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The Scale of Observation and Modeling in Soil Hydrology

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LECTURE NOTES

The Scale of Observation and Modeling in Soil Hydrology

Extended text of the textbook
Soil Hydrology, 1994 by M. Kutílek and D.R. Nielsen

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1.2 CONCEPTS OF SOIL HYDROLOGY

All studies in soil hydrology eventually have a unique aim - a better understanding and description of hydrological processes. The individual elementary processes of infiltration, redistribution, drainage, evaporation and evapotranspiration are first analyzed and subsequently considered in combination during a particular sequence of events or season. Transport of solutes is also considered as an integral part of those processes. All such processes occur in soils and under actual meteorological situations. A proper physical understanding of them requires several levels of approximative studies.

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. Only when the physical interpretation of some phenomena requires a detailed discussion at the microscopic level will we temporarily abandon laws and equations based on a macroscopic scale of observation.

The elementary hydrologic processes for simply modeled soils and for trivial boundary conditions are described by analytical solutions of the basic macroscopic equations. The advantage of analytical solutions is a full understanding of the physical processes. 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. At this 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. We properly interpret the data physically by applying the knowledge we gained at the first approximation level.

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 megascopic scale, larger than Darcian, is usually denoted as catchment scale. See Fig. 1.1. Considering the principles of soil mapping, it is advisable to differentiate between two new categories within the catchment scale: (1) the pedotop scale

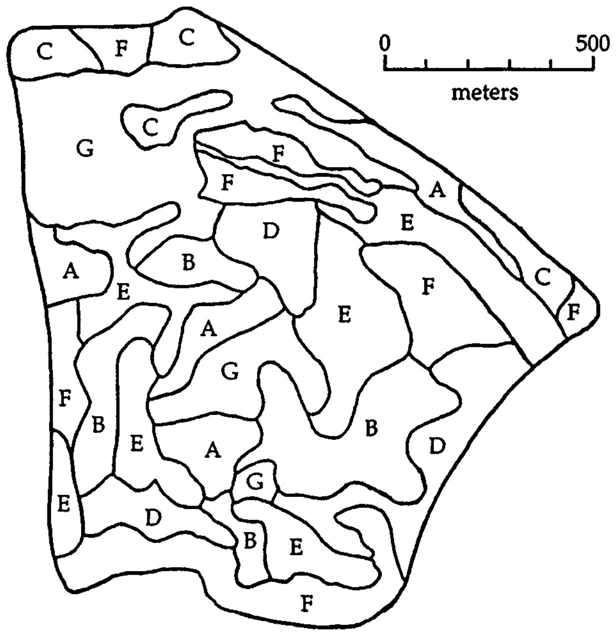


Figure 1.2. Pedologic map delineating seven pedotops (designated A through G) within a mapping unit associated with a 100-ha farm.

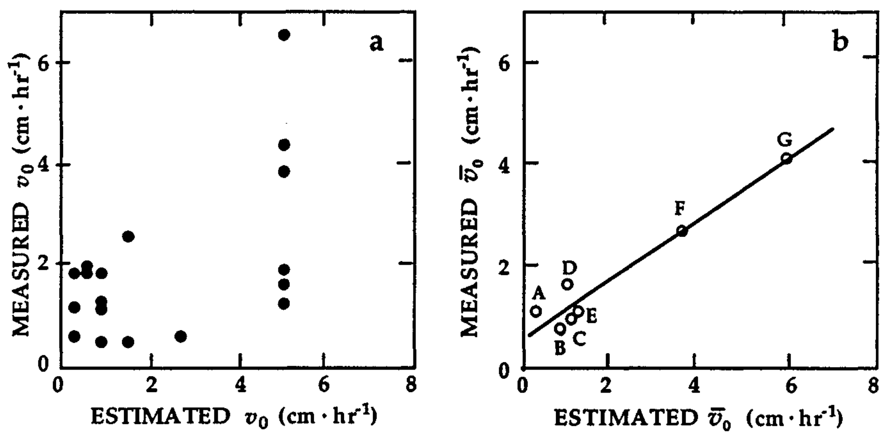


Figure 1.3. Measured quasi-steady state infiltration rates for the seven pedotops illustrated in Fig. 1.2 versus those estimated from soil texture: a. measured and estimated values v_0 at each location within the farm without considering pedotops, and b. measured mean and estimated mean values $\bar{v}_0$ within each pedotop.

