick et al, 1977). However, analysis of field data suggests that a scaling factor can not account for all of the variability in the field (Jury et al., 1987). However, because of its simplicity, the scaling approach has wide application in simulation studies of water flow and transport in heterogeneous fields (Russo, 1991; Tseng et al., 1993).

Parallel columns model.

The stochastic continuum model can be simplified by assuming that the correlation length scale in vertical direction is infinite. This type of model is justified for domains which are homogeneous vertically, for formations whose vertical extent is smaller compared to the vertical scale of heterogeneity, and for formations where the vertical variability is small compared to the horizontal one. Finally, in many cases, although variability may exist in the vertical direction, the determination of soil hydraulic properties through field methods such as drainage experiments(Libardi et al., 1980) homogenize the properties vertically, giving effective parameters , thus eliminating the variability in the vertical direction in the practical sense (Rubin et al., 1993). This model has been utilized by Dagan and Bresler (1979, 1983), Hopmans et al. (1988), Rubin an Or (1993), and Chen et al. (1994).

Perfect stratification model

The perfect stratification model is a type of stochastic continuum model that assumes the horizontal correlation length scale is infinite. This is justified to a certain extent, since in general, soil properties tend to be correlated horizontally over much larger distances than in the vertical direction. This model has been utilized by Destouni(1992), Yeh et al. (1989) and Indelman et al. (1993).

1.4.3 Steady-state flow in unsaturated media

Parallel to the work on saturated flow phenomena, studies have developed a stochastic approach to flow in the unsaturated zone(Dagan and Bresler, 1979; Yeh et al., 1985 a.b.c; Yeh, 1989). While in general the approaches for saturated and unsaturated flow modeling are similar in the sense that the soil hydraulic properties are viewed as random functions and a differential flow equation is used to derive the moments of dependent variables, modeling flow in the unsaturated zone has unique aspects. The dependence of hydraulic conductivity on the pressure head complicates the problem. However, under some conditions the flow can be treated reasonably well as one dimensional in the vertical direction(Dagan and Bresler, 1979; Russo and Bresler, 1981; Yeh, 1989; Protopapas and Bras, 1991; Rubin and Or, 1993; Indelman et al., 1993).

Yeh et al. (1985) used spectral representation to derive the variance of soil-water pressure head and the effective hydraulic conductivity of a stochastic random media under steady state infiltration conditions. The results of their studies showed that the head variance was mean-dependent and increased with mean soil-water pressure head. The effective hydraulic conductivity was shown to be a second-rank tensor and anisotropic. The ratio of the horizontal to the vertical hydraulic conductivity depends on the soil water saturation. This indicates that the mean of water flux, $\langle q(x) \rangle$, is non-local and non-Darcian. The study by Yeh (1989) was based on Monte Carlo simulation for one-dimensional steady-state infiltration in heterogeneous soils. The simulation was in good agreement with the analytical results.

The study by Yeh at al. (1985a,b) assumed that the hydraulic head changes slowly along the profile relative to the heterogeneous Ks(x) (local stationarity of the hydraulic head), in order to use Fourier-Stieljes integral representations. The assumption is valid for the case of average vertical infiltration in an unbounded region where the mean hydraulic gradient is constant (J=1). However, for bounded cases, such as flow approaching a water table, the average gradient is not constant.

Indelman et al. (1993) extended the small perturbation technique to steady-state flow through bounded horizontally homogeneous and vertically heterogeneous formations. The expansion of expression of hydraulic head to the second-order leads to the analytical solution for the mean (second order) and variance (first-order) of hydraulic head for generic soil water properties; including the Gardner soil. The agreement between moments predicted by the model and Monte Carlo simulation was satisfactory but the variances of the Y and α was small. In the nonstationary region of the profile, the dependence of pressure head variance on mean pressure head was sensitive to both the value of the water flux and the variability of soil properties. The stationary variance of pressure head (at large time) exhibited a strong dependence on the flux boundary condition and on the cross correlation between Y and $\ln(\alpha)$. In the absence of cross correlation, it increased monotonically with the reduction in q; when there is perfect correlation between Y and $\ln(\alpha)$, however, it has a minimum at mean pressure head.

Rubin et al. (1993) studied the same problem for horizontally heterogeneous and vertically homogeneous formations with plant water uptake. These authors used the first order perturbation to derive the mean and variances of the water content and pressure head for plant water uptake exponentially decaying with depth.

1.4.4 Flow in unsaturated media for transient flow

A general method, which applies to saturated, and unsaturated flow is Monte Carlo simulation combined with the numerical or analytical solution of the flow equations for a large number of realizations of the heterogeneous medium. The starting point is now the given statistical structure, i.e. the joint probability distribution function of the properties values at different points. The flow domain Ω is partitioned into elements ω and by the Monte Carlo generation process the value of the property in each element becomes a constant but random across the domain Ω. Once the flow problem is solved in each realization, various statistical moments can be easily evaluated. The simplest way to preserve the given statistical structure of the hydraulic conductivity or other properties is with a sufficiently dense partitioning, i.e. one in which the numerical elements are small compared to the heterogeneity scale. However, this approach has formidable difficulties: it requires considerable computing capacity and severe numerical problems are encountered for large spatial gradient. Furthermore, the level of information obtained this way is too detailed and much of it is redundant (Indelman, 1993)

Dagan and Bresler (1983) were the first attempt to study the stochastic flow for infiltration and redistribution. They assumed that the flow was one-dimensional and adopted the parallel column model. Their approach to incorporate with spatial variability is similar to the Monte Carlo approach, with a different way of carrying out integrations for the mean and variance. They concluded that the stochastic approach leads to an accurate value of the expectation and variance of the flow variables, even if a simplified model such as piston flow is adopted. However, their approach applies only to sufficiently heterogeneous soils where the variance of log saturated hydraulic conductivity is greater than 1. The variance of log Ks of many soils is less than 1(Sudicky, 1986; Russo et al., 1992). Furthermore, their approach requires numerical integration which can be computationally demanding when there are more than one hydraulic parameters treated as random space functions.

Mantoglou and Gelhar (1987) analyzed unsaturated flow in heterogeneous media. They introduced a small perturbation of additional soil water capacity, and derived a large-scale flow equation with the same form as the local Richards' equation. Thus q(x) is Darcian. However, the effective hydraulic conductivity is non-local, depending on the mean soil properties, the stochastic properties of the soil fluctuations (large scale effect of the local properties and their fluctuations), the mean flow characteristics (a nonlinear flow model), and the time history of the model output (a hysteresis of the effective parameter).The traditional one-dimensional flow model or the steady-state stochastic models can not predict these effects, because they do not account for the spatial variability of the local properties, the three dimensionality of the local flow processes, and the parametric nonlinearity of the local governing flow equation. They linearized the fluctuation equation and solved it using the spectral representation, after assuming one-dimensional mean flow and unbounded flow domain (far from the boundary). The results of their studies also indicated that water content dependent anisotropy shows significant hysteresis, depending on the mean flow conditions (wetting or drying).

Chen et al.(1994) presented an upscaled equation to describe water flow for infiltration. The upscaled equation only involves the means and variance of Ks, and the equation can be solved once to obtain the average behavior.

1.5 Objectives

The general goal of this thesis is to further our understanding the movement of water during infiltration and drainage through heterogeneous field soils. The focus is on effective one-dimensional water flow with a constant flux (infiltration) or no flow (drainage) surface boundary condition. The objectives of this thesis are:

(1) To develop an improved field method of measuring quickly and non-destructively the in situ average , variance, and spatial structure of hydraulic properties, including hysteresis.

(2) To present a new analytical solution for transient water storage for a fixed depth under constant water flux. The solution allows any general soil hydraulic function to be used and is directly applicable to the field method in objective (1).

(3). To develop and evaluate inverse procedures for identification of hydraulic parameters, from measurements and prediction of transient infiltration in objectives (1) and (2).

(4) To evaluate and incorporate the influence of hysteresis in hydraulic parameter identification from transient infiltration and drainage measurements and predictions.

(5) To develop a unified stochastic analytical solution for transient infiltration and drainage of water in heterogeneous soils. The influence of the average, variance, and integral length scales of Ks and α, on the average, variance, and integral scale of transient soil water content and storage are examined.

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Chapter 2

Measurement of hydraulic properties and prediction of soil water storage during constant flux infiltration: field average

Abstract

A series of infiltration experiments in Borden, Ontario, were conducted with a green house irrigation system. Using multipurpose TDR probes, we were able to determine the local flux at each TDR probe, based on the fact that the rate of increase in water storage measured by a vertically-installed TDR probe is linear with time before the wetting front passed the end of TDR probes. Our experiments showed that for different application rates, water flow was approximately vertical within the measurement volume of TDR. This provided experimental evidence of the stream tube model of Dagan and Bresler (1983).

By employing the unit gradient assumption with each depth increment, we were able to obtain the hydraulic conductivity at equilibrium phase of constant flux infiltration from locally measured flux and water content. With measured water matrix potential by multipurpose TDR probes at equilibrium, we obtained the water retention curve at the same location.

With the measured apparent $K(\theta)$ and $\psi(\theta)$ curves for the field, the predicted water storage using Parkin's solution (1992) was remarkable compared to the measured field-averaged water storage for 20 cm and 40 cm long probes during constant rainfall infiltration, indicating that the measured $K(\theta)$ and $\psi(\theta)$ by multipurpose TDR probes represented the

field behavior.

Introduction

A quantitative description of water infiltration under constant flux boundary conditions in unsaturated soils is fundamental to understanding water balance, irrigation, movement of chemicals and, more generally, transport processes occurring in surface soils. Analytical solutions of Richards' equation for constant flux water infiltration into homogeneous soil profiles have been developed using integral procedures (Parlange, 1972; Philip and Knight, 1974; White et al., 1979; Perroux et al., 1981), Kirchhoff, Hopft-Cole and Storm transformations (Broadbridge et al., 1988; Broadbridge and White, 1988; Warrick et al., 1990) and by reciprocal Bäcklund transforms (Sander et al., 1988, 1991; Barry and Sander, 1991). These analytical solutions are very useful for assessing the accuracy of numerical models and estimating soil hydraulic properties by inverse procedures. Analytical solutions can also be used to test inverse techniques for non-uniqueness and identifiability of hydraulic parameters of interest.

Significant advances have recently been made in the measurement technology for field infiltration experiments. Time Domain Reflectometry (TDR) is potentially useful for measuring both volumetric water content (Topp et al., 1980) and vertical solute mass flux in a nondestructive and rapid fashion during field infiltration experiment (Kachanoski et al., 1992). Vertically installed TDR probes measure the volume averaged water content, or water storage from the surface to bottom of the probes. Parkin et al. (1992, 1995a) presented quasi-analytical solutions for cumulative water storage to a fixed depth of soil by integration of the parametric water content-depth relationships presented by Broadbridge and White (1988) for constant flux infiltration and by Warrick et al. (1990) for drainage. However, the solutions require particular forms of the hydraulic conductivity function, $K(\theta)$ and diffusivity function, $D(\theta)$.

Parkin et al. (1995b) used TDR probes installed vertically at the soil surface under a constant-rate rainfall simulator to measure cumulative water storage with time. They estimated the local infiltration rate from the slope of water storage versus time during early time before the wetting front reached the bottom of the TDR probe. Assuming a unit gradient and utilizing the spatial variability in local infiltration rate, they estimated directly the unsaturated hydraulic conductivity over a wide range of water contents using only two water application rates. They also concluded that an unique estimate of $K(\theta)$ and $\theta(\psi)$ with three unknown parameters was not possible from measurements of only soil water storage with time. Additional measurements of ψ are an obvious choice to reduce non-uniqueness. However, spatial variability may limit the usefulness of ψ measurements taken at spatial locations different from the soil water measurements. Baumgartner et al. (1994) developed a soil water TDR probe which measures ψ and soil water storage at the same horizontal location. However, the probe has not been used in field applications, to our knowledge.

The objectives of this paper were to extend the method of Parkin et al. (1995b) to estimate not only the field average $K(\theta)$, but also the field average water retention characteristic, $\psi(\theta)$, during constant flux infiltration. In addition, utilizing the estimated field averaged parameters, we compare the solution of Parkin et al (1992) to in-situ measured values of soil water storage as a function of time during constant flux infiltration. The new multipurpose TDR probes of Barmgartner et al. (1994) were used in a field experiment with a rainfall simulator to fulfill the objectives.

Theory

Measurement of unsaturated hydraulic properties

The cumulative storage of water (m^3 m^{-2}) to depth L, W(L,t), is measured by vertically installed TDR probes and is given by

$$W(L,t) = \int_0^L \theta(z,t)dz$$

where θ(t) is the average water content (m^3 m^{-3}) over the probe length, L (m). The abrupt change of water content at the wetting front does not have significant effect on the measurement of water storage (Topp et al., 1982).

During the period before the wetting front first reaches L under constant water application, the derivative of cumulative storage of water measured by TDR with respect to

$$W(L,t) = \bar{\theta}(t)L \qquad [2\text{-}1]$$

time should equal the local water flux at the soil surface, $q_{w|0}$ (Parkin et al., 1995b). Assuming conservation of mass, one dimensional flow, and the applied water has not reached depth L, yet, then

$$q_{w|0} = \frac{dW(L,t)}{dt} \qquad [2\text{-}2]$$

Eq. [2-2] allows us to calculate the local water flux during the early stage of constant flux infiltration. After a long time, the average water content from the soil surface to depth L reaches a constant value θ and a corresponding steady-state ψ measurement can be taken from the multi-purpose TDR probe.

Solution of Parkin et al. (1992).

Broadbridge and White (BW) (1988) and Sander et al (1988) independently developed an analytical solution for constant flux infiltration. The BW solution is based on the following parameterization of hydraulic conductivity and diffusivity functions

$$K(\Theta) = Ks \frac{(C-1)\ \Theta^2}{C-\Theta} \qquad [2\text{-}3]$$

$$D(\Theta) = \frac{Ks\ C\ (C-1)}{\alpha\ \Delta\theta\ (C-\Theta)^2} \qquad [2\text{-}4]$$

where $\Delta\theta=\theta_s-\theta_r$ and $\Theta=(\theta-\theta_r)/\Delta\theta$. θ_s and θ_r are the saturated water content and residual water content, respectively. Ks, α, and C are the saturated hydraulic conductivity, inverse capillary length scale (Philip, 1985), and a constant introduced by BW, respectively. By definition,

$$D(\Theta) = K(\Theta)\ \frac{d\psi}{d\theta} \qquad [2\text{-}5]$$

we have,

$$\psi(\theta) = \int_{\theta}^{\theta_s} D(\Theta)/K(\Theta)\ d\theta \qquad [2\text{-}6]$$

Substitution of Eq. [2-3] and Eq. [2-4] into Eq. [2-6] and integration yields

$$\psi_0 - \psi(\Theta) = \frac{1}{\alpha}\left[\frac{1-\Theta}{\Theta} + \frac{1}{C}\ln\left(\frac{C-\Theta}{\Theta(C-1)}\right)\right] \qquad [2\text{-}7]$$

where ψ_0 is an integration constant. Following BW, we set ψ_0=0.

We consider nonhysteretic vertical flow and seek to find expression for time dependence for water storage to a fixed depth. The flow of water may be described in this process by the continuity equation,

$$\frac{\partial\theta}{\partial t} = -\frac{\partial q}{\partial z} \qquad [2\text{-}8]$$

and Darcy's Law,

$$q(\theta,t) = -D(\theta)\frac{\partial\theta}{\partial z} + K(\theta) \qquad [2\text{-}9]$$

where, t is time, z is vertical coordinate, θ is the volume water content, q is the volumetric flux of water, and D(θ) is the water-content dependent soil-water diffusivity.

Substitution of Eq.[2-9] into Eq.[2-8] yields the nonlinear Richards' equation used to describe one-dimensional nonhysteretic flow in idea soil:

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial z}\left(D(\theta)\frac{\partial\theta}{\partial z}\right) - \frac{dK(\theta)}{d\theta}\frac{d\theta}{dz} \qquad [2\text{-}10]$$

The initial and boundary condition considered here are

$$\theta(z,0) = \theta_0; \qquad z \geq 0 \qquad [2\text{-}11]$$

$$-D(\Theta)\frac{\partial \theta}{\partial z} + K(\Theta) = R \qquad [2\text{-}12]$$

where R is the constant application rate on soil surface. Utilizing Eq. [2-1] and Eq. [2-2], through a series of transforms (i.e. Kirchhoff, Storm, and Hopf and Cole transforms), BW derived an analytical solution as

$$\Theta(\zeta,t) = C[1-(1+2\rho-u(\zeta,t)^{-1}\frac{\partial u(\zeta,t)}{\partial \zeta})^{-1}] \qquad [2\text{-}13]$$

and

$$z(\zeta,t) = (C\alpha)^{-1}[\rho(\rho+1)\tau+(2\rho+1)\zeta-\ln(u(\zeta,t))] \qquad [2\text{-}14]$$

where ζ is a parameter connecting Eq. [2-13] and Eq. [2-14], $u(\zeta,t)$ is given by Eq. [43] of BW, and

$$\rho = \frac{R}{4C(C-1)Ks} \qquad \tau = \frac{4C(C-1)\ \alpha K_s t}{\Delta\theta} \qquad [2\text{-}15]$$

By change of variable of integration, Parkin et al. (1992) obtained an analytical solution for water storage to depth L for constant flux infiltration,

$$W(L,t) = \frac{\Delta\theta}{\alpha}[2\rho\ \zeta(L,t) + \ln(\frac{u(0,t)}{u(\zeta,t)})] + \theta_r L \qquad [2\text{-}16]$$

A more versatile hydraulic model is the van Genuchten form(Eq.[2-17] for soil-water characteristic and Burdine form (Eq. [2-18]) for hydraulic conductivity (van Genuchten, 1980).

$$\Theta = (\frac{1}{1+(\alpha_{VG}\psi)^n})^{-m} \qquad [2\text{-}17]$$

with m=1-2/n, and

$$K(\Theta) = K_s\ \Theta^2(1-(1-\Theta^{1/m})^m) \qquad [2\text{-}18]$$

where α_{VG} and n are fitting parameters.

Materials and methods

Site description

The field infiltration measurements were conducted at the Canadian Forces Base Borden, Ontario, Canada. Extensive hydro-geological research, including a large scale, natural-gradient tracer test and forced gradient test have been conducted by University of Waterloo on this site. Details about this site can be found in Sudicky (1986). The spatial variability of saturated hydraulic conductivity (Ks) in the saturated zone has been characterized in detail by Sudicky (1986) using 1275 undisturbed cores and re-examined by Woodbury and Sudicky (1991). Turcke et al. (1996) used 642 undisturbed cores sampled near the site of Sudicky (1986). The study site at Borden was an area where the water table was greater than 4.5 m below the surface. The site was prepared by removing the top 0.5 m thick layer of surface soil over an area 4 × 9.5 m^2.The area was covered with a greenhouse to prevent effects of wind, precipitation and evaporation. Within the sampling area, multi-purpose TDR probes for a given depth were installed every 0.15 m in a 7.5 m long transect for a total of 50 probe per depth. This was repeated in parallel transects 0.1 m apart for each of 4 depths (0.2, 0.4, 0.6, and 0.8 m) for a total of 200 TDR probes (Fig. 2-1).

Each multi-purpose TDR probe consisted of two stainless steel rods constructed in a manner similar to Baumgartner et al. (1994). One of the rods was a hollow stainless steel tube (6 mm internal diameter) with a porous stainless steel cup threaded on the bottom (Mott Metallurgical Corp, Farmington, Connecticut. Air entry: 175 cm). The second rod was solid stainless steel with the same length as the hollow rod plus the porous cup. The rods were 5 cm apart perpendicular to the transects. The top of the hollow stainless steel rod had a 5 cm long transparent plastic tube connected using epoxy resin. The hollow steel tube was filled with water to within 2 cm of the top of the plastic tube and a rubber septum was installed to seal the top and create the tensiometer. Each pair of steal rods (hollow, solid) were connected to shielded parallel antenna cable to create a TDR wave guide. Groups of 25 probe were attached to common access boxes allowing rapid and frequent scanning of all probes.

Water applications.

An array of eight flat spray nozzles was constructed. The spray pattern of a single nozzle suspended 0.5 m above the surface approximates a narrow rectangle 1.2×0.2 m^2. The nozzles were installed on the linear array at 0.1 m intervals with their spray axis aligned. This produced a uniform narrow wetted area of approximately 0.2×2 m^2. The nozzle array was attached 0.5 m above the soil surface to a commercially available, programmable water application system designed for green houses (model DCA, Monorail Boom Spray System, Waterford, Ontario). The system has a single pressure regulator, electric solenoid valve, and microprocessor unit attached to a hanging track and conveyor belt. The hanging track is mounted to the top of the greenhouse and allows the nozzle array to go smoothly back and forth along a straight line (9 m long) with programmable delay time at either end of the line. The water can be turned on or off, at either end of the line. The system produces a uniform wetted area 2 m wide by 9 m long centered over the TDR instrumented transects (Fig. 2-1.).

Six different infiltration rates were applied over a 60 day period (Table 2-1.). After each infiltration rate the soil was allowed to drain until daily changes in soil water storage were negligible relative to the next infiltration rate. Measurements were taken during drainage, but are not described in this paper. The uniformity of the water application system was checked by placing 100 cups (12 mm high by 9 mm interior diameter) along the transects and collecting applied water for 1 hour. The water application was very uniform with the coefficient of variation less than 1.5 % (Fig. 2-2.). For example, at the rate of 0.9 cm hr^{-1}, the minimum and maximum measured rate was 0.87 cm hr^{-1} and 0.92 cm hr^{-1}, respectively.

Measurement of water storage and ψ

Soil water content was measured using the TDR method of Topp et al. (1980). The readings were taken manually from the display screen of two pre-calibrated Tektronix(1502 C) metallic cable tester by four operators. The readings were taken just prior to the start of water application and every 5-30 minutes depending on infiltration rate and rate of change of θ, for all the 200 multipurpose TDR probes. After the wetting front was beyond the 80 cm depth and all θ measurements indicated little or no change with time, the pressure head ψ measurements were taken using two tensimeters (Soil Measurement System, Tucson, Arizona). The ψ measurements were taken for application rate=0.21, 0.9, 3.3 cm hr^{-1}. At other rates, we found the ψ was small from the above three rates and the ψ measurements were not made. We also took ψ measurements at the initial condition before we started the infiltration experiment for application rate = 6.22 cm hr^{-1}.

Estimation of the hydraulic parameters

The optimization utilized simultaneous fit of model parameters to observed retention and hydraulic conductivity. The objective function is:

$$O(b|\theta) = \sum_{i=1}^{N}[\psi_i - \overline{\psi_i}(b|\theta))]^2 + \sum_{j=1}^{M} G_j[K_j - \overline{K_j}(b|\theta)]^2 \qquad [2\text{-}19]$$

where b is the parameter vector (Ks, α, C) for BW model or (Ks, α, and n) for VG model. M and N are the number of observations of ψ and K, respectively. G is the weight assigned to the hydraulic conductivity in order to prevent ψ dominating the K data solely because of its larger numerical values. Since ψ value is generally ten times bigger than K, we set G=10. Several nonlinear programs such as secant, Gauss-Newton, Marquardt, steepest decent methods (SAS/Stat vol 2, 1994) were adopted and different initial values were tried to ensure a global minimum. We assume that auto-correlations among the measurement errors in $K(\theta)$ and $\psi(\theta)$ are negligible, since they were measured by different equipment and at different times.

Result and discussion

An example of measured water content as a function of time for individual TDR probes is shown in Figure 2-3. The water content measurements are multiplied by the probe length, L, to obtain water storage with time which is an estimate of the net water flux along the TDR probe. Generally, there existed a linear relationship between W(L,t) and t for early time measurements (i.e. before the wetting front moves beyond the ends of the probes) (Fig. 2-2). This suggests that local water flux was relatively constant with depth, for a particular probe. For one-dimensional infiltration, the values of the measured water flux should equal the applied water application rate and be the same for all TDR probes. The average of measured local water flux was very similar to the applied rate (Table 2-1.). However, there was significant horizontal variability of the water flux for individual probes (Table 2-1). The absolute variance of local water flux increased as the water application rate increased for all the four depths. This is in agreement with Yeh et al. (1989) for higher rate steady-state flow in heterogeneous soils with positively correlated saturated hydraulic conductivity, Ks, and macroscopic capillary length scale, α. The variability of local water flux under constant water application rate indicates flow is not one-dimensional. However, the strong linear relationship between W(L,t) and early time suggests that applied water is redistributing in the first few centimeters of the soil surface, and subsequently establishing constant, but different local vertical water fluxes in the horizontal plane. This is similar to the stream-tube assumptions of Dagan and Bresler (1979, 1983).

The average steady-state soil water content decreased as expected with a decrease in application rate (Table 2-2.). The variance of steady-state water content first increased, then decreased with increasing water application rate, thus, increasing average water content for depth 0-0.2, 0-0.6, and 0-0.8 m . This is, again, similar to the theoretical analysis given by Yeh et al. (1989) for steady-state flow in heterogeneous soils with positively correlated saturated hydraulic conductivity, Ks, and macroscopic capillary length scale, α. For 0-0.4 m depth, however, the variance of water content did not change much as the average water content increased. The standard deviation (STD) of the water content for 0-0.4 m (Table 2-2.) is similar to the measurement error of water content by TDR (STD=0.013, Topp et al, 1980). Therefore, the measurement error may mask the spatial variability for this depth. The average steady state water content for 0-0.2 m is similar to that of 0-40 cm. However, the average water content for 0-0.6 and 0-0.8 m decreased significantly for the same application rate. Given the steady state flow, the difference of steady-state water contents at different depth is a reflection of vertical variability of soil hydraulic properties. Therefore, the hydraulic properties of 0.4-0.6 and 0.6-0.8 m should be treated differently from that of 0-0.2 and 0.2 and 0.4 m. Based on mass balance, the steady state water content for 0.2-0.4, 0.4-0.6, and 0.6-0.8 m were calculated (Table 2-2.). The average steady-state water content at the same application rate has a difference as large as 0.11 along the vertical direction, further indicating the significant change of hydraulic properties along the profile. Even with this, the flow is still approximately one dimensional and the flux along a probe remains constant (Fig. 2-3).

In a manner similar to Parkin et al. (1995), the variability in measured local water fluxes are utilized to estimate the field average hydraulic conductivity. Constant water flux along each TDR probe represents an individual stream-tube with local but different one-dimensional flow. At long times a unit gradient is assumed along each TDR probe and the measured local water flux (from early time measurements) is set equal to the hydraulic conductivity value associated with the steady-state local soil water content and pressure head measurements for each multi-purpose TDR probes. These measurements (L=0.2 m) are graphed in Fig. 2-4 and Fig. 2-5. By fixing the residual water content, θ_r =0.05, the nonlinear optimization procedure NONLIN (SAS, 1994) was used to estimate the parameters K_s, C, α, and θ_s for BW model and Ks, m,n, θ_s for VGB model. The fitted 4-parameter van Genuchten and Burdine model (VGB) (Eq.[2-17] and Eq. [2-18]) and Broadbridge and White model, BW (Eq.[2-3] and Eq.[2-4]) are very similar. The parameters for the models are given in Table 2-3. The fitted θ_s is close to the saturated water content for sandy soils (Carsel and Parish, 1988). The C parameter is in the range of in-situ soils as indicated by White and Broadbridge (1988). The estimated Ks is in the range of sandy soils, but smaller than the average value of underground aquifer (Sudicky, 1986).

In the same manner, the average soil hydraulic conductivity as a function of steady-state water content for depths 0.2-0.4, 0.4-0.6, and 0.6-0.8 m can be obtained from Table 2-2, by assuming the application rate equal the hydraulic conductivity at steady state (Fig. 2-6). The hydraulic conductivities for 0-0.2, and 0.2-0.4 m are quite similar except for water content close to saturation. However, the hydraulic conductivity for 0.4-0.6 and 0.6-0.8 deviate significantly from the curve for 0-0.2 m depth. The change of hydraulic conductivity with water content becomes sharper for 0.4-0.6 and 0.6-0.8 m, revealing that the pore size distribution becomes narrower for the two depths. This agrees with visual observation of the material in the soil profile. In the same manner, the average water characteristic curves at depth=0.2 and 0.4 m are compared with the fitted curve (Fig. 2-6). The average of measured pressure head versus the average of measured steady state water content agree with the fitted curve, further indicating the homogeneity of the soil in 0-0.4 m.

The estimated BW parameters in Table 2-2 were used in the BW solution (Eq. [2-16]) to predict field average water storage versus time for the 0-0.2 and 0- 0.4 m depth during constant flux infiltration for the 4 application rates. The predicted water storage was very similar to measured values (Fig. 2-7; Fig. 2-8). For 0-0.2 m depth, the predictions for rate=0.9, 3.3, and 6.22 cm h^{-1} were remarkably similar to the measurements , while a little overestimation occurs for application rate = 1.5, and 3.3 cm h^{-1} . For 0-0.4 m depth, the prediction underestimates the water storage for rate =0.9, and 1.5 cm h^{-1} , but overestimates the W(t) for rate=2.59, 3.3, and 6.22 cm h^{-1} . However, in general, the regression of predicted versus measured storage among all rates were highly significant(R^2= 0.95,1,1,0.99 and 1 for application rate= 0.90, 1.5, 2.59, 3.3, and 6.22 cm h^{-1}, respectively). The average prediction error for water content was ± 0.005 with a standard deviation of 0.006, which is less than the measurement error of the TDR method (Topp, et al., 1980). We notice that the prediction can be further improved by adopting an infiltration rate obtained from the regression of W(t) versus time for early time measurements, as listed in Table 2-1.

Summary and Conclusions

A series of infiltration experiments in Borden, Ontario were conducted with a greenhouse irrigation system. By using multipurpose TDR probes, we were able to determine the local flux at each TDR probe, based on the fact that the rate of increase in water storage for vertically-installed TDR probes is linear with time before the wetting front passes the end of TDR probes. Our experiments showed that for different application rates, water flow was approximately vertical within the measurement volume of TDR. This provided experimental evidence of the stream tube model of Dagan and Bresler (1983).

By employing the unit gradient assumption, we were able to obtain the hydraulic conductivity at equilibrium phase of constant flux infiltration from locally measured flux and water content. With measured water matric potential by multipurpose TDR probes at equilibrium, we obtained the water retention curve.

With measured apparent $K(\theta)$ and $\psi(\theta)$ curves for the field, the predicted water storage from Parkin et al.(1992) solution, was remarkably similar to the measured field-averaged water storage during constant rainfall infiltration, indicating that the measured $K(\theta)$ and $\psi(\theta)$ by multipurpose TDR probes and the solution represented the field behavior.

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Table 2-1. Applied water application rates and measured water fluxes.

	Average measured water flux							
	Local flux averaging‡				Local storage averaging§			
Applied rate	0-0.2 m	0.0.4 m	0-0.6 m	0-0.8 m	0-0.2 m	0-0.4 m	0-0.6 m	0-0.8 m
$cm\ hr^{-1}$	$cm\ hr^{-1}$				$cm\ hr^{-1}$			
0.9	0.84(0.15)†	0.81(0.08)	0.94(0.09)	0.96(0.12)	0.74	0.87	0.87	0.88
1.50	1.41(0.19)	1.51(0.13)	1.52(0.14)	1.56(0.17)	1.40	1.43	1.55	1.62
2.59	2.34(0.20)	2.59(0.22)	2.59(0.32)	2.61(0.34)	2.38	2.40	2.46	2.44
3.30	3.20(0.45)	3.29(0.30)	3.44(0.50)	3.41(0.63)	2.97	3.29	3.22	3.19
6.22	5.47(0.80)	6.19(0.44)	6.03(0.89)	6.19(0.80)	6.26	6.07	6.53	6.23

† Values in brackets (.) are standard deviations for the transect.

‡ Average of all local measured water fluxes.

§ Water flux calculated from the rate of change of average soil water storage.

Table 2-2. Steady state soil water content and pressure head under constant water application.

	Pressure head		Soil water content				Incremental soil water content‡		
Applic. rate	0.2 m	0.4 m	0-0.2 m	0-0.4 m	0-0.6 m	0-0.8 m	0.2-0.4 m	0.4-0.6 m	0.6-0.8 m
$cm\ hr^{-1}$	cm		$cm^3\ cm^{-3}$				$cm^3\ cm^{-3}$		
Initial	-82 (6.0)†	-74 (5.9)	0.11 (0.016)†	0.13 (0.019)	0.14 (0.010)	0.14 (0.010)	0.15	0.16	0.14
0.21	-30 (5.2)	-27 (5.0)	0.21 (0.018)	0.21 (0.020)	0.21 (0.010)	0.21 (0.014)	0.21	0.21	0.21
0.9	-22 (4.8)	-13 (4.8)	0.27 (0.029)	0.28 (0.017)	0.28 (0.018)	0.27 (0.019)	0.29	0.27	0.24
1.5	N/A§	N/A	0.31 (0.028)	0.31 (0.018)	0.31 (0.025)	0.29 (0.021)	0.32	0.29	0.25
2.59	N/A	N/A	0.34 (0.026)	0.34 (0.012)	0.32 (0.020)	0.31 (0.026)	0.34	0.28	0.26
3.30	-4.3 (2.6)	-4.5 (3.8)	0.38 (0.022)	0.37 (0.019)	0.35 (0.019)	0.33 (0.029)	0.36	0.31	0.27
6.22	-8.7 (3.4)	-3.5 (6.2)	0.41 (0.024)	0.40 (0.017)	0.38 (0.014)	0.36 (0.020)	0.39	0.34	0.30

† Values in brackets (.) are standard deviations along the transect.
‡ Calculated by mass balance from average water storage for each TDR probe length
§ Not measured.

Table 2-3. Fitted parameters for Broadbridge & White model (BW) and van Genuchten & Burdine model (VGB).

Model	Hydraulic parameter				
	Ks	**α**	**θ_s**	**C/n**	**m**
	cm hr^{-1}	cm-1	cm3 cm-3		
BW	7.18	0.0978	0.42	1.27	N/A*
VGB	8.94	0.056	0.45	1.64	0.76

Note: *N/A, not applicable.

