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Journal of Hydrology 184 (1996) 35–55

Journal of Hydrology

Surface soil water content regimes: opportunities in soil science

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Received 7 June 1995; accepted 29 October 1995

Abstract

With the qualities and properties of soil not being uniformly distributed across continents, soils are classified according to their morphological features, genesis and soil-forming processes. Because properties of soils vary across the landscape, a relationship observed at one location may not be applicable for other locations. Hence, measured data and deduced relationships are location specific and should be interpreted with information regarding the particular soil type according to the discipline of soil science. To better understand the role of water in land–atmosphere interactions and the role of land–atmosphere interactions in regional and global climate, spatial and temporal observations of water in the soil surface can be more comprehensively analyzed with a knowledge of soil science. On the other hand, an opportunity to strengthen the discipline of soil science (with its various branches of soil physics, soil chemistry, soil microbiology, etc.) exists if spatial and temporal observations of water in the soil surface at different scales are considered. Anticipating that such observations of soil water will eventually become more abundantly available through satellite imagery, we discuss how they can be used to improve our understanding and application of soil science.

1. Prologue of soil science

Soil develops under mutually interacting climatic, biotic, topographic, geologic and temporal influences. Pedology, the conceptual framework upon which soil science is based, integrates and quantifies the formation, morphology and classification of soils. Pedologists study soil development and identify distribution patterns of soils and soil properties across the landscape. The movement of soil water during infiltration,

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SSDI 0022-1694(95)02967-2

redistribution, drainage, evaporation and transpiration has a profound influence on soil development and is often the mechanism that controls the rate of many reactions occurring within soil profiles. Soil water plays a dominant role in the transport of solutes over both short and long distances. Suspended soil particles, primarily of clay size, transported over short distances by water contribute to the formation of illuvial horizons. Microbial and biological processes are closely coupled with water transport. Hence, a huge number of chemical and physical phenomena seldom if ever in equilibrium with each other exist within soil profiles driven by ever-changing meteorological conditions.

Owing to the action of climate and soil organisms, horizons within a soil profile are formed according to topography and soil parent material. Horizons are relatively thin layers having a thickness of the order of 10 cm and are typically characterized by their macro- and micromorphological features. Each horizon manifests its own processes of transformation and accumulation of substances. Thus, along the vertical dimension of a soil we find a regular arrangement of heterogeneity. As a result of this arrangement, soil hydraulic theories applied to field situations must account for the fact that soil profiles are indeed layered.

According to pedologists, the basic element of a soil is the pedon, a three-dimensional body having a geographical surface area of 1–10 m^2. Its morphology is usually described on a two-dimensional, vertical cross-section of a soil profile, i.e. on the wall of an excavated pit. The pedon scale as well as the laboratory scale are macroscopic in size and are commonly denoted as the Darcian scale. Most formulations of the retention and flux of water, heat and solutes at the soil surface are Darcian. Kutílek and Nielsen (1994) preferred to differentiate between laboratory and pedon Darcian scales. The laboratory Darcian scale is related to artificially prepared samples of ground, sieved soil material packed into laboratory columns, or small soil core samples (usually of a size smaller than that of the representative elementary volume of the field from which they were taken) studied in the laboratory. These two subclasses of the laboratory Darcian scale may differ substantially. In the case of the ground, sieved material, a well-defined distribution of soil pores exists that can be described immediately with a probability distribution function. In the case of soil cores samples, the hydraulic function of macropores is usually deformed, with the continuity of interaggregate micropores and macropores being disrupted. Consequently, the saturated hydraulic conductivity and the unsaturated hydraulic conductivity function for each of the two subclasses differ significantly.

Positions of individual pedons across the landscape are usually identified on maps of scale 1:2000 or 1:5000. With the pedon classified according to the lowest level of the taxonomic system, we obtain the abstract form—a pedotop, which is the lowest taxonomic unit of the soil mantle. On geographically large-scale maps, we approximate the boundary of the domain of each pedotop either by simple interpolation or with the help of geostatistics. If the soil body consists of more than one contiguous pedon, it is termed a polypedon. The domain of one pedotop may contain inclusions of polypedons. In such cases a pedotop is polymorphic. A monomorphic pedotop has no inclusions of neighboring pedotops and polypedons.

When the area of a mapped region is orders of magnitude greater than that of an average district of one pedotop (i.e. if the scale of the map is decreased by orders of magnitude compared with that of pedotop maps), the soil cannot be depicted in all details of all districts of pedotops. The lowest taxonomic units, the pedotops, are then clustered either according to the hierarchical structure of the classification system into higher taxonomic units or are grouped with regard to a close similarity of specified properties. Thus, we obtain higher mapping units denoted sometimes as pedochors and pedocomplexes. In a given higher mapping unit, the occurrence of polypedons frequently depends upon topography, e.g. hydromorphic soils occur in depressions of alluvia whereas around the depressions, at slightly higher elevations of the alluvium, semihydromorphic soils occur, and on the next higher terrace, lithogenic soils can occur without features of hydromorphism. These gradual transitions within higher mapping units are called catena. The term catena suggests that soils across the landscape are related as links in a chain, and with pedogenic processes being in concert with hydrologic processes, it is expected that soil water behavior at any one location has spatial and temporal covariance structures with a multitude of landscape attributes.

For studies of soil hydrology, the largest scales of pedotops are most appropriate. The random variation of soil hydrologic properties in each pedotop should be statistically well defined within this scale. Within smaller scales of higher mapping units, the variation of soil hydrologic properties consists of two components. One component is the random variation of soil physical characteristics within each of the pedotops composing a unit of higher mapping unit scale. The second is the variation having a deterministic character owing to the heterogeneity of the landscape, parent rock or microclimate, which may predestine a specific soil evolution towards a specific pedotop. The origin of a pedotop is therefore determined by known factors and the heterogeneity caused by this type of variation of pedotops is predictable. Among soil physicists, there is a tendency to estimate the soil hydraulic functions by regression analysis on the higher mapping unit scale. Soil hydraulic functions are correlated to simply obtainable data (e.g. textural components, bulk density, organic matter content and measures of soil structure). However, a detailed preliminary study of the mutual relationships in the given region is indispensable and the knowledge gained is not simply transferable to other higher mapping units. Efforts to apply a general relationship (pedotransfer function) of small scale to soil hydrological studies into various pedoregions have been futile.