and (2) the mapping unit scale. Both categories belong to megascopic observations in soil hydology 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 mapping unit scale, variability is both stochastic and deterministic. We illustrate this behavior of spatial variability in Fig. 1.2 which depicts seven pedotops located deterministically within a mapping unit across the landscape of a farm. The pedotops were mapped based on data from 293 bore holes taken approximately at 60-m intervals across the entire 100-ha farm. Measured values of surface water infiltration rates within each pedotop were found to be log-normally distributed. Estimates of infiltration rates were derived using soil survey interpretation methods (U. S. Dept. of Agr., 1951) 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. 1.3a). 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. 1.3b).

At the pedotop 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 mapping unit scale remains sufficiently inadequate to preclude any generalizations.

Analogous to these briefly introduced concepts of soil hydrology, we proceed further into the content of the book.

SCALES OF STUDIES IN SOIL HYDROLOGY:

1. Pore scale: Navier-Stokes eq. Fractals, fractal fragmentation, percolation. Gradual transition to Darcian scale.
2. Darcian scale
   2.1. Surrogate soil scale: Artificial porous materials, laboratory columns filled by repacked soil. Darcy-Buckingham eq., Richards eq.
   2.2.Pedon scale. Darcy-Buckingham eq., Richards eq.
3. Pedotop scale: Geostatistics. Scaling applied to physical soil properties. Scaling applied to boundary conditions of elementary soil hydrologic processes. Probability density function (PDF) of estimates of soil hydraulic characteristics, see next table. Semivariance on „pedotop" scale..
4. Mapping unit scale, **SH**, Fig 1.2. and 1.3., p. 14. Combined approaches, in Fig. next page. (Rogowski, Wolf, 1994).
5. Watershed scale.
6. Regional scale.

For scales > pedotop scale see Figs. 7.2 - 7.4. (Rogowski, Wolf, 1994)

SCALE: ONE PEDOTOP

PDF of saturated hydraulic conductivity K_S [LT^{-1}] and of sorptivity S [$LT^{-1/2}$] estimated from ponded infiltration test by various infiltration equations

	arenic chernozem		ferralsol		
	short set	full set	A-B	C-D	full set
K_S					
Philip, 2-parameters	LG	-	LG	E	LG
3-parameters	W	B	LG	E	LG
Swartzendruber	B	W	LG	E	LG
Green-Ampt	-	-	LG	G	E
Brutsaert	W	-	LG	LG	LG
S					
Philip, 2-parameters	LG	W	G	N	N
3-parameters	LG	E	G	N	E
Swartzendruber	LG	E	G	N	E
Brutsaert	LG	-	LG	G	E

Types of PDF: N - normal
LG - log-normal
W - Weibull
G - gamma
B - beta
E - Erlang