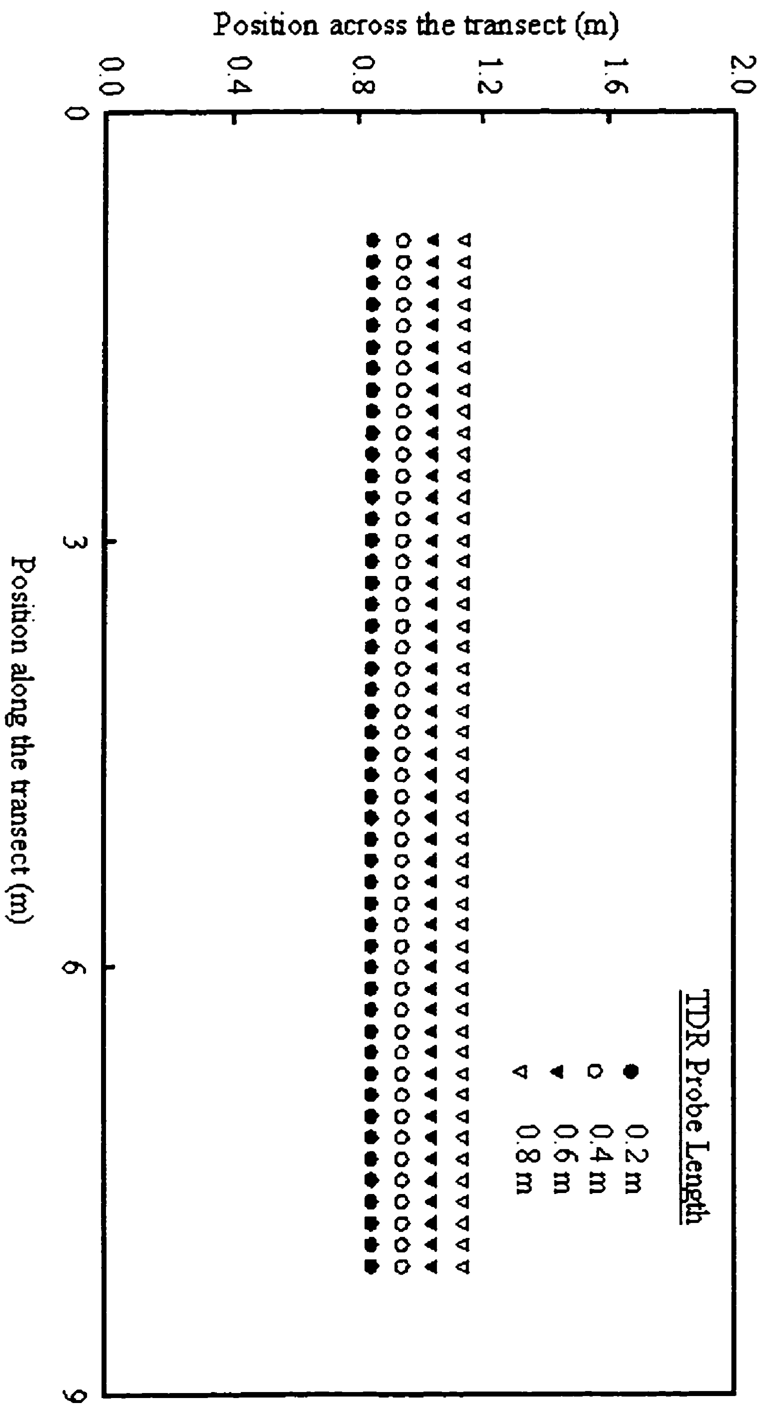

Figure 2-1. Diagram of wetted sample area(2×9 m^2) and locations of multipurpose TDR probes.

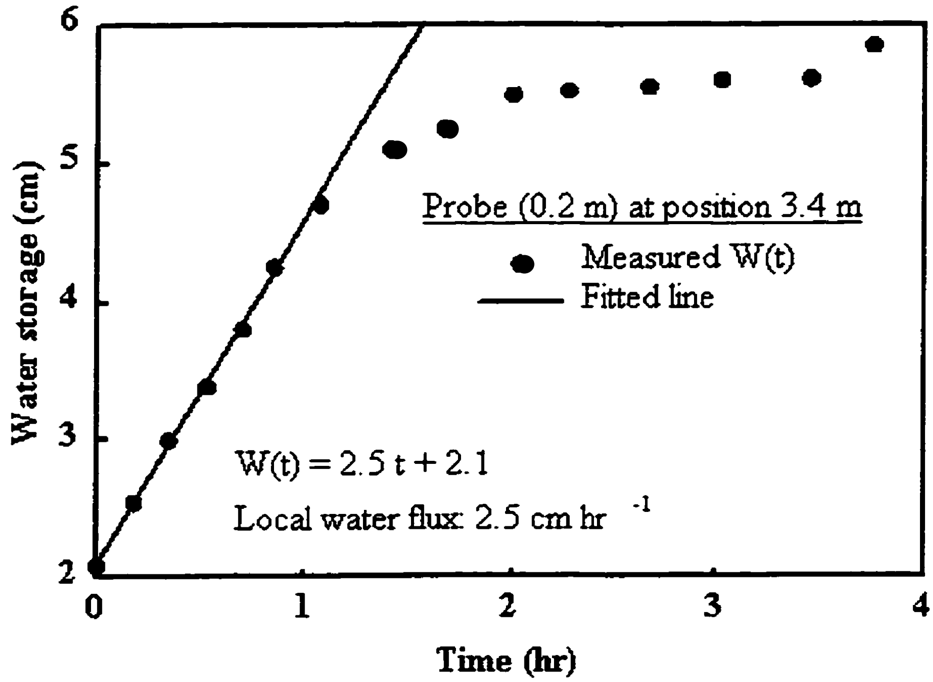

Fig. 2-2. Illustration of the of linear relationship at early time before the wetting front pass the end of TDR rod at position 3.4 m. The first five points were used in the regression.

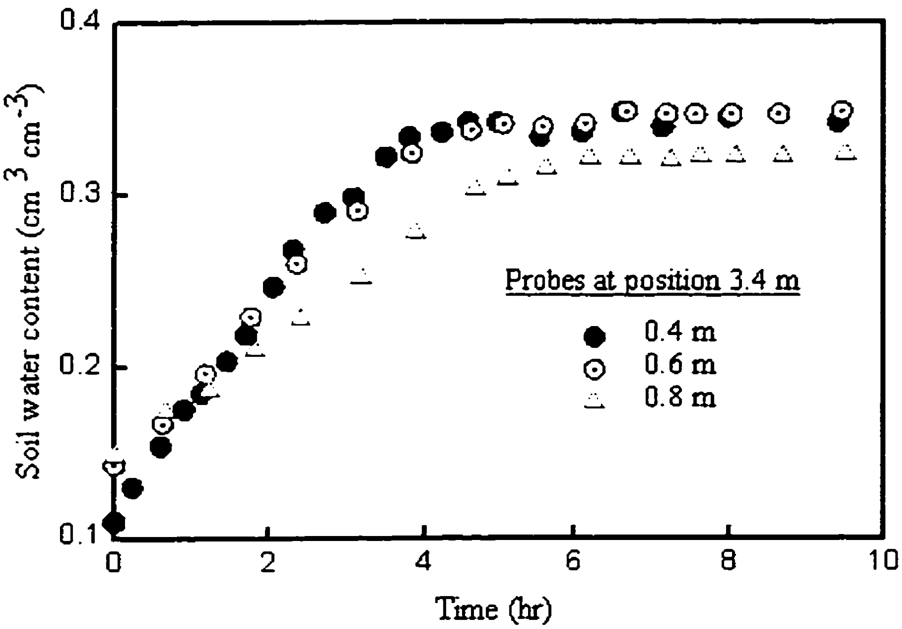

Fig. 2-3. Water content versus time for 40, 60, and 80 cm probe in position #35

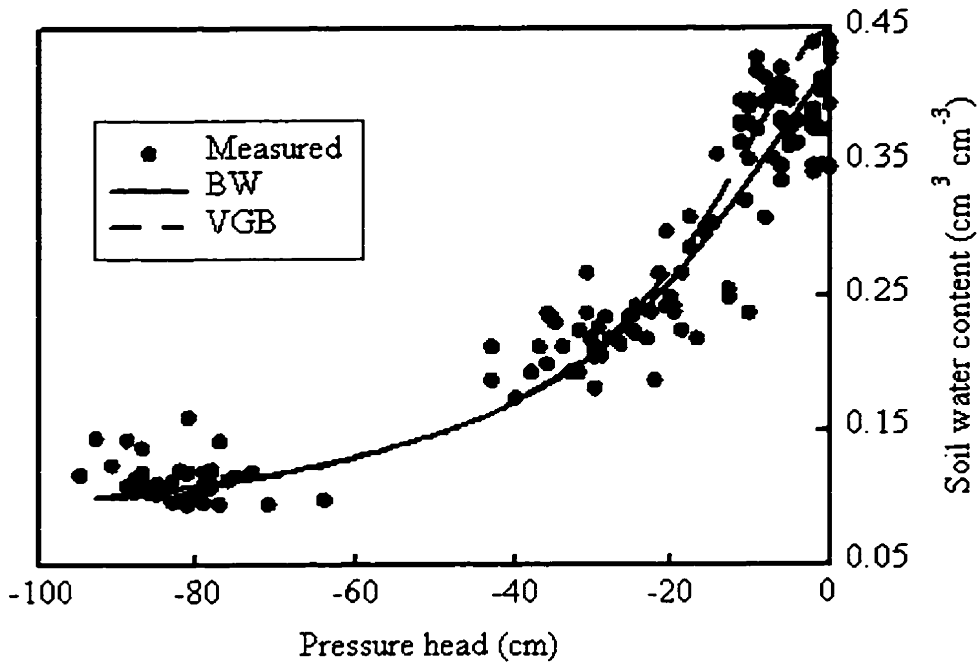

Fig. 2-4. Measured and fitted water retention curves for 0-20 cm depth.

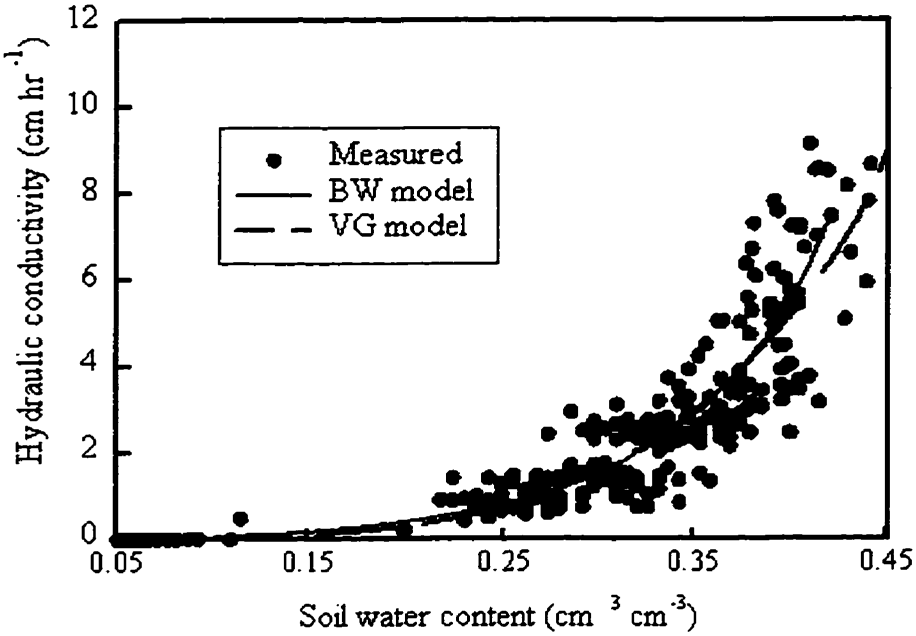

Fig. 2-5 Measured and fitted hydraulic conductivity curves for 0-20 cm depth.

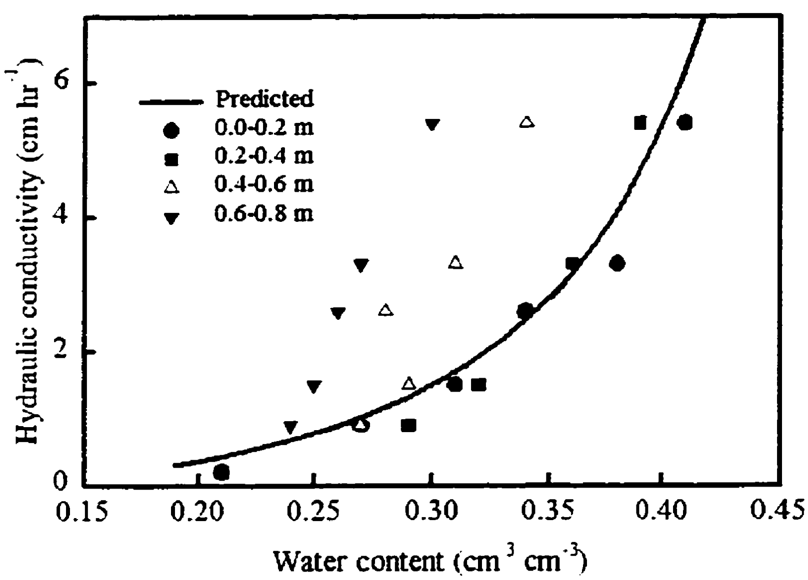

Fig. 2-6. Measured hydraulic conductivity as a function of water content for depth 0-0.2, 0.2-0.4, 0.4-0.6, and 0.6-0.8 m.

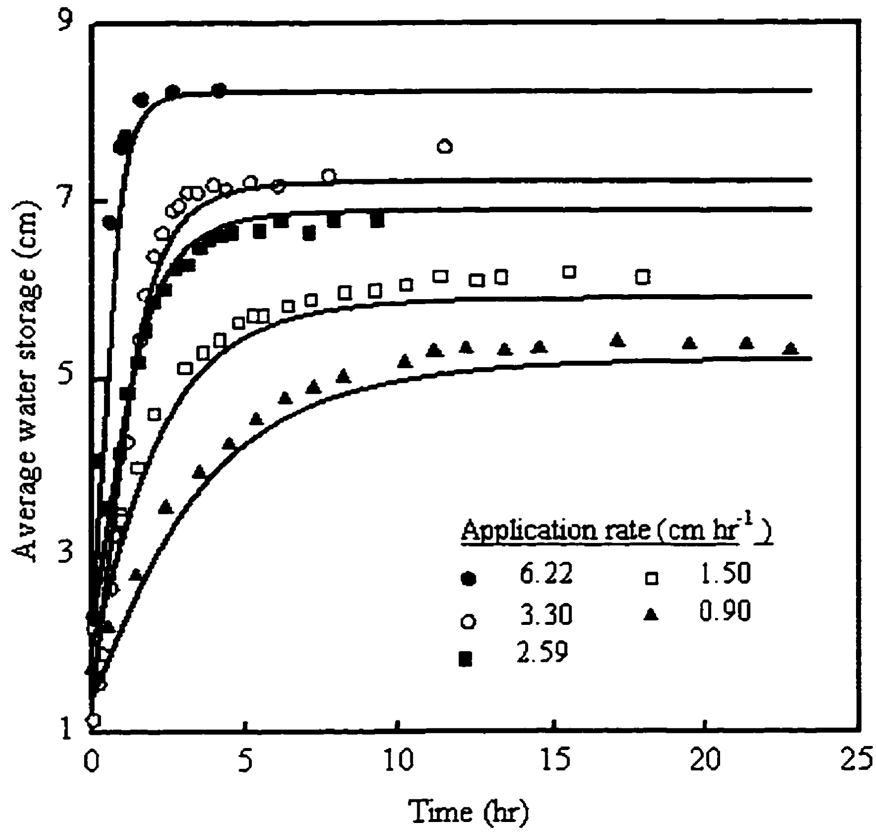

Fig. 2-7. Measured and predicted water storage versus time for application rate=0.9, 1.5, 2.59, 3.3, and 6.22 cm hr^{-1} for 0-0.2 m.

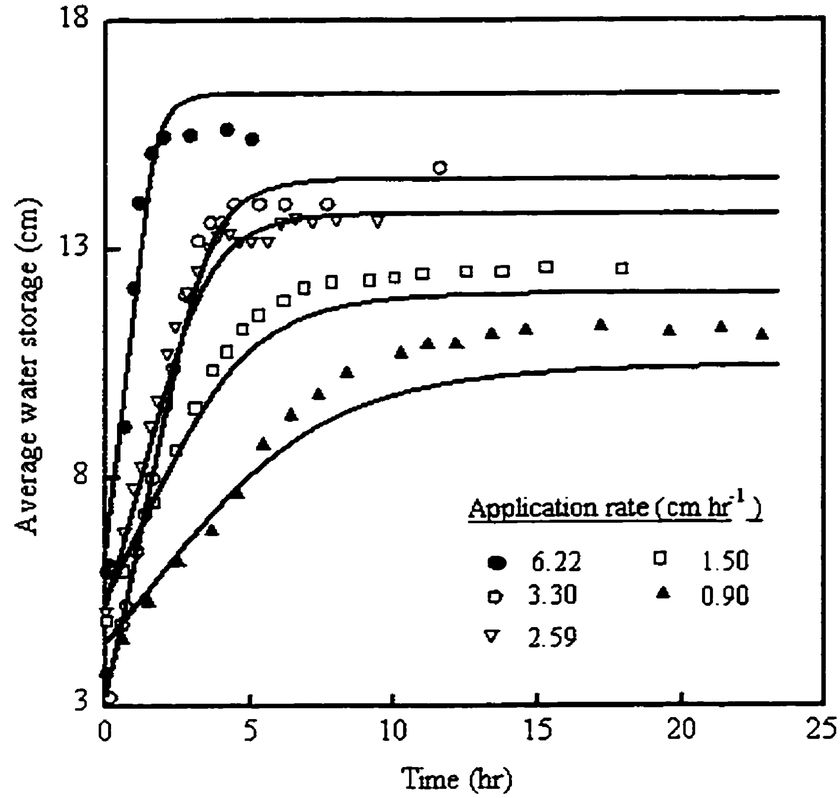

Fig. 2-8. Measured and predicted water storage versus time for application rate=0.9, 1.5, 2.59, 3.3, and 6.22 cm hr^{-1} for 0-0.4 m.

Chapter 3

Estimating the soil hydraulic properties from measurements of multi-purpose TDR probes using inverse procedure

Abstract

There is a need for accurate and cost-effective methods to estimate the hydraulic properties of soils. Past work indicated measurements of a single hydraulic response will not necessarily result in unique and stable estimates of hydraulic parameters when the number of unknown is more than two. Prior information regarding the parameters or additional measurements are needed for the estimation problem to be well-posed. However, accurate prior information is seldom available due to variations of the hydraulic properties in space and time. This paper presents a method for estimating hydraulic properties from simultaneous measurements of soil water storage to a fixed depth as a function of time during constant flux infiltration and steady-state pressure head readings using vertically installed multi-purpose TDR probes (MTDR). MTDR probes have a porous steel cup at their ends allowing soil water storage and ψ to be simultaneously measured at the same location. Our parameter estimation is formulated by an inverse procedure which combines a weighted nonlinear least square method with analytical solutions for soil water content and pressure head as functions of depth and time during one dimensional infiltration. We analyze the possibility of using water storage data combined with the initial and steady-state pressure head readings for the purpose of estimating soil hydraulic properties. The uniqueness

problem was analyzed by studying the behavior of response surfaces. The combination of water storage measurements during constant flux infiltration with an initial and a steady-state pressure head reading yielded unique and stable solutions of the inverse problem. The utility of the parameter estimation procedure is demonstrated using experimental and theoretical data.

Introduction

In efforts to better monitor and manage the migration of chemicals in the vadose zone, scientists and engineers over the past several decades have developed analytical and numerical models describing the movement of water and chemicals into and through the unsaturated zone. These models have become indispensable tools in research for quantifying and integrating the most pertinent physical and chemical processes in the unsaturated soil zone. The application of these models to field-scale flow and transport problems relies heavily on the quality of the model parameters, especially the unsaturated hydraulic properties.

For accurately describing soil unsaturated hydraulic conductivity, $K(\theta)$, and soil pressure head, $\psi(\theta)$, relationships over a wide range of soil water contents, θ, the equations of Brooks & Corey (Brooks and Corey, 1963), van Genuchten & Mualem(van Genuchten, 1980) and Broadbridge &White (Broadbridge and White, 1988) are good choices (van

Genuchten and Nielsen, 1985; White and Broadbridge, 1988). These equations have four to five independent parameters, which vary considerably among soils and are not readily available.

Inverse procedures can be used to estimate the parameters of hydraulic functions (Dane and Hruska, 1983; Zachmann et al., 1982; Kool et al., 1985, 1988; Russo et al., 1991; Simunek et al., 1996). For given initial and boundary conditions, Richards' equation can be solved with appropriate analytical or numerical methods. Particular constitutive functions for the hydraulic properties are assumed. The parameters in these hydraulic functions are estimated by minimizing the difference between the predicted and observed hydraulic responses, such as pressure head, ψ, water content θ, flow rate, or other flow attributes. The approach is attractive because few restrictions are posed upon the experimental conditions, allowing relatively simple experimental designs.

A serious problem encountered in the estimation of hydraulic functions stems from their over-parametrization, or inclusion of unidentifiable parameters. For example, Parker et al.(1985) indicated that the inverse problem for a one-step outflow experiment is non-unique when the number of unknown parameters is three and only outflow volume is measured. Russo et al.(1991) concluded the same for ponded infiltration when only infiltration rate is recorded. Steady-state measurements of infiltration rate for a tension infiltrometer is also not enough to obtain unique estimation of saturated hydraulic conductivity Ks, and two other shape parameters for van Genuchten equations(Simunek et al., 1996). To solve the identification problem, additional information regarding the parameters must be provided. There are usually two types of information: (1) additional measurements of one or more response variables such as ψ measurements as in the case of Parker et al.(1985), or another set of experiments (van Dam et al., 1992; Parkin et al., 1995); (2) prior information about the hydraulic parameters, such as the saturated hydraulic conductivity K_s and one of the shape parameters (Russo et al., 1991).

Prior information about the parameters is a very effective method to remove nonuniqueness. Prior information usually takes the form of an initial guess of the parameter values and range based on easily measured soil properties. The actual value of the parameter identified in the inverse problem can be different from this initial guess. However, this pre-specified and approximate value constrains the parameter within the range. An inverse problem is always unique if accurate prior information about all the parameters is available and an appropriate estimation procedure is adopted (Abaspour et al., 1997). Prior information about saturated water content θ_s can be obtained through bulk density, and soil particle size distribution. Accurate prior information about the shape parameters and K_s is seldom available, because the parameters are highly variable in field conditions. It is usually easier to take additional measurements of a response variable such as ψ than to have accurate prior information about these hydraulic parameters.

Not all additional response measurements are useful for improving well-posedness of an inverse problem. The usefulness of additional measurements depends on its sensitivity to the hydraulic parameters , independence of the existing measurements, and measurement error. For example, measurement during transient conditions can be added to steady-state measurements of the disk tension infiltrometer for inverse parameter identification(Simunek et al., 1997). The effort needed to take the measurements is also an important factor.

Pressure head is a good choice for additional measurements if only water flux or water content have been measured (Kool and Parker, 1988; Parker et al., 1985). The standard methods to measure ψ is to install a tensiometer at a spatial location different from the soil water measurements. This may introduce significant error in spatially varying soils (Tseng and Jury, 1993).

Recently, vertically-installed multi-purpose TDR probes developed by Baumgartner et al. (1994) were utilized to measure simultaneously soil water storage and pressure head at the same spatial location during constant flux infiltration(Chapter 2). This effectively alleviates the error due to measurements taken at different locations. The approach of Parkin et al. (1995) was used to measure directly the field average $K(\theta)$. The approach utilized the spatial variability of vertical soil water flux under constant water application at different rates. Multipurpose TDR probes were used to measure field average $\psi(\theta)$ after steady-state had been reached. Despite the simplicity, these methods (Parkin et al., 1995; Chapter 2) have the following disadvantages: (1) multiple water application rates are required. (2) only field average $K(\theta)$ and $\psi(\theta)$ are obtained. (3) The method does not make use of transient information on the depth integrated shape of the wetting front collected from water storage measurements at each TDR probe.

The objectives of this paper are to extend the method of Chapter 2 to estimate the hydraulic parameters at a single location (TDR probe) from multipurpose TDR measurements of water storage W and ψ during a single constant flux infiltration experiment. The method was formulated as an inverse problem and the full set of transient water storage measurements are utilized in the estimation process. The need for ψ

measurements, to guarantee unique parameter estimates are examined from the response surfaces for different combinations of parameter spaces. Analytical solutions for transient soil water storage, W(t), and ψ under constant flux infiltration (Parkin et al., 1992) are utilized with the realistic hydraulic function of Broadbridge and White (1988). The utility of the parameter estimation procedure is demonstrated using experimental and theoretical data.

Theory

Statement of the estimation problem

A typical curve of soil water storage as a function of time, W(t), to a fixed depth as measured by TDR during constant flux infiltration is shown in Fig. 3-1. This curve can be partitioned into three distinct pieces of information. The first piece is the water storage during the period that the wetting front remains within the length of the TDR probe. In this period, assuming approximate one dimensional flow, the water storage increases linearly with the time. The rate of change of W(t) during this time is equal to the local infiltration rate at this location. The second piece of information is the shape (curvature) of the soil water storage curve from the time when the wetting front just reaches the end of TDR rod to the time when the wetting front completely passes the TDR rod. This section contains the depth integrated transient shape of the wetting front and represents the nonlinearity of water flow in soil during constant flux infiltration. The third piece of information is the water storage value at steady state.

Under field conditions, uniformly applied water can redistribute in the first few centimeters of the soil surface, and subsequently establish relatively constant, but different local vertical water fluxes in the horizontal plane (Chapter 2). Therefore, the water flux at a point is a priori unknown. The proposed method includes two steps. The first step is to estimate the local infiltration rate R from the first piece of the W(t) curve. With R known, the second step is to estimate the hydraulic parameters by best fitting the measured water storage as a function of time to the analytical solution of Parkin et al. (1992).

In this paper, the hydraulic parameters Ks, α, C, and θ_s are treated as unknowns. The purpose is to estimate Ks, α, C, and θ_s given the measurements of the full W(t) curve , a priori information about θ_s and the easily-measured ψ at the initial condition and the final steady state condition. Here, the prior information about θ_s is utilized, because the prior θ_s is easy to obtain. Our intention is not to analyze the influence of prior information on the parameter estimation, but rather to use as much information as possible in the estimation problem based on the Bayesian philosophy(Box and Tiao, 1973). The influence of additional measurements of steady- state ψ are examined.

Parametrization of soil hydraulic properties.

Broadbridge and White (BW) (1988) and Sander et al.(1988) independently developed an analytical solution for constant flux infiltration boundary. The BW solution is based on the following parametrization of hydraulic conductivity, $K(\Theta)$ (cm hr^{-1}) and diffusivity function, $D(\Theta)$ (cm^2 hr^{-1})

$$K(\Theta) = K_s \frac{(C-1)\ \Theta^2}{C-\Theta} \qquad [3\text{-}1]$$

$$D(\Theta) = \frac{K_s\ C\ (C-1)}{\alpha\ \Delta\theta\ (C-\Theta)^2} \qquad [3\text{-}2]$$

where $\Delta\theta=\theta_s-\theta_r$ and $\Theta=(\theta-\theta_r)/\Delta\theta$. θ_s and θ_r are the saturated and residual water content ($cm^3\ cm^{-3}$), respectively. K_s (cm hr^{-1}) and α (cm^{-1}) are the saturated hydraulic conductivity and inverse capillary length scale (Philip, 1985), respectively. C is a shape constant introduce by BW. By definition,

$$D(\Theta) = K(\Theta) \frac{d\psi}{d\theta} \qquad [3\text{-}3]$$

we have,

$$\psi(\Theta)-\psi_0 = \Delta\theta\int_0^{\Theta} D(\Theta)/K(\Theta)\ d\Theta \qquad [3\text{-}4]$$

By assuming ψ_0 as zero as did Broadbridge and White (1988), substitution of Eq. [3-1] and Eq. [3-2] into Eq. [3-4] and integration yields

$$\psi = \frac{1}{\alpha}[\frac{1-\Theta}{\Theta}+\frac{1}{C}\ln(\frac{C-\Theta}{\Theta(C-1)})] \qquad [3\text{-}5]$$

Forward problem

Richards' equation used to describe one-dimensional nonhysteretic flow in idea soil is given by

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial z}(D(\theta)\frac{\partial\theta}{\partial z}) - \frac{dK(\theta)}{d\theta}\frac{d\theta}{dz} \qquad [3\text{-}6]$$

where θ(z,t) is the volumetric water content, z (m) is the depth and t(s) is the time. The initial and boundary conditions considered here are

$$(-D(\theta)\frac{\partial\theta}{\partial z} + K(\theta))|_{z=0} = R \quad ; \quad t>0 \qquad [3\text{-}7]$$

$$\theta(z,0) = \theta_0 \qquad [3\text{-}8]$$

where R is the application rate (cm hr^{-1}) at the soil surface and θ_0 is the initial soil water content (cm^3 cm^{-3}). Utilizing Eq. [3-1] and Eq. [3-2], through a series of transforms (i.e. Kirkhoff, Storm, and Hopf and Cole transforms), BW derived an analytical solution as

$$\Theta(\zeta,t) = C[1-(1+2\rho-u(\zeta,t)^{-1}\frac{\partial u(\zeta,t)}{\partial\zeta})^{-1}] \qquad [3\text{-}9]$$

and

$$z(\zeta,t) = (C\alpha)^{-1}[\rho(\rho+1)\tau+(2\rho+1)\zeta-\ln(u(\zeta,t))] \qquad [3\text{-}10]$$

where ζ is a parameter connecting Eq. [3-9] and Eq. [3-10], u(ζ,t) is given by Eq. [43] of BW, and

$$\rho = \frac{R}{4C(C-1)Ks} \qquad \tau = \frac{4C(C-1)\ \alpha K_s t}{\Delta\theta} \qquad [3\text{-}11]$$

By change of variable of integration, Parkin *et al.* (1992,1995) derived analytical solutions for water storage for infiltration and drainage, respectively. Using the unified solution of Warrick et al. (1990) for soil water content profile, a unified water storage solution for both infiltration and drainage can be obtained as following,

$$W(L,t) = \frac{\Delta\theta}{\alpha}[2\rho\ \zeta(L,t) + \ln(\frac{u(0,t)}{u(\zeta,t)})] + \theta_r L \qquad [3\text{-}12]$$

Eq.[3-12] provides the basic formula for estimation of soil hydraulic parameters.

Formulation of the inverse problem.

The inverse problem is to obtain parameter vector $\beta = \{K_s, \alpha, C, \theta_s\}$ by best fitting Eq. [3-12] to measured water storage W(L,t)*. This is repeated under the constraint of prior information about θ_s and additional measurements of steady-state ψ (Eq. [3-5]). To obtain a good estimate of a particular hydraulic parameter, we need to define an estimator. A good estimator minimizes the discrepancy between the measurement and predicted response, while best reflecting the hydraulic properties of the medium. A general, intuitively appealing and theoretically sound estimator is the maximum a posteriori estimator, which incorporates additional measurements and prior information into the estimator (Bard, 1974). In this way, the obtained parameters are guaranteed physically meaningful and may convert a degenerate equation into a non-degenerate case (Bard, 1974). Assuming the measurement errors asymptotically follow multi-variate normal distributions, the likelihood function, $L(\beta|y^*)$, can be formulated as

$$L(\beta|Y^*) = f(Y|\beta) = (2\pi)^{-n/2}\det[G]^{-1/2}\exp(-\frac{1}{2}(Y(\beta)-Y^*)^T G^{-1}(Y(\beta)-Y^*)) \qquad [3\text{-}13]$$

where n is the number of observations, det[ ] indicates determinant,

$$G = \begin{matrix} G_W & 0 & 0 \\ 0 & G_\psi & 0 \\ 0 & 0 & G_\beta \end{matrix}$$

and $Y=\{W, \psi, p\}$, $Y^*=\{W^*, \psi^*, \beta^*\}$; The values of transient water storage W, and pressure head ψ are those predicted by Eq. [3-12], and Eq. [3-5] at those times associated with the measurements; G_w, G_ψ, and G_p are the covariance matrices of W, ψ, and prior information, respectively. The independence between W, ψ, and prior information are assumed, as indicated by zero non-diagonal terms in the covariance matrix . This is a reasonable assumption, because (1), the measurements of water storage and hydraulic head are taken by different instrumentation and measured at different times; (2) the prior information is usually a good guess from other source of information or an approximation according to characteristics of the solution. Therefore the measurement error associated with the hydraulic head or the water storage are not the dominant factor controlling the error of prior information. Since the logarithm is a monotonic increasing function of its argument, the value of β that maximizes $L(\beta)$ also maximizes $\log(L(\beta))$. Since log L is frequently a simpler function than L, the maximum likelihood estimator is obtained by minimizing the negative log of the a posterior likelihood function,

$$\varphi = -2\log(L(\beta|y)) = n\ln(2\pi) + \ln(\det[G]) + [(W-W^*)^T G_W (W-W^*)]$$

$$+[(\psi-\psi^*)^T G_\psi (\psi-\psi^*)] + [(\beta-\beta^*)^T G_\beta (\beta-\beta^*)] \qquad [3\text{-}14]$$

Assuming uniform measurement error (constant variance) and prior information available only for θ_s, minimizing Eq. [3-14] is equivalent to minimizing the following weighted nonlinear least squares estimator

$$S = \sum (W-W^*)^2 + \frac{\sigma_W^2}{\sigma_\psi^2}\sum(\psi-\psi^*)^2 + \frac{\sigma_W^2}{\sigma_\theta^2}(\theta_s-\theta_s^*)^2 \qquad [3\text{-}15]$$

where σ_W^2, σ_ψ^2, and σ_θ^2 are the variances of measurement error in W, of measurement error in ψ, and of estimation error in θ_s respectively. The inverse problem is to minimize S with respect to β given W*, ψ* and prior information about θ_s, θ_s*. Usually, σ_w, σ_ψ, and σ_θ are unknown, and could be treated as unknown parameters in minimizing Eq. [3-15]. However, this introduces more parameters and uncertainty in the inverse problem, which is not recommended. Therefore, σ_w, σ_ψ, and σ_θ are selected empirically from other source of information or experience (Bayesian philosophy), which is subjective. A smaller σ_ψ means a heavier weight on the ψ measurement and the resulting parameters fit the ψ measurement better at the cost of fitting W or prior information worse. Too much weight on one kind of measurement is a waste of information of the other kinds. Therefore, improper selection of weights will lead to an ill-posed inverse problem.

An inverse problem is ill posed if (1) the solution does not exist, (2) is not unique, (3) not stable, which means small change in the response can cause large change in the parameters. For this problem, the possibility of ill-posedness is reduced because:

(1) As shown by Broadbridge and White (1988), the BW form is fairly realistic and capable of incorporating soil properties ranging from those of the weakly nonlinear Burgers' equation to those of a highly nonlinear Green-Ampt-like model. Thus, the parametrization is simple enough to yield well-posed problem but complex enough to capture the salient features of the change of pressure head and hydraulic conductivity or diffusivity with water content.

(2) Three (K_s, α, θ_s) of four parameters in the BW model have clear physical meaning, thus more information about the parameters can be projected into the model according to the properties of the soil, such as organic mater, bulk density, etc.