As a first approximation, we model the soil as a simple, homogeneous porous body, temporarily forgetting the existence of horizons within its profile and the horizontal variation of its properties. In some instances, a soil profile consisting of two horizons is modeled simply by considering a layer of a homogeneous soil overlain by a second having different hydraulic properties. For studying the behavior of soil water including flow and transport of matter, we use phenomenological (or macroscopic) descriptions. We describe what we can 'see' with our apparatuses and we denote the scale where the phenomenological approach is applied as Darcian. A physical interpretation of some phenomena requires a detailed discussion at atomic, microscopic, human or global scale.

Elementary hydrologic processes for simply modeled soils and for trivial boundary conditions are described by analytical solutions of basic macroscopic equations. Parallel to such mathematical analyses are carefully conducted experiments performed on repacked soil columns or on model porous materials under precise conditions in the laboratory.

The next level of approximation is the quantification of processes for real soils, i.e. field soils. Although the scale remains Darcian, we speak of it as the pedon scale. The main differences in hydraulic characteristics of the laboratory and pedon Darcian scales are related to differences within the porous systems of both, as mentioned above. In addition to them, at the pedon-scale level, the boundary conditions are usually less trivial than those used in the first level, and if they are sufficiently complex, numerical methods are applied to achieve particular solutions. These results, similar to an accurately performed field experiment, are regularly verified by field experimentation. The advantage of numerical simulation is the rapid production of a large number of 'computer experiments' which partially substitute for tedious, time-consuming field experiments. Alternatively, numerical procedures allow us to study specific features of a process which are not accessible or readily observed by existing experimental techniques.

From these pedon studies (often called 'point-scale' studies) we try to extend the results to the larger scale of a field or catchment. This scale, larger than Darcian, is usually denoted as catchment scale. Considering the principles of soil mapping, it is advisable to differentiate between two new categories within the catchment scale: (1) the pedotop scale; (2) the higher mapping unit scale. Both categories belong to observations in soil hydrology but they differ in the structure of the soil mantle and therefore in the nature of the variability of soil physical properties. Within the pedotop scale, variability is strictly stochastic. Within the higher mapping unit scale, it is both stochastic and deterministic. We illustrate this behavior of spatial variability in Fig. 1, which depicts seven pedotops located deterministically within a higher mapping unit across the landscape of a farm.

Mapping of the pedotops was based on data from 293 bore holes taken at approximately 60 m intervals across the entire 100 ha farm. Measured values of surface water infiltration

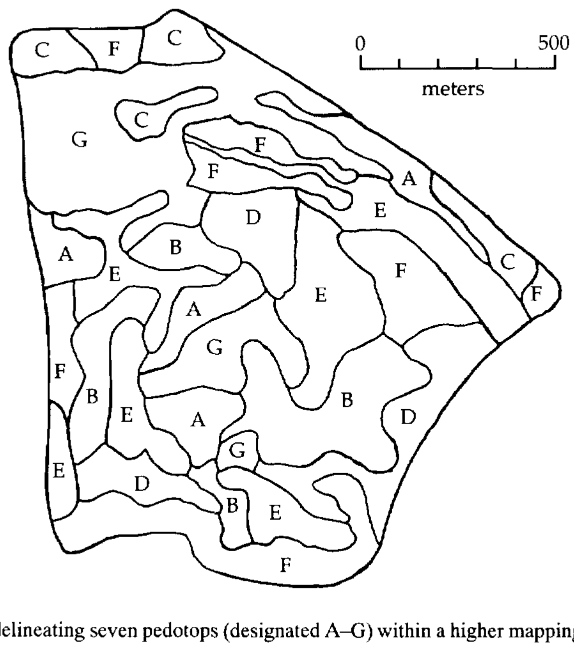

Fig. 1. Pedologic map delineating seven pedotops (designated A–G) within a higher mapping unit associated with a 100 ha farm.

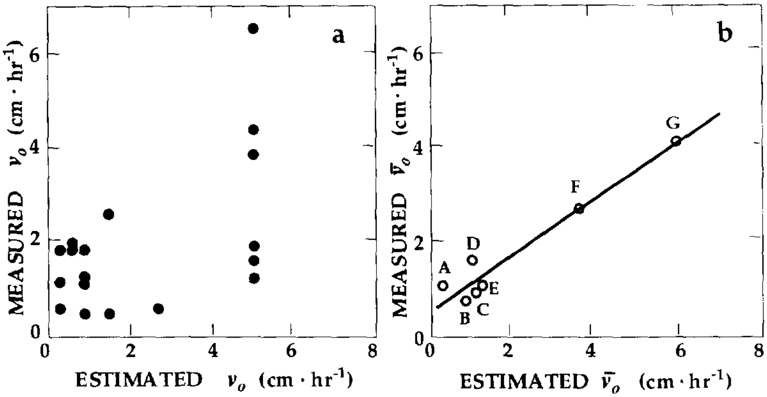

Fig. 2. Measured infiltration rates v_0 for the seven pedotops illustrated in Fig. 1 versus those estimated from soil texture. (a) Measured and estimated values v_0 at each location within the farm without considering pedotops. (b) Measured mean and estimated mean values v_0 within each pedotop.

rates within each pedotop were found to be log-normally distributed. Estimates of infiltration rates were derived using soil survey interpretation methods based upon the texture of the surface soil where each infiltration rate was measured. If the seven pedotops are ignored, there is no relation between measured and estimated values of infiltration (Fig. 2(a)). On the other hand, if the infiltration rates are grouped together by pedotop, their measured and estimated geometric mean values are highly correlated with $r^2 = 0.936$ (Fig. 2(b)).

At the pedon scale, methods used at the Darcian scale need to be modified with stochastic characteristics entering our equations and procedures. The stochastic structure of these hydraulic properties of field soils is studied by specific procedures. In some instances, we obtain a set of deterministic pedon-scale observations spatially distributed across the field or catchment to define a newly formed stochastic or regionalized variable. In other instances, entirely new approaches are developed applicable only to the pedotop scale. Experience with the higher mapping unit scale remains sufficiently inadequate to preclude any generalizations, yet it is at this scale that we expect the greatest improvement of our knowledge regarding land–atmosphere interactions.

2. Present-day soil science opportunities

Because soil is the interlayer between the atmosphere and the geosphere, soil scientists frequently utilize expertise and knowledge on the margins of their discipline to study fundamental concepts of soil development as well as the management of soil resources in relation to agriculture and other professional activities related to the landscape. Scientific inquiry embraces the cognate sciences of physics, chemistry and biology as well as the various interdisciplines of biochemistry and biophysics, ecology, limnology and others.