$PDF(A) \neq PDF(A + e_i)$

$(A + e_i)$ is our estimate

15b

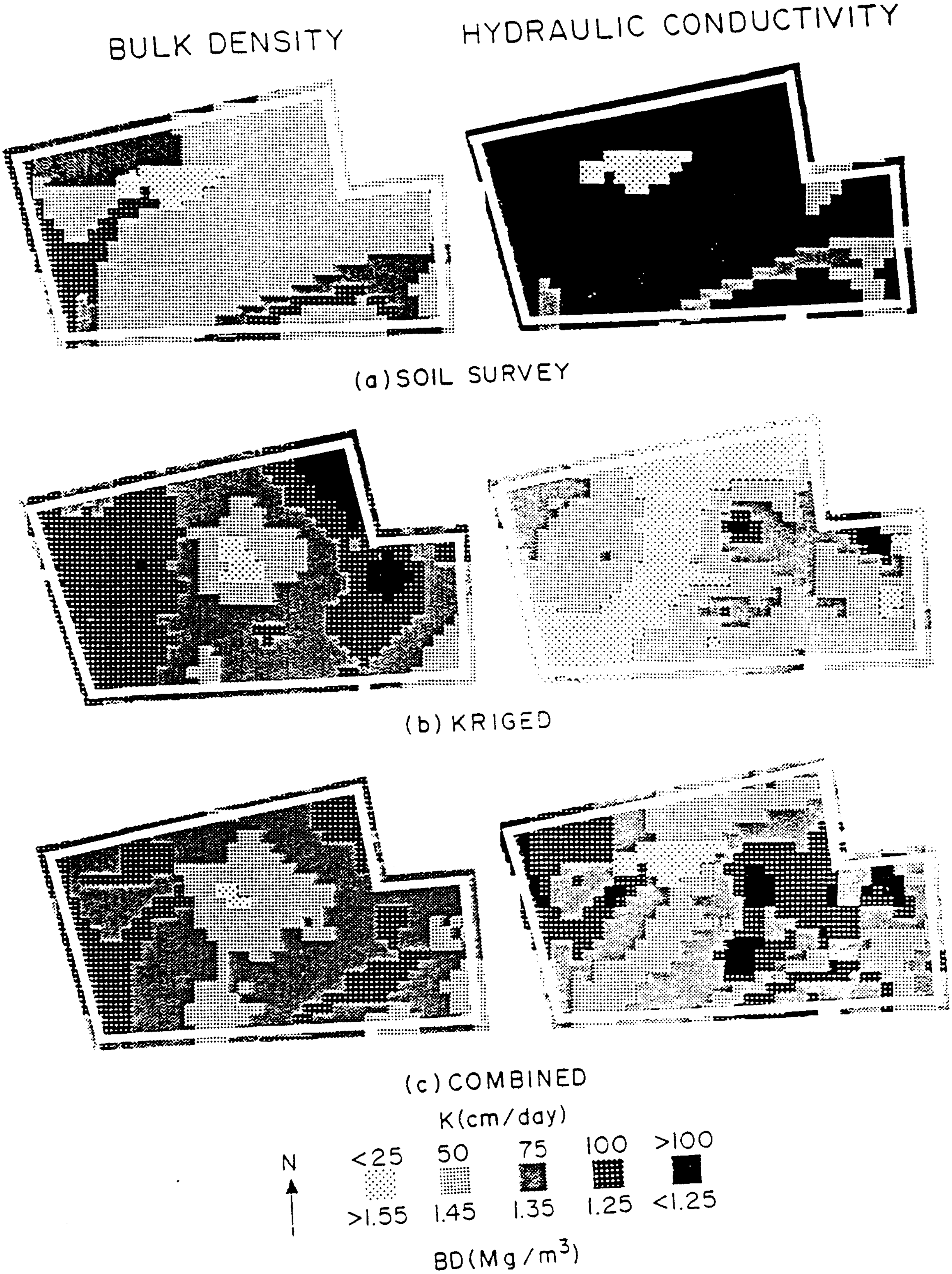