(3) Adopting an advanced technology such as the multipurpose TDR probe allowing repeated measurements, measurement error of the response should be reduced.

(4) An exact analytical solution is used and the model error or the numerical error due to discretization in space and time should be minimized.

(5) Flux boundary conditions are easy to control (Chapter 2) and more sensitive to the hydraulic parameters (McLaughlin et al., 1996).

(6). Local application rate, R*, can be calculated from the solution characteristics: The rate of increase in water storage at initial stage equals the local water flux. In this way, the local infiltration rate can be obtained, and one unknown reduced from the inverse problem.

Analysis

Sensitivity coefficients

To find the approximate range of applied infiltration rate over which the parameters have the maximum sensitivity to the water storage W(L,t). The sum sensitivity coefficients over time at specific infiltration rate R were calculated using the finite difference method as follows (Yeh, 1986).

$$\lambda_j = \frac{\partial[\sum_{i=1}^{m} W(\beta;t_i)]}{\partial\beta_j} = \frac{\sum_{i=1}^{m}[W(\beta+\Delta\beta e_j;t_i)-W(\beta;t_i)]}{\Delta\beta_j}$$

Where e_j is the jth unit vector and m is the number of measurements. In this paper, only the sensitivity coefficients of λ as a function of R were calculated and the numerical calculations were carried out using the software package Mathcad (version 6, Mathsoft Inc.).

Uniqueness and stability analysis

To investigate the question of nonuniqueness, the global properties of the prediction error were examined. If the prediction error surface has a single minimum point, the solution is unique. If it has more than one minimum points, the solution is nonunique, and additional information must be added to resolve the indeterminacy. When the number of unknown parameters is 2 , it may be possible to investigate the shape of the surface by graphical techniques(Menke, 1989).

Thus, the uniqueness of the inverse problem was evaluated from the two-dimensional response surfaces of the objective function as a function of pairs of soil-hydraulic parameters. This contour analysis applies only to the case where there are two unknown parameters. Because of our human limitation of understanding in higher dimensions, the uniqueness analysis for problems with three unknowns or more is usually carried out in two-dimension, by fixing one or more of the other parameters. However, the information provided by the contours are nonconclusive regarding the well-posedness, but conclusive regarding the ill-posedness of a inverse problem. To confirm the above results obtained by analyzing response surfaces, we use the Statistical Analysis System(SAS/Stat User's Guide, volume 2, 1994) procedure NONLIN to numerically find the global minimum of the objective functions for different scenarios. To analyze the cases where there are more than two unknowns, the above graphical analysis is not conclusive and the problem has to be solved several times with different initial parameter estimates, to have confidence. A program named FIT_BW.sas written in SAS language was used to carried out the numerical inversion. The program makes use of a modified Gauss-Newton nonlinear optimization methods. Because of the complicated nature of the derivatives of water storage with respective to the parameters Ks, α, and C, a numerical derivative was used.

Simulated soil water storage for a sandy soil.

A simulated case for a sandy soil with a uniform initial condition of Θ=0.1 and a flux boundary condition of R=2 cm hr^{-1} is used as an example. Parameter values for C, Ks, α, and θ_s, and θ_r for a typical sandy soil are assumed to be 1.24, 5 cm hr^{-1}, 0.08 cm^{-1}, 0.41 cm^3 cm^{-3}, and 0.06 cm^3 cm^{-3}, respectively. Water storage data was generated at a time interval of 0.15

hr from 0 to 7.5 hr using Eq. [3-12] for a TDR probe of length L=20 cm. The generated data is error-free, in the sense that it is identical to the predicted data. The generated water storage versus time is shown in Fig. [3-3] for error-free water storage measurement.

In practice, measurements of soil water properties are subject to error. For water storage measured with TDR, the measurement error mainly come from improper delineation of the reflection point, calibration error, improperly installed TDR probe and so on. A normally-distributed measurement error source $N(0,\sigma)$ is used to represent the true measurement error for the water storage measurement by TDR. The approximate standard error σ associated with a measurement of water storage given by TDR needs to be defined. After examining many mineral soils, Topp at al (1980) indicated that the water content measurement given by TDR had a standard error of 0.013 when the three term Topp's calibration equation was used. Thus, for a 20 cm probe, the water storage measurement would have an approximate standard error of 0.26 cm, if the same calibration equation is used. To investigate the effect of measurement error on the inverse solution, we considered the case where the water storage data are subject to random measurement error represented as a $N(0, \sigma)\times L$ where σ=0.013 cm and L is the length of TDR rods. Theoretically generated water storage data for the typical sandy soil example is also shown in Fig. 3-3.

For the sandy soil example, the error response surface as a function parameter pair was calculated according Eq. [3-14], while keeping other parameters at the "true" value. The calculation were carried out with and without error in the water storage measurements. Response surface contour lines were drawn by Surfer (Golden software, 1995) using the inverse distance interpolation algorithm. Response surface were also calculated with prior average θ_s estimated at 0.41 with standard deviation=0.09 (Carsel et al., 1989). Finally, response surfaces were calculated assuming either a ψ measurement was available: $\psi(\Theta=0.3)=91$ cm, or both a final and an initial $\psi(\Theta=0.3)=91$ cm and $\psi(\Theta=0.2)=20$ c m are available. We assumed that the σ^2_ψ is three times bigger than σ^2_w Therefore, all the unknowns in Eq. [3-15] are known and the response surface for different scenarios can be constructed.

Field experiment

The experiment was conducted at Borden, Ontario, Canada. A detailed description can be found in Si et al. (1998). Briefly, the experimental surface area was covered with a greenhouse to prevent effects of wind, precipitation and evaporation. Within the sampling area, multi-purpose 20 cm TDR probes for a given depth were installed every 0.15 m in a 7.5 m long transect for a total of 50 probes. A hanging track system with spray nozzles was used to provide uniform application of water along the transect. The nozzles were installed on the linear array at 10 cm intervals with their spray axis aligned perpendicular to the transect. This produced a uniform narrow wetted area of approximately 0.2×2 m^2. The nozzle array was attached 0.5 m above the soil surface to a commercially available, programmable water application system designed for green houses (model DCA, Monorail Boom Spray System, Waterford, Ontario). The system has a single pressure regulator, electric solenoid valve, and microprocessor unit attached to a hanging track and conveyor belt. The hanging track is mounted to the top of the greenhouse and allows the nozzle array to go smoothly back and forth along a straight line (9 m long) with programmable delay time at either end of the line. The water can be turned on or off, at either end of the line. The system produces a uniform wetted area 2 m wide by 9 m long centered over the TDR instrumented transects

Soil water content was measured using the TDR method of Topp et al (1980). The readings were taken manually from the display screen of two pre-calibrated Tektronix(1502 C) metallic cable tester by four operators. The readings were taken just prior to the start of water application and every 5-30 minutes depending on infiltration rate and rate of change of θ. After the wetting front was beyond the 80 cm depth and all θ measurements indicated little or no change with time, the pressure head ψ measurements were taken using two tensimeters (Soil Measurement System, Tucson, Arizona). The ψ measurements were taken for application rate=0.21, 0.9, 3.3 cm h^{-1}. Infiltration experiments were conducted for 6 water application rates. After each application, the profile was allowed to drain. We also took ψ measurements at the initial condition before we started an infiltration experiment for application rate = 6.22 cm h^{-1} .

The estimated $K(\theta)$ and $\psi(\theta)$ functions from the inverse procedure and single rate were compared with those estimated from steady state measurements from all 6 application rates (Chapter 2). The average water storage measurements for the single application rate=3.3 cm h^{-1} was used as W* data.

Results and discussion

Sensitivity analysis

The sensitivity of the objective function to the hydraulic parameter, Ks, C, and α is shown in Fig. 3-2. The maximum sensitivity for Ks occurs when the water application rate R=0.8 Ks. The sensitivity to Ks increases linearly for $R \leq 0.25$ Ks and then starts to plateau with almost maximum sensitivity for R≥ 0.5 Ks and then decreases again for R > 0.8 Ks. Sensitivity to C and α is maximal at approximately R=0.3 Ks, and decreases with higher or lower application rates. At approximately R=0.4 Ks, there is very good sensitivity to all 3 parameters. Thus for sandy soils, approximate constant application rate equal to 0.4 Ks is likely optimal for hydraulic parameter estimation.

For clay soils, a separate analysis (not shown here) indicates that the sensitivity coefficient is maximal at application rate close to 0.5 Ks. Thus, different soils have approximately the same optimal application rate for identification of soil hydraulic parameters.

Uniqueness and stability analysis

Response surface analysis in two-dimensional parameter planes

Fig. 3-4 shows the response surfaces of the objective function S(W) with error-free water storage data for the three different parameter planes, K_s-C, K_s-α, and C-α. The K_s-α response surface shows a single well-defined minimum, at the true parameter values. Since the objective function is the negative logarithm of the joint probability density of K_s and α at a given value of C, the contour line also reflected the reciprocal of the probability of the combination of the two parameters. The width of the contour reflects the spread of the probability distribution about the mean of the parameter. Since the contour is elliptical, the uncertainty associated with α is bigger than that of the K_s. Thus, W is more sensitive to K_s relative to α. In addition, the contour ellipses are tilted, which means large values of K_s are especially probable if α is large. Consequently, an increase in K_s will likely result in an increase in α and vice versa. This suggests α and K_s are positively correlated. The same is true for the response curve in the C-α plane since the contours are tilted ellipses. Again, a large α, will likely have a corresponding large C. The response surface in the K_s-C plane shows a well-defined valley which starts at high K_s and low C values and extended linearly through nearly the entire parameter space. This suggests that increases in Ks and decreases in C will lead to very similar values of the objective function. This indicates possible difficulty in finding a unique inverse solution. The absence of a well-defined minimum in the response surface in Fig. 3-4 suggests that identical water storage curves can be generated by an infinite number of combinations of parameters, α, C, and K_s. Thus, the parameter C and K_s can not be estimated simultaneously from the water storage measurement only.

Figure 3-4 suggests that all the parameters are possibly correlated. The correlation would be reflected in the parameter covariance matrix, if the nonlinear least square regression were carried out. For a good estimation, we require not only a simpler covariance matrix of the residual error, but a simpler covariance matrix of the parameter as well. This means that the best model has best fit to the experimental data, least number of parameters, and least correlation among parameters (Williams, et al, 1996). We need to remove or reduce the correlation among the K_s, C, and α as much as possible, in order to get a good estimate of a parameter.

When measurement error is introduced, the K_s-C response plane (similar to Fig.3-4b) has a well-defined valley, which suggests the solution is nonunique (Fig. 3-5). Similar to Fig. 3-4q and Fig. 3-4c, the Ks-α plane and α-C plane have a well defined minimum, but severely deviated from the true values of the parameters. This is possibly due to the strong sensitivity of all the three parameters to the error in the response variable -water storage. A small change in the water storage measurement results in a big change in the estimated parameters, revealing the strong instability of this objective function. In this scenario, even if a minimum of the objective function can be located by an algorithm, it can be severely biased and the resulting parameters may not have any physical meaning, or may be difficult to interpret. This strongly suggests additional information is needed for determining uniquely the parameters from the water storage measurements.

The response surface for K_s-C, K_s-α, and C-α planes for the error-free measurements with an additional ψ measurement at the steady state for 0.2 m depth are shown in Fig. 3-6. All the objective functions have well-defined minimums. The shape of the contours for K_s-α, and α-C are almost circular, indicating that the sensitivity of α has been improved by introducing the ψ measurement. The correlation between the parameters is also reduced, since especially large values of K_s or C are no more or less likely if α is large or small. Considerable improvement in the uniqueness was also obtained in the K_s-C plane. The long valley across the parameter space in Fig. 3-4 is not present and a single well-defined minimum appears at the true parameter values. This is because ψ provides another constraint on C, reducing the interdependence of C on K_s. This suggests that the solution provided by the objective function S(W,ψ) is likely unique. The resulting parameters K_s and C may be slightly negatively correlated because the elliptical contours are tilted on the K_s-C plane.

When measurement error with zero mean and a standard error of 0.26 cm was introduced in the water storage measurements, for the case with an additional ψ measurement, the uniqueness is generally not affected (Fig. 3-7). There was little migration in the minimum of the objective function, and good approximations to the true values are obtained. Therefore, the solution provided by $S(W,\psi)$ is likely unique and stable even with errors in the measurements of the water storage when there are two unknowns.

Numerical optimization analysis

Since the contour analysis of the response surface is not conclusive when there are three unknown parameters, parameter values were sought by numerical minimization of S with different initial parameter values. Validation of the contour analysis in two-dimensional plane was also carried out.

For the first scenario with error-free water storage measurements, the program converged nicely to the true values when only Ks and α, or α and C were considered unknown (Table 3-1a). However, the program hits the upper bounds set for C for the case where only K_s and C were treated as unknown, indicating no minimum existed in the parameter space. Furthermore, the Jacobian matrix is singular, suggesting high colinearity between K_s and C. There are also moderate positive correlation between parameter K_s and α, and between α and C, confirming the graphical analysis of the contour ellipses. It is not surprising to see that when all three parameters were treated as unknown, the program converged to a local minimum, with negative correlation between K_s and α, and between K_s and C, and positive correlation between α and C. When measurement error was introduced, all the three combinations converged to local minimums. When all three parameter were treated as unknown, the program took 182 iterations and converged to unacceptable results.

For the second scenario, where one steady-state ψ measurement was available, all cases converge nicely to the true values, including the case where all three parameters treated as unknown (Table 3-1b). When error was introduced, all cases with two unknown parameters converged. However the case with three unknowns converged to an unacceptable values, suggesting that the problem is not stable with the introduced error.

When an additional initial ψ measured, the case with three unknown parameters converges to the true values with relative error less than 2 %, which is acceptable for most practical purpose (Table 31-b). This is expected, since the simultaneously measured pressure head and water content data at two states should directly define the general shape of the water retention curve, and the saturated hydraulic conductivity becomes the main unknown parameter in the inverse problem. Compared to the other cases with three unknown parameters, the correlations between Ks and α, Ks and C were reduced. However, the correlation between C and α is still high, suggesting more information such as prior information on K_s would producer a better estimate.

Inversion of in-situ data

We conclude our paper by illustrating the performance of our proposed methodology. Water storage data from the average of all the 50 probes (L=20 cm; R=2.59 cm h^{-1}) are shown in Fig. 3-8. As shown in Table 3-2, with only water storage data, the inverse solution converged to an unacceptable result, even though the resulting parameters still gave a good fit to the measured data (small residual sum of square).

With only one steady-state ψ measurement available, the inverse procedure converged to the values close to the estimated true values, despite different initial guesses.

This is similar to our second theoretical scenario without measurement error. This may be because our data is the average of 50 probes and the error was reduced $50^{0.5}$ times. The correlation matrix was higher than expected, indicating a larger measurement error would turn the correlation matrix singular, and the estimated parameters may not be correct. In practice, the inverse solution response function depend on the relative measurement error and not the absolute measurement error. Since the relative error of soil water content changes with TDR are significantly less than 0.013 (Topp et al., 1980). The inverse solution may give accurate relative estimates with only one ψ measurement.

With two ψ measurements, the estimated parameters were very close to the values measured using direct method and have small asymptotic standard errors. The correlation matrix of estimated parameters is also reasonable, suggesting a good estimation.

The estimated parameters in Table 3-2 were used as input to Eq. [3-12] to predict water storage as a function of time for application rate =2.59 cm hr^{-1} (Fig. 3-8). The prediction has an excellent agreement with the measurement. The coefficient of determination was r^2=0.999 and the standard deviation of prediction is 0.0036 cm^3 cm^{-3} for the average of water content across the probe length. The prediction error is within the measurement error suggested by TDR (Topp et al., 1980).

Summary

MTDR combined with inverse procedure provides an accurate, fast, and nondestructive way to estimate the hydraulic properties of the soil during constant flux infiltration. Water storage and ψ measurement are made in the same volume, consequently, reducing the error associated with the spatial variability in the horizontal direction. Major conclusions are

(1). Water storage measurements and a priori θ_s during one-rate constant infiltration won't yield unique estimates of hydraulic parameters in the BW form, because of the interactive nature between K_s and C in the solution.

(2) Water storage combined with a steady-state ψ and a priori θ_s gave unique estimates of hydraulic parameters, but the inverse solution is not stable with high measurement error.

(3) Water storage and a priori θ_s combined with an initial and steady-state pressure head measurements resulted in unique and stable estimates of the parameters.

The results can be further improved if we have prior information about K_s, or additional measurements using a different water application rate. In the paper, only the hydraulic parameters of BW form were estimated by taking advantage of the analytical solution of constant flux infiltration the BW form. Parameters for other forms such as those of van Genuchten and Brooks and Corey can be used if a numerical or quasi-analytical solution is used. The procedure proposed in this paper can also apply to the drainage process.

The analysis in this paper was based on the assumption that the measurement error is random. In reality, the three-term equation of Topp et al. (1980) may systematically underestimate or overestimate the soil water content from TDR measured dielectric constant. The effect of this systematic bias on the estimation of hydraulic parameters from measured soil water storage should be examined also.

The variance of the measurement or prior information has significant influence on the well-posedness of an inverse problem. If the variance of prior information is much bigger than the measurement error of soil water storage, the inclusion of prior information would be of little use for improving the well-posedness of an inverse problem. In addition, if the measurement error is much bigger, the inverse (conditioning) method would not be able to improve the precision of the parameters based on prior information. However, our results in this paper are very conservative. The variance of measurement error for soil water storage and prior information about θ_s were estimated for a wide range of soils. A good TDR calibration equation and prior θ_s is likely much more accurate than we have assumed. Therefore, better uniqueness and stability of the inverse problem and more accurate parameter estimates can be expected in most field application. The correlation matrix in Table [3-2] is the asymptotic behavior which derived from the Cramer-Rao bounds. It will hold only approximately in the vicinity of the true parameter values where the linear approximation applies (Bard, 1974).

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Table 3-1a .Results of inversion for scenario 1.

Information	Unknowns	Estimates				Correlation Coefficient		
		Ks	α	C	θ_s	Ks-α	Ks-C	α-C
		cm hr^{-1}	cm^{-1}					
W(t) Only	Ks,α	5.00	0.08	-	-	0.75	-	-
	Ks,C	3.58	-	60.00	-	-	0.00	-
	α,C	-	0.08	1.30	-	-	-	0.83
	Ks,α,C	5.87	0.07	1.20	-	-0.81	-0.78	1.00
	Ks,α,C,θ_s	7.57	0.11	1.53	0.48	-1.00	-1.00	1.00
W(t)+Error	Ks,α	5.40	0.12	-	-	0.60	-	-
	Ks,C	28.80	-	1.02	-	-	0.00	-
	α,C	-	0.13	1.38	-	-	-	0.67
	Ks,α,C	17.10	0.08	1.00	-	1.00	-1.00	1.00
	Ks,α,C,θ_s	8.20	0.18	2.38	0.55	1.00	-1.00	1.00

Note: * Jacobian matrix is singular

- Not applicable

Table 3-1b .Results of inversion for scenario 2 and 3.

Information	Unknowns	Estimates				Correlation Coefficient		
		Ks (cm hr^{-1})	α (cm^{-1})	C	θ_s	Ks-α	Ks-C	α-C
W(t)+ψ	Ks,α	5.00	0.08	-	-	0.17	-	-
	Ks,C	5.00	-	1.30	-		-0.49	
	α,C	-	0.08	1.30	-	-	-	-0.75
	Ks,α,C	5.00	0.08	1.30	-	0.94	-0.95	-0.97
	Ks,α,C,θ_s	8.90	0.13	1.68	0.53	0.94	-0.95	-0.97
W(t)+ψ+error	Ks,α	5.06	0.08	-	-	0.12	-	-
	Ks,C	5.07	-	1.30	-	-	-0.50	-
	α,C	-	0.08	1.28	-	-	-	-0.87
	Ks,α,C	6.48	0.11	1.18	-	0.97	-0.97	-0.99
	Ks,α,C,θ_s	8.72	0.18	2.38	-	0.99	-0.99	-0.99
W(t)+2ψ+error	Ks,α,C	5.13	0.08	1.30	-	0.80	-0.82	-0.97
	Ks,α,C,θ_s	5.15	0.08	1.25	0.40	0.69	-0.47	-0.89

Note: * Jacobian matrix is singular

- Not applicable

Table 3-2.Estimated hydraulic parameters from the inverse solution of measured water storage.

	Information		
Parameter Estimates	W(t) Only	W(t)+ψ_1	W(t)+ ψ_1+ψ_2
Ks (cm hr^{-1})	8.12±25675	6.64±0.40	6.71±0.38
C	1.27±712	1.32±0.17	1.38±0.005
α (cm^{-1})	0.09*	0.0832±0.02	0.0894±0.002
θ_s	0.43±210	0.41±0.021	0.42±0.005
Correlation Matrix			
Ks-α	1.00	0.40	0.95
Ks-C	1.00	0.16	-0.68
α-C	1.00	0.96	-0.71
θ_s-Ks	1.00	0.38	0.39
θ_s-C	1.00	0.97	0.39
θ_s-α	1.00	0.98	0.32

Note: *Jacobian matrix is singular.

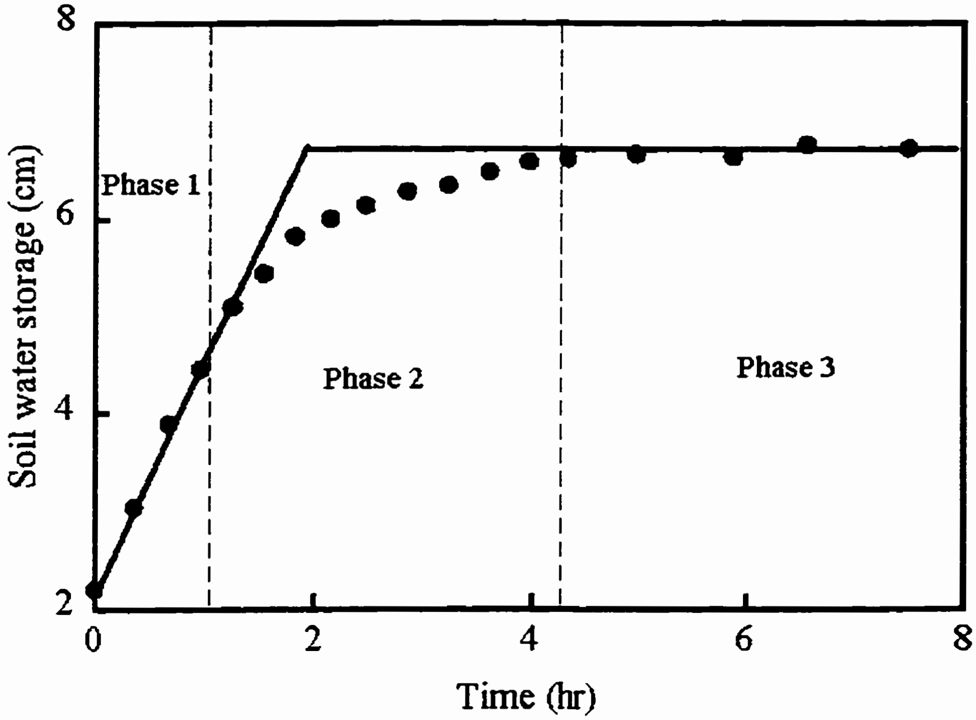

Fig. 3-1. Delineation of soil water storage curve into different regions (phases): Phase 1 (Water storage increases linearly with time), Phase 2 (water storage breakthrough phase), and Phase 3 (steady-state flow phase).

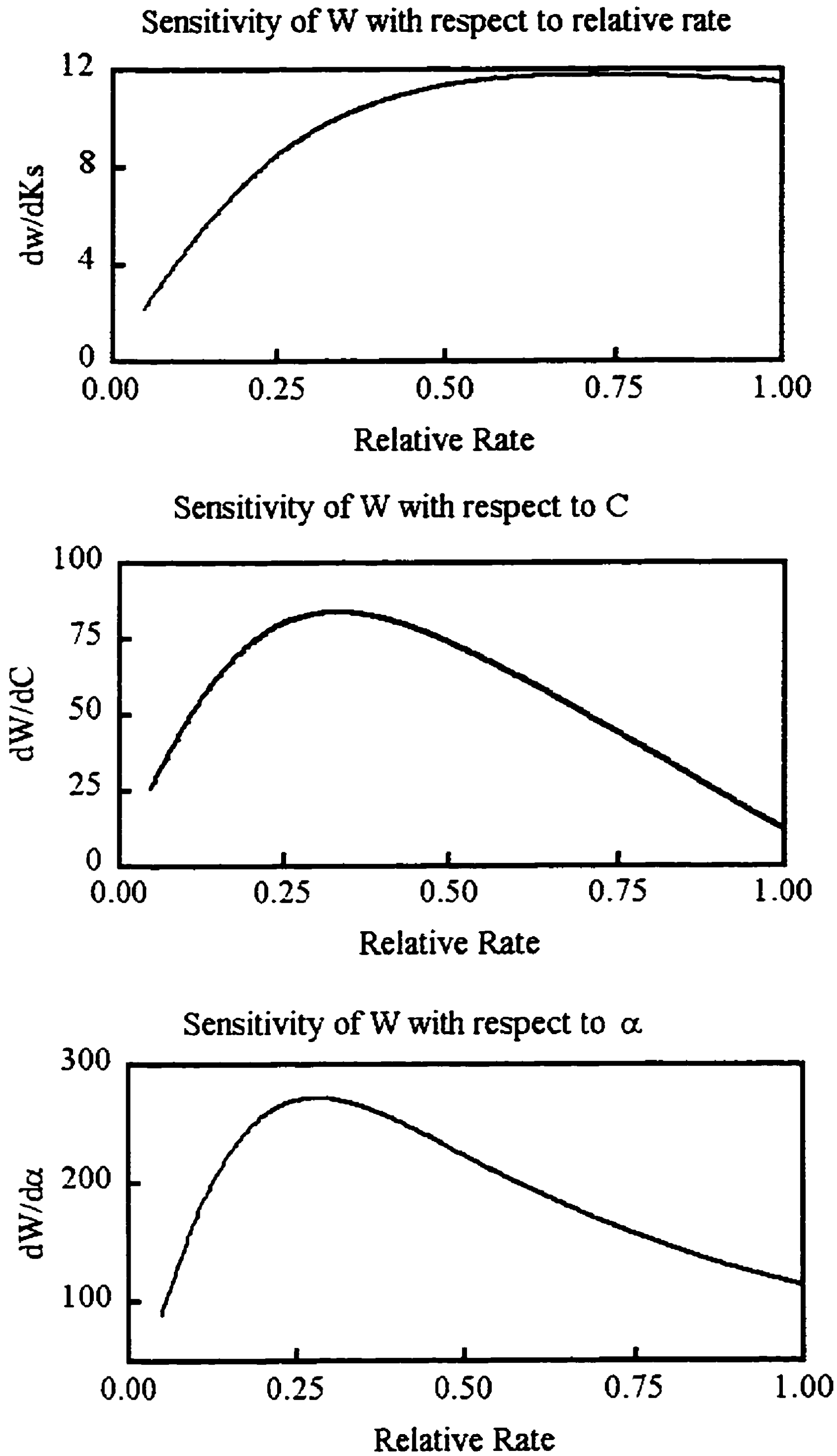

Fig. 3-2. Sensitivity of the φ(W) with respect to (a) Ks, (b) C, and (c) α to the change of relative application rate R/ Ks.

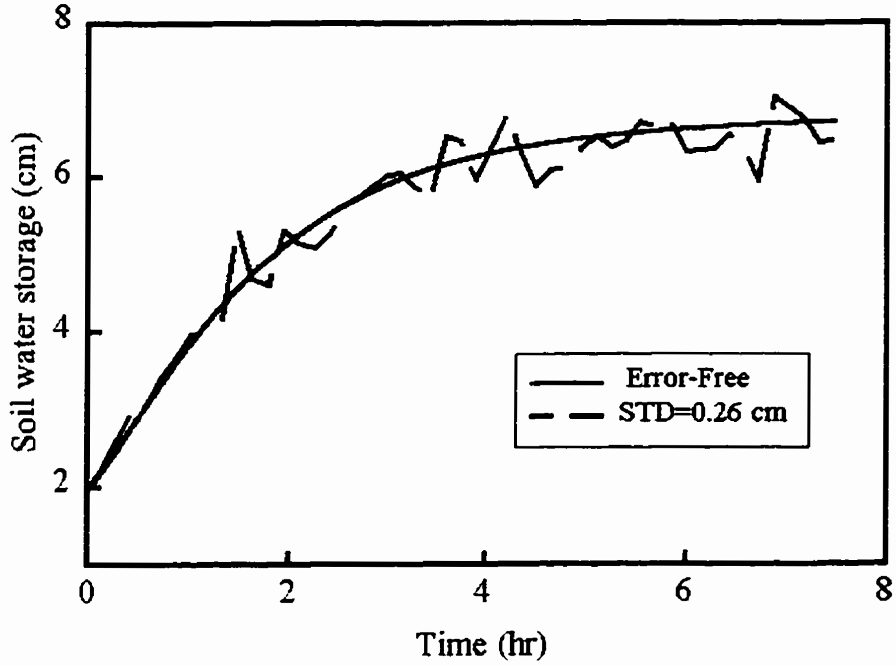

Fig. 3-3. Calculated soil water storage vs time for error-free measurments (solid curve) and measurements with error (STD=0.26 cm) (dashed line).

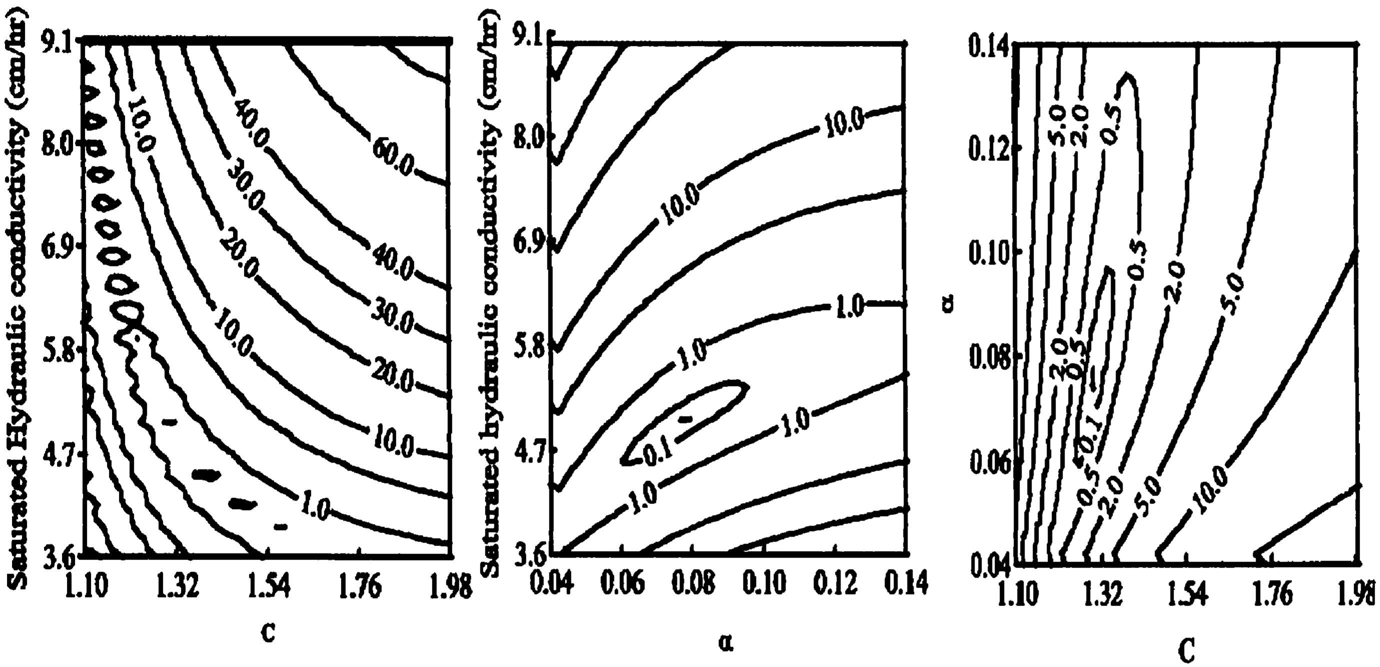

Fig. 3-4. Contours of φ for error-free water storage data as a function of (a). Ks and α, (b) Ks and C, and (c) α and C.

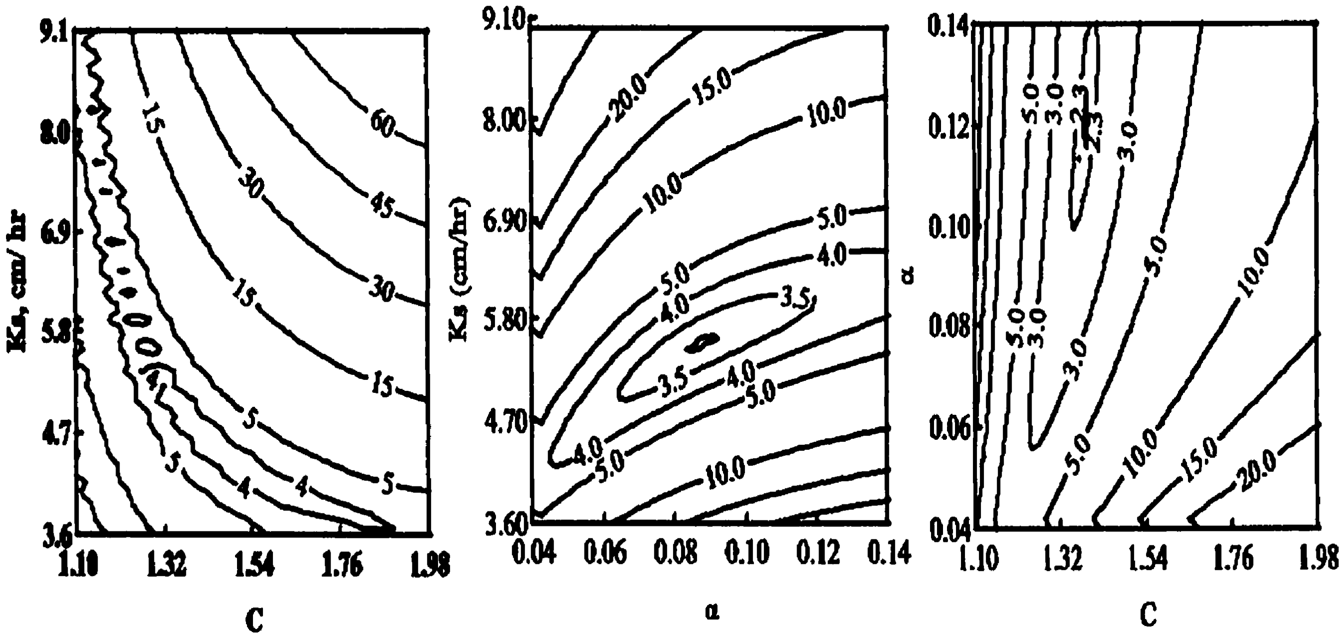

Fig. 3-5. Contours of φ for water storage data contaminated by an error of STD=0.058 as a function of (a). Ks and α, (b) Ks and C, and (c) α and C.