We tend to believe that soil processes included in many theoretical descriptions too often match the academic specialty of the scientist rather than an on-site assessment of a spectrum of soil processes having various levels of importance that indeed affect a particular field soil or land–atmosphere interaction. We also note that the choice of a particular model (e.g. chemical equilibrium vs. nonequilibrium, mobile vs. immobile soil water, zero-order vs. higher-order kinetic reactions) or a set of dependent equations is somewhat arbitrary and often made on the basis of criteria not specifically applicable to a given soil. Justification for the adoption of empirical functions for the description of soil properties and related parameters remains inadequate and awaits improvement in the majority of field studies. An optimal frequency in time and space for making observations of a soil attribute remains an enigma for almost all scientists. This puzzle persists owing to our inadequate characterization within fields of spatial and temporal variances which embrace the uncertainties of our measurement methods and those of soil taxonomy.

Opportunities based upon spatial and temporal distributions of surface soil water content to enhance our understanding of soil science and its application to regional and global environmental issues are plentiful. Here we outline briefly some previously published results coupled with our conjecture of the benefit of such distributions relative to enhancing soil science and its application to related disciplines that contribute to our understanding of the land–atmosphere interface.

2.1. Soil genesis and pedology

Being unaware of statistical and mathematical algorithms to quantify the variance structure of soil attributes within the landscape, pedologists established hierarchical classification and soil mapping schemes based upon modal (most frequently observed) soil properties within spatial domains, especially those subjectively described in terms of clay mineralogy, chemistry and microbiology. With their primary interest in soil genesis, plant growth and agriculture, pedologists from different parts of the world developed classification schemes strongly influenced by their different national cultures. Today, soil taxonomy, a soil classification scheme recognized world wide, provides a scientific basis for identifying the location and expected properties of soils across continental landscapes. Soil taxonomy, together with voluminous soil information cataloged in each and every country of the world, provides an excellent but imperfect contribution to the development of a new Earth system science aimed to improve our understanding of the Earth as an integrated whole, the objective of the International Geosphere–Biosphere Program.

During the past decade, those soil scientists aware of regionalized variable analysis have contributed to a better understanding of criteria used to delineate soil mapping units and have accelerated efforts to quantify soil spatial variability (Nielsen and Bouma, 1985; Webster and Oliver, 1990; Mausbach and Wilding, 1991) in relation to its genetic development as well as land use.

2.2. Locating soil boundaries

Data from measuring field soil properties generally exhibit both short- and long-range variations, are highly irregular and are multivariate. Various methods for obtaining optimal sampling strategies for mapping soil types based upon spatial distribution functions are commonly available. Here we illustrate a split moving window technique along a

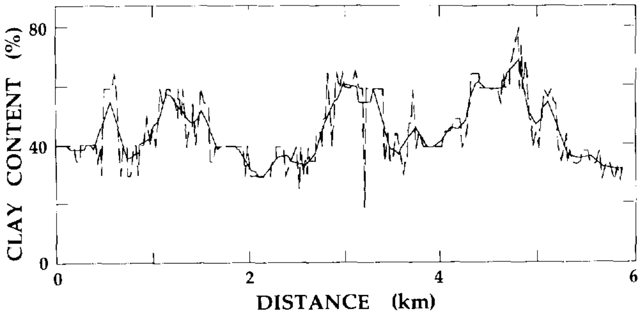

Fig. 3. Clay content of topsoil plotted against distance along a transect. The original data are represented by the broken line, and a nine-point simple moving average is shown by the continuous line.

transect of the upper Thames Valley of 6 km length sampled at 20 m intervals to a 1 m depth. Values of 27 properties of the soil profile were ascertained at each location. One property, the clay content, is depicted in Fig. 3.

Webster (1973), expecting a boundary somewhere in the middle of a selected portion of such data, divided the sampling points in that portion into two groups, those on one side and those on the other. This effect was assessed by comparing the difference between the two groups with the variation within them. The greater the difference between the groups and the less the variation within them the more effective is the division. To identify the best position to divide the portion, he used Mahalanobis' generalized distance D calculated from

$$D^2 = (\bar{x}_1 - \bar{x}_2' W^{-1} (\bar{x}_1 - \bar{x}_2) \qquad (1)$$

where $\bar{x}^1$ and $\bar{x}^2$ are the mean vectors of the principal component scores of the two halves of the window and W is the pooled within-halves variance–covariance matrix. If it is assumed that correlations between the principal components within any portion of the transect are negligible, eqn (1) reduces to

$$D^2 = \sum_{i=1}^{p} \frac{d_i^2}{s_i^2} \qquad (2)$$

where d is the difference between means, s^2 the pooled within-halves variance and p the number of components. Values of D^2 for the Thames Valley transect are presented in the top portion of Fig. 4, with soil types recognized in the field judged on soil taxonomy and airphoto evidence presented in the bottom portion of Fig. 4. The heights of the D^2 peaks leave little doubt about the positions of the boundaries. The initial choice of the length of transect portion was based upon autocorrelation analysis inasmuch as the lag distance over which the correlation decays is related to the average distance between boundaries.

It should be obvious that soil types A–F above, as well as those shown previously in Fig. 1, have different soil water properties that yield vertical distributions of soil water which influence the partitioning of sensible and latent heat at their surfaces. Such information analyzed by soil physicists and available in taxonomic descriptions of soils should be utilized to enhance our understanding of the land–atmosphere interface. The quality of

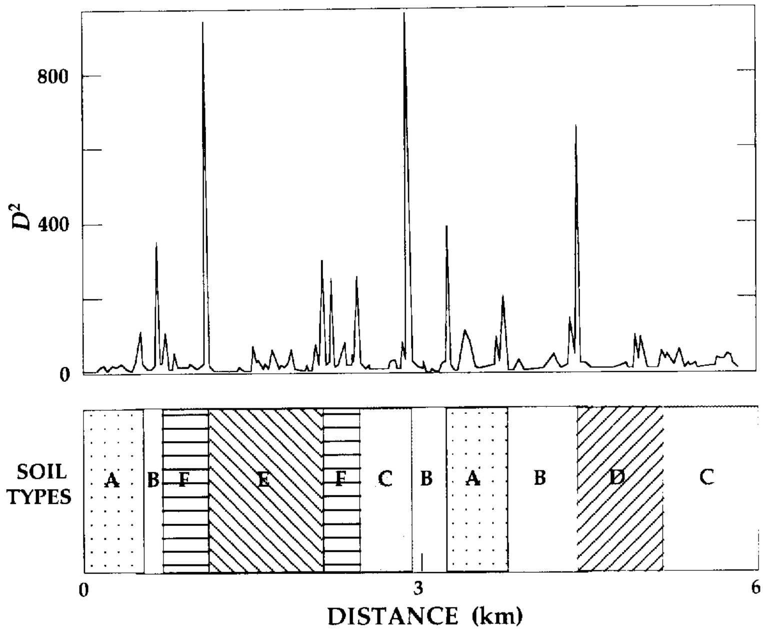

Fig. 4. The partition of the Thames Valley transect. The top graph shows Mahalanobis' D^2 for a split window width of 280 m. The bottom portion shows boundaries between soil types: A, deep brown, more or less calcareous loam over limestone gravel; B, grayish brown, mottled clay loam over clay; C, gravelly calcareous brown loam over limestone gravel at about 0.5 m; D, medium to heavy textured, dark gray, mottled soil over old alluvium; E, dark gray or grayish brown mottled clay, river alluvium; F, deep brown calcareous medium textured soil with mottling at depths over limestone.

soil maps in terms of (1) the proportion of soil boundaries that remain undetected as a result of point samples and (2) the accuracy of their locations is seldom provided.