Figure: Combined approaches in mapping unit scale

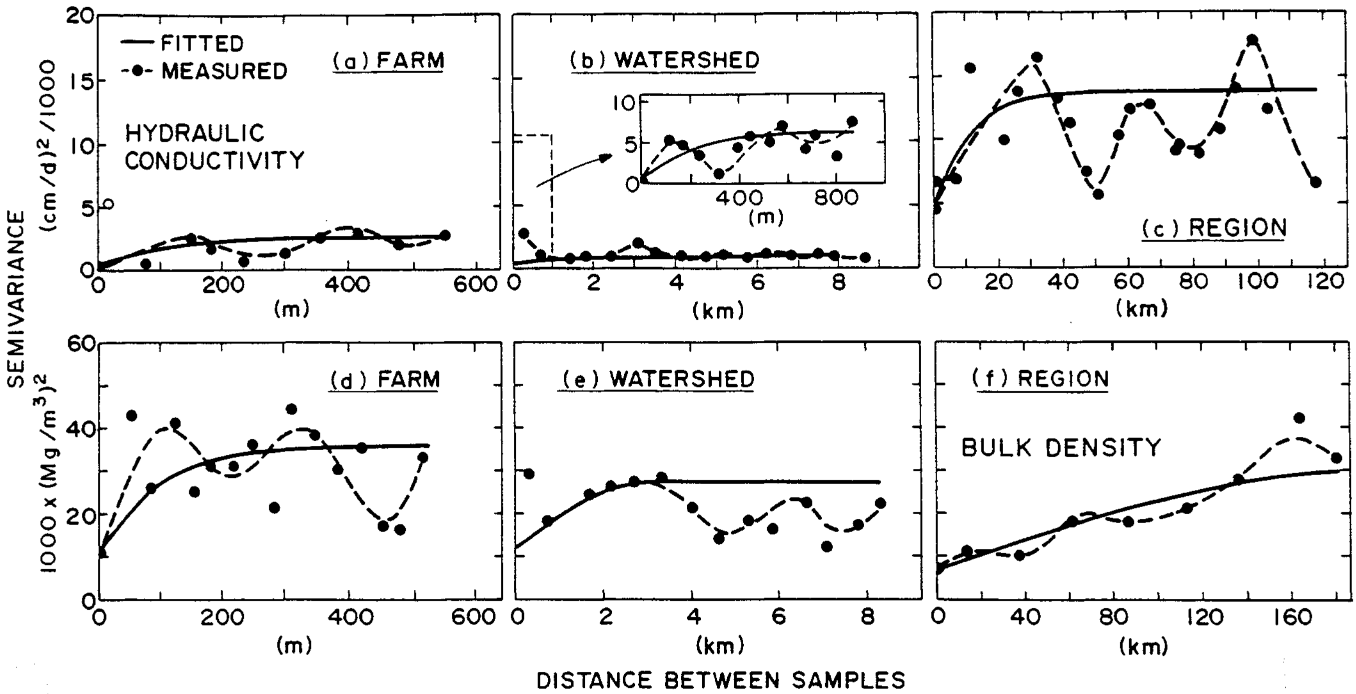
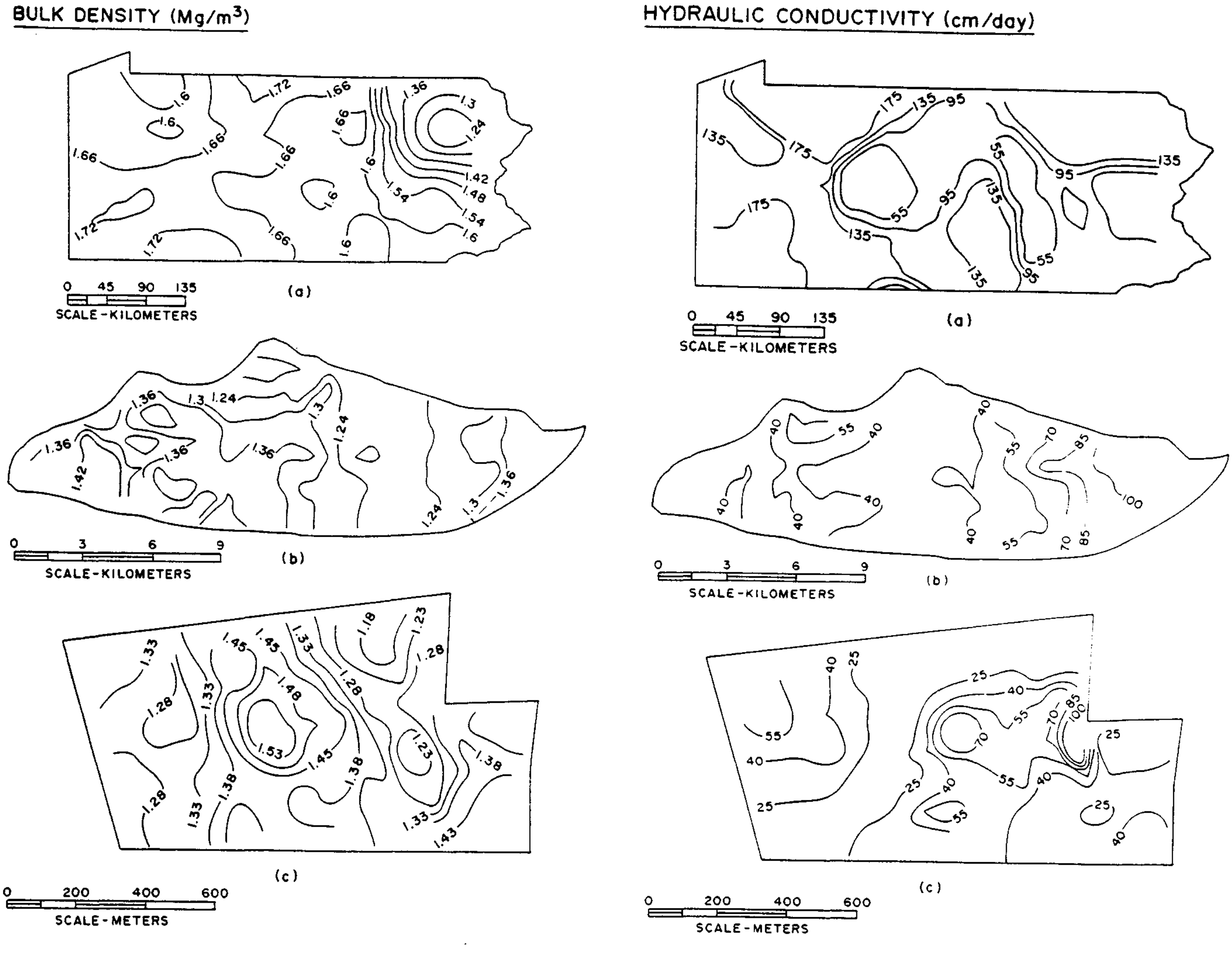