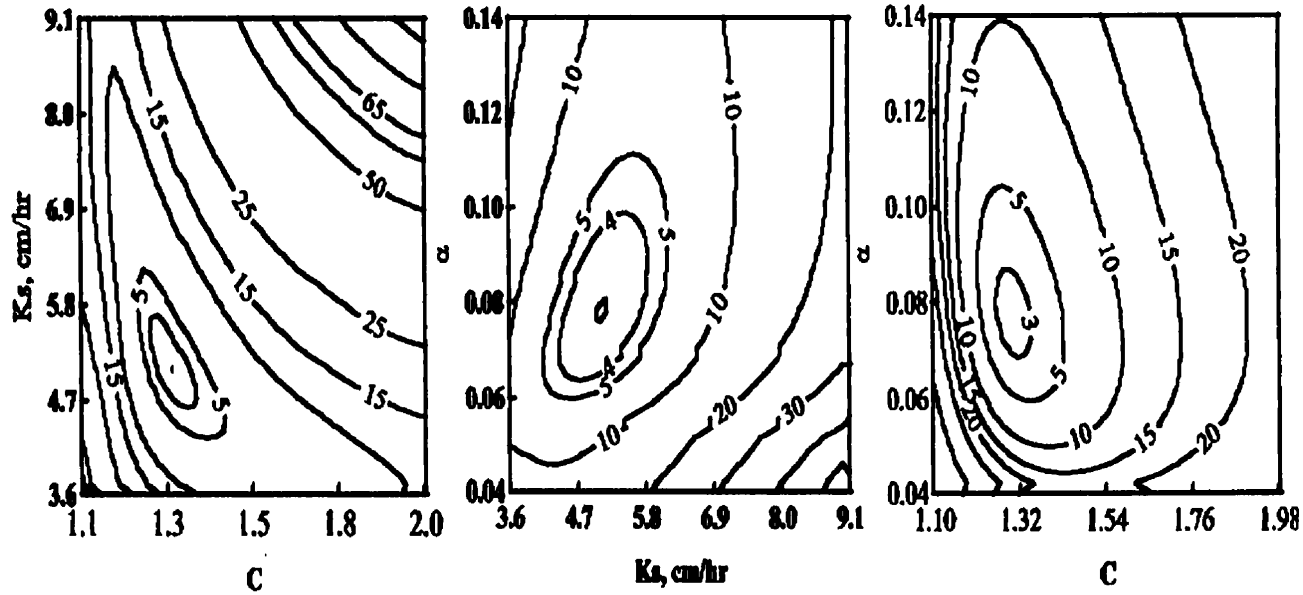

Fig. 3-6. Contours of φ with an additional ψ measurement for error-free water storage data as a function of (a). Ks and α, (b) Ks and C, and (c) α and C.

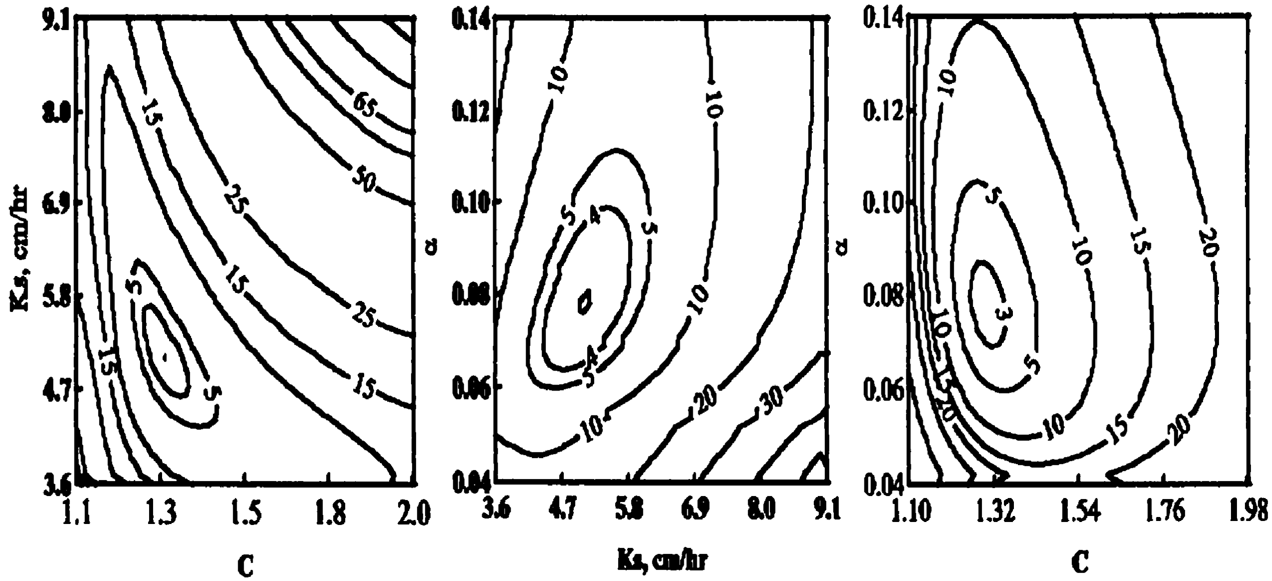

Fig. 3-7. Contours of φ with an additional ψ measurement for water storage data with an error of STD=0.058 cm as a function of (a). Ks and α, (b) Ks and C, and (c) α and C.

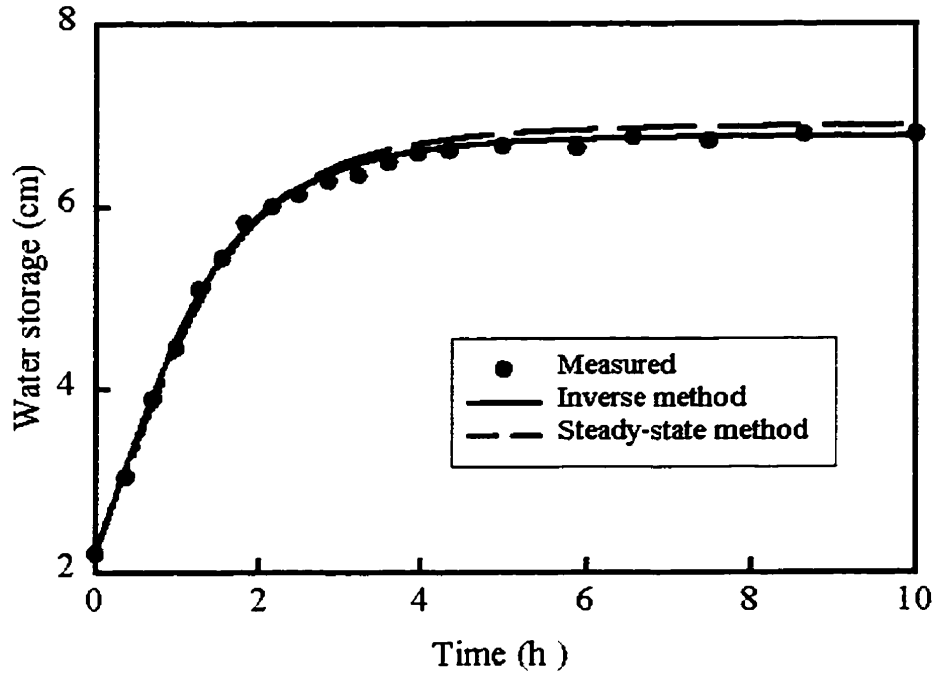

Figure 3-8. Measured and predicted water storage versus time (L=20 cm; R=2.59 cm h^{-1}).

Chapter 4

A new solution for water storage to a fixed depth for constant flux infiltration

Abstract

A new quasi-analytical solution for water storage to a fixed depth is presented. The proposed solution allows general soil hydraulic properties, such as the versatile van Genuchten form of hydraulic properties functions to be used . The solution is based on the flux concentration relationship of Philip (1973) and the approximate flux concentration relationship of White et al. (1979) for a linear soil. The solution is similar to that of Parkin et al.(1992) for a wide range of realistic hydraulic properties, but does not require the Broadbridge and White (1988) form of hydraulic functions. The solution was applied to a field soil. Using independently measured soil hydraulic properties, the solution predictions were essentially identical to that of Parkin et al.(1992) and to the measurements using the approximate $F(\Theta_0)$ relationship of White et al. (1979) for linear soils.

Introduction

A quantitative description of water infiltration under constant flux boundary conditions in unsaturated soils is fundamental to understanding water balance, irrigation, movement of chemicals and, more generally, transport processes occurring in surface soils. Despite the success of numerical solutions, analytical solutions have received considerable attention. Analytical solutions are very useful for assessing the accuracy of numerical models and provide insight into the physics of flow phenomena. Additionally, analytical solutions can be used to test inverse techniques for non-uniqueness and identifiability of hydraulic parameters of interest. In the past thirty years, analytical solutions of Richards' equation for constant flux water infiltration into homogeneous soil profiles have been developed using approximate integral procedures (Parlange, 1972; Philip and Knight, 1974; White et al., 1979), and exact transform methods such as Kirchhoff, Hopf-Cole and Storm transformations(Broadbridge and White, 1988; Warrick et al., 1990) and reciprocal Bäcklund transform by Sander et al. (1988, 1990).

The nonlinear Richards' equation was solved by Parlange (1972), who described an approximate integral procedure for the solution of infiltration by exploiting the rapid change of diffusivity with water content. Philip and Knight(1974) showed how Parlange's method could be improved to any desired accuracy through the use of a concept called the flux-concentration relation (Philip, 1973). The use of the flux-concentration relation, in principle, permits quasi-analytical solution of the highly nonlinear flow equation to be found for a wide range of flow phenomena in soils. White at al. (1979) analyzed constant flux adsorption using an approximate flux-concentration relation. Experiments using a fine sand validated the approach and indicated both the surface water content and the water content profile could be predicted accurately for the horizontal adsorption of water supplied to the sand at a wide range of constant flux rates. Perroux et al. (1981) extended the solution to constant flux infiltration and concluded that sufficiently accurate predictions of soil water profile development can be made by using the simple adsorption analysis of White et al. (1979). Boulier et al. (1984) confirmed the ability and the versatility of the flux-concentration relation-based approach to predict water infiltration into soils.

Exact solutions for infiltration were developed for linear soils (Braester, 1973). Such a linearized solution can only be expected to predict, approximately, the integral properties of the soil-water system. Parlange (1976) pointed out a significant disparity between surface water contents calculated from this linearized solution and those calculated numerically. In addition, the linear convection term does not permit the development of a traveling wave solution at large infiltration times. This problem does not arise in the exactly solvable Burgers' equation with its weakly nonlinear convection term. The solution to Burgers' equation satisfactorily described rainfall infiltration in an undisturbed field soil (Clothier et al., 1981). However, like the linear soil, Burgers' solution treats diffusivity as constant, even though soil water diffusivity varies over several orders of magnitude across the water content range of interest. Broadbridge and White(BW) (1988) and Sander et al. (1988) independently presented exact analytical solutions for constant flux infiltration based on realistic nonlinear dependence of unsaturated hydraulic conductivity and diffusivity on soil water content. These solutions not only predict water infiltration accurately, but also produce all the salient features of water flow during constant flux infiltration including the traveling wave solution.

Parkin et al. (1992) derived an analytical solution for water storage to a fixed depth based on the analytical solution of Broadbridge and White (1988) and Sander et al. (1988). The model result can be used directly to interpret the measurement of water storage from vertically installed TDR probes. However, the solutions of Parkin et al.(1992) requires specific forms of diffusivity and hydraulic conductivity dependence of water content in the Broadbridge and White (1988) solution. This limits its applications where hydraulic parameters are known only for other forms of hydraulic properties such as the van Genuchten and Mualem (van Genuchten, 1980), Brooks and Corey (Brooks and Corey, 1966), and Gardener and Russo forms (Russo, 1988). The objective of this paper is to present a quasi-analytical solution for water storage to a fixed depth during constant flux infiltration based on the solution of White et al. (1979). This solution allows functions for general soil hydraulic properties. We compare our solution with the solution of Parkin et al. (1992) and with the measurements from a field experiment.

Theory

We consider nonhysteretic vertical soil water flow under constant water application at the soil surface and seek to find an expression for time dependence of water storage to a fixed depth. The flow of water is described in this process by the continuity equation,

$$\frac{\partial \theta}{\partial t} = -\frac{\partial q}{\partial z} \qquad [4\text{-}1]$$

and Darcy's Law,

$$q(\theta,t) = -D(\theta)\frac{\partial \theta}{\partial z} + K(\theta) \qquad [4\text{-}2]$$

where, t(s) is time, z(m) is the vertical coordinate, $\theta(m^3\,m^{-3})$ is the volume water content, $q(m^{-3}\,m^{-2}\,s^{-1})$ is the volumetric flux of water, $D(\theta)$ $(m^2\,s^{-1})$ is the water-content dependent soil-water diffusivity, and $K(\theta)$ $(m\,s^{-1})$ is the hydraulic conductivity.

Substitution of Eq.[4-2] into Eq.[4-1] yields the nonlinear Richards' equation used to describe one-dimensional nonhysteretic flow in idea soil:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(D(\theta)\frac{\partial \theta}{\partial z}\right) - \frac{dK(\theta)}{d\theta}\frac{d\theta}{dz} \qquad [4\text{-}3]$$

$$\theta(z,0) = \theta_n \;; \qquad t=0; \qquad z \geq 0 \qquad [4\text{-}4]$$

$$-D(\theta)\frac{\partial \theta}{\partial z} + K(\theta) = R \;; \qquad z = 0\;;\; t \geq 0;\; R \leq Ks \qquad [4\text{-}5]$$

The initial and boundary conditions considered here are the uniform initial water content, θ_n, the constant surface water application rate $R(m^{-3}\,m^{-2}\,s^{-1})$ on the soil surface with Ks $(m^{-3}\,m^{-2}\,s^{-1})$, the saturated hydraulic conductivity.

An analytical solution based on White et al. (1979).

Philip(1973) introduced the flux-concentration relation, $F(\Theta_0,t)$ as

$$F(\Theta_0,t) = \frac{q(\theta,t)-K_n}{R-K_n} \qquad [4\text{-}6]$$

where $\Theta_0=(\theta-\theta_n)/(\theta_0-\theta_n)$, θ_0 is the surface water content. And $K_n(m^{-3}\ m^{-2}\ s^{-1})$ is the initial soil hydraulic conductivity. Substitution of Eq. [4-6] into [4-2] and integration with respect to θ gives (White et al, 1979):

$$(R-K_n)\ z(\theta,t) = \int_{\theta}^{\theta_0(t)} \frac{D(\theta)\ d\theta}{F(\Theta_0,t)\ -\ (K(\theta)\ -\ K_n)\ /\ (R\ -\ K_n)} \qquad [4\text{-}7]$$

We use the identity

$$\left(\frac{\partial\theta}{\partial t}\right)_z \cdot \left(\frac{\partial z}{\partial\theta}\right)_t = -\left(\frac{\partial z}{\partial t}\right)_\theta \qquad [4\text{-}8]$$

to transform Eq. [4-1] to

$$\frac{\partial z(\theta,t)}{\partial t} = \frac{\partial q}{\partial\theta} \qquad [4\text{-}9]$$

Integrating with respect to θ, we obtain

$$\frac{\partial}{\partial t}\int_{\theta_n}^{\theta_0(t)} z(\theta,t)\ d\theta = R\ -\ K_n \qquad [4\text{-}10]$$

Substituting for z(θ,t) from Eq. [4-7] into Eq. [4-10] and integrating by parts yields

$$(R - K_n)^2 t = \int_{\theta_n}^{\theta_0(t)} \frac{(\theta - \theta_n)\ D(\theta)\ d\theta}{F(\Theta_0,t) - [K(\theta) - K_n]/(R\ -\ K_n)} \qquad [4\text{-}11]$$

Water storage at time t, W(L,t) to a fixed depth L, may be obtained by integrating $z(\theta,t)$ with respect to θ :

$$W(L,t) = \int_{\theta_L(t)}^{\theta_0(t)} z(\theta,t)\ d\theta + \theta_L(t)\ L \qquad [4\text{-}12]$$

Where $\theta_L(t)$ is the water content at depth L as a function of time t. Substitution for $z(\theta,t)$ from Eq. [4-7] into Eq. [4-12], and integration by parts leads to

$$W(L,t) = \int_{\theta_L(t)}^{\theta_0(t)} \frac{(\theta - \theta_n)\ D(\theta)\ d\theta}{F(\Theta_0,t)\ (R\ -\ K_n) - K(\theta) + K_n} + \theta_n\ L \qquad [4\text{-}13]$$

Equations. [4-7], Eq.[4-11], and Eq.[4-13], together give a quasi-analytical solution for constant flux infiltration. If $F(\Theta,t)$ is known, Eq.[4-7] and Eq. [4-11] can be used to predict the time dependence of the surface soil water content $\theta_0(t)$and the water content at depth z, respectively. With $\theta_0(t)$ and $\theta_L(t)$ known, Eq. [4-13] can be used to predict the change of water storage with time. This quasi-analytical solution for water storage to a fixed depth L is general in terms of the form of $D(\Theta)$ and $K(\Theta)$. It allows us to use the more versatile van Genuchten (VG) water retention curve (Eq. [4-14]) combined with the Burdine hydraulic conductivity function (Eq. [4-15]) (van Genuchten, 1980)

$$\Theta = \left(\frac{1}{1+(\alpha_{VG}\psi)^n}\right)^{-m} \qquad [4-14]$$

$$K = K_s\, \Theta^2[1-(1-\Theta^{1/m})^m] \qquad [4-15]$$

with m=1-2/n, where n and α_{VG} are fitting parameters, respectively. Ks is the saturated hydraulic conductivity.

This solution is for constant flux infiltration into soil of uniform initial water content, however, it can also apply to constant flux infiltration into a soil of non-uniform initial water content with modification of $F(\Theta_0,t)$, $\theta_0(t)$, and $\theta_L(t)$.

Generally, we need the iterative procedure of Philip and Knight(1974) to obtain $F(\Theta_0,t)$. However, it is well known that the time dependence of $F(\Theta_0,t)$ is negligible. The extreme cases of soil hydraulic properties are those of constant diffusivity(Linear soil and Burgers' soil) and a Dirac function(Green & Ampt soil). For linear soil, $F(\Theta_0)$ is exact and can be approximated by $F(\Theta_0)= \Theta_0^{\,2-4/\pi}$. For Green&Ampt soil, $F(\Theta_0)$ is also exact and equal to Θ_0 for constant concentration adsorption. Philip (1973) conjectured that for constant flux infiltration, $F(\Theta_0)$ lies in the narrow band bounded by $F(\Theta_0)=\Theta_0$ and $F(\Theta_0) = \Theta_0^{\,2-4/\pi}$.

Solution of Parkin et al. (1992).

Broadbridge and White (BW) (1988) and Sander et al. (1988) independently developed analytical solutions for constant flux infiltration. The BW solution is based on the following parametrization of hydraulic conductivity and diffusivity functions

$$K(\Theta) = Ks \frac{(C-1)\ \Theta^2}{C-\Theta} \qquad [4\text{-}16]$$

$$D(\Theta) = \frac{Ks\ C\ (C-1)}{\alpha\ \Delta\theta\ (C-\Theta)^2} \qquad [4\text{-}17]$$

where $\Delta\theta=\theta_s-\theta_r$ and $\Theta=(\theta-\theta_r)/\Delta\theta$. θ_s and θ_r are the saturated water content and residual water content, respectively. Ks, α , and C are the saturated hydraulic conductivity, inverse capillary length scale (Philip, 1985), and a constant introduced by BW. By definition,

$$D(\Theta) = K(\Theta) \frac{d\psi}{d\theta} \qquad [4\text{-}18]$$

we have,

$$\psi(\theta) = \int_{\theta}^{\theta_s} D(\Theta)/K(\Theta)\ d\theta \qquad [4\text{-}19]$$

Substitution of Eq. [4-16] and Eq. [4-17] into Eq. [4-19] and integration yields

$$\psi(\Theta)-\psi_0 = \frac{1}{\alpha}[\frac{1-\Theta}{\Theta} + \frac{1}{C}\ln(\frac{C-\Theta}{\Theta(C-1)})] \qquad [4\text{-}20]$$

where ψ_0 is an integration constant. Following BW, we set ψ_0=0.

Utilizing Eq. [4-16] and Eq. [4-17], through a series of transforms (i.e. Kirchhoff, Storm, and Hopf and Cole transforms), BW solved Eq.[4-3], Eq. [4-4], and Eq. [4-5] and derived an analytical solution as

$$\Theta(\zeta,t) = C[1-(1+2\rho-u(\zeta,t)^{-1}\frac{\partial u(\zeta,t)}{\partial\zeta})^{-1}] \qquad [4\text{-}21]$$

and

$$z(\zeta,t) = (C\alpha)^{-1}[\rho(\rho+1)\tau+(2\rho+1)\zeta-\ln(u(\zeta,t))] \qquad [4\text{-}22]$$

where ζ is a parameter connecting Eq. [4-21] and Eq. [4-22], $u(\zeta,t)$ is given by Eq. [43] of BW, and

$$\rho = \frac{R}{4C(C-1)Ks} \qquad \tau = \frac{4C(C-1)\ \alpha K_s t}{\Delta\theta} \qquad [4\text{-}23]$$

By change of variable of integration, Parkin et al. (1992) obtained an analytical solution for water storage to depth L for constant flux infiltration,

$$W(L,t) = \frac{\Delta\theta}{\alpha}[2\rho\ \zeta(L,t)+\ln(\frac{u(0,t)}{u(\zeta,t)})]+\theta_r L \qquad [4\text{-}24]$$

The BW model encompasses a wide range of realistic soil hydraulic properties by varying the C parameter. As C goes to infinity, the model reduces to the weakly nonlinear Burgers' equation, which has been applied in certain field conditions. At the other end of the range as C approaches 1, the BW model approaches the Green-Ampt-like model (White and Broadbridge, 1988).

Materials and methods

Field infiltration measurements were conducted at the Canadian Forces Base Borden, Ontario, Canada. Extensive hydro-geological research, including a large scale, natural-gradient tracer test and forced gradient test have been conducted by University of Waterloo on this site. Details about this site can be found in Sudicky(1986). Water was applied to an instrumented transect(7.5 m long) inside a greenhouse using a hanging track and nozzle system(see chapter 2). Multi-purpose TDR probes were installed every 0.15 m at each of 4 depths (0.2, 0.4, 0.6, and 0.8 m) for a total of 200 TDR probes. Five different water application rates were used. Soil water content was measured using the TDR method of Topp et al. (1980). The readings were taken manually from the display screen of two pre-calibrated Tektronix(1502 C) metallic cable testers by four operators. The readings were taken just prior to the start of water application and every 5-30 minutes depending on infiltration rate and rate of change of θ, for all the 200 multipurpose TDR probes. Here, we use the site average of the 50 probes for the 20 cm depth as a illustration. A fit of VG and BW models to measured data is given in Fig. 2-4, and Fig. 2-5.

In the following, we take advantage of the dimensionless variables

$$t^{*} = \frac{K_s\, t\, \alpha}{\Delta\theta} \qquad L^{*} = L\, \alpha \qquad W^{*} = \frac{(W - \theta_n L)\, \alpha}{\Delta\theta}$$

This transforms both the BW and our solution into equations only involving t*, L*, W*, and

C parameters. Therefore, the sensitivity of $F(\Theta_0)$ to different soils can be examined through the changes of the C value.

Results and discussion

Figure. 4-1(a, b, c) and Fig. 4-2 (a,b,c) depict dimensionless water storage-time functions for the new solution and the Parkin et al. (1992) solution for the limiting conditions; C=1.01, appropriate for a repacked coarse material (Green & Ampt soils); C=15, appropriate for soils with a wide range of pore sizes. The initial increase in storage is clearly linear for all soils, reflecting the constant surface applied infiltration rate. As the wetting front moves below L, the rate of change of storage gradually decreases for the Burgers' soil and abruptly reaches equilibrium for the Green & Ampt soils.

For C=1.01, 1.02, and 1.10, the new solutions with $F(\Theta_0)=\Theta_0$ and $F(\Theta_0)=\Theta_0{}^{2-4/\pi}$ are essentially identical to each other and to the solution of Parkin et al.(1992) when the BW forms of $K(\Theta)$ and $D(\Theta)$ are used. This suggests that the $F(\Theta_0)$, for either a linear soil or the Green & Ampt soil, is accurate enough to predict water storage during constant flux infiltration. It also indicates the new solution is not sensitive to the value of $F(\Theta_0)$ at small C. This is reasonable, since diffusivity changes abruptly with water content as the value of C gets close to 1. Thus, the selection of $F(\Theta_0)$ from the narrow band is not critical. However, when C increases to 1.5 as in Fig 4-2a, diffusivity changes gradually with water content and the gravity effect becomes significant. Thus, the dominance of $D(\Theta)$ over $F(\Theta_0)$ is lost and the influence of different $F(\Theta_0)$ in the new solution becomes significant. This becomes obvious at C=5 (Fig. 4-2b) and C=15(Fig. 4-2c). Different $F(\Theta_0)$ results in significant differences in the predicted water storage in the middle curve region. For these C values, the new solution with $F(\Theta_0)= \Theta_0^{2-4/\pi}$ for linear soil is essentially identical to the solution of Parkin et al. (1992), while the new solution with $F(\Theta_0)=\Theta_0$ significantly underestimate the water storage relative to the solution of Parkin et al.(1992). As expected, the predictions at initial time and large time are identical for all C values, since the increase of water storage with time is a reflection of applied flux density, while the prediction at large time reflects the water content θ at $K(\theta)=q$. Thus, the main difference in the models are reflected in the curvature of W(L,t).

White (1979) found that the time dependence of $F(\Theta_0,t)$ for constant flux adsorption into Bangendore fine sand was negligible and that the measured $F(\Theta_0,t)$ lies only slightly above the line $F(\Theta_0)=\Theta_0$. Boulier et al (1984) pointed out that the measured flux concentration relation can be well approximated by $F(\Theta_0)=\Theta_0$ and the time dependence is not significant. These experiments were based on repacked coarse materials and it is reasonable to infer that the C values for the materials would be close to 1. Thus, it is not difficult to understand why the predictions using both $F(\Theta_0)=\Theta_0$ and $F(\Theta_0) = \Theta_0^{2-4/\pi}$ were successful for the prediction of surface water content and the water content profile during constant flux adsorption and vertical infiltration (White et al., 1979; Perroux et al, 1979; Boulier et al., 1984). However, based on the above analysis, we suggest that $F(\Theta_0)=\Theta_0^{2-4/\pi}$ be used since it applies to most field soils, while $F(\Theta_0)=\Theta_0$ only applies to repacked laboratory and coarse field soils.

Application to field data.

For $F(\Theta_0) =\Theta_0^{2-4/\pi}$, the new $F(\Theta_0)$ solution(Eq.[4-7], Eq.[4-11], and Eq.[4-13]) using either BW or VG parameters in Table 2-3 gives almost identical predictions of water storage versus time to the measurements and to the BW solutions (Eq. [4-24]) (Fig. 4-3a). The predictions from all models are highly correlated with the measurements (Table 4-1). The underestimation using VGB model is more than that using the BW model, suggesting that different forms of hydraulic model have different sensitivity to the form of $F(\Theta_0)$. The major difference in the solutions, as expected, are in the middle curved regions, which reflect the integrated effect of the wetting front shape. An alternative choice of $F(\Theta_0)$ could be made by using $F(\Theta_0)=\Theta_0^{\ \beta}$ where $0<\beta<1$ (Kutilek ,1980). An optimal β could be calculated by matching the BW solution and the new solution presented here. The average difference between predicted and measured average water content (water storage divided by the length of TDR rods) is less than 0.01 for all solutions, which is smaller than the measurement error of TDR(Topp et al., 1980).

Summary and conclusion

A new quasi-analytical solution for water storage to a fixed depth was presented. The solution is based on the flux concentration relationship of Philip (1973). Using the approximate $F(\Theta_0)$ relationship of White et al. (1979) for linear soil, the solution is essentially identical to that of Parkin et al.(1992), however, for a wide range of realistic hydraulic properties. The solution was applied to a field soil. Using independently measured soil hydraulic properties, the predictions were essentially identical to the measurements.

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Table 4-1. Statistics for measured versus the predicted water storage (W) to depth L=20 cm using the solution of Parkin et al. (1992) (Parkin), the new solution with BW model (BW) and the new solution with VG model (VG) for $F=\Theta_0$ and $F=\Theta_0^{\,2-4/\pi}$.

	Parkin	BW		VG	
		$F=\Theta_0^{\,2-4/\pi}$	$F=\Theta_0$	$F=\Theta_0^{\,2-4/\pi}$	$F=\Theta_0$
R^2	0.999	0.999	0.995	0.996	0.981
AVG ($cm^3\ cm^{-3}$)	-0.0056	-0.0052	0.0015	-0.0018	0.0083
RMSE ($cm^3\ cm^{-3}$)	0.0066	0.0057	0.0050	0.0054	0.013
MAX ($cm^3\ cm^{-3}$)	0.011	0.0098	0.011	0.0092	0.025
MIN ($cm^3\ cm^{-3}$)	0.0	0.0	0.0	0.0	0.00

Note: R^2--- coefficient of determination; AVG--- Average of the difference between measured and predicted depth-averaged water content(W/L); RMSE--- Root mean square error; MAX--- Maximum of the absolute difference between measured and predicted depth-averaged water content (W/L); MIN--- Minimum of the absolute difference between measured and predicted depth-averaged water content.

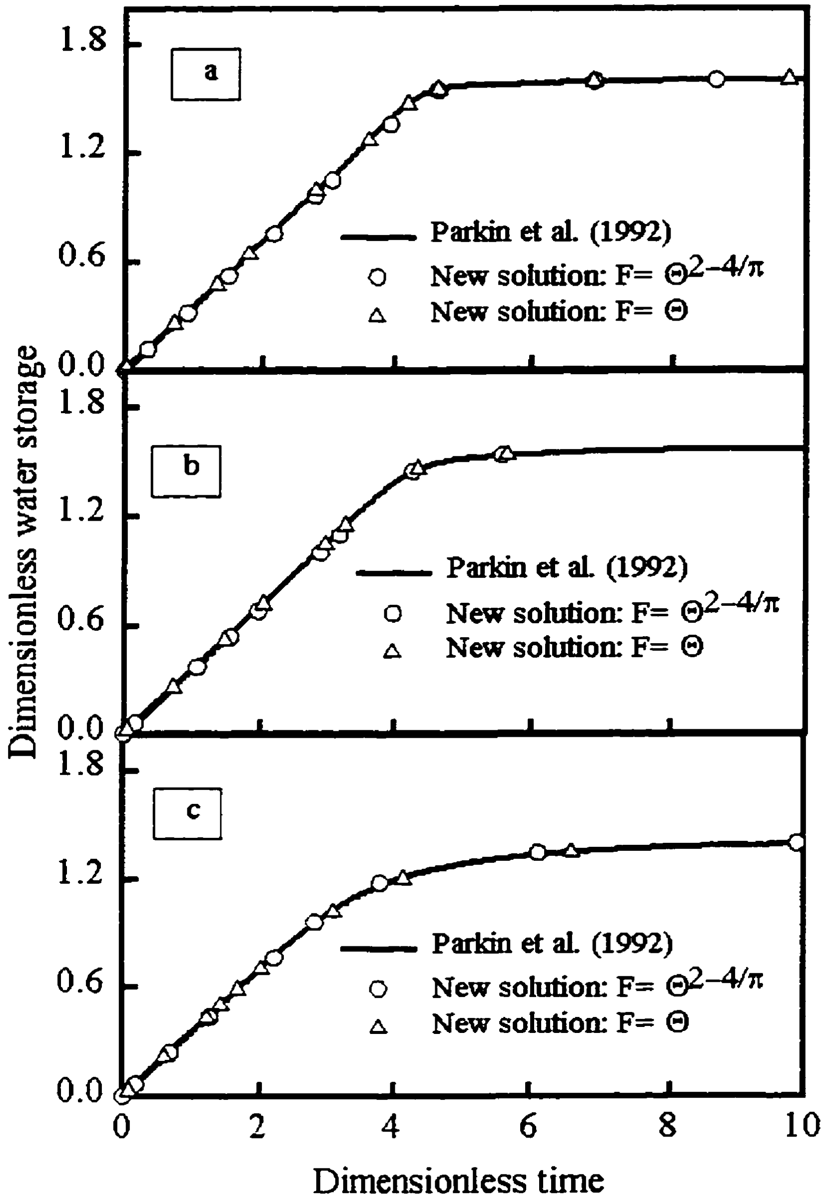

Figure 4-1. Comparison of the new solution using $F(\Theta_0)=\Theta_0^{2-4/\pi}$ and $F(\Theta_0)=\Theta_0$ and with the solution of Parkin et al. (1992) for (a) C=1.01, (b) C=1.02, and (c) C=1.10.