Risk functions and sampling intervals for surface soil water behavior based upon field measurements are only beginning to emerge is soil science research. Estimates of soil hydraulic characteristics are usually method dependent, and at the pedon scale their probability distribution functions are usually not identical if one characteristic is measured by several methods simultaneously. Even when one experimental method is used to evaluate the parameters associated with different kinds of theoretical approximations, the probability distribution functions of the parameters markedly differ. For example, values of the sorptivity S $[L\,T^{-1/2}]$ and saturated hydraulic conductivity K_S $[L\,T^{-1/2}]$ were determined by ponded infiltration tests (Kupcová, 1989; Krejča, 1991). The field data on cumulative infiltration were fitted to four different infiltration equations based upon different simplifying assumptions: Philip's two-term algebraic equation (P2), Philip's three-term series equation (P3), Swartzendruber's equation in a simplified form (Sw) and Brutsaert's equation (Br). On a chernozem, they found a log-normal distribution of S(P2), S(P3), S(Br) and K_S(P2), whereas K_S(P3) and K_S(Br) manifested a Weibull distribution and K_S(Sw) manifested a Beta distribution with S(Sw) being identical to S(P3). In other sets of infiltration experiments performed on oxisols, they also found in some instances normal, Erlang's and Gamma types of distributions. Hence, the error

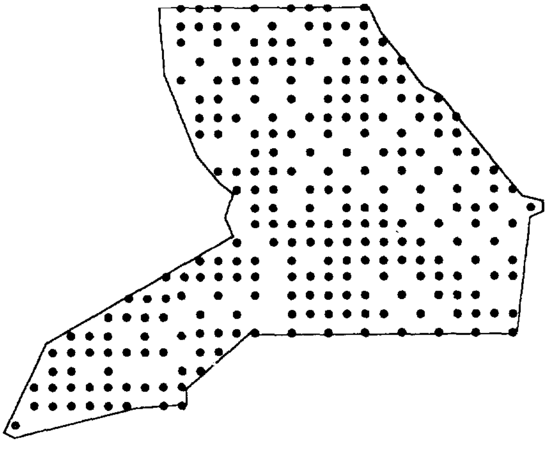

Fig. 5. Location of 1 km grid soil sampling sites on a single soil series in Sudan.

owing to the nature of the approximation in the evaluation procedure deforms the theoretical distribution of the soil hydraulic attribute being investigated.

2.3. Soil properties within pedotops

The relative size of different soil mapping units appropriate to land–atmosphere interactions varies greatly within different landscapes. In Fig. 1 and Fig. 2, the distance between boundaries was of the order of 10–100 m. Fig. 5 shows a 1 km grid of soil sampling locations on a single soil series in Sudan (Uehara et al., 1985) extending over an area of about 400 km^2.

Surface soil samples collected at each location were analyzed for exchangeable sodium percentage inasmuch as that soil attribute was judged to be most likely to limit sugarcane production. One measure of the spatial variance structure of the exchangeable sodium percentage within the soil expressed as a semi-variogram is given in Fig. 6. The variogram

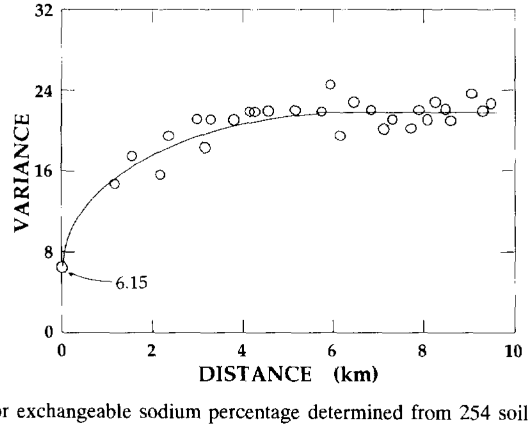

Fig. 6. Semivariogram for exchangeable sodium percentage determined from 254 soil samples collected from locations shown in Fig. 5.

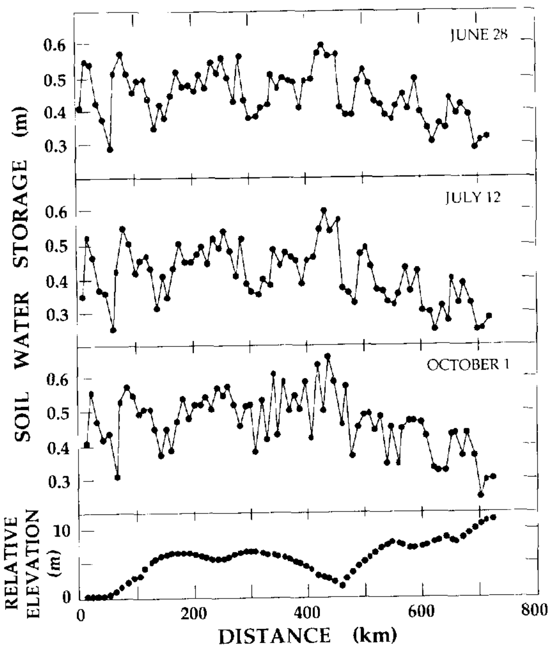

Fig. 7. Measured soil water storage and relative elevation of the experimental site.

has a nugget of 6.15, a range of 3 km and a sill and sample variance of 21.6. Kriged contours of exchangeable sodium percentage having values between 5 and 21% had a mean estimation variance of 10.5.