Fig. ? Semivariances of (a, b, and c) hydraulic conductivity and (d, e, and f) bulk density on farm, watershed, and regional scales, respectively.

KRIGING



PEDOGENETIC SCALES

Hoosbeek, M.R. and R.B. Bryant, 1992. Towards the quantitative modelling of pedogenesis. Geoderma, 55:183-210

Scale	Unit
$i+4$	Region
$i+3$	Interacting catchment
$i+2$	Catena or catchment
$i+1$	Field (polypedon)
i	Pedon
$i-1$	Profile horizon
$i-2$	Peds, aggregates
$i-3$	Mixtures
$i-4$	Molecular

POSTSCRIPT

For our readers who have the intention of getting engaged in modeling hydrological events related to soils, we felt obliged to write this postscript. In the nine chapters of the text, we divided the complex reality of soil hydrology into sections which we considered more lucid for individually dealing with each of the main problems. We simplified reality and distinctly described formulations that can be and are currently used in models. The strict physical interpretation of various phenomena as they were discussed in this text are not only beneficial in modeling hydrological events but without their conceptual understanding the modeling of long term hydrological processes would degenerate into more or less sophisticated computer games.

All of our descriptions of the phenomena in nature are more or less approximate, and if their outputs have a quantitative character, the term models is appropriate. Soil hydrologic models can be defined as systems which describe the reality of hydrologic processes (to a certain degree of approximation) in soils for long periods of time such as those associated with a vegetative season, a hydrologic year or a climatic era. In such cases the spatial scale usually must be greater than that of the pedon and the time scale is extended far beyond the time of one isolated elementary hydrologic process. When compared with the processes and events discussed in the previous chapters, the systems are extended or extrapolated in both space and time. If soil hydrologic models are defined in such a way, our text does not cover all of the essential features of modeling soil hydrology. An instructive, comprehensive text on modeling would inevitably include details on numerical procedures, the theory of systems analysis and formulations applicable to spatial scales greater than that of the pedon. For such content, our book would have increased in volume and themes far beyond our goal to offer basic information on soil hydrology. Hence, this postscript.

We are offering here just some introductory notes for a general orientation in the subject. The notes are accompanied by examples selected from the literature. In the discussion we demonstrate how the complexity of the nature in a watershed modifies the processes described earlier in isolated forms.

MODELS OF SOIL HYDROLOGY

We distinguish between physical, analog and mathematical models. A *physical model* is that of a porous medium, e. g. a Hele-Shaw model or a column of glass beads or soil studied in the laboratory. These models frequently have a smaller scale than reality. *Analog models* are based on the similarity of the flow of water in soil to other transport phenomenon, e. g. the flow of electricity through a conductor. Although somewhat common in groundwater studies, these models presently are rarely applied in soil hydrology. *Mathematical models*, the subject matter of this chapter, commonly require computer methods for investigating a specific problem.

Mathematical models in soil hydrology can be classified either according to the principles of the methods applied or according to the subjects modeled.