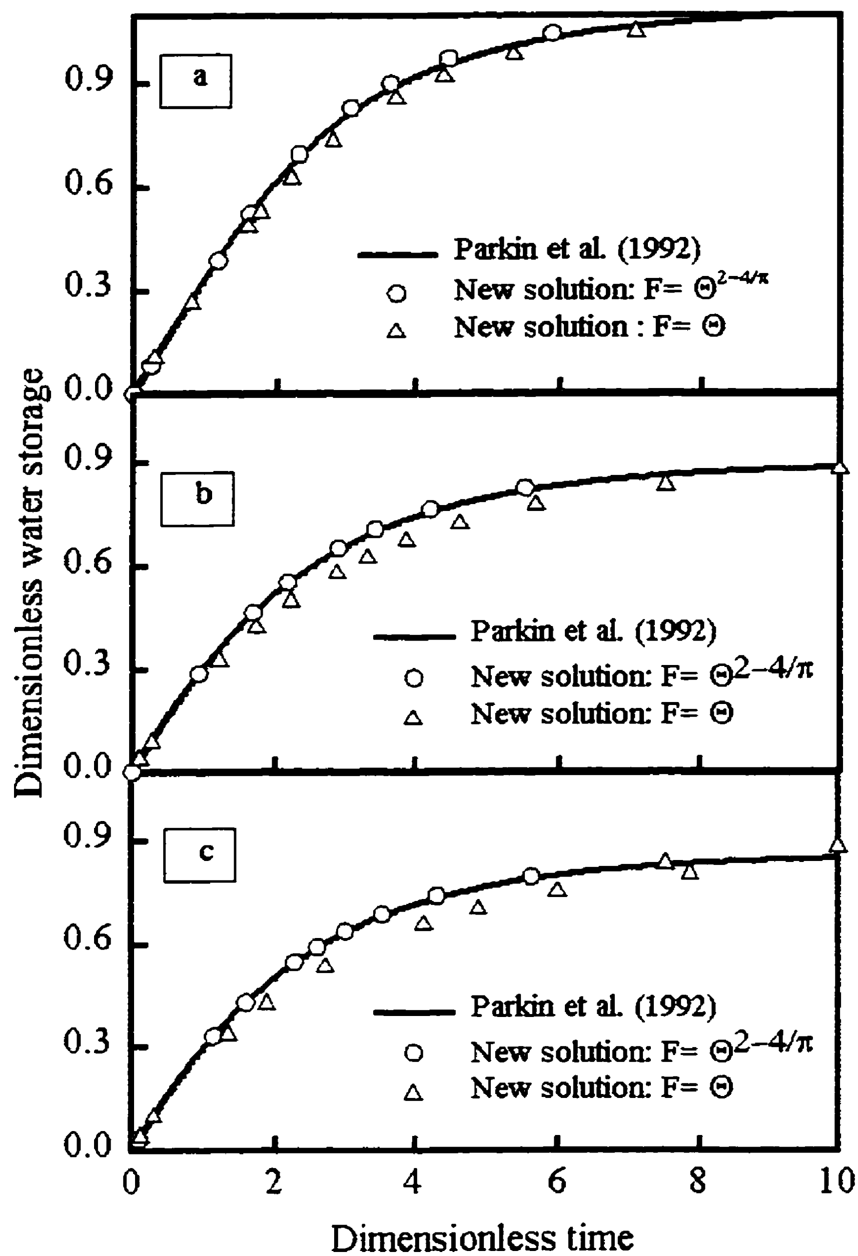

Figure 4-2. Comparison of the new solution using $F(\Theta_0)=\Theta_0^{2-4/\pi}$ and $F(\Theta_0)=\Theta_0$ and with the solution of Parkin et al. (1992) for (a) C=1.5, (b) C=5, and (c) C=15.

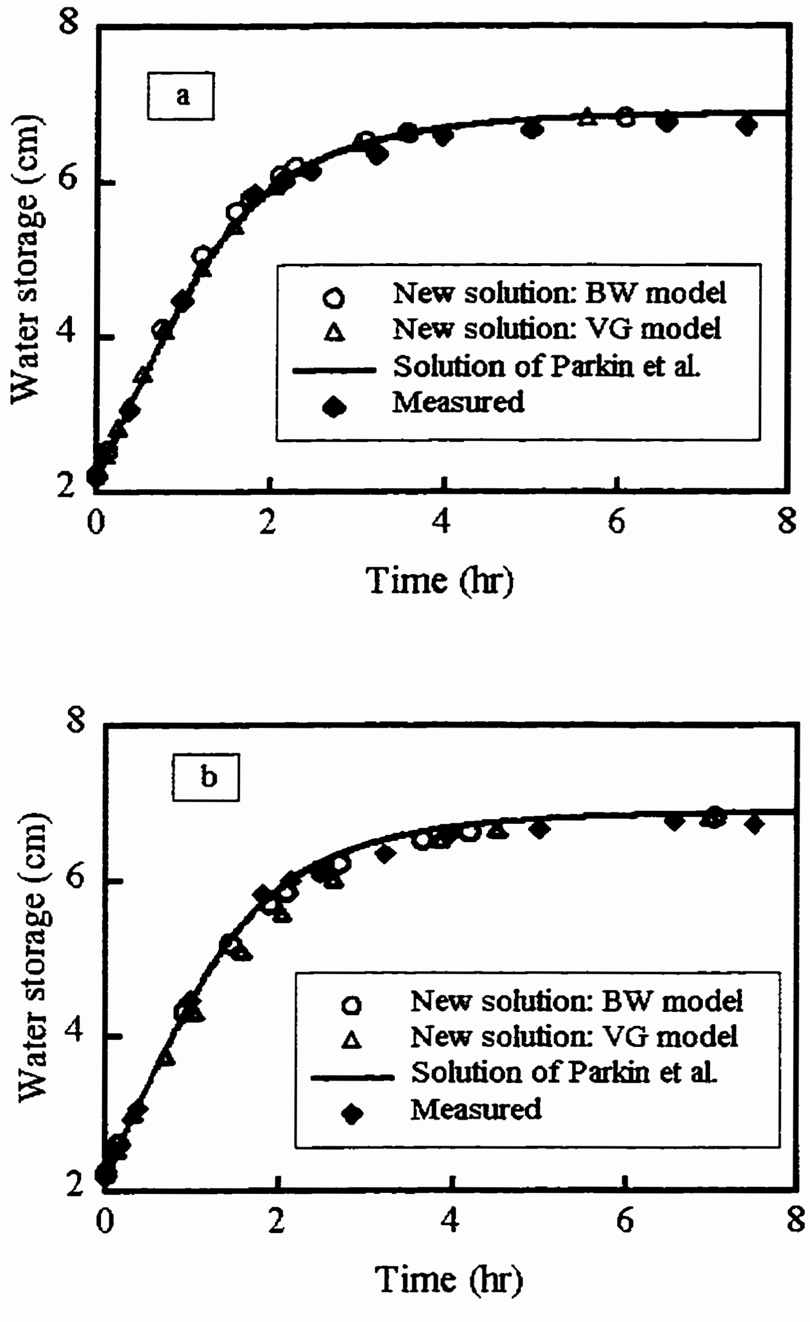

Figure 4-3. Water storage to depth L=20 cm measured in filed and predicted as a function of time for the new solution with BW model and VGB model and for the solution of Parkin et al. (1992) in the case of (a) $F(\Theta_0)=\Theta_0^{2-4/\pi}$ and (b) $F(\Theta_0)=\Theta_0$.

Chapter 5

Prediction of drainage from infiltration with hysteresis

Abstract

Prediction of drainage from infiltration with hysteresis has practical significance. A Haines' Jump model of hysteresis is proposed which is combined with the Broadbridge & White (1988) form of $K(\theta)$ and $D(\theta)$ and allows unified analytical solution for infiltration and drainage. The model accounts for all of the hysteresis by making the inverse macroscopic capillary length scale, α, hysteretic. Neglecting hysteresis resulted in poor prediction of water storage during drainage based on hydraulic parameters estimated from infiltration. This was especially true for drainage with high initial water content. Incorporating the proposed hysteresis model resulted in prediction error less than measurement error.

A method of a priori estimating the hysteretic nature of α was proposed. The hysteretic change in α was based on $\theta(\psi)$ hysteresis models proposed by either Parlange (1976) or Mualem (1984), in combination with the Broadbridge and White (1988) hydraulic functions. The predicted hysteresis in α was similar to that obtained from inverse procedures.

Introduction

A quantitative description of water infiltration under constant flux boundary conditions in unsaturated soils is fundamental to understanding water balance, irrigation, movement of chemicals and, more generally, transport processes occurring in surface soils. Analytical solutions of Richards' equation for constant flux water infiltration into homogeneous soil profiles have been developed using the integral procedures(Parlange, 1972; Philip and Knight, 1974; White et al., 1979), Kirchhoff, Hopf-Cole and Storm transforms (Broadbrodge and White, 1988; Warrick et al., 1990, 1991) and reciprocal Bäckland transform(Sander et al., 1988, 1991; Barry and Sander, 1991). Parkin et al. (1992,1995) presented analytical solutions for water storage to a fixed depth based on solutions of Broadbrodge and White (1988) and Warrick et al. (1990). These analytical solutions are very useful for assessing the accuracy of numerical models and to estimate soil hydraulic properties by inverse procedures. Analytical solutions can also be used to test various inverse techniques for uniqueness and identifiability of various hydraulic parameters of interest. The model results of Parkin et al. (1992, 1995) are directly utilizable to interpret time-domain reflectrometry measurements.

To quantitatively predict the movement of water through variably saturated soils detailed knowledge of the hydraulic properties of the soil are needed. The unsaturated hydraulic conductivity, K, expressed as a function of the soil water content θ, or the soil water pressure head, ψ, and the relation between θ and ψ must be specified before analytical or numerical models can accurately predict water flow during infiltration, evaporation or drainage. Unfortunately, because of hysteresis, even in stable, non-swelling soils, these relationships are not simple functions, but rather show a great deal of variation between wetting and drying cycles. Hysteresis exists in both $\psi(\theta)$ and $K(\psi)$ (Haines, 1930; Staple, 1969; Kool and Parker, 1987; Jaynes, 1992). However, studies suggest that when the hydraulic conductivity is expected as a function of water content instead of pressure head, there is little hysteresis or it is so slight as to be masked by the error of the measurements and can be ignored (Gillham et al., 1976; Topp, 1971).

Considerable effort has been put into the analysis and description of hysteretic soil hydraulic properties. This has led to numerous models for describing hysteresis in $\theta(\psi)$ (Gillham et al., 1976; Scott et al.,1983; Mualem, 1974, 1984; Kool and Parker, 1987; Parlange, 1976; Hogarth et al., 1988). These models provide a simple means for determining any scanning curve from a limited amount of data, such as the main wetting and drying hysteresis curves. The models of Parlange (1976) and Mualem (1984) need only one branch of the loop to predict all the scanning curves. Viaene et al.(1994), compared different models of hysteresis using ten measured scanning curves, and concluded that the best models were the conceptual models needing two branches for calibration. Simulation studies carried out by Jaynes (1984, 1992) have shown that none of the models were consistently better than the others. Numerical simulations (Kool and Parker, 1987) of flow during transient infiltration and redistribution using a variety of hysteresis models did not differ greatly and agreed reasonably well with experimental water distribution, even when the scanning curves were not described very accurately.

Unfortunately, all the models, empirical or theoretical, do not allow exact unified analytical solutions of infiltration and drainage, even though the hydraulic models of BW and Sander allow exact solution independently for infiltration and drainage. As a result, completely different sets of parameters have to be used for infiltration and drainage. This greatly inhibits the use of the analytical solution and our understanding of role of hysteresis in the application of infiltration and drainage. In addition, the effect of hysteresis on water storage to a fixed depth has not been reported so far. In this paper, we present a model of hysteresis which connects the analytical solution of infiltration with that of drainage, thus allowing a unified solution of both drainage and infiltration. We apply the model to field measured water storage during infiltration and drainage. To test the approach, the hydraulic parameters estimated from infiltration are used to predicted the measured soil water storage during drainage.

Theory

Parametrization of soil hydraulic properties

Broadbridge and White (BW) (1988) and Sander et al. (SA) (1988) independently developed analytical solutions for constant flux infiltration boundary. The SA solution is based on the following parametrization of the hydraulic conductivity K(Θ) and diffusivity D(Θ) functions,

$$K(\Theta) = \frac{K_1 + K_2 \cdot \Theta + K_3 \cdot \Theta^2}{1 - v \cdot \Theta} \qquad [5\text{-}1]$$

$$D(\Theta) = \frac{D_0}{(1 - v \cdot \Theta)^2} \qquad [5\text{-}2]$$

where $\Delta\theta=\theta_s-\theta_r$ and $\Theta=(\theta - \theta_r)/\Delta\theta$. θs and θ_r are the saturated water content and residual water content, respectively. K_1, K_2, K_3, v, and D_0 are parameters. Sander et al. (1988) reduced the parameter number from four to two by taking into account two conditions on $K(\Theta)$. These are that $K(0) = 0$, which implies that $K_1 = 0$, and $K(1) = Ks$ where K_s is the saturated conductivity. This second condition gives K_2 in terms of K_3 and K_s or:

$$K_2 = K_s \cdot (1 - v) - K_3$$

By definition,

$$D(\Theta) = K(\Theta) \frac{d\psi}{d\theta} \qquad [5\text{-}3]$$

we have,

$$\psi - \psi_0 = \int_0^\theta D(\Theta)/K(\Theta) \; d\theta \qquad [5\text{-}4]$$

Substitution of Eq. [5-1] and Eq. [5-2] into Eq. [5-3] and integration yields (Sander, et al., 1988)

$$D_0^{-1}(\psi-\psi_e) = K_2^{-1}\cdot\ln(\Theta)+\frac{v}{v\cdot K_2+K_3}\cdot\ln[\frac{1-v}{1-v\cdot\Theta}]+\frac{K_3}{K_2\cdot(K_3+v\cdot K_2)}\ln[\frac{K_2+K_3}{K_2+K_3\cdot\Theta}] \qquad [5\text{-}5]$$

It can be shown that if $K_3=0$ this model reduces to the SA model and if $K_2=0$, this model reduce to the BW model:

$$K(\Theta) = Ks\,\frac{(C-1)\,\Theta^2}{C-\Theta} \qquad [5\text{-}6]$$

$$\psi(\Theta) = \frac{1}{\alpha}[\frac{1-\Theta}{\Theta}+\frac{1}{C}\ln(\frac{C-\Theta}{\Theta(C-1)})] \qquad [5\text{-}7]$$

where $C=1/v$ and $D_0= Ks\,(C-1)/\alpha/(\theta_s-\theta_r)$ (Parkin et al., 1995).

Analytical solution

The nonlinear Richards' equation used to describe one-dimensional nonhysteretic flow in idea soil is given by

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial z}(D(\theta)\frac{\partial\theta}{\partial z})-\frac{dK(\theta)}{d\theta}\frac{d\theta}{dz} \qquad [5\text{-}8]$$

where θ is the volumetric water content, z is the depth and t is the time. The initial and boundary conditions considered here are

$$\theta(z,0) = \theta_0 \qquad [5\text{-}9]$$

$$-D(\theta)\frac{\partial\theta}{\partial z}+K(\theta) = R \;; \qquad z = 0 \;; \quad t > 0 \qquad [5\text{-}10]$$

where R is the water application rate and θ_0 is the initial water content. By utilizing Eq. [5-1] and Eq. [5-2], through a series of transforms (i.e. Kirkhoff, Storm, and Hopf and Cole transforms), the following analytical solution can be derived:

$$\Theta(\zeta,t) = \frac{1}{\nu}[1-\frac{A\cdot D_0}{\nu}(B-2u(\zeta,t)^{-1}\frac{\partial u(\zeta,t)}{\partial\zeta})^{-1}] \qquad [5\text{-}11]$$

and

$$z(\zeta,t) = \frac{\nu}{A\cdot\sqrt{D_0}}[2\lambda\tau+B\zeta-2\ln(u(\zeta,t))] \qquad [5\text{-}12]$$

where

$$A = \frac{2\nu^2}{D_0\sqrt{D_0}}(K_1+\frac{K_2}{\nu}+\frac{K_3}{\nu^2}) \qquad B = \frac{1}{\sqrt{D_0}}(\frac{2K_3}{\nu}+K_2+\nu R)$$

$$\lambda = \frac{B^2}{4}-\frac{K_3\sqrt{D_0}A}{2\nu^2}$$

$$u(\zeta,t) = 0.5\exp(-\frac{\zeta^2}{4t})[f(0.5\zeta\cdot t^{-0.5}-\sqrt{\lambda t})+f(0.5\zeta\cdot t^{-0.5}+\sqrt{\lambda\cdot t})+$$

$$+f(-A_0\cdot t^{0.5}-0.5\zeta\cdot t^{-0.5})-f(-A_0\cdot t^{0.5}+0.5\zeta\cdot t^{-0.5})] \qquad [5\text{-}13]$$

$$f(x) = \exp(x^2)\cdot erfc(x) \qquad A_0 = 0.5[B-\frac{A\cdot D_0}{v}(1-v\Theta_0)^{-1}]$$

By change of variable of integration, a unified water storage solution for both infiltration and drainage was obtained as following,

$$W(L,t) = \frac{\theta_s-\theta_r}{A\cdot D_0^{0.5}}[2\cdot\lambda\cdot t+(B-\frac{A\cdot D_0}{v})\cdot\zeta(L,t)-2\cdot\ln[u(\zeta(L,t),t)]]+\theta_r\cdot L \qquad [5\text{-}14]$$

Eq.[5-14] was derived using a different series of transforms from that used by SA. It is derived from the same series of transforms derived as used by BW. However, the form of K(θ) and D(θ) used are similar to that of SA. The equation is a unified solution (both drainage and infiltration) that is general for both SA and BW, depending on the definition of D_0 (Eq. [5-5].

Hysteresis Models

Haines' Jump hysteresis model

Hysteresis is caused by a change of energy status of water when a wetting process is switched to a drying process or vice versa. The energy status can be measured by the capillary matric pressure (i.e, a "Haines Jump", Miller and Miller, 1956). We assume that the change of capillary pressure is abrupt when the process is switched. The scale of the change of capillary pressure is modeled by adding a constant change to the macroscopic inverse capillary length scale, α. Thus, if we assume that the change of energy status is immediate and abrupt, then the α value must jump to another value immediately after the process is switched. Since this model of hysteresis does not change the form of $K(\theta)$ and $D(\theta)$, the original analytical solution still exists. However, the predicted value of ψ from the solution (see Eq. [5-7]) is scaled by the value of α^{-1}, which changes depending on the process (drainage, infiltration). This approach is conceptually consistent with the notion of a change in "effective pore size" associated with the reversal of the flow process(wetting, drying) and the use of α as an integrated macroscopic effective capillary length(Philip, 1985; Miller and Miller, 1956).

It is possible to equate our proposed Haines Jump approach to any model of hysteresis such as Parlange (1976) model at least at an integral scale. An analogy is the Green-Ampt integral approximation of the $K(\psi)$ and $\theta(\psi)$ curves. According to Eq. [5-7], assuming no hysteresis of C, the value of the effective inverse macroscopic capillary length scale α is given by

$$\alpha = [f(\theta)\cdot\psi(\Theta)]^{-1} \qquad [5\text{-}15]$$

where $f(\theta)$ is a constant non hysteretic function. It follows that an average effective α_d* for any drainage scanning curve in form of α_w for infiltration can be given by

$$\alpha_d^* = \alpha_w \cdot \frac{\int_{-\infty}^{\psi_f} \psi_w(\Theta)d\Theta}{\int_{-\infty}^{\psi_f} \psi_d(\Theta)d\Theta} \qquad [5\text{-}16]$$

where ψ_f is the matric pressure at the reversal point. Thus, the value of α_d* can be a priori predicted for each initial condition, if α_w is known(or vice versa). The Haines Jump is given by $(\alpha_w^{-1}-\alpha_d^{-1})\cdot f(\theta)$. Equation [5-16] can be used to calculate "effective Haines Jump" given any other model which relates $\psi_w(\theta)$ to $\psi_d(\theta)$. In addition, any other existing hysteresis model can be used to a priori estimate the "effective Haines Jump". Two examples, which are subsequently discussed, are models by Parlange (1976) and Mualem (1984). Some hysteresis models may not be compatible with this approach. For example, the Scott et al. (1983) model results in a Haines Jump, which is not reversible (Kool et al., 1987). That is, an instantaneous switch from drying to wetting and then back to drying would not leave the value of α_d the same.

Parlange Model. The drying and wetting scanning curves can be related by

$$\theta_d(\psi,\psi_i) = \theta_w(\psi) - (\psi - \psi_i)\frac{d\theta_w}{d\psi} \qquad [5\text{-}17]$$

where subscripts d and w refer to drying and wetting and subscript i designates the point on the wetting curve where the drying curve is starting. Thus, knowing one scanning curve (θ_d or θ_w) the other can be calculated. Comparison with experiments shows that if the shape of the drying scanning curves varies smoothly, then the drying boundary of the loop is sufficient to predict all scanning curves (Parlange, 1976).

The Parlange (1976) hysteresis model has no additional parameter and gives an a priori prediction of the $\psi(\theta)$ drying curve from $\psi(\theta)$ wetting curve. Unfortunately, the $\psi(\theta)$ wetting curve now has a form that does not lead itself to an analytical solution of Richards' equation. However, the functional relationship between $\psi_w(\theta)$ and $\psi_d(\theta)$ can be substituted into Eq. [5-16] to calculate an " effective Haines Jump".

Mualem universal model.

Assuming the distribution functions of water in the pore domains for drying and wetting are the same for the independent domain model, Mualem (1984) presented a universal relationship between the two main curves:

$$\Theta_d(\psi,\psi_i) = \Theta_w(\psi_i)+[1-\Theta_w(\psi)]\Theta_w(\psi) \qquad [5\text{-}18]$$

where ψ_i is the value of pressure head for the starting point of drainage. The predicted drying curve provided a lower boundary of the hysteresis domain for 6 disturbed soils studied by Mualem (1984). For field soil, there may be less pore water blockage against air entry, since there is usually well-developed structure and a wide range of pore size. Therefore, we expect this model will be more accurate for field soils. In a manner similar to the Parlange (1976) model, it is possible to a priori predict an "effective Haines jump" using Eq. [5-16].

First order error analysis

The mean E[•] and variance var[•] of a function f(u) can be derived from its uncertainty parameter vector, u, through a first order Taylor expansion:

$$f(u) = f(\bar{u}) + \sum_i \frac{\partial f(\bar{u})}{\partial u_i}(u_i - \bar{u}_i) \qquad [5\text{-}19]$$

where is the vector of estimated parameter values. Using the expected value operator, E[•], on both side of this expression, we obtain

$$E[f(u)] = f(\bar{u}) \qquad [5\text{-}20]$$

and

$$Var[f(u)] = \sum_i \sum_j \frac{\partial f(\bar{u})}{\partial u_i} \frac{\partial f(\bar{u})}{\partial u_j} Cov[u_i, u_j] \qquad [5\text{-}21]$$

For linear dependence of f(u) upon u, Eq. [5-20] and Eq.[5-21] are exact. For nonlinear relationship, Eq. [5-20] and Eq. [5-21] are good approximations provided the coefficients of variation of u are small. This first order analysis provides a way to evaluate the effect of uncertainty in the parameters on the function f(u). The derivatives in Eq. [5-21] were calculated numerically using the software package Mathcad (version 6, Math Soft Inc, 1995).

Including the effect of uncertainty in the parameter on the estimated soil water storage allows a confidence interval to be placed on predicted water storage. Thus, the necessity of including a connection in α for hysteresis can be checked by comparing predicted water storage during drainage, from parameters with uncertainty obtained by inverse procedures from infiltration. If measured water storage during drainage is outside of the 95 % confidence interval of predictions, then the discrepancy cannot be related to uncertainty in parameters estimated from infiltration (Table 5-1). Thus, the discrepancy is likely from a change in parameters due to hysteresis.

Materials and methods

Field Experiments

Field infiltration experiments were conducted at the Canadian Forces Base Borden, Ontario, Canada and have been described in detail earlier. Extensive hydro-geological research, including a large scale, natural-gradient tracer test and forced gradient test have been conducted by University of Waterloo on this site. Details about this site can be found in Sudicky (1986). Water was applied to an instrumented transect(7.5 m long) inside a greenhouse using a hanging track and nozzle system. Multi-purpose TDR probes were installed every 0.15 m at each of 4 depths (0.2, 0.4, 0.6, and 0.8 m) for a total of 200 TDR probes. Five different water application rates were used. Soil water content was measured using the TDR method of Topp et al. (1980). The readings were taken manually from the display screen of two pre-calibrated Tektronix(1502 C) metallic cable tester by four operators. The readings were taken just prior to the start of water application and every 5-30 minutes depending on infiltration rate and rate of change of θ, for all the 200 multipurpose TDR probes. Here, we use the site average of the 50 probes for 20 cm as a illustration. At the end of each infiltration rate (i.e., after steady-state water content was established in the soil profile), the water application was stopped and the soil allowed to drain. TDR reading were taken at regular intervals during the drainage until soil water content changes were small.

A single set of hydraulic parameters with their uncertainty were obtained independently from the infiltration measurements using inverse procedures described earlier (Chapter 3). Since hysteresis in the K(θ) function is assumed to be negligible, the values of Ks and C from the infiltration data were used as known values to estimate a new value of α for each drainage event (i.e., α_d). The value of α_d was obtained using a similar inverse procedure and measurements of soil water storage during drainage. The need to incorporating hysteresis was examined by comparing predicted and measured soil water storage during the drainage and from the change in estimated α using infiltration verses drainage data. The comparison involves an envelope of the uncertainty of water storage introduced by the uncertainty associated with the input parameters and general TDR measurement error(see discussion of Eq. [5-20]). Finally, measured values of α during drainage (i.e., α_d) from different initial conditions were compared to "effective Haines jump values of α_d* estimated a priori using Eq. [5-16] using the hysteresis models of Parlange (1976) and Mualem (1984) as examples.

Results and discussion

Table 5-1 gives the hydraulic parameters and their covariance matrix estimated from measured K(θ) and ψ(θ) during the infiltration phase of the experiment(Chapter 2). Figure 5-1 shows the measured water storage (0-0.2 m) during drainage for three initial conditions (θ_i=0.38, 0.31 and 0.27), and the water storage predicted by direct substitution of the hydraulic parameters for infiltration (Table 5-1) into Eq. [5-14]. For the wetter initial conditions (θ_i=0.38, 0.31), the prediction using infiltration parameters underestimates measured water storage during drainage. At the driest initial condition, the measured and predicted values are similar. At θ_i=0.38, the measured values exceed the upper 95 % prediction limits based on uncertainty (from the first order perturbation approximation). This suggests the differences are from a change in hydraulic parameters (most likely hysteresis). The Root Mean Square error(RMS) of prediction for depth averaged soil water content was 0.031, 0.014, and 0.015 for θ_i=0.38, 0.31 and 0.27, respectively. This error is greater than the average estimated TDR error for absolute soil water content (0.01-0.015, Topp et al, 1980). Relative measurement error using TDR, as would be relevant here, would be significantly lower. This also suggests that TDR measurement error cannot account for the discrepancy. In combination, the parameter uncertainty error and TDR measurement error may account for the discrepancy of predicted verses measured.

The analytical solution for drainage (R=0) (Eq. [5-14]) was fitted to the measured water storage during drainage for each of the three initial conditions. The inverse capillary length scale α_d was the only free-varying parameter. The α_d values from the inverse procedure(0.037, 0.054, and 0.054 cm^{-1} for θ_0= 0.27, 0.31, and 0.38, respectively) are all considerable smaller than the value obtained from for infiltration (α =0.098 cm^{-1}) and exceed the lower 95 % confidence interval of α=0.098 cm^{-1} for infiltration (Table 5-1). The α_d values also depend on the initial condition. This again suggests that the discrepancy in predicted soil water storage (Fig. 5-1) is from hysteresis. Thus, the α parameter is hysteretic.

Figure 5-2 shows the predicted water storage curves using the best-fit α_d value for each of the three initial conditions. The agreement with measured water storage is quite good for all times. The calculated Root Mean Square Errors (RMS) for depth-averaged water content (W/L) were 0.0087, 0.006, and 0.006 for $\theta_0 = 0.38$, 0.31, and 0.27, respectively, and are substantially less than the expected measurement error (0.013 cm^3 cm^{-3}) of TDR (Topp et al., 1980) and much lower than the RMS using α_w for infiltration.

Application of Parlange (1976) model

The values of effective α_d* predicted using Eq. [5-16], the Parlange (1976) hysteresis model and α_w=0.098 cm^{-1} are 0.049, 0.058, and 0.061 cm^{-1}, for initial conditions $\theta_i = 0.38$, 0.31 and 0.27. These values are only slightly higher than the best-fit α_d values (0.037, 0.054 and 0.054 cm^{-1}) from inverse procedures. Fig. 5-3 shows the drying scanning curves predicted from the original Parlange (1976) model and those predicted by the Haines Jump model (with effective α_d using Eq. [5-16]). As an example, the Parlange (1976) model underestimates W compared to the Haines Jump model at high soil water content and overestimates at low soil water content. However, at the integral scale the curves are identical. Fig. 5-3a show a comparison of the drying scanning curve obtained with the Haines jump model using α_d from soil water storage during drainage using an inverse procedure, and α_d * predicted a priori using Eq. [5-16](with Parlange (1976) model). The slight difference in α_d and α_d * results in negligible difference in estimated drying scanning curves.

In addition, the water storage values(during drainage) as predicted from the Haines Jump hysteresis model using α_d* values from Eq. [5-16] and the Parlange(1976) model are in good agreement with measured values(Fig. 5-4), though a slight consistent underestimation of water storage occurs. The calculated RMS values of depth-averaged water content are 0.012, 0.006, and 0.008 $cm^3\ cm^{-3}$ for θ_0= 0.38, 0.31, and 0.27 $cm^3\ cm^{-3}$, respectively. The RMS values are lower than TDR measurement error, significantly lower than RMS using α_i =0.098, and only slightly higher than the RMS using α_d from the best fit inverse procedures. The calculation of confidence interval for the predicted water storage in Fig. 5-4 is complicated because the estimation error for α_d* is generally unknown. However, if we assume no error is introduced when matching the Parlange predicted curve with the Haines Jump model, we are assuming α_d has perfect correlation with α_w. Since the area under the $\theta(\psi)$ is proportional to $1/\alpha$, the relationship between α_d and α_w is linear. Thus, the estimated variance of α_d can be approximated by the variance of α_w divided by $(\alpha_w^* / \alpha_d^*)^2$, since the correlation matrix would be the same as in Table 5-1 (due to the perfect correlation between α_d and α_w). Assuming the estimated confidence interval in α_d* is correct, the calculated confidence interval of W was calculated and is shown in Fig. 5-3. All the measured water storage values fall inside of the 95 % confidence region (Fig. 5-3). This suggests that the proposed Haines jump model, with a priori prediction of effective α_d* from α_w* (or vice versa) using Eq. [5-16] with the Parlange(1976) model, may be an accurate way of incorporating hysteresis in the unified analytical solution for infiltration and drainage. This would allow the development of a single unified inverse procedure for estimating hydraulic parameters from combined infiltration and drainage measurements.

Application of Mualem's universal model(Mualem, 1984)

The estimated α_d* values from Eq. [5-16] using the Mualem (1984) model are 0.0595, 0.0705, and 0.076 cm^{-1}, for θ_i = 0.38, 0.31 and 0.27. The values are slightly higher than α_d* from the Parlange (1976) model and less similar to the α_d value from the inverse procedures. Thus, as an example, predictions of water storage using the Mualem α_d* values are not as good as the Parlange (1976) model(Figure not given). The calculated RMSs are 0.019, 0.009, and 0.011 cm^3 cm^{-3} for θ_i= 0.38, 0.31, and 0.27 cm^3 cm^{-3}. About half of the measurements fall outside of the 95 % confidence interval. The predictions are still better than using the value of α_w =0.09875 cm^{-1} from infiltration. The Mualem (1984) model may be less accurate because it is a universal model for the lower boundary of hysteresis (Mualem, 1984). The result is consistent with the finding of Viaene et al. (1994) that the one-branch Parlange (1976) model fitted ten soil retention curves better than the Mualem Universal model.

For practical purposes, the combination of the Haines' jump model with the prediction of α_d* from α_w(or vice versa) from Eq. [5-16] and either the Parlange (1976) model or Mualem(1984) model is likely satisfactory. The RMS error would be about 1- 2 % of water storage, which is within the measurement error of water storage by TDR. This substantiates the conclusion obtained by Jaynes(1985), that simple hysteresis models usually give similar results as complicated models. Totally ignoring hysteresis is unacceptable.

Conclusion

A Haines' Jump model of hysteresis is proposed and can be combined with a unified analytical solution for soil water storage to a fixed depth as a function of time during infiltration and drainage. The model accounts for hysteresis by making the inverse macroscopic capillary length scale, α, hysteretic. Neglecting hysteresis resulted in poor prediction of water storage during drainage based on hydraulic parameters estimated from infiltration. This was especially true for drainage with high initial water content. Incorporating the proposed hysteresis model resulted in prediction error less than measurement error.

A method of a priori estimating the hysteretic nature of α was proposed. The method was tested using hysteretic models proposed by Parlange (1976) and Mualem (1984). The predicted hysteresis in α was similar to that obtained from best fit inverse procedures applied independently to soil water storage measurement during infiltration and drainage.

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Table 5-1. Estimated hydraulic parameters and their correlation matrix from measured hydraulic properties during a serries of steady state infiltration experiments.

	Estimate value	Standard Deviation of error	Correlation matrix			
			Ks	α	C	θ_s
Ks (cm hr^{-1})	7.18	0.41	1			
α (cm^{-1})	0.098	0.006	0.44	1		
C	1.27	0.03	-0.32	-0.52	1	
θ_s(cm^3 cm^{-3})	0.42	0.005	0.77	0.20	0.22	1

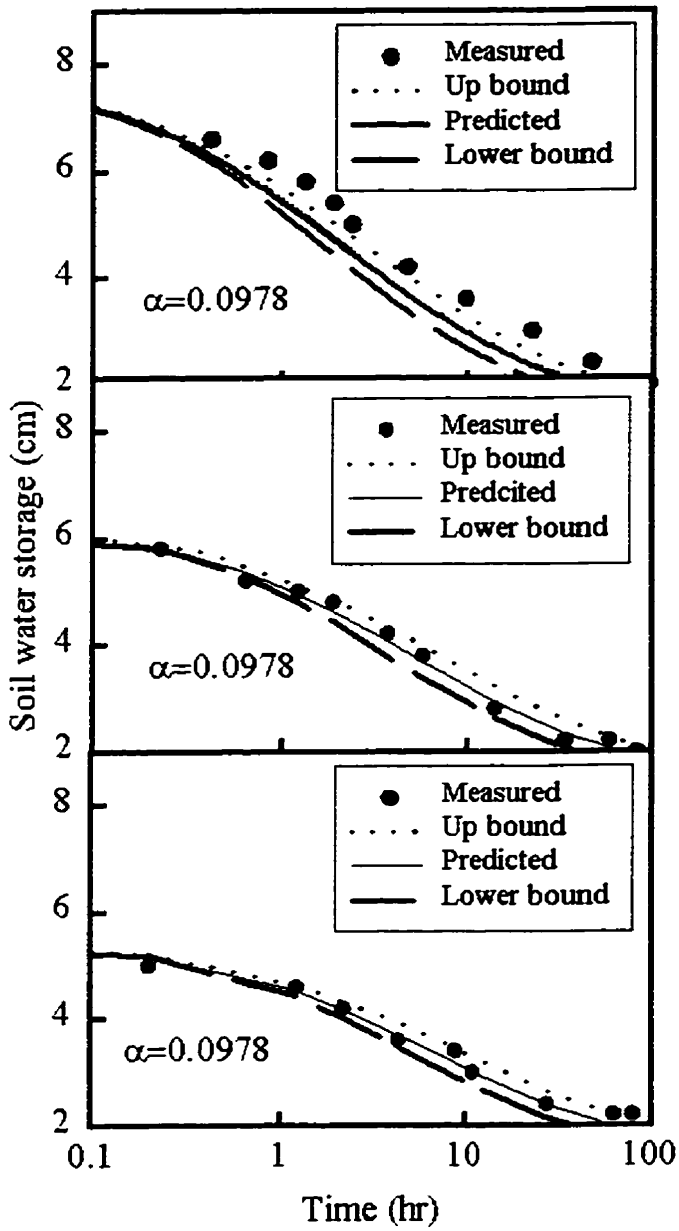

Figure 5-1. A comparison of measured and predicted soil water storage during drainage using unified solution with no hysteresis, and the value of α from infiltration.