Although the domain shown in Fig. 5 is within a single soil mapping unit according to soil taxonomy, local variations in exchangeable sodium percentage occurring at distances less than 4 km will cause different levels of sugarcane growth and evapotranspiration. Regardless of the vegetative cover of this domain, major differences in water evaporating at the soil surface will be manifested owing to soil water diffusivity and unsaturated hydraulic conductivity values being deterministically dependent upon exchangeable sodium percentage. For the same soil water content, their values would change by one order of magnitude for the levels of exchangeable sodium percentage observed in the field. Coupling soil water properties to other soil profile attributes through cross-variograms and cokriging (Vauclin et al., 1983) provides opportunities not yet fully realized by those interested in land–atmosphere interaction.

2.4. Time stability within pedotops

Time stability was defined by Vachaud et al. (1985) as the time-invariant association between spatial locations and classical statistical parametric values of soil properties. It appears promising especially for soil water behavior at the Earth's surface. Vachaud et al. tested the concept on measured water stored in a soil profile and suggested that time stability will occur if covariances exist between a spatial variable of interest and a deterministic factor such as soil texture or topography.

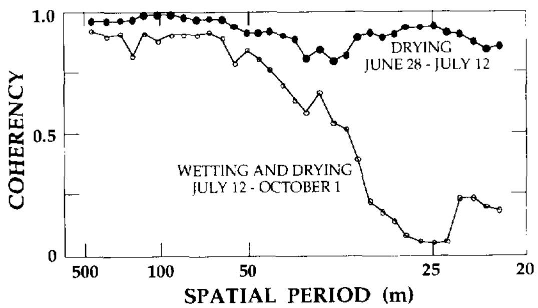

Fig. 8. Coherency spectra for the drying period (28 June–12 July) and recharge period (12 July–1 October).

Kachanoski and De Jong (1988) explored the above idea by analyzing the power spectrum and coherency of soil water stored in the soil profile along a 720 m transect of a fine-textured, moderately calcareous soil (classified as Typic Haploboroll according to soil taxonomy) between a period of time involving only evapotranspiration and another period during which both evapotranspiration and precipitation as rainfall occurred. Fig. 7 shows the depth of water stored in the 2 m soil surface measured with neutron probes at 10 m intervals across the transect having a relative elevation that undulates within a range of 12 m. Soil water stored is plotted versus distance along the transect for 28 June, 12 July and 1 October. Between the first two dates, no precipitation occurred, and between the last two dates, precipitation was sufficient to significantly recharge the amount of water stored in the profile.

The coherency spectrum for the drying period (28 June–12 July) being highly significant for all spatial scales indicates the presence of a linear correlation and thus temporal stability across all spatial scales (see Fig. 8). On the other hand, the coherency spectrum for the recharge period being significant only at the larger spatial scales indicates that temporal stability was present for scales greater than 40 m, and indeed was shown to be related to the spatial pattern of the soil surface curvature across the transect. During wet periods topography was related to soil water storage, and during drying periods it had little to do with soil water loss. The nature of this scale-dependent time stability of the specific processes of infiltration, recharge and evaporation has not been investigated within pedotops or higher mapping units. Evaluating the nature of its existence across the landscape would not only help quantify land–atmosphere interactions but would provide additional criteria to identify mapping units within soil taxonomic concepts.

Summarizing from the above examples and others not cited, we envision water content distributions near the soil surface at various scales of space and time to enhance research in soil genesis and pedology that relates to the following: (1) development of criteria for soil mapping units based upon spatial and temporal variance structures of physical, chemical and biological state variables; (2) possible consistency of covariance structures of soil water properties with present-day soil mapping units; (3) determination of the most promising opportunities to quantify covariance structures of soil water properties with soil profile and landscape attributes; (4) identification of scales of observation most useful or informative for different soil and land processes consistent with soil taxonomy and their application.

2.5. Soil physics

Soil physicists are now being joined by other soil scientists, atmospheric scientists, ecologists, geologists, hydrologists, engineers and other investigators interested in ascertaining naturally occurring and anthropogenically induced rates of change in landscape and subsurface attributes of our environment. That interest, coupled with new and continually improving opportunities for instrumentation and data acquisition, renders the topic of this workshop intellectually stimulating and a challenge to each and every soil physicist. They recognize the need for new approaches for simultaneously examining (1) alternative formulations of differential equations to describe soil processes, (2) alternative functions for soil parameters contained in those equations, (3) alternative frequencies of spatial and temporal measurements to match the theoretical considerations in (1) and (2), and (4) the adequacy of accepting different levels of uncertainty always inherent in observation instruments and their calibration including human errors.

2.6. Quantification of soil water transport

The surface energy balance for an infinitesimally small layer (e.g. bare soil surface) can be written

$$R_{\mathrm{n}} - G = H + LE \tag{3}$$

where R_{n} is the net radiation (incoming longwave and shortwave, outgoing longwave and reflected short wave), G the soil heat flux, H the sensible heat flux and LE the latent heat flux. In soil moisture balance studies, LE enters directly into the soil storage equation:

$$\frac{\mathrm{d}W}{\mathrm{d}t} = P - E - (D + R) \tag{4}$$

where the time rate of change of soil water content W depends on P the precipitation, E the evaporation, and $(D+R)$ a combination of deep drainage and runoff. The soil water content W for some layer at the soil–atmosphere interface plays an important role in the partitioning of the available energy $(R_{\mathrm{n}}-G)$ into latent heat and sensible heat. The quantity (amount) of water in this layer of course depends on the precipitation forcing and is then ultimately linked to how much is evaporated into the atmosphere. It is well known that in natural landscapes as well as agricultural settings, more than half of the precipitation is partitioned as evaporation, and therefore any estimate of $(D+R)$, for instance, will depend on the success of specifying E. With soil water retention being inextricably linked to physical, chemical and biological processes occurring within the soil profile, the spatial and temporal characteristics of the entire profile play a major role in the loss of water from the soil into the atmosphere, a role no less important than the atmospheric boundary layer profile above the land surface. A simple solution of Richards' equation for a drying land surface is $E = De\, t^{1/2}$, where De is the desorptivity. The desorptivity is a soil hydraulic characteristic which depends upon soil water content. It is related to the soil water diffusivity and unsaturated soil hydraulic conductivity functions. Here we present a few examples of using applied time series with experimental observations in the field to link the response of surface soil water content to precipitation and evaporation, estimate soil water transport functions, and analyze the nature of vertical and horizontal soil heterogeneity as it affects our estimates of soil water behavior at the pedotop scale.