Further consideration reveals that the nature of either method tends to be empirical, deterministic or stochastic. Inasmuch as the different kinds of models are frequently merged into larger model structures, sharp boundaries between them do not exist. A broadly used classification of mathematical models in soil hydrology originally proposed for leaching models by Addiscot and Wagenet (1985) is:

- I. Deterministic models
  - A. Mechanistic (usually based on rate parameters)
    - 1. Analytical
    - 2. Numerical
  - B. Functional (usually based on capacity parameters)
    - 1. Partially analytical
    - 2. Soil layers and other simple approaches
- II. Stochastic models
  - A. Mechanistic
  - B. Non-mechanistic

Models of agro-ecosystems have been classified into the following groups (Rohdenburg, 1989):

- I. Empirical/mathematical
- II. Deterministic-analytical

According to Rohdenburg, the stochastic nature of agro-ecosystems is not explicitly included in the formulation of their processes but enters implicitly through the spatial variance structure of the deterministic formulation.

The unique character of each of the two classifications above stems from different conceptualizations. The first starts with a Darcian-scale soil column and subsequent broadening of the model brings new and stochastic features into the model. Accepted at the outset that ecosystem processes are phenomena in spatially heterogeneous media, the stochastic characteristics in the second classification stem just from the initial descriptive part of the system.

If mathematical models are placed into only three categories (empirical, deterministic and stochastic), we must remind ourselves that all three have deterministic origins. Additionally, only the deterministic models adhere strictly to a mathematically rigorous, unique formulation of each of the process rates.

From a pragmatic point of view, we distinguish between research-oriented and practice-oriented models. Here we consider not only a requirement for scientific accuracy, but the entire structure of the model and its aim. Recognizing these requirements, we avoid useless questions (e. g. "How do you imagine that we obtain the required population of soil parameters?" and "Do you expect us to make Swiss cheese of our watershed to obtain enough samples?"). And we also avoid arguments from an opposite group (e. g. "This kind of simplification does not comply with our scientific background"). Recently, Reiniger et al. (1990) found that simpler models (compared with more sophisticated models) were either adequate or even more appropriate for describing the transport of nitrates in agricultural soils. Their results should not suggest that simple models be given higher priority automatically. Our recent uncertainty in the quantification of some detailed processes and the uncertainty in estimating some physical characteristics including their statistical character provide even a greater challenge to develop comprehensive models having either a research-oriented or practice-oriented utility.

Reading the literature on models published during the last decade we are reminded of the "rule of 90 percents". Ninety percent of the models presented in papers are not developed sufficiently for others to use them. Of the remaining 10%, 90% of the models are used by only their creators. And of the remaining 10% which are used by others, 90% of the models are never verified. A similar rule also applies to all scientific publications. Although the "rule of 90 percents" is perhaps sad or cynical, it offends neither innovative modelers nor productive scientists.

Empirical Models

We neglect "completely black box" models which represent the roughest form of empiricism. Inasmuch as they are generally not transferable or applicable on a broader scale either in practice or for research, we do not recommend or discuss them here.

The simplest empirical models are eventually based on the empirical concepts of field capacity and wilting point. The balance of inputs (precipitation or irrigation) and outputs (evapotranspiration) is computed at regular time intervals. Field capacity θ_{FC} is considered the maximum water stored within the soil profile during the time interval. If rainfall or irrigation exceeds the disposable unfilled water storage capacity, the excess water drains from the profile. The disposable water storage *DWS* is calculated from

$$DWS = \int_0^Z (\theta_{FC} - \theta_i) dz$$

where Z is the soil depth at the lower boundary of the balanced profile. This empirical model is sometimes denoted as the capacitance model (Addiscot and Wagenet, 1985).

Rainfall or irrigation is assumed to either fully or partly infiltrate into the surface. The first assumption is generally fulfilled by small, flat areas. For the second assumption, the ratio of infiltration to runoff is either verified with the calibration of the model or is obtained analytically or semi-analytically (section 6.2.3). With evapotranspiration commonly formulated by Penman's or Penman-Monteith's equations, the soil water regime for a season is obtained. The reduction of potential to actual evapotranspiration is achieved with the principles formulated in (6.153a) through (6.153d). Or, alternatively, the balance of soil water storage is used to determine the actual evapotranspiration. The soil profile is usually subdivided into layers or "compartments". If cumulative infiltration exceeds the *DWS* of the top layer, the excess is considered as filling the next lower layer. This system of soil water reservoirs occurring in a layered series was first assumed to fill instantaneously without retardation. Later, more realistic rates of soil water movement were formulated using the hydraulic conductivity of each soil layer or "compartment". For example, with each successive compartment first being filled to saturation, the infiltrating water moves through each of water-saturated series of compartments at rate K_S until the cumulative infiltration is accommodated. At that time redistribution of soil water from θ_S to θ_{FC} occurs at a "redistribution rate $q = K(\theta_{FC})$. Various other more complicated modifications exist. Such refinements have the features of deterministic modeling. Even in its simplest form, this model is being successfully used in irrigated agriculture.