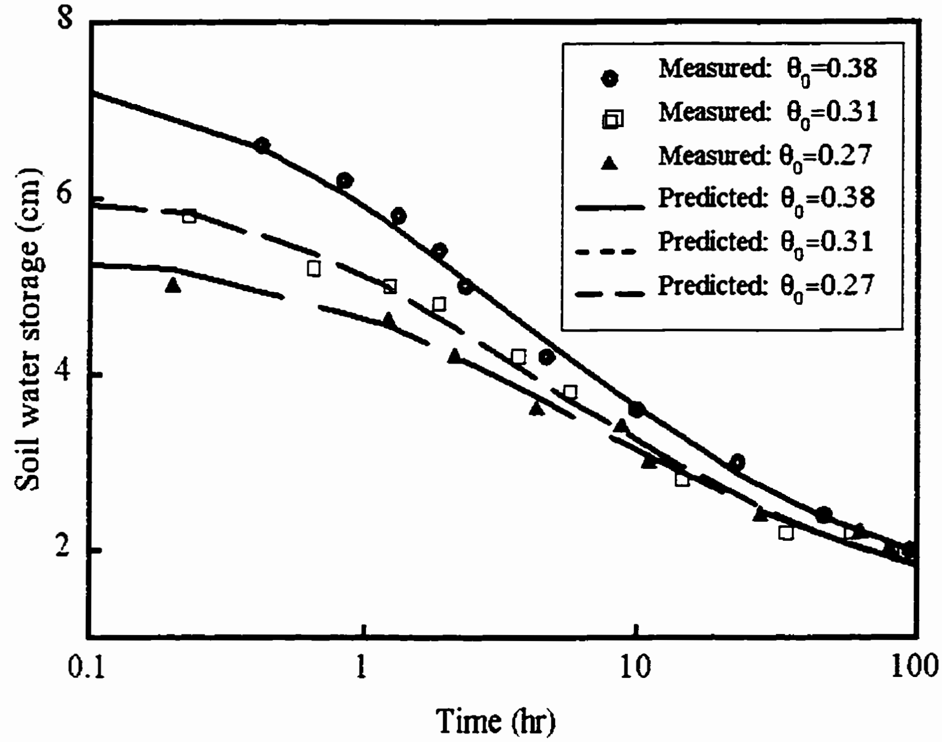

Figure 5-2. A comparison of measured and predicted soil water storage during drainage using the Haines Jump hysteresis model, and the value of α_d from inverse procedures.

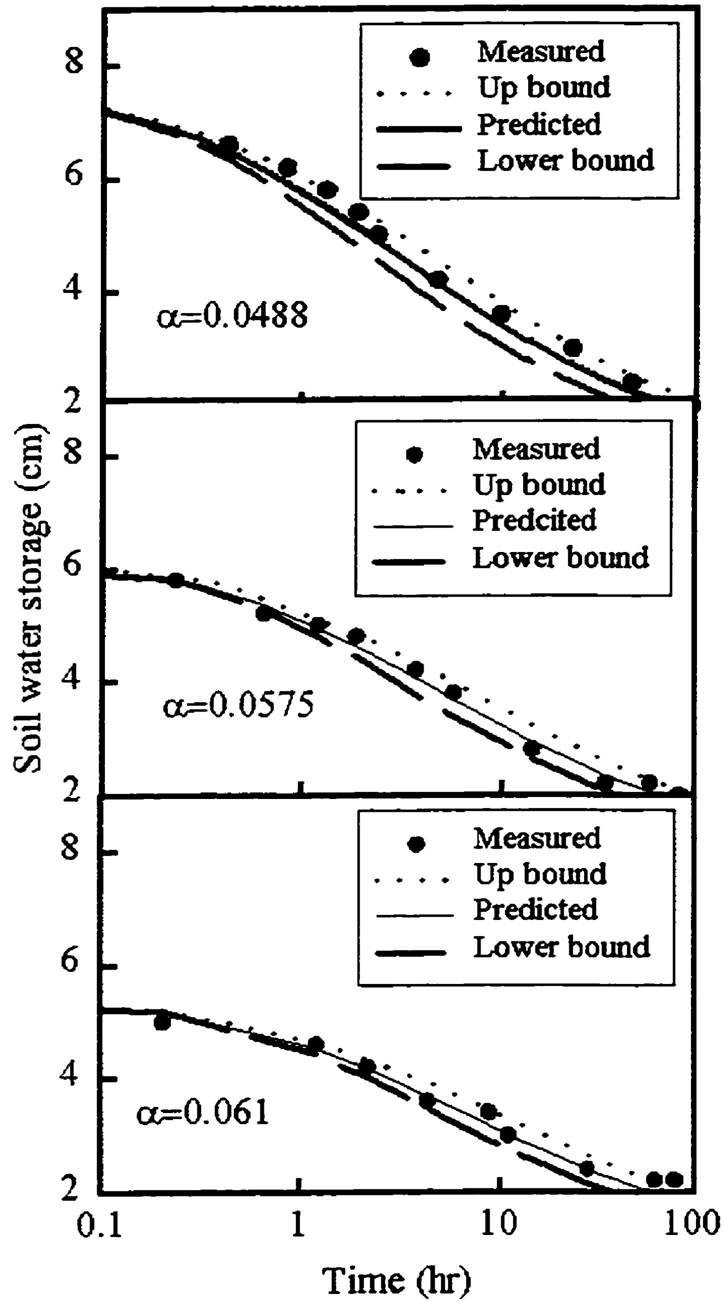

Figure 5-3. A comparison of measured and predicted soil water storage during drainage using the Haines Jump hysteresis model, and a priori value of α estimated from Eq. [] and the Parlange 91976) model.

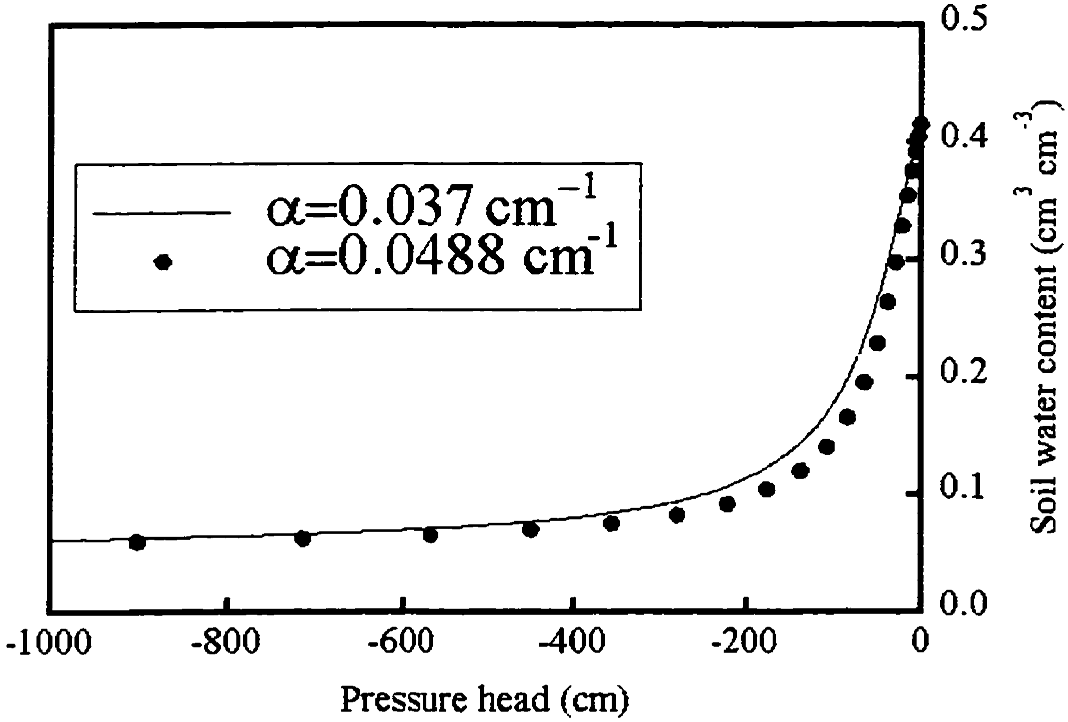

Fig. 5-3a. A comparison of the drying scanning curve obtained with the Haines jump model using an inverse procedure (α=0.037 cm^{-1}) and the effective (α_d^* =0.0488 cm^{-1}) predicted using Parlange (1976) model.

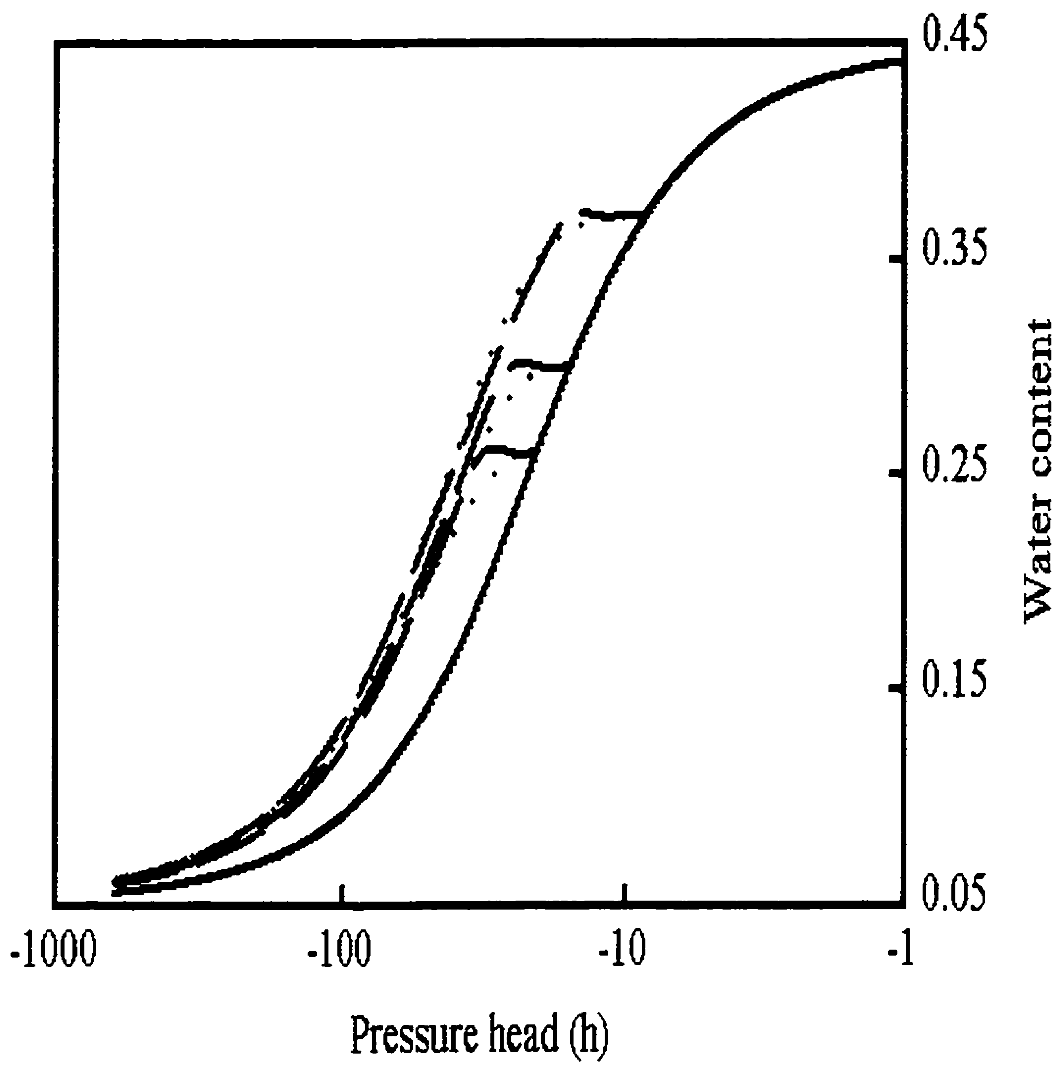

Figure 5-4.Comparison of the predicted drying scanning curves from the Parlange (1976) model (Dashed line) and corresponding Haines Jump hysteresis model(dotted line) for initial water content =0.38, 0.31, and 0.27.

Chapter 6

Analytical stochastic solution for constant flux infiltration and drainage in heterogeneous soils

ABSTRACT

A unified stochastic-analytical solution for soil water storage (W) as a function of depth and time was developed for both infiltration and drainage. The solution is a small perturbation of Parkin et al. (1992) for homogeneous soils and has excellent agreement with Monte Carlo simulations for moderate variance of log hydraulic conductivity, inverse capillary length scale, and the spatially random but temporally constant surface flux. The predicted expected value of soil water storage to a fixed depth for a constant flux boundary in a spatially variable field depends on the averages of hydraulic parameters only. Therefore, average of soil water storage, $\langle W \rangle$, of a heterogeneous field is identical to that of a homogeneous soil with hydraulic parameters equal to the average hydraulic parameters. The variance of soil water storage increases with the increase in $\langle W \rangle$. The auto-correlation coefficient of soil water storage is positive and decays with the separation distance. For infiltration, the integral scale of soil water storage does not change with time and is identical to that of log hydraulic conductivity. For drainage, it is time-dependent. The random surface flux, being constant temporally and varying horizontally, has no significant effect on $\langle W \rangle$, but enhances the spatial variability in soil water storage during infiltration.

Introduction

Infiltration and drainage are important processes occurring in surface soils. Numerous analytical and numerical solutions have been proposed to solve the infiltration equation. Despite their success in repacked soil columns, their application in field soils has been hindered by the spatial variability of soil hydraulic properties and scarcity of measurements. In recent years, stochastic approaches have been proposed, which consider hydraulic properties as random space functions (RSFs). These approaches have been very successful in saturated aquifers (Dagan, 1989). In the unsaturated zone, the dependence of hydraulic conductivity and diffusivity on the water content complicates the mathematical treatment of the problem. However, with some assumptions, solutions have been obtained. For example, in some conditions the flow can be treat reasonably well as one dimensional in the vertical direction (Dagan and Bresler, 1979, 1983; Yeh , 1989; Protopapas and Bras, 1991; Rubin and Or, 1993).

Dagan and Bresler (1983) examined stochastic infiltration and redistribution. They assumed that water flow is one-dimensional and the spatial hydraulic properties do not change along any vertical profile, but vary considerably in the horizontal plane. They concluded the stochastic approach leads to a quite accurate value of the expectation and variance of the flow variables even if a simplified model such as piston flow is adopted. However, their approach applies only to sufficiently heterogeneous soils in which the variance of log saturated hydraulic conductivity is greater than 1. Many soils have a variance less than 1 (Sudicky, 1986; Russo and Bresler, 1982; Russo et al., 1992). Furthermore, their approach needs numerical integration and is very time consuming when more than one hydraulic parameters are treated as random space functions (RSFs).

Mantoglou and Gelhar (1987) analyzed three-dimensional unsaturated flow in heterogeneous media. Introducing a small perturbation of soil water capacity, they obtained a large scale equation of the same form as Richards' equation. However, the fluctuation equation is nonlinear and can only be solved numerically. To obtain a closed solution, they linearized the fluctuation equation and solved it using the spectral representation, after assuming one-dimensional mean flow and an unbounded flow domain (far from the boundary). Although useful results were derived for transient conditions, their results only apply to flow under quasi-steady state conditions.

Chen et al.(1994) presented an upscaled equation describing water flow during infiltration. The upscaled equation involves only the average and variance of Ks, and can be solved to obtain the average behavior. Their approach is numerically efficient compared to Monte Carlo simulation, but still requires numerical solution and the solution may not converge (Chen et al., 1994).

In general, past works for heterogeneous transient flow during infiltration and drainage used numerical calculations. For models employing the stream-tube model, a common assumption is that local flux density in each individual stream tube is identical to each other and to the application rate, under constant flux boundary. Variability arises from the variability of water velocity and shape of the wetting front. However, field measurements suggest that applied water can redistribute in the first few centimeters of the soil surface, and subsequently establish constant, but different local vertical water fluxes in the horizontal plane space (Parkin et al., 1995; Chapter 2). The objective of this paper is to present a unified(infiltration and drainage) stochastic analytical solution for soil water storage to a fixed depth as a function of time in heterogeneous soils. The solution is the small perturbation of the unified solution developed by Parkin et al. (1992) and modified in Chapter 2. We compare our solution with the Monte Carlo solution on simulated fields. The effect of variations in Ks, α and the application rate, R, on the mean and covariance of water storage as s function of time are examined.

Theory

Broadbridge and White (BW) (1988) and Sander et al. (1988) independently developed an analytical solution for constant flux infiltration. The BW solution is based on the following parameterization of hydraulic conductivity (m s^{-1}), K(Θ), and diffusivity functions(m^2 s^{-1}), D(Θ),

$$K(\Theta) = Ks \frac{(C-1)\ \Theta^2}{C-\Theta} \qquad [6\text{-}1]$$

$$D(\Theta) = \frac{Ks\ C\ (C-1)}{\alpha\ \Delta\theta\ (C-\Theta)^2} \qquad [6\text{-}2]$$

where $\Delta\theta=\theta_s-\theta_r$ and $\Theta=(\theta-\theta_r)/\Delta\theta$. θ_s, θ_r and θ are the saturated water content, residual water content, and soil water content, respectively. Ks, α, and C are the saturated hydraulic conductivity (m s^{-1}), inverse capillary length scale(m^{-1}) (Philip, 1985), and a constant introduced by BW, respectively.

Richards' equation for one-dimensional nonhysteretic flow in a uniform soil is:

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial z}(D(\theta)\frac{\partial\theta}{\partial z}) - \frac{dK(\theta)}{d\theta}\frac{d\theta}{dz} \qquad [6\text{-}3]$$

where z is the depth and t is the time.

The initial and boundary condition considered here are

$$\theta = \theta_0 \ ; \qquad t=0 \ ; \qquad z\geq 0; \qquad [6\text{-}4]$$

$$-D(\theta)\frac{\partial\theta}{\partial z} + K(\theta) = R \ ; \qquad 0<t<t_p \ ; \qquad z=0 \qquad [6\text{-}5]$$

where R, θ_0 and t_p are the water application rate at the surface(z=0), the initial water content and ponding time, respectively. If R=0, the flow is a gravity drainage process. Utilizing Eq. [6-1] and Eq. [6-2], through a series of transforms (i.e. Kirchhoff, Storm, and Hopf and Cole transforms), following Broadbridge and White (1988), Warrick et al. (1990) derived an analytical solution as

$$\Theta(\zeta,t) = C[1-(1+2\rho-u(\zeta,t)^{-1}\frac{\partial u(\zeta,t)}{\partial\zeta})^{-1}] \qquad [6\text{-}6]$$

and

$$z(\zeta,t) = (C\alpha)^{-1}[\rho(\rho+1)\tau+(2\rho+1)\zeta-\ln(u(\zeta,t))] \qquad [6\text{-}7]$$

where ζ is a parameter connecting Eq. [6-9] and Eq. [6-10] and

$$\rho = \frac{R}{4C(C-1)Ks} \qquad \tau = \frac{4C(C-1)\ \alpha K_s t}{\Delta\theta} \qquad [6\text{-}8]$$

$$u(\zeta,t)=U1(\zeta,t)+U2(\zeta,t) \qquad [6\text{-}9]$$

$$U1=0.5\exp(-\frac{\zeta}{\tau})[f(\zeta\tau^{0.5}-(\rho(\rho+1)\tau)^{0.5})+f(\zeta\tau^{0.5}+(\rho(\rho+1)\tau)^{0.5})] \qquad [6\text{-}10]$$

$$U2=0.5\exp(-\frac{\zeta}{\tau})[f(-0.5A_0\tau^{0.5}-\zeta\tau^{-0.5})+f(-0.5A_0\tau^{-0.5}+\zeta\tau^{0.5})] \qquad [6\text{-}11]$$

$$A_0=1+2\rho-C/(C-\Theta_0) \qquad [6\text{-}12]$$

By change of variable of integration, a unified analytical solution for both water storage to depth L for constant flux infiltration and drainage was obtained (Chapter 2),

$$W(L,t) = \frac{\Delta\theta}{\alpha}[2\rho\ \zeta(L,t) + \ln(\frac{u(0,t)}{u(\zeta,t)})] + \theta_r L \qquad [6\text{-}13]$$

Stochastic characterization of heterogeneity.

For unsaturated flow, there are five parameters in the hydraulic functions (Ks, C, α, θ_s, and θ_r), and each one of them exhibits spatial variation. While some parameters are highly variable, like Ks, others are less variable, such as θ_s and θ_r. The variation of C is not well known. Without loss of generality, we focus on two of them, Ks, and α, because their properties are best known, and because Ks represents the influence of gravity on water flow and α represents the ratio of capillary force and gravity (Philip, 1985). The following assumptions are adopted concerning the heterogeneous parameters:

(1). The log saturated hydraulic conductivity, Y(x)=ln(Ks(x)), is assumed to be a multi-normal random function that is expressed through its stationary mean <Y> and a spatial covariance with a finite integral scale. Its spatial structure is modeled by the isotropic exponential model:

$$C_Y(r) = \langle Y'(x)Y'(x+r)\rangle = C_y(r) = \sigma_Y\ e^{-r/I_Y} \qquad [6\text{-}14]$$

where, C_Y is covariance of Y, σ_Y is the variance of Y and r is the lag distance between two points, and I_Y is the integral scale of Y. This choice of model is supported by field studies (Freeze, 1975; Sudicky, 1986).

(2). The parameter α is also treated as a random spatial function and is assumed to be statistically homogeneous and isotropic with constant mean $<\alpha>$, variance σ_α, integral scale

I_α and a similar spatial structure as Eq.[6-14].

(3) The α field is assumed to be either perfectly correlated or uncorrelated with the log saturated hydraulic conductivity field Y(x) (Yeh et al., 1985). For perfectly correlated field, there may be positive correlation and negative correlation. While some field experiments suggests that higher Ks values are associated with coarser media, which in turn are characterized by large α (Unlu et al., 1990; White and Sully, 1992; Russo et al., 1997), there is field evidence that $\alpha(x)$ is not correlated with Y(x) (Russo et al., 1992). However, no experimental evidence supports a negative correlation. Thus, we consider two cases: perfectly positively correlated and the uncorrelated α-Y fields.

(4). The flow domain is much bigger than I_Y or I_α such that the ergodicity assumption can be invoked. Under this assumption, the spatial average and ensemble average can be exchanged.

(5). The flow domain is assumed to be composed of homogeneous soil columns, each with different soil properties (Ks, and α).This assumption was adopted by Dagan and Bresler (1983) and Rubin and Or (1993).

To account for erratic spatial variability and for the uncertainty associated with their estimation, the hydraulic parameters are expressed as random functions, each composed of an expected value and a random fluctuation:

$$Y = \langle Y \rangle + Y' \qquad \langle Y' \rangle = 0 \qquad [6\text{-}15]$$

$$\alpha = \langle \alpha \rangle + \alpha' \qquad \langle \alpha' \rangle = 0 \qquad [6\text{-}16]$$

where angle brackets denote the expected value operator. Since soil water storage W is function of Y and α, we may expand W around the means of Y and α according to Taylor's series

$$W(Y,\alpha) = W(\exp(\langle Y\rangle,\langle\alpha\rangle) + \frac{\partial W(\exp(\langle Y\rangle,\langle\alpha\rangle)}{\partial\langle\alpha\rangle}\alpha' + \frac{\partial W(\exp(\langle Y\rangle,\langle\alpha\rangle)}{\partial\langle Y\rangle}Y' + \frac{1}{2}\frac{\partial^2 W(\exp(\langle Y\rangle),\langle\alpha\rangle)}{\partial\langle\alpha\rangle^2}(\alpha')^2 +$$

$$\frac{1}{2}\frac{\partial^2 W(\exp(\langle Y\rangle,\langle\alpha\rangle)}{\partial\langle Y\rangle}Y'Y' + \frac{\partial^2 W(\exp(\langle Y\rangle,\langle\alpha\rangle))}{\partial\langle\alpha\rangle\partial\langle Y\rangle}\alpha' Y' \qquad [6\text{-}17]$$

Taking the expectation of the above, an approximate formula for the mean and variance for W as a function of depth z and time t, W(L,t) can be expressed to the first order as

$$\langle W(Y,\alpha)\rangle = W(\exp\langle Y\rangle,\langle\alpha\rangle) \qquad [6\text{-}18]$$

and the covariance as

$$C_W(L,t;r) = F_1^2(L,t)C_Y(r) + F_2(L,t)C_\alpha(r) + 2F_1(L,t)F_2(L,t)C_{\alpha Y}(r) \qquad [6\text{-}19]$$

Where r is the separation distance between two points, and

$$F_1(z,t) = \frac{\partial\langle W(z,t)\rangle}{\partial\langle Y\rangle} \qquad F_2(z,t) = \frac{\partial\langle W(z,t)\rangle}{\partial\langle\alpha\rangle}$$

Using Eq. [6-13] and Eq. [6-7], the derivatives F1 and F2 can be obtained as

$$F_1 = \frac{\Delta\theta/\langle\alpha\rangle}{(2\bar{\rho}+1)\cdot\bar{U}-F_3}[\bar{\rho}\cdot F_4 - \bar{\tau}\cdot F_5 - \bar{\rho}^2\cdot\bar{\tau}\cdot\bar{U} - 2\bar{\rho}\cdot\bar{\zeta}\cdot\bar{U}] \qquad [6\text{-}20]$$

$$F_2 = -\frac{\langle W\rangle - \theta_r L}{\langle\alpha\rangle} + \frac{\Delta\theta}{\langle\alpha\rangle}[CL - \bar{\rho}(\frac{1/\bar{U}\cdot F_5 + CL - \bar{\rho}(\bar{\rho}+1)\bar{\tau}/\langle\alpha\rangle}{2\bar{\rho}+1-1/\bar{U}\cdot F_3})] \qquad [6\text{-}21]$$

where

$$F_3 = \frac{\partial\bar{U}}{\partial\bar{\zeta}} = \overline{A_0 U_2} - 2\sqrt{\bar{\rho}(\bar{\rho}+1)}\cdot\overline{U_1} + \exp(-\frac{\bar{\zeta}^2}{\bar{\tau}})[2\sqrt{\bar{\rho}(\bar{\rho}+1)}f(\overline{A_2}) + \overline{A_0}f(\overline{B2})] \qquad [6\text{-}22]$$

$$F_4 = \frac{\partial\bar{U}}{\partial\bar{\rho}} = (2\bar{\rho}+1)[(\frac{\zeta}{\sqrt{\bar{\rho}(\bar{\rho}+1)}} - \bar{\tau})\overline{U_1} + \frac{\zeta}{\sqrt{\bar{\rho}(\bar{\rho}+1)}}f(\overline{A_2})] - 2\sqrt{\bar{\tau}}[\overline{B_1}\ \overline{U_2} + \exp(-\frac{\zeta^2}{\bar{\tau}})] \qquad [6\text{-}23]$$

and

$$F_5 = \frac{\partial\bar{u}}{\partial\bar{\tau}} = \bar{\rho}(\bar{\rho}+1)\overline{U_1} + 0.25\overline{A_0^2}\,\overline{U_2} \qquad [6\text{-}24]$$

$$\bar{\rho} = \frac{\langle R\rangle}{4C(C-1)\exp(\langle Y\rangle)} \qquad \bar{\tau} = \frac{4C(C-1)\langle\alpha\rangle\exp(\langle Y\rangle)\cdot t}{\Delta\theta} \qquad [6\text{-}25]$$

$$f(x) = \exp(x^2)\cdot erfc(x)$$

where erfc(x) is the complimentary error function. Average ζ is the root of the following function.

$$(C(\alpha))^{-1}[\bar{\rho}\cdot(\bar{\rho}+1)\cdot\bar{\tau}+(2\bar{\rho}+1)\cdot\bar{\zeta}-\ln(\bar{U}))]-L=0$$

$$\bar{U}=\bar{U}_1+\bar{U}_2 \qquad [6\text{-}26]$$

$$\bar{U}_1=0.5\exp(-\frac{\bar{\zeta}}{\bar{\tau}})[f(\bar{A}_1)+f(\bar{A}_2)] \qquad [6\text{-}27]$$

$$\bar{U}_2=0.5\exp(-\frac{\zeta}{\bar{\tau}})[f(\bar{B}_1)+f(\bar{B}_2)] \qquad [6\text{-}28]$$

$$\bar{A}_1=\bar{\zeta}\cdot\bar{\tau}^{0.5}-(\bar{\rho}\cdot(\bar{\rho}+1)\cdot\bar{\tau})^{0.5} \qquad \bar{A}_2=\bar{\zeta}\cdot\bar{\tau}^{0.5}+(\bar{\rho}\cdot(\bar{\rho}+1)\cdot\bar{\tau})^{0.5} \qquad [6\text{-}29]$$

$$\bar{B}_1=-0.5\cdot\bar{A}_0\cdot\bar{\tau}^{0.5}-\bar{\zeta}\cdot\bar{\tau}^{-0.5} \qquad \bar{B}_2=-0.5\cdot\bar{A}_0\cdot\bar{\tau}^{-0.5}+\bar{\zeta}\cdot\bar{\tau}^{0.5} \qquad [6\text{-}30]$$

$$\bar{A}_0=1+2\bar{\rho}-C/(C-\Theta_0) \qquad [6\text{-}31]$$

Effects of unevenly distributed surface flux density

There are two approaches to assess the influence of spatially random but temporally constant surface water flux R, with a mean $\langle R \rangle$ and variance σ^2_R. Here we only deal with the effect of R on the mean and variance of W(L,t). One approach is the small perturbation approximation. The mean and variance of W is simply

$$\langle W(L,t) \rangle = \frac{\Delta\theta}{\langle\alpha\rangle}[2\cdot\bar{\rho}\cdot\zeta + \bar{\rho}\cdot(\bar{\rho}+1)\cdot\bar{\tau} - \ln(\bar{U})] + \theta_r \cdot L \qquad [6\text{-}32]$$

and

$$\sigma^2_W(L,t) = \frac{\partial\langle W(L,t)\rangle}{\partial\langle R\rangle}\sigma^2_R + C_W(L,t;0) \qquad [6\text{-}33]$$

where

$$\frac{\partial\langle W\rangle}{\partial\langle R\rangle} = -\frac{\Delta\theta}{\langle\alpha\rangle\langle R\rangle}\frac{\bar{\rho}/\bar{U}\cdot F_4 - [(2\bar{\rho}+1)\bar{\rho}\cdot\bar{\tau} + 2\bar{\rho}\cdot\zeta]}{2\bar{\rho}+1-1/\bar{U}\cdot F_3}$$

The other approach to derive the mean and variance is to use the probability density distribution. For an independently distributed flux density R, the mean and variance of the dependent variable W can be expressed as:

$$\overline{W} = \int_0^\infty W(R)\cdot P(R)\cdot dR \qquad [6\text{-}34]$$

and

$$\langle (W-\overline{W})^2 \rangle = \int_0^\infty \sigma^2_W \cdot P(R) \cdot dR + \int_0^\infty (W-\overline{W})^2 \cdot P(R) \cdot dR \qquad [6\text{-}35]$$

This approach was used by van Wensenbeek and Kachanoski (1994) for solute breakthrough in heterogeneous soils. The differences between Eq.[6-31] and Eq. [6-34] are that: (1) the first one is approximate while the second one is exact for given W(R); (2) the first one is quasi-analytical while the second one is generally fully numerical.

Monte Carlo simulations.

A realization of the two-dimensional Gaussian random field(g(x))on a grid 100×100 m^2 with standard normal distribution N(0,1), which reproduced a prescribed mean, variance and correlation structure of Y and α (with appropriate correlation), was generated using the turning bands methods. The program TB3D given in Deutsch and Journel (1992) was employed. The realization was transformed to a normally distributed variate:

$$g(x) = \sigma_y (x) + \langle Y \rangle \Rightarrow N(\langle Y \rangle, \sigma^2)$$

and then subsequently transformed to lognormality:

$$Ks(x) = e^{y(x)} = e^{\langle Y \rangle} e^{\sigma_Y (x)}$$

The α(x) field was generated using the first two steps. For perfectly-correlated α field and Y field, the same Gaussian random field, g(x), was used. For uncorrelated fields, different seed numbers were used to generate Ks and α fields. We used I_Y=5 m and I_α=3 m for uncorrelated α-Y fields and $I_Y=I_\alpha= I_{\alpha Y}$=5 m for perfectly correlated α-Y fields.

Ks and α values on each node are used as input to Eq. [6-13] to produce W on that node. The W values of the simulated fields were then used to calculate the moments of W by invoking the ergodicty assumption. Semivariances of Θ and W were calculated using GS⁺(Gamma Design Software, Plainweel, USA).

Results and discussion

Infiltration

The analytical solution for W, which included its expected value and spatial covariance is given in Eq. [6-18] and Eq. [6-19], respectively. The solution is expressed in terms of the input soil parameters and the boundary conditions. Parameter statistics used for illustration are given in Table 1. The analytical and Monte Carlo, MC, simulated $\langle W \rangle$ and σ_W are shown in Fig. 6-1 at three depths.The case of perfectly correlated α-Y fields are considered for all the three depths and the case of uncorrelated α-Y fields is considered only for L=100 cm. $\langle W \rangle$ increases linearly at small times with a slope equal to the uniform application rate R and gradually reaches a constant value for both correlated flow and uncorrelated flow (Fig. 6-1b). This constant values equals the product of the steady-state water content and length of TDR rods. The first order approximation to $\langle W \rangle$ depends only on the means of α and Y, and not on the variances and covariance of α and Y (Eq. [6-18]). The result of this approximation is essentially identical to the MC simulation for both correlated and uncorrelated α-Y fields (Fig. 6-1b).

The variance of water storage at small time remains practically zero for both correlated and uncorrelated flow. This is because the wetting front is still located completely within the depth L, and the water storage deterministically equals the amount of water supplied on surface: $W(L,t)=R \cdot t$. Therefore, σ_W equals zero. As the length increases, the time σ_W remains zero increases, because it takes longer for the wetting front to reach L (Fig. 6-1a). As the wetting front passes depth L, σ_W increases quickly and then gradually reaches the asymptotic limit for both cases of correlated flow and uncorrelated α-Y fields.