2.6.1. Example 1

Parlange et al. (1992) presented a simple daily hydrologic balance in which only three governing components at a daily time step interact: applied water, evaporation, and change in soil water content. The field experiment over a uniform and flat bare soil field was designed to insure that only those three hydrologic parameters were interacting when the applied irrigation water was known. Under those conditions, Parlange et al. studied the interaction between soil water storage and evaporation into the atmosphere, and showed (with the above simplified Richards' equation and the hydrologic balance) that the Markovian AR(1) process used by Manabe and Delworth (1990) could be derived from physical considerations. They compared the derived AR(1) model with daily measured soil water content data obtained from neutron-scattering. They modeled the relationship between soil water content and soil water diffusivity, hysteresis owing to wetting and drying, and assumptions regarding the second stage of evaporation with a random stochastic shock for daily time increments that is small compared with the applied water forcing. They demonstrated that the AR(1) model transfer parameter is related to the soil water diffusivity function. Fig. 9 shows a summary of their results with forecast soil water storage, measured soil water storage and irrigation events as a function of time during the 100 day experiment.

The assumptions leading to the AR(1) equation were primarily simplifications to the soil water transport equation while retaining mass conservation as the governing mechanism in the soil–atmosphere system. Owing to nonlinearities in the dynamics of soil water flow, the simplifying assumptions would not be valid over short time periods of minutes or hours. The soil water diffusivity calculated from the AR(1) model parameter

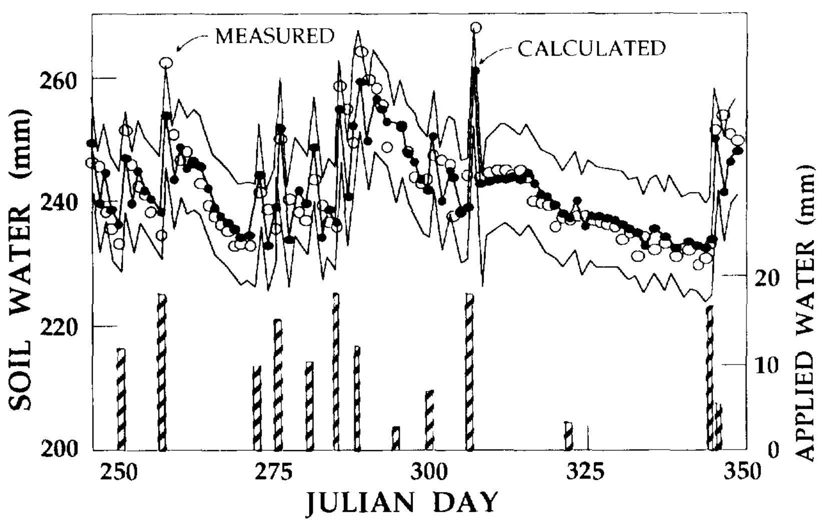

Fig. 9. AR(1) predictions and neutron probe measurements of stored soil water during evaporation.

was comparable to those measured in the field and in the laboratory on the same soil. For other soils, the evaporation occurring would be similarly dependent upon the diffusivity function, which has been studied for nearly 50 years by soil physicists. It is well recognized that the function, which is strongly dependent upon soil water content, is also sensitive to water quality and temperature as well as local variations of other soil properties. These functions, uncataloged for virtually all field soils and yet necessary to partition the available energy (R_n–G) into latent heat and sensible heat, could be readily obtained for the major global pedotops or higher mapping units from a sequence of surface soil water content distributions.

2.6.2. Example 2

Following a procedure similar to that for the first example above, the diffusivity function was calculated with the Kalman filter assuming that the observation variance can be estimated from spatially averaging neutron probe readings that measure the stored soil water at different locations within the same pedotop. The details of the experimental setup, located near the site of the first example described above, have been fully described by Parlange et al. (1993). Five neutron access tubes positioned every 18 m along a transect allowed soil water content to be monitored with a neutron probe at 15 cm depth intervals within the soil profile at each location. The level site was free of vegetation and equipped with a sprinkler irrigation system that was used to apply 15 small irrigations (each less than 20 mm) during a period from 4 September to 12 December. In addition to the neutron probe measurements of soil water to estimate evaporation, 20 min weighings of a lysimeter of 50 t capacity in the same field were integrated to obtain daily values of evaporation.

Evaporation and infiltration from the applied water are the primary physical processes that create changes in stored water, and those changes occur primarily in the 0–22.5 cm depth. Variations in soil water stored in the top 22.5 cm of the profile as a function of time as well as location are shown in Fig. 10.

It can be seen in Fig. 11 that the observation variance is much larger than the neutron probe calibration variance. Values of A and B (the parameters of the assumed exponential

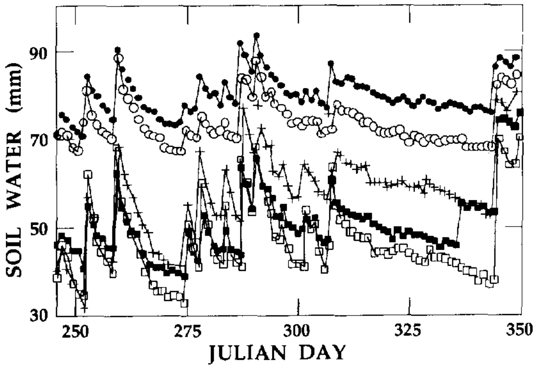

Fig. 10. Depths of water stored within the 0–22.5 cm topsoil at each of five field locations measured with a neutron probe.

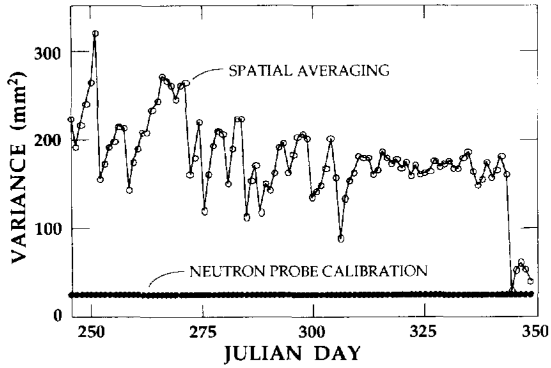

Fig. 11. Observation variance owing to spatial averaging of measured soil water storage for the 0–22.5 cm topsoil as well as the neutron probe calibration variance.

soil water diffusivity function) were estimated to be 0.0292 mm^2 day^{-1} and 32.59 cm^{-1}, respectively, with the state variance per unit time Q being 18.87 mm^2 day^{-1}. The value of Q is of the same order of magnitude as the neutron probe calibration variance, and the model uncertainty for stored water prediction on a daily basis is within the neutron probe noise.

The agreement found between the Kalman filter estimation of cumulative evaporation and that measured with the lysimeter (r^2 = 0.98) indicates that the estimated diffusivity function provides an adequate description of evaporation, and the flow equation by Gardner (1962) may be satisfactorily extended to the field with variable water content. There remains an additional task of defining soil water diffusivity functions appropriate to each pedotop and ascertaining their limitations relative to local and regional soil variabilities.