The simplest form without flow rates has an advantage over numerical deterministic models. A numerical solution of partial differential equations with a sink term requires small time steps in order to converge. Unfortunately, routine meteorological data do not provide adequate time-dependent information. Therefore, simple water budget models have real value for practical use and are easily used owing to their simple structure. Because water budget models were in initiated early when computers were not available, they have been comprehensively developed with personal computers during the last two decades (e. g. Baier et al., 1979; Petrovič, 1984; Chopart and Vauclin, 1990).

A different subclass of empirical models are those using correlation analysis between the input and the searched output. For example, adequate soil water storage is merely estimated by correlating meteorological characteristics during periods decisive for optimal crop yields. Such empirical relations are associated with soil mapping units without analyzing the physical processes of water within the soil profile.

Deterministic Models

Deterministic models are based on the assumption that a quantitative physical predictability of processes is attainable when events defined on a boundary or within the profile are considered. The outcome (e. g. the flux to the water table or surface runoff) is thus determined by events occurring earlier than those predicted. For example, if we consider the soil water regime [$\theta(z, t)$ or $\theta(x, y, z, t)$] as an outcome, its prediction is realized through a solution of the Richards' equation with a sink term. Here the upper boundary condition at $z = 0$ is defined from meteorological conditions and the lower boundary at $z = Z$ is defined approximately to match field reality. Three different types of conditions can be found at $z = Z$. (i) The Dirichlet condition with soil water pressure head prescribed at the soil surface and connected to the ground water level. (ii) The Neuman condition as a defined flux at the soil surface usually associated with a unit total potential head gradient when the ground water level is absent or is well below depth Z. (iii) The Cauchy condition as a combination of flux and soil water head relations when the fluxes in the unsaturated soil influence and are influenced by regional groundwater flow.

In a sense, the analytical and approximate solutions of elementary soil hydrological processes (Chapter 6) belong to the simplest class of deterministic models and are classified in the subclass as analytical models. We have already pointed out that analytical models are no doubt instructive for understanding processes but they are restrictive regarding direct application to field situations even for distinct and well-defined 1-dimensional elementary hydrologic processes. Soil profile characteristics as well as θ_i are neither constant with depth nor easily defined analytically.

We describe as Pedon Hydrological Models (PHM) those models which are restricted to the scale of a pedon and related to a time scale larger than just one meteorological event. See publications of field tests for soil water regimes during one or more vegetative seasons (e. g. Renger et al., 1970; Vachaud, 1979). In the vast majority of PHM, the method of finite differences is applied to the solution of Richards' equation with the sink term (Feddes et al., 1978). The model SWATRE (Belmans et al., 1983) is an example of a commonly used PHM.

A numerical PHM applied for large time periods (e. g. a cultivated season or a hydrological year) is troubled with problems related to time discretization. In order to achieve stability and convergence of the numerical scheme, small time steps are required. But this requirement is generally not compatible with routinely available meteorological input data. Feddes et al. (1978) and Belmans et al. (1983) tackled the problem in their early finite difference models. And authors of more recent Galerkin models face the problem by posing different time discretizations in finite difference schemes of time. Some PHMs having no universal or generic character are problem oriented. For example, the Dutch simulation model LAMOS (Bouma et al., 1980) predicts the change of soil water regimes and the occurrence of soil water deficits owing to a lowering of the ground water level.

When the study area is substantially greater than that of a pedon, we must deal with soil heterogeneity. If we assume hypothetically that the heterogeneity is only of a deterministic nature, we could use the finite element method. In such a case, with each node point of the grid theoretically being associated with unique and different values of soil hydraulic parameters, the known heterogeneity is projected into the numerical grid. In practice, this advantage is hardly usable inasmuch as sufficiently detailed data are seldom available to represent the soil spatial heterogeneity. And even when they are available, the scale of the computational grid generally does not correspond with that of the measured soil heterogeneity. Moreover, some soil parameters typically vary by orders of magnitude within distances smaller than the spacing of neighboring grid nodes selected to model a simple hydrologic catchment. This difference in scales lead to the concept of equivalent soils – a concept sometimes not explicitly stated.