The dependence of σ_W on $\langle W \rangle$ is very clear from Fig. 6-1a and Eq. [6-19]. As $\langle W \rangle$ increases at small time, σ_W increases and as $\langle W \rangle$ reaches the asymptotic limit, so does σ_W. The stationarity of σ_W is achieved when $\langle W \rangle$ attains stationarity and the flow is steady-state. Similar results were obtained for steady-state pressure head in a bounded domain (Indelman et al., 1993). The duration for zero σ^2_W is very short. Thus, the estimated application rate from the slope of increase in $\langle W \rangle$ with time is underestimated at moderate to long times (Chapter 2)

Water storage variance σ^2_W increases with time more sharply for uncorrelated α-Y fields than for correlated α-Y. σ^2_W decreases with the increase in σ^2_α for perfectly correlated α-Y fields. This can be explained from Eq. [6-19]. The absolute value of the derivative of W with respective to Y, dW/dY, and σ_W are greater than that of dW/dα and σ_α , respectively. Morever, dW/dα is always less than or equal to zero, and the increase in σ_α increases the covariance between α and Ks, $\sigma_{Y\alpha}$ for perfectly-correlated flow. Thus, the increase in the value of the second term in Eq.[6-19] is smaller than the decrease in the third term. Consequently, an increase in σ_α results in a decrease in the variance of W for perfectly correlated flow. However, at large times, because dW/dα is zero, the variance of W remains practically the same regardless of the variation of α.

σ_W increases with an increase in σ_α for uncorrelated α-Y field, because the third term in Eq. [6-19] is zero and the second term increases with the increase in σ_α. The difference between the correlated and uncorrelated cases is relatively small for application rate =2 cm day^{-1}. However, the difference can be as large as one half of the STD of W{L,t} for correlated flow for application rate=8 cm day^{-1} (Fig. 6-1b for C=1.2). The curves for dependence of σ_W on $\langle W \rangle$ for correlated and uncorrelated α-Y fields merges at the largest $\langle W \rangle$ value (Fig. 6-1b). This suggests the influence of correlation between α and Y disappears as $\langle W \rangle$ reaches its largest value (i.e., the flow reaches steady state)

The dependence of σ_W on $\langle W \rangle$ is influenced by the value of the C parameters. At C=1.05, which is typical for a sandy soil (White and Broadbridge, 1988), σ_W increases with $\langle W \rangle$ at smaller $\langle W \rangle$ and reaches its highest value at $\langle W \rangle$=6.8, and subsequently decreases with $\langle W \rangle$. However, at C=2.5, which may represent a loamy clay soil, σ_W increases with $\langle W \rangle$ monotonically. At the same $\langle W \rangle$, σ_W always increases with an increase in C.

The agreements between MC simulation and the analytical solution are excellent for different combinations of variances of α and Y for perfectly correlated α-Y fields (Fig. 6-2). This indicates that variances of Y and α do not have significant influence on the prediction of average storage within this range. This is consistent with Eq. [6-1a]. However, for σ_Y <0.5, σ_Y has no effect on the agreement between MC and the analytical solution for σ_W. For σ_Y >0.5, σ_Y has an effect on the agreement between MC and the analytical solution for σ_W. As expected, an increase in σ_α does not lead to overestimation of σ_W at large time, regardless of the magnitude of σ_α, because the derivative of W with respective to α is zero at large time. Therefore, as expected, α has no role in steady-state flow in a semi-infinite system. This is different from the results for a bounded system (Rubin and Or, 1993). Practically speaking, the agreement between the analytical prediction and MC simulated values for the mean and variance of W is very good, even though the predicted variance is more sensitive to σ_α^2 and σ_Y^2 than the predicted mean of water storage.

Figure. 6-3 and Fig. 6-4 show the effect of application rate on the predicted mean and variance of water storage for correlated and uncorrelated α-Y fields. As application rate increases, the analytical solution and MC simulated results for $\langle W \rangle$ are essentially identical to each other. This suggests the analytical solution is not sensitive to σ^2_R for both correlated and uncorrelated α-Y fields. For perfectly correlated α-Y fields, the variance of W increases smoothly with time for all rates. For the uncorrelated α-Y field, at low application rates(0.2 and 2 cm day^{-1}), σ_W increases smoothly with time. However, for high application rates (10 and 16 cm day^{-1}), σ_W increases abruptly at the beginning, reaches a highest point , and subsequently decreases to a constant value.

At large time, σ^2_W increases with an increase of application rate from R=0.2 to 0.2 cm day^{-1} and then decreases with the increase of application rate from R=2 to 10 to 16 cm day^{-1}. This behavior is for a specific class of soils, namely, coarse textured soils. To examine this in more detail, we study the large time behavior of water content. At large time, or steady-state,

$$q = \frac{K_s(C-1)\Theta^2}{C-\Theta} \qquad [6\text{-}36]$$

Taking the first order derivative Θ with respective to Ks, yields

$$\frac{\partial \Theta}{\partial K_s} = -\frac{(C-1)\Theta^2}{2K_s(C-1)\Theta + q} \qquad [6\text{-}37]$$

Substitution of Eq. [6-36] into Eq. [6-37], leads to

$$\frac{\partial \Theta}{\partial K_s} = -\frac{1}{K_s}\frac{\Theta(C-\Theta)}{2C-\Theta}$$

Taking the partial derivative with respect to Θ, we have

$$\frac{\partial}{\partial \Theta}\left(\frac{\partial \Theta}{\partial K_s}\right) = \frac{1}{K_s}\left[-\frac{C-2\Theta}{2C-\Theta} - \frac{\Theta(C-\Theta)}{(2C-\Theta)^2}\right] \qquad [6\text{-}38]$$

Assuming there is a maximum of Eq. [6-38] in the range $0< \Theta \leq 1$. Eq. [6-38] can be set to zero. The maximum of the absolute value of ∂Θ/∂Ks is then located at

$$\Theta = C(2-\sqrt{2}) \approx 0.6C \qquad [6\text{-}39]$$

Since C>1.0, then Θ>0.6. If Θ=1 (maximum possible), then C=1/0.6 = 1.67. Thus, for C> 1.67, or Θ<0.6, the variance of Θ would increase with application rate continuously, and the maximum is outside of the admissive Θ range.

Figure 6-5 shows the analytical solution and MC simulated semivariance $\gamma(h)$ of water storage at different times. The agreement is excellent. $\gamma(h)$ increases with the increase in separation distance (h) for h<15 m and then gradually reaches a constant, indicating the existence of a finite integral scale. The auto correlation function is shown in Fig. 6-6 for uncorrelated Y and α with I_Y=15 m and I_α =3 m. Clearly, the integral scales of water storage at different times are very similar with each other and with the integral scale of Y. This can be explained from Eq.[6-19] where the first term dominates the others. Similar results were obtained by Rubin and Or (1993) for steady-state water content at depth far from the water table. This is of practical significance, because I_Y can be determined directly from the integral scale of water storage to a fixed depth at any time. This will reduce the number of unknowns and greatly improve the uniqueness of the inverse problem in which the spatial structure of the Y field is determined from structure of measured water storage.

Effect of variation in flux on water storage.

Experimental evidence indicated that uniformly applied surface flux redistributes in the first few centimeters and then remains constant (Chapter 2). The significance of this variation in R in the evaluation of σ^2_W and $\langle W \rangle$ is examined next . We assume that R is normally distributed with a mean $\langle R \rangle$ and variance of σ^2_R, independent of Y and α. In this example, $\langle R \rangle$=2 cm day^{-1} and σ_R=0.1, 0.2, 0.4 and 0.8 cm day^{-1}, which represent a coefficient of variation (CV) of 5, 10, 20, and 40 %. The first order approximation to $\langle W \rangle$ is only a function of $\langle R \rangle$, irrelevant of σ^2_R (Eq. [6-32]) and σ_W increases as the variation in R increases (Eq. [6-33]). Figure 6-7 shows the theoretical and MC simulated $\langle W \rangle$ and σ^2_W.

The variation in R increases the steepness of the increase of σ^2_W during early time flow. For σ_W =2.0 cm day^{-1}. It needs 18, 12, 7, and 5 days for σ_R=0, 0.1, 0.2, 0.4 and 0.8 cm day^{-1} respectively. The effect of σ_R on σ_W is not obvious at σ_R =0.1 and 0.2 cm day^{-1}. However, as σ_R increases to 0.8 cm day^{-1}, the large time σ_W increased significantly from the value of σ^2_W at σ_R =0. Another interesting point at σ_R =0.8 is that σ^2_W increases with time initially, and then decreases with the increase of time to the asymptotic limit. This indicates that the variation in R enhances the spreading of wetting fronts in the field. When σ_W is small, the variation in Y dominates the variation in W. For the field in Borden (Chapter 1) where the CV of q is less than 20 %, the variation can be neglected, and consequently, the field can be treated as homogeneous in terms of surface flux.

Drainage

For drainage, as expected, $\langle W \rangle$ decreases with time and the rate of decrease is large at small time and slows down at large time (Fig. 6-8). σ^2_W increases sharply with time at the beginning of the drainage and reaches its largest value shortly thereafter. Subsequently, σ^2_W decreases with time. σ^2_W=0 at t=0 for a uniform initial condition. At large time, as soil water content becomes very low, and the variability of soil water content becomes smaller and so does the water storage variance.

The dependence of σ^2_W on $\langle W \rangle$ exhibits a bell-shape (Fig. 6-9). Different from that of infiltration, the positive correlation between α and Y fields increases σ^2_W, because the derivative of W with respective to α is positive for drainage (Eq. [6-19]).

Figure 6-10 shows the comparison of results of Eq. [6-19] with that of Monte Carlo simulation for different combinations of variances of Y and α. Similar to the result for infiltration, analytical drainage predictions for $\langle W \rangle$ are identical to that of Monte Carlo simulation. For σ_W, the agreement is good, indicating the solution is accurate. However, σ^2_W is more sensitive to σ^2_α than to σ^2_Y for large time and the opposite is true for small time (Fig. 6-10). This is because the flow is a gravity-dominated process (Y is more important) for small time and a diffusion-dominated process (α is more important) for large time.

Figure 6-11 shows the auto-correlation coefficient as a function of lag distance, $\rho(h)$ for different times for uncorrelated α-Y field. Initially, $\rho(h)$ is similar to that of Y. However, $\rho(h)$ deviates from that of Y with time towards that of α, further indicating the influence of α.

Summary and conclusions

In this, paper, we presented a unified stochastic analytical solution for soil water storage to a fixed depth for both infiltration and drainage. The solution is the small perturbation of those presented by Parkin et al. (1992) for homogeneous soils. Our analysis leads to the following major conclusions.

1. The expected value of soil water storage to a fixed depth for a constant flux boundary in a spatially variable field depends on the mean values of hydraulic parameters only. Therefore, $\langle W \rangle$ of a heterogeneous field is identical to that of a homogeneous soil column. This conclusion holds for constant flux infiltration and drainage.

2. The variance of soil water storage is time-dependent and depends on $\langle W \rangle$. The dependence of variance of soil water storage is influenced by the correlation between α and Y fields, the value of the C parameter, and the flow process (either constant flux infiltration or drainage).

3. The auto-correlation coefficient of soil water storage is positive and decays with the separation distance. The integral scale of soil water storage does not change with time and is identical to that of log hydraulic conductivity for infiltration. However, for drainage, the integral scale of W is time dependent.

4. The surface flux, being constant temporally and varying horizontally, has no significant influence on $\langle W \rangle$, but increases the spatial variability in soil water storage.

5. The first order solutions to the mean, variance and covariance for soil water storage, W(L,t) have excellent agreement with Monte Carlo simulations for moderate variance of log hydraulic conductivity for both infiltration and drainage.

The proposed solution can serve as a useful tool for validation of numerical codes simulating unsaturated transient infiltration in horizontally heterogeneous soils. The moments of water storage can also be used for deriving the moments of solute evolution during constant flux infiltration. The solution has applications for inverse procedures to estimate the spatial structures of hydraulic parameters from transient measured water storage to a fixed depth through vertically-installed TDR probes.

In the field, the initial conditions for different columns may be different and exhibit spatial variability. This variation may have an effect on the average and variance of soil water storage during drainage. We neglected this effect by assuming uniform initial conditions across the field. However, the effect can be examined using the small perturbation technique as we did for infiltration with spatially variable surface flux.

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Table 6-1. Statistical parameters, initial and boundary conditions for illustration.

	Constant					Variable	
	θ_r $cm^3\,cm^{-3}$	θ_s $cm^3\,cm^{-3}$	θ_0 $cm^3\,cm^{-3}$	R cm/d	C	α cm^{-1}	Y ln(cm/d)
Mean	0.06	0.42	0.06	2.0	1.2	0.03	3
Variance	0	0	0	0	0	2.5×10^{-5}	0.25
Integral scale (m)	∞	∞	∞	∞	∞	5.0	5.0

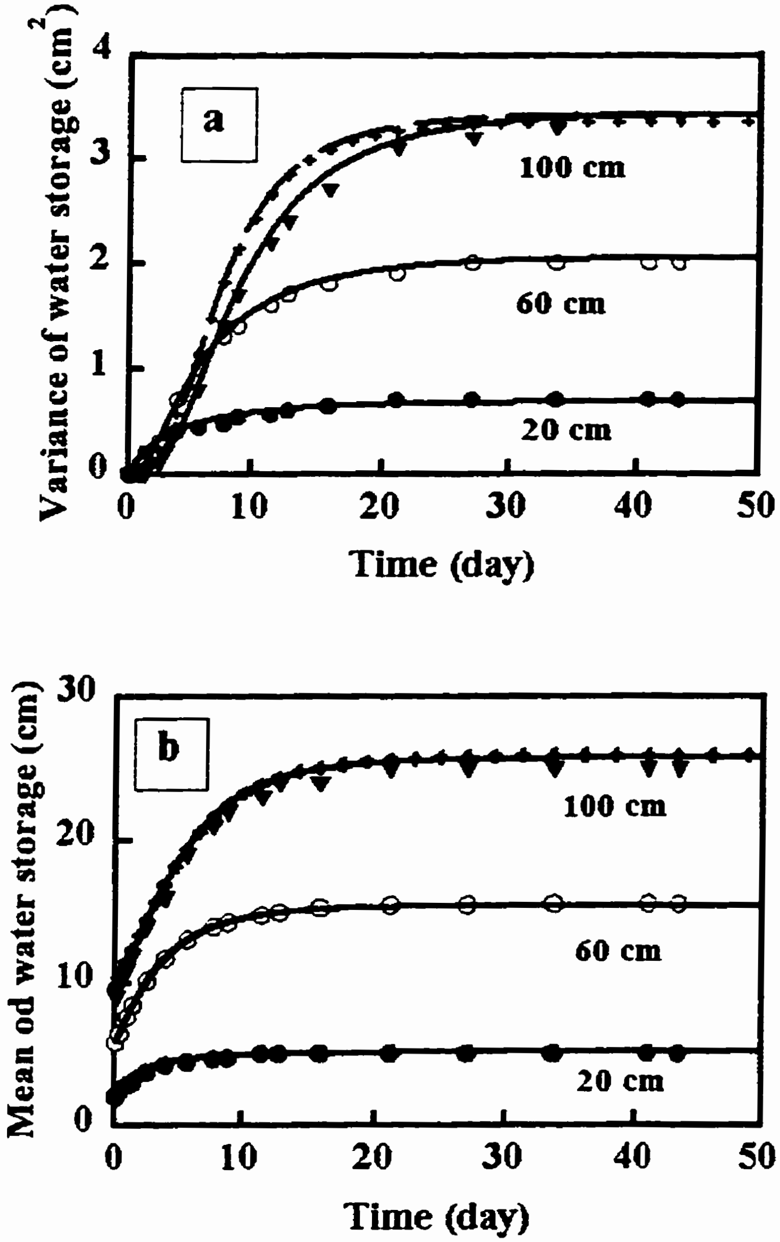


Fig. 6-1. Theoretical (solid) and MC-simulated (symbols) results of temporal change of (a)σ_W and (b) ⟨W⟩ to depth L=20, 60, and 100 cm for perfectly correlated α-Y fields during infiltration under constant flux boundary. The theoretical (dashed line) and MC-simulated (cross) results of temporal change of (a)σ_W and (b) ⟨W⟩ to depth L=100 for uncorrelated α-Y fields are also shown.

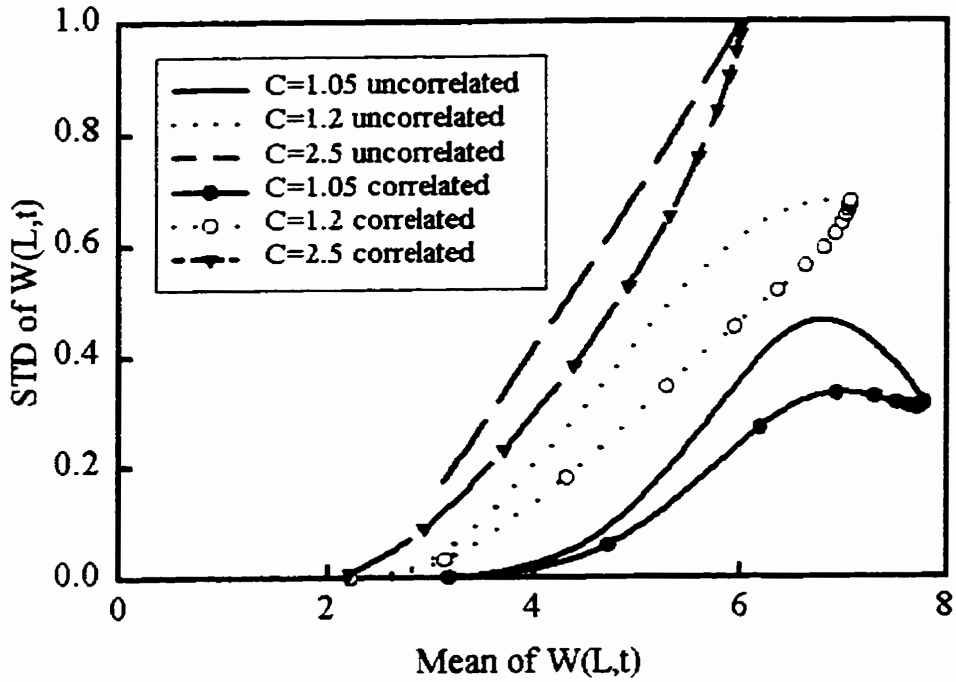


Fig. 6-1a. The dependence of variance on mean of soil water storage for perfectly correlated and uncorrelated α-Y fields for constant flux infiltration with application rate = 8 cm day^{-1} and different C values.

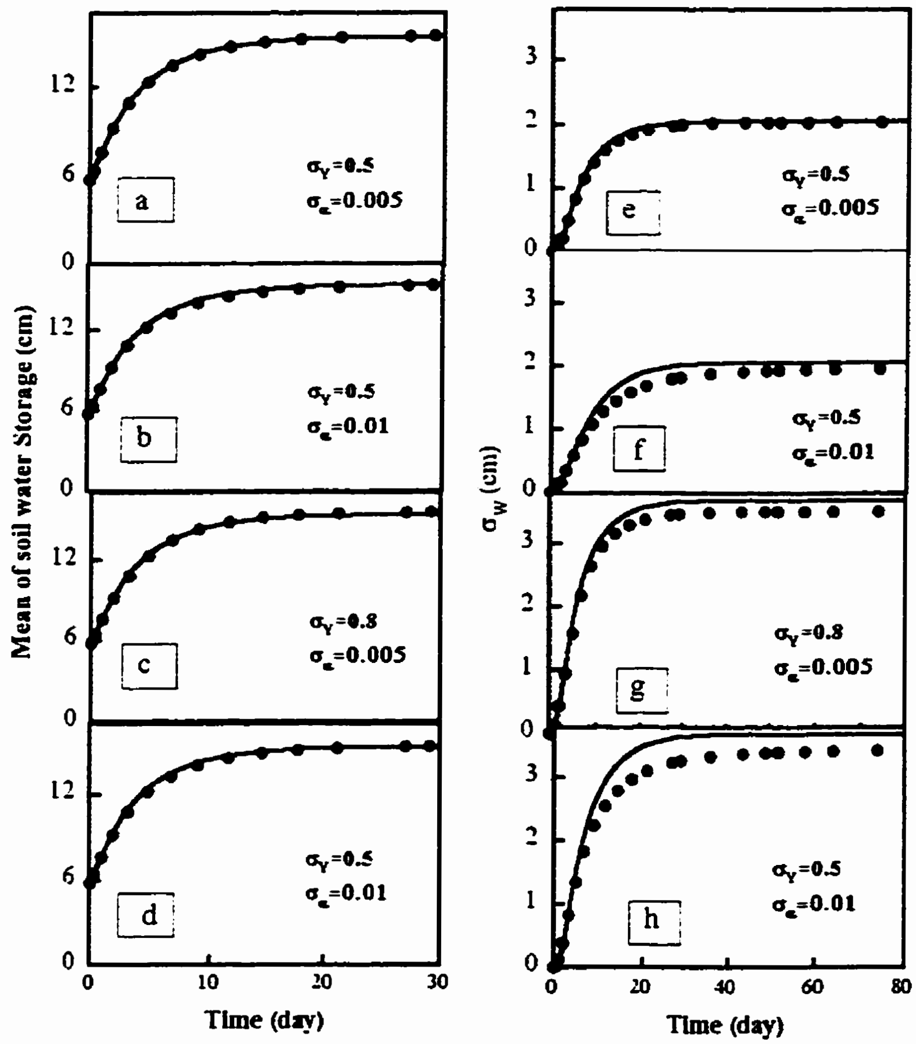


Fig. 6-2. Theoretical (Solid) and MC simulated (symbol) temporal change of ⟨W⟩ and σ_W to depth L=60 cm for infiltration under constant surface application rate R=0.2, 2, 10 and 16 cm day^{-1} for perfectly correlated α-Y fields with different variances of σ_Y and σ_α.

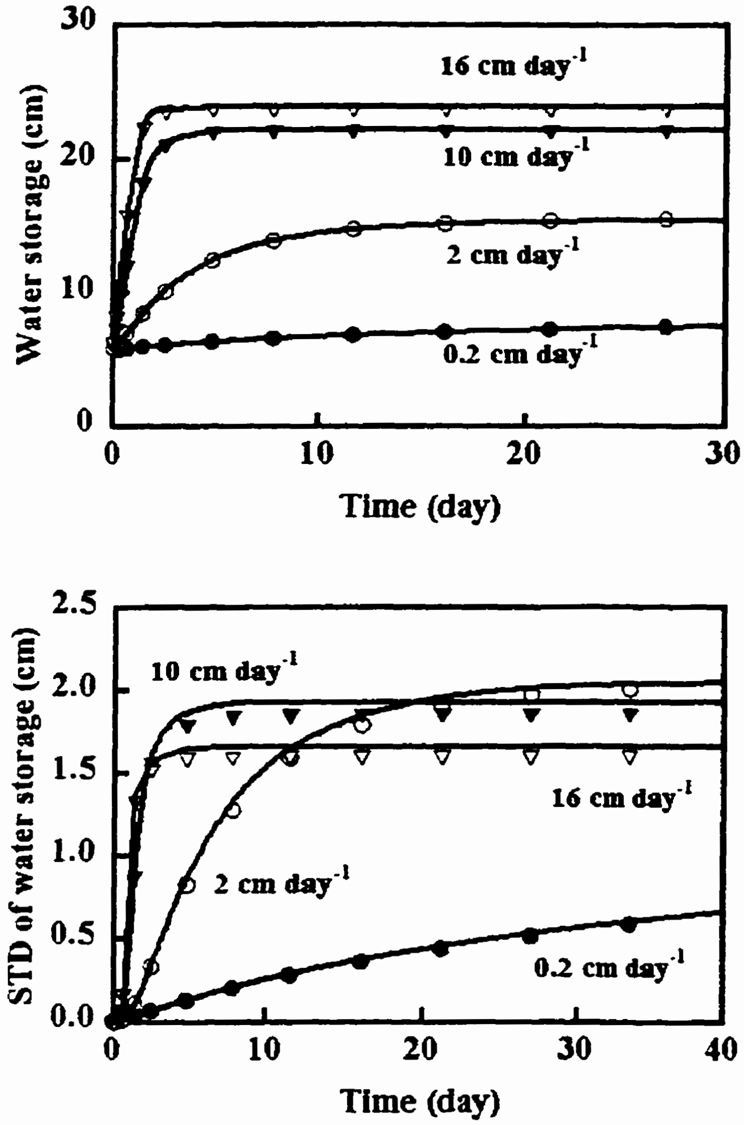
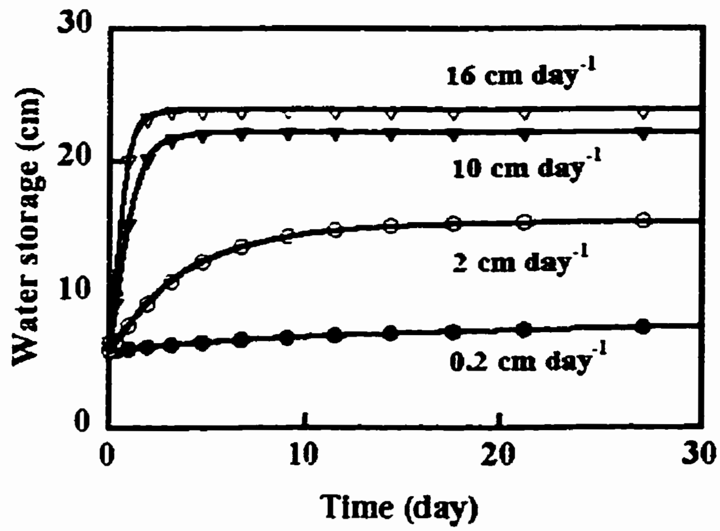


Fig. 6-3. Analytical (Solid) and MC simulated (symbol) temporal change of ⟨W⟩ and σ_W to depth L=60 cm for infiltration under constant surface application rate R=0.2, 2, 10 and 16 cm day^{-1} for perfectly correlated α-Y fields.



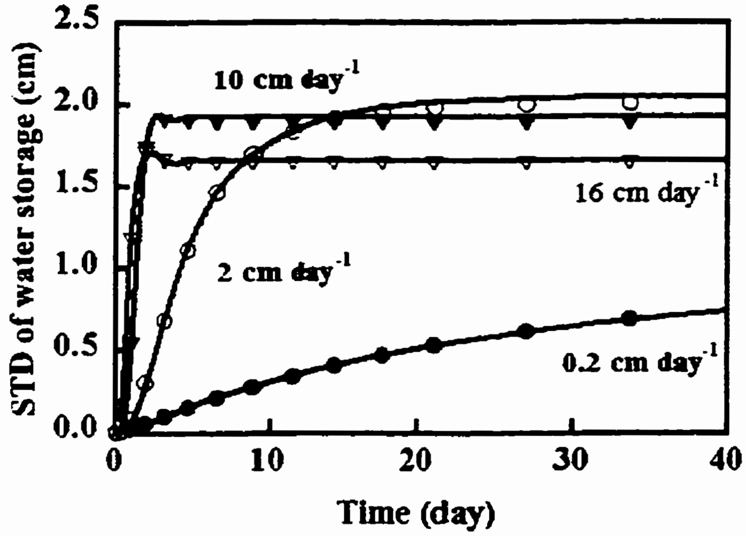


Fig. 6-4. Theoretical (Solid) and MC simulated (symbol) temporal change of $\langle W \rangle$ and σ_W to depth L=60 cm for infiltration under constant surface application rate R=0.2, 2, 10 and 16 cm day^{-1} for uncorrelated α-Y fields.

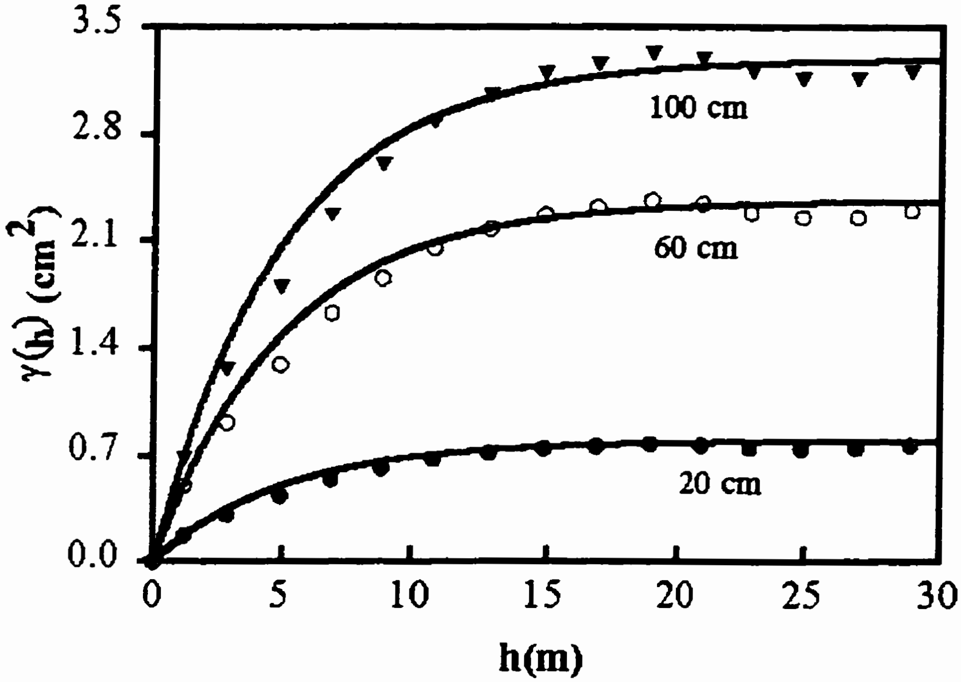


Fig. 6-5. Theoretical (Solid) and MC simulated (symbol) semivariance (γ) of water storage to depth L=20, 60, and 100 cm for infiltration under constant surface flux rate R= 2 cm day^{-1} for perfectly correlated α-Y fields.

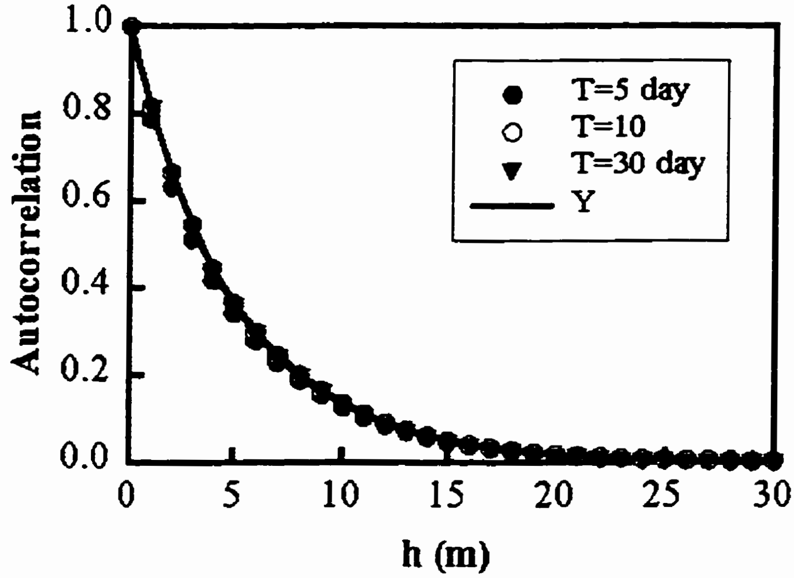


Fig. 6-6. Theoretical autocorrelation functions as a function of separation distance for soil water storage to depth L=60 cm at time T=5, 10 and 30 days of infiltration under constant surface flux R=2 cm day^{-1} for uncorrelated α-Y field. Solid line is the autocorrelation coefficient of Y. Integral scale of Y and α are 5 and 3 m respectively.

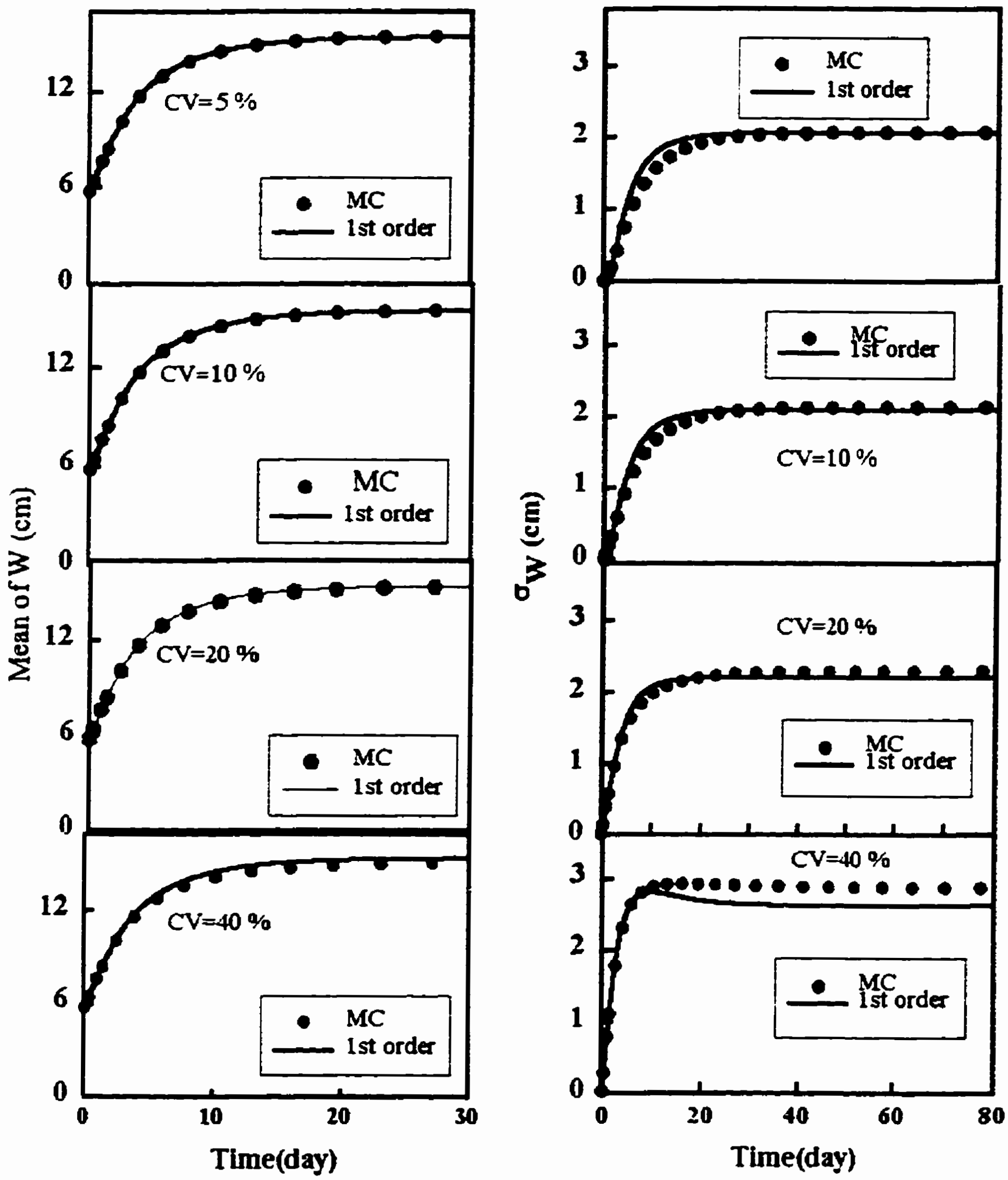


Fig.6-7. Theoretical (Solid) and MC simulated (symbol) temporal change of ⟨W⟩ and σ_W to depth L=60 cm for infiltration under spatially-random but temporally constant surface flux rate R= 2 cm day^{-1} with coefficient of variation (CV) =5, 10, 20 and 40 % for perfectly correlated α-Y fields.