2.6.3. Example 3

Description of infiltration and drainage in unsaturated soils is generally complicated by uncertainties in estimating the hydraulic conductivity relation $K(\theta)$. The sources of uncertainty in estimating the hydraulic conductivity function at a particular location in a field include (1) simplifying the description of the physical processes that are used indirectly to infer the hydraulic conductivity function, and (2) the measurements used to determine the hydraulic conductivity function.

Katul et al. (1993) constructed a nonlinear filter that provides hydraulic conductivity function parameters that minimize the mean square error of a differential equation describing the redistribution of soil water content relative to measured soil water content in an unsaturated drainage experiment (Milly, 1986; Milly and Kabala, 1986; Gardner, 1990; Parlange et al., 1993). Simplifying Richards' equation for one-dimensional soil water flow to an equation in terms of stored water W, we have

$$\frac{\partial W}{\partial t} = -K(W)\left(\frac{\partial H}{\partial z}\right)_{z=b} \tag{5}$$

where $K(W)$ is the hydraulic conductivity function. In the derivation of Eq. (5), the following assumptions were made: (1) horizontal transport is neglected; (2) a linear relationship exists between depth-averaged soil water content θ^* and the soil water content

Table 1
Values of parameters A and B of the hydraulic conductivity function $K(W) = A\exp(BW)$ estimated by the five methods

Method	A (cm day^{-1})	B (cm^{-1})
Nonlinear filter	1.24×10^{-8}	1.625
Classical	1.20×10^{-9}	1.872
Flux	1.56×10^{-9}	1.865
Theta	2.45×10^{-9}	1.818
CGA	8.13×10^{-11}	2.212

θ at z; (3) thermal and salinity effects on $K(W)$ are neglected. Here we assume that $K(\theta)$ is of the form $A\exp(B\theta)$, but the results can be generalized for any analytic form of the function. A simple scheme accounts for both measurement and system uncertainty for processing and updating the time sequence of measurements of soil water content θ and hydraulic gradient dH/dz. The method presumes that the simplifying assumptions for the soil water transport equation result in a random noise to an initial value differential equation characterizing the water stored within the soil profile. The hydraulic conductivity parameters stemming from discrete stored water and hydraulic gradient measurements can then be determined iteratively from a sequence of prediction-updating steps to maximize a defined objective function (the likelihood function).

The details of the experimental setup have been fully described by Katul et al. (1993). After an infiltration period of 10 days on small field plot of Yolo light clay, the soil surface was covered with a plastic sheet to impose a no-flux surface boundary condition and allow soil water storage to be decreased only through vertical downward drainage. Neutron probe and tensiometric observations were used to monitor the stored water in the surface 22.5 cm of the soil profile and the hydraulic gradient at the 22.5 cm depth, respectively. Observations were recorded every 6 h for the first day and every 12 h afterwards for a total period of 43 days.

The parameters A and B estimated by the nonlinear Kalman filter are given in Table 1, together with those estimated by the Theta, Flux and CGA methods (Libardi et al., 1980), and the classical method (Jones and Wagenet, 1984). The Flux, Theta and CGA methods assume a unit hydraulic gradient and only require soil water content observations, whereas the classical method also requires matric potential observations. A major disadvantage of all four methods is the fact that an arbitrarily smoothed monotonically decreasing relation between q and t is required. The raw soil water content and matric potential data were smoothed by eye for the four methods. The smoothing insured a monotonic decrease in soil water content with time, and an attempt was made to preserve local trends observed in the data. With the exception of the CGA method, all the methods provided comparable estimates of A and B, with those of the classical method being well within the 67% confidence band of the Kalman filter predictions of $P(t)$ for all of the observed soil water content ranges (Fig. 12). The CGA, Theta and Flux methods resulted in larger hydraulic conductivity values than those from the Kalman filter and the classical method, especially for $\theta^* > 0.43$. These differences were attributed to deviations from the unit gradient assumed for the CGA, Theta and Flux methods.

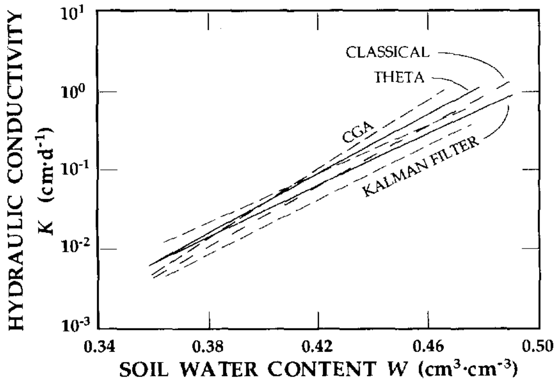

Fig. 12. Comparison of various field methods for determining the hydraulic conductivity function. The predicted standard deviation using the nonlinear Kalman filter is the shaded area.

Unlike current field methods, which provide $K(\theta)$ relations in the mean from arbitrarily smoothed field observations, this example of Kalman filtering provides mean estimates of $K(\theta)$ as an exponential function of soil water content and their variances based on direct raw measurements. It also allowed a quantitative assessment of the validity of Eq. (5) on a daily basis, based on the state variance per unit time. For a daily time step, the isothermal and nonhysteretic assumptions invoked were not inappropriate for this transient field experiment. An interesting possibility for different soils and land–atmosphere interface conditions would be the examination of the depth b to which Eq. (5) could be successfully integrated.

2.6.4. Example 4

Cahill et al. (1996) have recently examined the spatial and spectral characteristics of near-surface soil water content as influenced by applied water and evaporation. A transect, 50 m in length and equipped with neutron probe access tubes every 1 m, was used to monitor the evolution of soil water content measured daily at each of the 50 locations for 120 days. These measurements permitted explicit evaluation in the changes of the spatial structure of soil water content owing to evaporation and infiltration.

Applied water events were used to force the soil system and induce high evaporation rates that switch from climate controlled to soil controlled under dry conditions. The influence of applied water and subsequent evaporation on the statistical structure of soil water content in the 15 cm topsoil was analyzed in the frequency domain using power spectra and in the space domain using autoregressive models. Cahill et al. found that the applied water events attenuated the spectral peaks of the soil water content at all wavenumbers. In physical space, the applied water events increased the correlation between neighboring locations by more than 30%. The evaporation rate increased the magnitude of the spectral peaks of soil water content at the small wavenumber end of the spectrum with little influence on the larger wavenumbers. This increase indicated that the evaporation rate affects the 'field'-scale soil water content rather than that at the 'local' scale, whereas applied water events affected all scales ('local' and 'field').

These results are only the beginning of more meaningful investigations at the land–atmosphere interface that would merge the discipline of atmospheric science with that of soil physics. Being cognizant of local and regional scales within and outside higher mapping units would provide additional criteria for ascertaining optimal sampling strategies.

Summarizing from the concepts of the above examples, we envision water content distributions near the soil surface at various scales of space and time to enhance research in soil physics that relates to the following: (1) ascertainment of soil physical properties and conditions within soil profiles based upon surface soil water content distributions; (2) quantification of correlation lengths of soil water content in time and space relative to precipitation and evaporation events; (3) determination of whether there is a useful covariance structure between soil water properties and those associated with water and heat fluxes at the land–atmosphere interface identifiable at the pedotop or higher mapping unit scale; (4) determination of whether vertical and horizontal fluxes of energy and matter in gaseous and liquid phases below the soil surface can be ascertained from surface soil water distributions

2.7. Soil microbiology

Soil microbiology is the subdiscipline of soil science that offers the greatest opportunity to utilize surface soil water content distributions. To date, there has not been an adequate systematic approach to categorize different scales at which soil microbial ecology is studied or linked to other Earth sciences. The diversity of soil microbial communities staggers our imagination. Ten grams of soil may contain as many bacteria as the world has citizens. Different species of bacteria, fungi, protozoa, algae and other microscopic plants and fauna, together with soil organisms and the roots of higher plants, symbiotically and competitively coexist in soils. The pathways of energy and matter exchange between all of them are at best only qualitatively known. Soil microbiologists study individual organisms over scales ranging from molecules to regional or global biomes. An opportunity to focus on populations of particular kinds of microbes at a vertical scale the size of the thickness of a soil horizon exists and is promising. Analyzing the impact of perturbations of the state variables soil water and soil temperature on such populations would allow us to quantify and enhance our present understanding of various soil microbial processes.

Applications of soil microbiology have long been linked with agriculture, owing to its relevance to soil fertility and plant nutrient cycling. Every soil microbiologist knows a great deal about the biochemistry of terrestrial nitrogen, phosphorus, sulfur, iron and other cycles. Although the water cycle mediates and sometimes even controls the rates occurring in these cycles, the impact of the time rate of change of soil water content on biochemical reactions in those cycles has been generally neglected. Soil microbiologists, mindful of the importance of the relative availability of water, especially in the nitrogen cycle, have usually studied and cataloged microbially induced chemical transformations under different levels of the amount of water present, owing to its implications for chemical transport in both the gas and liquid phases of the soil. Hence, we have terms such as nitrification and denitrification, dry and wet deposition, etc.

Rates of change occurring in the carbon cycle and those of other elements and inorganic and organic compounds mediated by soil microbes not necessarily associated with agriculture are actively being studied owing to implications of global climate change and proper environmental stewardship of the Earth. How do we monitor and analyze the myriad of soil microbial reactions continually in progress across the landscape? At what depth do we take a sample, and a sample of what? Over what increment of time should we sample? When do we pay attention to the genetic properties of soil pedotops and higher mapping units? How do we weigh the importance of different sources and sinks of microbially mediated matter integrated over particular scales of space and time? A field technology for soil microbiology is at its infancy. A step toward its maturation would be achieved if equations similar to Eq. (5) could be derived with one or two microbially based processes and the forcing of surface soil water content or temperature for different times analyzed. Any number of different time series methods could improve our knowledge of soil microbiology applied to field soils.

We envision water content distributions near the soil surface at various scales of space and time to enhance research in soil microbiology that relates to the following: (1) identification of state variables of microbiological populations related to surface soil water distributions; (2) whether rates of microbially induced transformations of organic materials are linked with surface soil water distributions, and whether they have a covariance structure according to soil taxonomy; (3) whether changes of microbial growth, metabolism and death can be associated with surface soil water distributions at different scales of time; (4) whether the mobility and persistence of soil-borne disease organisms are related to surface soil water distributions.

3. Discussion and conclusions

For analyzing field soil measurements we made an early assumption that retention and transfer processes are one dimensional. Many are not, and hence the above presentation starts out with that approximation. We also recognize that the details of many processes are sometimes best described with partial differential equations or even systems of such equations. However, information typically available from field observations seldom matches the data requirements to describe initial and boundary conditions or to fully utilize the rigor of the original partial differential equation, owing to a dearth of parameter values specific for the domain being investigated. Reducing to the use of ordinary differential equations is an observational and theoretical challenge to both 'practitioners' and 'theoreticians.' This reduction is achieved by adding more information, e.g. providing a functional behavior of transfer coefficients or utilizing pedotransfer functions from soil surveys, neglecting second-order or less important features of the processes, and deterministically defining magnitudes of more complicated initial and boundary conditions. With these and other approximations, the simplified ordinary differential equation is certainly not exact, but on the other hand, no equation is absolutely exact, particularly when it is used to describe a soil phenomenon related to environmental management or to the land–atmosphere interface. The advantage of the proposed approaches over almost all other field methods utilizing surface soil water content distributions is that we take advantage of soil taxonomy and acknowledge that equations are definitely approximate and contain model errors. Indeed, solving explicitly for the model variance, and through its examination, we ascertain the impact of our simplifications, and potentially identify improvements for a more realistic equation based on the potential availability of a particular data set.

A desirable feature is the inclusion of an observation error which can be treated as a known and measured quantity as was done above with the neutron probe calibration, or alternatively, treated as an unknown for which a solution is found in a numerical scheme. The magnitude of a known observation error allows a reconsideration of the state variable in the equation or an improvement in instrumentation or calibration. On the other hand, treating the observation error as an unknown, its behavior in space and time can be related to spatial and temporal correlation lengths that may manifest themselves within the domain of the field being studied. Such an opportunity exists when, for example, observations of surface soil water contents W derived from remote sensing procedures for a given pixel size are to be reconciled with direct neutron probe or TDR measurements of W at a much smaller scale. The problem of scale confounded with that of spatial heterogeneity has yet to be reconciled in terms of practical monitoring procedures.

Regardless of the instrument or field sampling technique used to observe a soil physical, chemical or biological process, most samples represent some sort of depth-averaged value. Hence, it is not only convenient but more correct to use equations that describe depth-averaged phenomena. We also expect that progress could be made using time-averaged equations to examine critical periods during which soil processes occur; these soil processes may be related to particular soil locations, mapping units or regions. A large array of combinations of state and observation variables together with different functions for parameter estimation provides attractive opportunities to enhance the maturation of our field technology in soil science and hasten its integration with other Earth and atmospheric sciences.

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