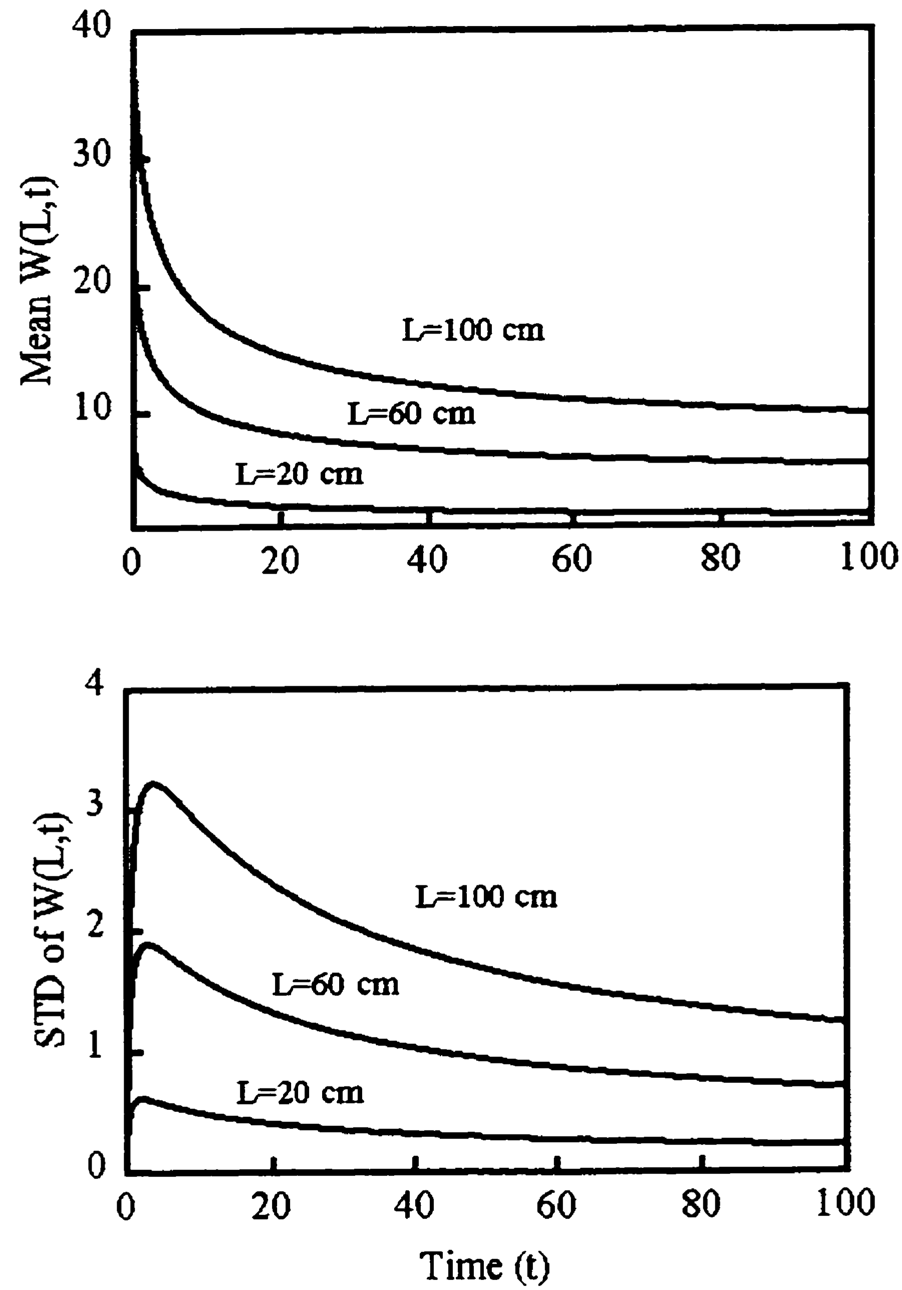


Fig. 6-8. Mean and variance of soil water storage to depth, W(L,t), for L=20, 60, and 100 cm for perfectly correlated α-Y fields during drainage.

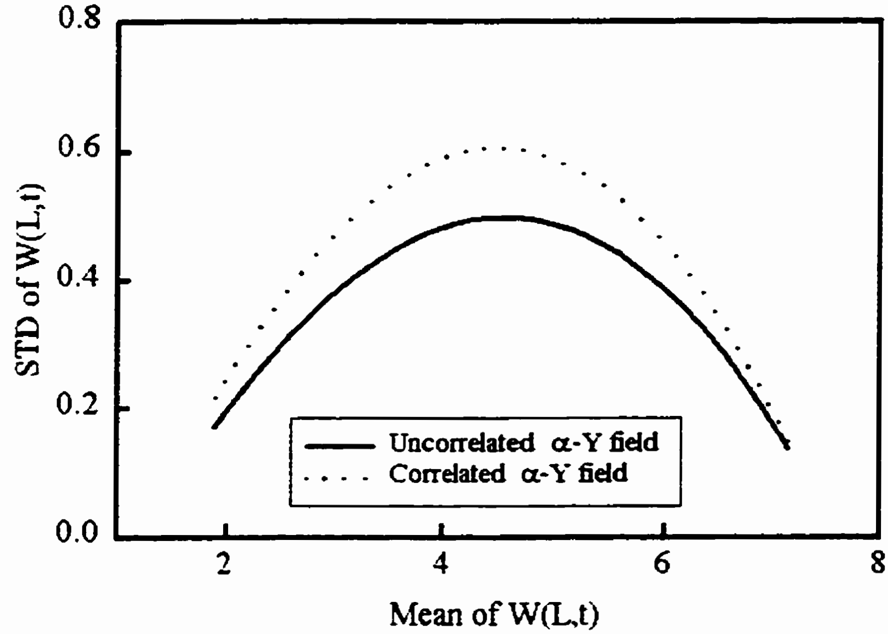


Fig. 6-9. The depdence of variance of soil water storage to depth L=20 cm, W(L,t), on the mean of W(L,t) for perfectly-correlated and uncorrelated α-Y fields during drainage (Θ_0 =0.9).

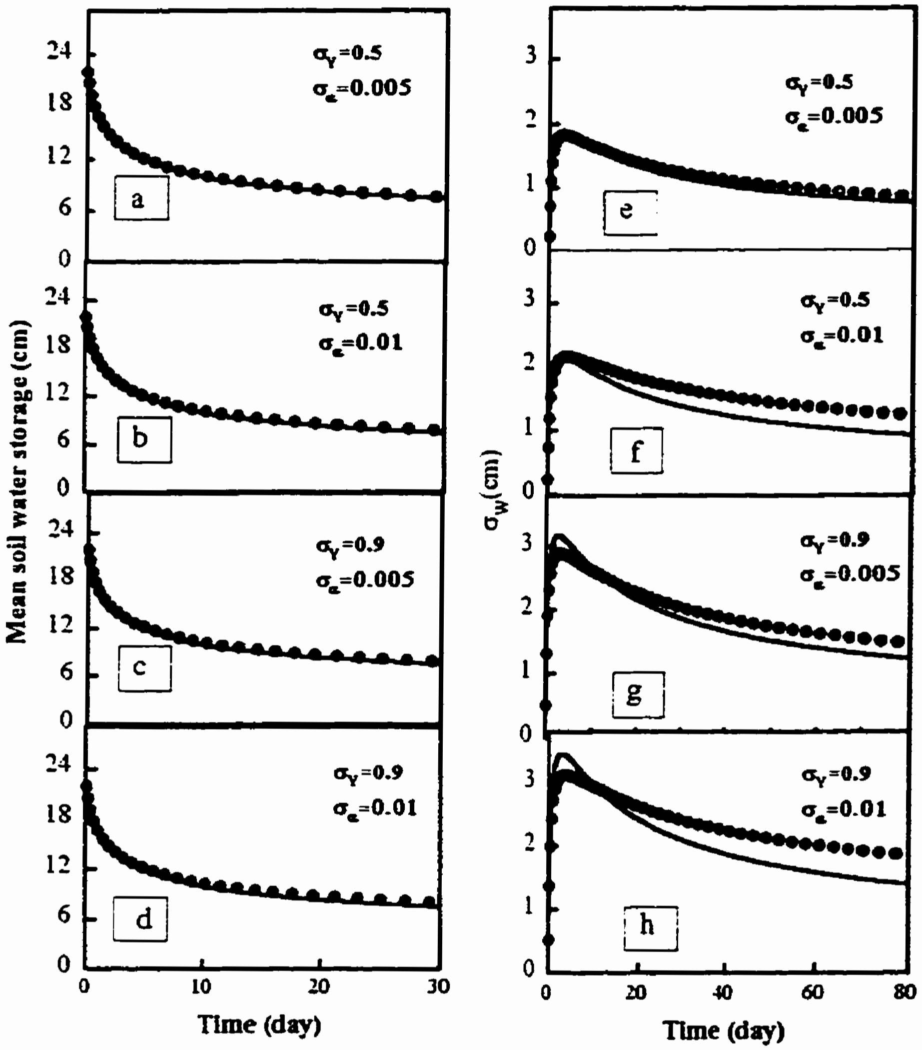


Fig. 6-10. Monte Carlo simulation and analytical result (Eq. [6-18] and Eq. [6-19]) for perfectly correlated α-Y fields during drainage (Θ_0 = 0.90).

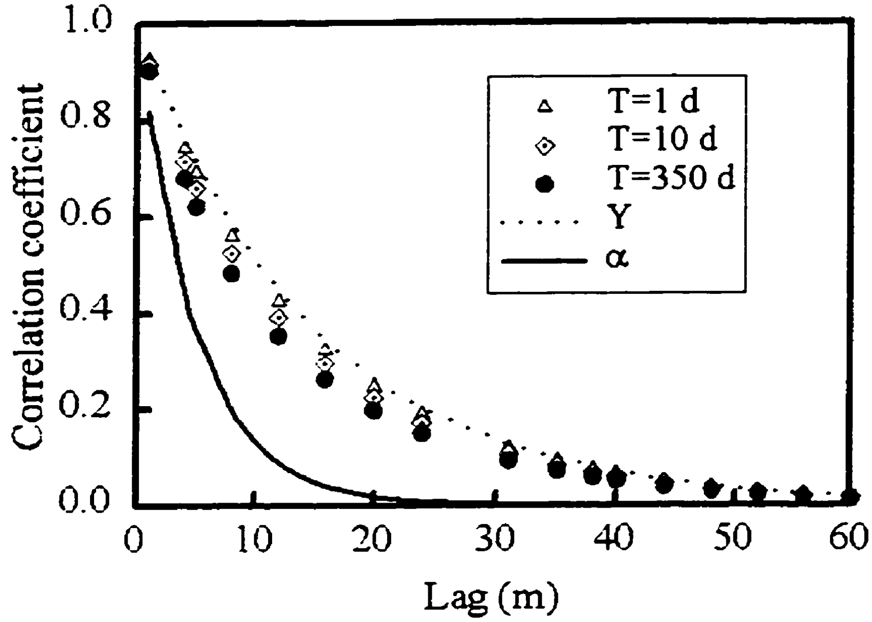


Fig.6-11. Dependence of auto-correlation of water storage to depth L=20 cm on time during drainage for uncorrelated α-Y fields (I_α =5 m and I_Y=15 m).

Chapter 7

Summary and conclusions

The major objective of this thesis was to further our understanding of the movement of water during infiltration and drainage through heterogeneous field soils. The focus was on effective one-dimensional water flow with a constant flux (infiltration) or no flow (drainage) surface boundary condition. The major contributions and conclusions of this thesis are:

1. An improved field method of measuring quickly and non-destructively the in situ average of hydraulic properties was presented. The method uses a series of multipurpose TDR probes that measure both θ and ψ at the same spatial location. The local water flux in each location was obtained through measured water storage during a series of constant flux infiltration studies. Assuming unit-gradient at steady state flow, the local hydraulic conductivity, ψ-θ relationships were obtained. In addition, our experiments showed that for different application rates, water flow was approximately vertical within the measurement volume of TDR. This provided experimental evidence of the stream tube model of Dagan and Bresler (1983).
2. A new analytical solution for transient water storage for a fixed depth under constant water flux was presented. The solution allows general soil hydraulic functions to be used and can be used directly to interpret the readings of vertically installed TDR probes. Therefore, the solution is directly applicable to the field method to measure

hydraulic properties.

3. Inverse procedures for identification of hydraulic parameters from measurement during transient infiltration were developed. The uniqueness and stability of the inverse problem from measured water storage to a fixed depth during constant flux infiltration and ψ measurements at initial and steady state were evaluated. The procedure was unique and stable and was applied to a field soil. The estimated parameters from the inverse problem were very similar to the parameters estimated from the in situ measured hydraulic properties.

4. The influence of hysteresis in hydraulic parameter identification was evaluated from transient infiltration and drainage measurements and predictions. A Hainess Jump model of hysteresis was presented. Combined with the prediction model of Parlange (1976) and Mualem (1984), the proposed model successfully predicted the soil water storage during drainage from parameters estimated from infiltration.

5. A unified stochastic analytical solution was developed for transient infiltration and drainage of water in heterogeneous soils. The influence of the average, variance, and integral length scale of Ks and α, on the average, variance, and integral scale of transient soil water content and storage are examined. The average soil water storage to a fixed depth, $\langle W \rangle$, in a heterogeneous soil is identical to that of a homogeneous soil with soil hydraulic properties equal to the means of the hydraulic properties in the heterogeneous soil. The variance of soil water storage to a fixed depth, however,

depends on $\langle W \rangle$ and variances of soil hydraulic properties. This dependence changes with time, water flux density, and cross-correlation of the soil hydraulic properties. The integral scale of W(L,t) is time-independent and can be approximated by the integral scale of log Ks during infiltration and is time-dependent and varying between the integral scale of Log Ks and the inverse capillary length scale α for drainage. For infiltration, the spatially variable, but temporally constant surface water flux as found in chapter1 has no significant influence on the mean or variance of water storage.

Future Research Needs

Measurement of soil hydraulic properties is fundamental to modeling hydraulic processes and evaluating models existing and under development. Numerous methods have been proposed to estimate the hydraulic properties of the unsaturated zone. Since soil hydraulic properties have strong spatial variability, information regarding the spatial statistics such as the mean, variance, covariance, and cross-covariance among soil hydraulic properties is critical for accessing numerical or analytical, deterministic or stochastic models. Future study should be conducted to use the inverse procedure presented in Chapter 3 to estimate those spatial statistics. Inversion of stochastic solutions to the flow problem like the one presented in Chapter 6 provides another alternative. Stochastic inversion may need fewer field measurements and lessnumerical computation. In addition, the calculation of the spatial statistics of hydraulic properties is straight forward. Future research should focus on evaluating the uniqueness and stability of the inversion of the stochastic solution and examining the correspondence with the methods provided in Chapter 2 and Chapter 3.

Chapter 2 indicated that one-dimensional flow was a good approximation to constant flux infiltration in field conditions. However, future work should examine the correspondence of hydraulic properties estimated using 1-dimensional methodology with those obtained from the 2-dimensional line source (at the same site).

With the spatial statistics known, effort should be made to understand the physical mechanism for the spatial redistribution of applied flux density during constant flux infiltration as shown in Chapter 2. The relation between the flux density at each individual column and the hydraulic properties may be established through correlation and spectral analysis.

Similar to water redistribution at the surface, resident solute mass also redistributes during water flow. Jury and Scotter (1994) postulated that there are two mechanisms; (1)The solute mass redistribution is proportional to the local flux, thus solute flux concentration is everywhere the same in the field.(2) The solute is uniformly redistributed on soil surface, such that each individual column receives the same amount of solute. Those assumptions, elegant and theoretically appealing, remain to be tested. With the method of measuring soil water flux density in Chapter 2 and the method of measuring solute flux (Kachanoski et al., 1992), along with the data base for soil water flux during infiltration and solute flux (not shown in this thesis), the relations between the solute mass redistribution and soil water flux density should be examined through cross-covariance among soil water flux density and solute flux density in each individual column.

APPENDIX I

Format of file containing measured soil water storage to depth 20 cm from the surface measured by vertically-installed TDR probe with length =20 cm during constant flux infiltration (R=0.9cm/hr).

time (min)	Location No. 1	2	3	4	5	6	7	8	9
0	1.80	1.96	1.39	1.44	1.08	0.96	1.13	1.57	1.39
27	2.02	2.42	2.05	1.99	1.93	1.79	1.54	2.12	1.82
81	2.37	3.01	2.27	2.45	2.15	2.13	1.87	2.58	2.27
141	2.60	3.75	2.98	3.17	2.74	2.95	2.44	3.18	2.98
209	2.96	4.12	3.72	3.66	3.34	3.56	3.04	3.92	3.59
266	3.57	4.62	4.09	3.66	3.84	4.06	4.02	4.42	4.33
316	4.19	5.12	4.59	4.03	4.71	4.68	4.64	5.16	4.95
376	4.56	5.73	5.08	4.65	5.45	5.42	5.39	5.89	5.45
434	4.69	5.85	5.33	4.90	5.81	5.79	5.75	6.25	5.81
496	4.69	5.97	5.33	5.02	5.69	6.03	5.87	6.25	5.93
612	4.81	6.20	5.45	5.39	5.93	6.14	5.99	6.48	6.05
667	4.69	5.97	5.57	5.27	5.81	6.14	5.99	6.37	6.05
731	4.81	6.20	5.57	5.39	5.93	6.14	6.11	6.48	6.17
801	4.94	6.32	5.70	5.27	6.05	6.26	6.23	6.37	6.05
871	4.94	6.20	5.57	5.39	6.17	6.26	6.23	6.60	6.05
1006	4.94	6.32	5.45	5.27	5.93	6.14	6.11	6.48	6.05
1166	4.69	6.08	5.33	5.15	5.81	6.26	6.11	6.48	6.29
1281	4.81	6.32	5.45	5.27	6.05	6.26	6.11	6.37	6.29
1366	4.81	6.32	5.57	5.27	6.05	6.14	6.11	6.37	6.05

APPENDIX II

Format of file containing measured soil water pressure head at depth 20 cm from the surface measured by vertically-installed multipurpose TDR probe with length =20 cm at steady-state infiltration (R=0.9 cm/hr)

	depth(cm)				
location		20	40	60	80
1	26.5	26.8	21.6	5.5	
2	37.5	11.5	25.5	22.5	
3	27.5	28.5	22.5	32.5	
4	31.5	6.5	19.5	17.5	
5	32.5	28.5	21.5	22.5	
6	41.5	27.5	17.5	14.5	
7	23.5	27.5	19.5	22.5	
8	35.5	29.5	24.5	20.5	
9	17.5	26.8	21.6	16.5	
10	35.5	31.5	12.5	12.5	
11	33.5	27.5	32.5	26.5	
12	34.5	28.5	14.5	28.5	
13	4.5	21.5	27.5	35.5	
14	31.5	27.5	24.5	23.5	
15	33.5	30.5	20.5	20.5	
16	27.5	32.5	24.5	29.5	
17	33.5	22.5	24.5	24.5	
18	34.5	30.5	25.5	12.5	
19	33.5	33.5	23.5	15.5	
20	38.5	34.5	22.5	33.5	
21	30.5	29.5	20.5	9.5	
22	32.5	27.5	29.5	22.6	
23	8.5	30.5	33.5	19.5	
24	34.5	19.5	28.5	40.5	
25	32.5	38.5	29.5	37.5	
26	23.5	26.8	21.6	22.6	
27	39.5	26.8	16.5	17.5	
28	13.5	29.5	11.5	32.5	
29	20.5	26.8	21.5	15.5	
30	33.5	17.5	18.5	22.6	
31	25.5	21.5	20.5	22.6	
32	35.5	10.5	7.5	14.5	
33	34.5	29.5	25.5	11.5	
34	26.5	28.5	21.6	22.6	
35	31.5	30.5	13.5	22.6	
36	25.5	22.5	36.5	26.5	
37	21.5	12.5	29.5	23.5	

APPENDIX III

Format of file containing measured soil water storage to depth 20 cm from the surface measured by vertically-installed TDR probe with length =20 cm during gravity drainage

	location								
time (hr)	1	2	3	4	5	6	7	8	9
0.00	7.96	7.96	7.96	7.96	7.96	7.96	7.96	7.96	7.96
0.02	7.65	7.65	7.65	7.65	7.65	7.65	7.65	7.65	7.65
0.40	7.12	7.12	7.12	7.12	7.12	7.12	7.12	7.12	7.12
0.83	6.79	6.79	6.79	6.79	6.79	6.79	6.79	6.79	6.79
1.32	6.67	6.67	6.67	6.67	6.67	6.67	6.67	6.67	6.67
1.90	6.33	6.33	6.33	6.33	6.33	6.33	6.33	6.33	6.33
2.02	6.09	6.09	6.09	6.09	6.09	6.09	6.09	6.09	6.09
4.70	5.24	5.24	5.24	5.24	5.24	5.24	5.24	5.24	5.24
9.92	4.87	4.87	4.87	4.87	4.87	4.87	4.87	4.87	4.87
22.37	4.25	4.25	4.25	4.25	4.25	4.25	4.25	4.25	4.25
47.20	3.88	3.88	3.88	3.88	3.88	3.88	3.88	3.88	3.88
94.87	3.63	3.63	3.63	3.63	3.63	3.63	3.63	3.63	3.63
190.95	3.51	3.51	3.51	3.51	3.51	3.51	3.51	3.51	3.51
270.62	3.39	3.39	3.39	3.39	3.39	3.39	3.39	3.39	3.39
505.10	3.63	3.63	3.63	3.63	3.63	3.63	3.63	3.63	3.63
1177.37	3.51	3.51	3.51	3.51	3.51	3.51	3.51	3.51	3.51

APPENDIX IV

A SAS program for fitting Broadbridge & White form of hydraulic functions to measured K(θ) and ψ(θ) data.

```
DATA FILE1;
  INFILE 'K_H_S.txt';
   INPUT ID $  theta  HK ;

PROC NLIN METHOD=DUD SMETHOD= CUBIC  converge=1E-10 MAXITER=300;
   PARMS C=1.1 alpha=0.1  Ks=9.0 thetas=0.42; thetar=0.05;
   psi0=0.0;
S=(theta-thetar)/(thetas-thetar);
if S<=0 then S=0.001;
IF S>=1 then S=1;
weight=17.2;
IF ID='h' THEN DO;
MODEL HK=1/alpha*(1-S)/S+1/C/alpha*log((C-S)/((C-1)*S))+psi0/alpha;
END;
ELSE IF ID='k' THEN DO;
HK=HK*weight;
MODEL HK=Ks*S*S*(C-1)/(C-S)*weight;
END;

BOUNDS 1.01 < C <20.1;
BOUNDS 0.01<alpha<0.6;
BOUNDS 3<Ks<150;
BOUNDS 0.26<thetas<=0.95;
OUTPUT out=est parms=C alpha Ks thetar thetas SSE=s P=predict;
```

APPENDIX V

A SAS program for fitting van Genuchten form of hydraulic functions to measured K(θ) and ψ(θ) data.

```
DATA FILE1;
  INFILE 'K_H_S.txt';
  INPUT ID $  theta HK;
PROC sort;  BY ID theta;

 PROC NLIN METHOD=DUD best=10 G4 maxiter=300   converge=1E-15;
   PARMS n=2.2 alpha=0.1 Ks=7.24 thetas=0.42 m=0.2; l=2;thetar=0.05;
 weight=17.2;
 S=(theta-thetar)/(thetas-thetar);
 IF S<=0 THEN S=0.001;
 IF S>=1 then S=0.999;
 IF ID='h' THEN DO;
   MODEL HK=(S**(-1/m)-1)**(1/n)/alpha;
 /**  DER.alpha=-(S**(-1/m)-1)**(1/n)/alpha/alpha;
   DER.n=-(S**(-1/m)-1)**(1/n)/alpha/n/n*(log(S**(-1/m)-1)-
          log(S)/n/m/m*S**(-1/m)/(S**(-1/m)-1));**/
  END;
 ELSE IF ID='k' THEN DO;
  HK=HK*weight;
  Y=1-S**(1/m);
  MODEL HK=weight*Ks*S**l*(1-Y**m);
  /**DER.Ks=S**l*(1-Y**m)**2*weight;
  DER.n=-2/n/n*Ks*S**l*(1-Y**m)*Y**m*(log(Y)+(1-Y)/m/Y*log(S))*weight;
  DER.l=Ks*S**l*(1-Y**m)**2*log(S)*weight;**/
END;
 BOUNDS 1.01<n<100;
 BOUNDS 0.00000001<alpha<1;
 BOUNDS 0.01<Ks<200;
 BOUNDS 0.25<thetas<0.6;
 OUTPUT out=est parms=n alpha Ks thetar thetas SSE=s P=predict;

 DATA _NULL_;
 FILE FN1;
 FILENAME FN1 'parms_BW.dat';

 PUT  n .2 alpha .3 Ks .2 thetar 0.2 thetas 0.2 s;
```

APPENDIX VI

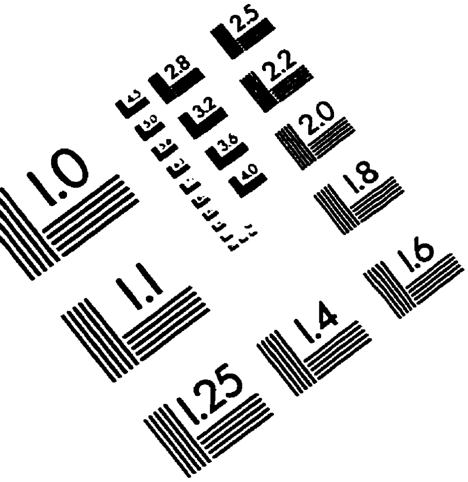
A SAS program for estimating hydraulic parameters of Broadbridge & White form of hydraulic functions from measured water storage data during constant flux infiltration or drainage.

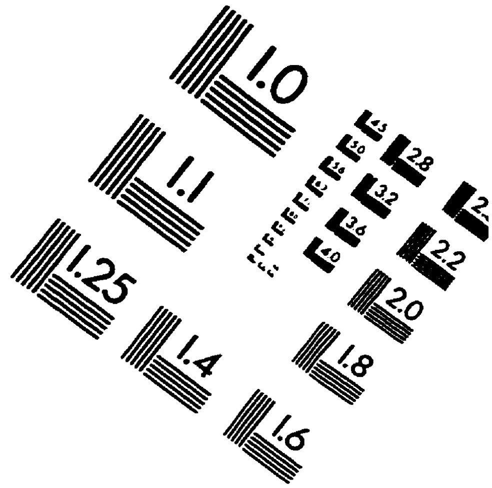
```
DATA FILE1;
 INFILE 'infil2.txt';
   INPUT ID $ T W ;
  if ID="w" then do; W=W*20;
   T=T/60;end;
 PROC NLIN METHOD=DUD SMETHOD= CUBIC maxiter=200 converge=1E-10;
   PARMS alpha=0.09 Ks=5 C=1.5 thets=0.41 ;
   weight=1;
   L=20 ;
   Q=1.59;
   thete=0.12;
   thetr=0.05;
   theta=(thete-thetr)/(thets-thetr);
   Rstar=Q/Ks;
   Tstar=T*alpha*Ks/(thets-thetr);
   mc=4*C*(C-1); rho=Rstar/mc; tau=mc*Tstar;
   lambda=rho*(rho+1);
   IF ID='w' then do;
   zeta=1; Z1=1; Zder=1; Tol=1e-5;/** convergence criterion for Root **/

/* Calculate Matric Flux Potential for BW Variable V=0 */
  U0=exp(lambda*tau);

/*----
  The following program used The Newton-Raphason Method to Find the
   parameter V which appears on the original Broadbridge & White Solution,
---*/

  DO WHILE (ABS(Z1) gt 0.000001) ;
   /*Criterion for Convergence of Newton Method*/
/*--The folowing variables are the intermediate variables for the matric flux
    potential U **/
   A0=1+2*rho-C/(C-theta);
```

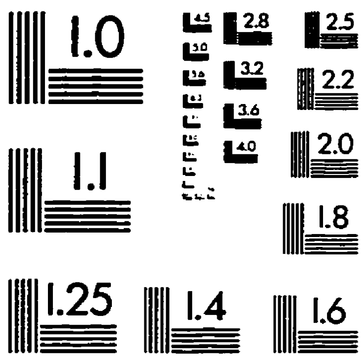
```
    A1=zeta/sqrt(tau)-sqrt(lambda*tau);
    A2=zeta/sqrt(tau)+sqrt(lambda*tau);
    B1=-0.5*A0*sqrt(tau)-zeta/sqrt(tau);
    B2=-0.5*A0*sqrt(tau)+zeta/sqrt(tau);
   IF A1<3.5 then DO; FA1=exp(A1*A1)*ERFC(A1); END;
   ELSE DO; FA1=(1-1/2/A1/A1+3/4/A1/A1/A1/A1
  - 5/8/A1**6+7/16/A1**8)/A1/sqrt(3.14);
   END;
   IF A2<3.5 then DO; FA2=exp(A2*A2)*ERFC(A2);END;
   ELSE DO; FA2=(1-1/(2*A2*A2)+3/4/A2/A2/A2/A2
   - 5/8/A2**6+7/16/A2**8)/A2/sqrt(3.14);
   END;
   IF B1<3.5 then DO; FB1=exp(B1*B1)*ERFC(B1);END;
   ELSE DO; FB1=(1-1/(2*B1*B1)+3/4/B1/B1/B1/B1
   -5/8/B1**6+7/16/B1**8)/B1/sqrt(3.14);
    END;
    IF B2<3.5 then DO; FB2=exp(B2*B2)*ERFC(B2);END;
   ELSE DO; FB2=(1-1/(2*B2*B2)+3/4/B2/B2/B2/B2
   -5/8/B2**6+7/16/B2**8)/B2/sqrt(3.14);
    END;
    U=0.5*exp(-zeta*zeta/tau)*(FA1+FA2+FB1-FB2);

    DU=exp(-zeta*zeta/tau)*(sqrt(lambda)*FA2+0.5*A0*FB2-sqrt(lambda)*FA1+
             +0.5*A0*FB1);
 /*-- Calculate the dimensionless Depth Z1 and its Derivative for NR--*/

    Z1=1/C*(lambda*tau+(2*rho+1)*zeta-LOG(U))-L*alpha;
    Zder=1/C*(2*rho+1-1/U*DU);
    Ratio=Z1/Zder;
    zeta=zeta-Ratio;
   END;
 MODEL W=1/alpha*(thets-thetr)*(2*rho*zeta+LOG(U0/U))+thetr*L;
_WEIGHT_=weight;
END;
ELSE IF ID='h' THEN DO;
S=(T-thetr)/(thets-thetr);
MODEL W=1/alpha*(1-S)/S+1/alpha/C*LOG((C-S)/S/(C-1));
_WEIGHT_=weight/5;
END;
ELSE IF ID='k' THEN DO;
 MODEL W=Ks*(C-1)*((T-thetr)/(thets-thetr))**2/(C-(T-thetr)/(thets-thetr));
_WEIGHT_=weight;
END;
```

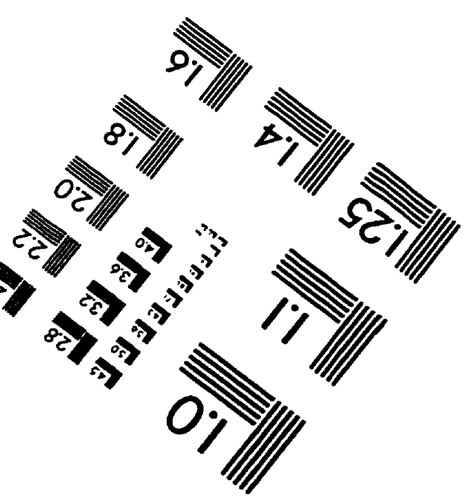
```
ELSE IF ID='p' THEN DO;
 MODEL W=thets*L/9;
 END;
BOUNDS 1.01 < C <60.1;
 BOUNDS 2.590 <Ks<15;
 BOUNDS 0.01<alpha<0.9;
 OUTPUT out=est parms=C alpha  yy  SSE=s P=predict;
```

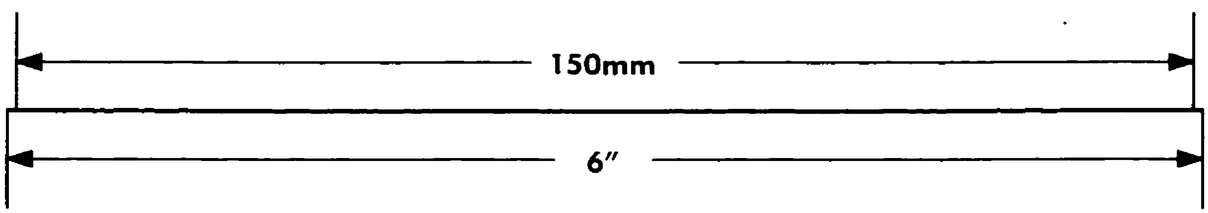
IMAGE EVALUATION TEST TARGET (QA-3)

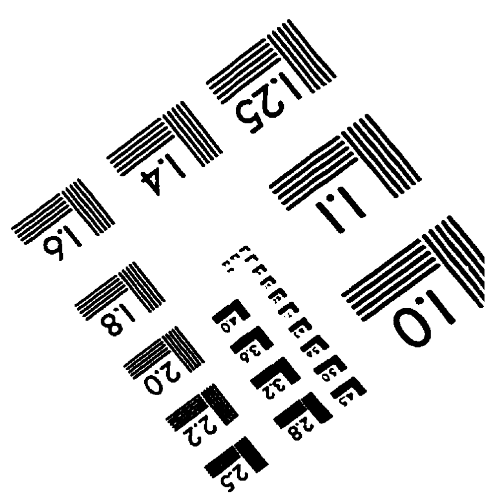












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