Finite element methods are often preferred for the solution of 2- and 3-dimensional soil hydrological problems. In many instances, 2-dimensional models suffice. For example, infiltration coupled with runoff and overland flow on a watershed is typically taken as a 2-dimensional problem over the (x, y)-plane. And the Galerkin finite element method with basic linear functions might be used to obtain the solution of the flow equations subject to imposed initial and boundary conditions. This method, now commonly used, is presented in detail in the literature (e. g. Neuman, 1975; Pinder and Grey, 1977). Because of the heterogeneous nature of field soils, the majority of problems described by a deterministic model requires stochastic entries which are next presented.

Stochastic Models

When the study area is substantially larger than that of a pedon, stochastic properties play an important role inasmuch as the pedons do not appear repetitiously across the landscape even if they belong to the area pedotop at the lowest level of soil taxonomy. Hence, we deal with a polypedon or with the pedotop hydrological model (PPHM).

A watershed or a large region usually consists of more than one pedotop and with lower level taxonomic units grouped into higher level units, we speak of pedochors or pedocomplexes. The gradation of pedotops within the watershed is defined as the land surface catena. And, within a pedocomplex or a catena we find predictable deterministic heterogeneity. When the boundaries of the pedotops are crossed, these deterministic soil hydraulic characteristics manifest different values.

The first approach to model unsaturated flow in spatially variable soils was to discretize the field or watershed into a series of 1-dimensional, non-interacting soil columns. This approach is frequently used to describe water regimes of specific regions (e. g. levels of water deficit within regions mapped by soil surveys. Stein et al. (1991) distinguish two procedures. In the first one, simulations are carried out for all points where soil parameters are available. By means of a statistical interpolation method the model output is predicted for the entire area. They describe the procedure as CI, "Calculate first and interpolate later". The method together with earlier similar procedures is given by Stein et al. (1991).

In the second procedure the variables needed for the model are pedologically and functionally clustered. The methods of clustering range from the traditional representative soil profiles found by detailed soil survey to the application of scaling methods. The simulation model is applied to the reference profile indicative of the pedological or functional cluster. This method is denoted by Stein et al. as IC, "Interpolate first and calculate later". Details can be found in publications of Wösten et al. (1985) and Wösten (1990). If scaling is applied with stochastic evaluation, the "accuracy" of the model output can be assessed.

PPHM consisting of vertical soil columns has been applied in theoretical studies of soil heterogeneity. Because the columns were assumed to be randomly located in the area but uniform in depth, we should speak of areal variation instead of spatial variation. In order to simplify the modeling procedure, it is frequently assumed that K_S is the random variable over the area while parameters of $h(\theta)$ and $K_r(\theta)$ remain constant or are simply shifted with a scale factor (Russo and Bresler, 1981; Binley et al., 1989; Aboujaoude, 1991). This kind of modeling for a simply defined heterogeneous block yields new results. If the concept of an equivalent soil representing the heterogeneous block is accepted, the PPHM of infiltration with Neuman's boundary condition for a flat terrain manifests a concave soil water content profile $\theta_R^*(z)$ rather than the convex deterministic profile $\theta_R(z)$ (Bresler, 1987).

For a sloping terrain, the model of vertical, mutually non-interconnected columns is hardly acceptable. It becomes somewhat more acceptable by considering the assumption of "runon". This term describes the redistribution of excess water on the sloping surface from locations of shorter ponding times (small values of K_S) to those downhill locations having larger ponding times (large values of K_S) (Smith and Hebbert, 1979). In addition to this surface interconnection, the interconnection on the basis of continuous saturated flow is sometimes considered. For example, the interconnection exists in the unsaturated zone component of the physically based distributed catchment model SHE (Système Hydrologique Européen, Abbott et al., 1986).

These types of models used for studying the applicability of an "effective soil" (or "effective soil parameters") in soil hydrology are based on the hypothesis that large scale soil heterogeneity can be successfully lumped into parameters descriptive of an "effective soil". Presently, the heterogeneity of unsaturated soils has only been studied through variations of K_S. Studies have shown that the concept of "effective soil" is restrictive and not generally applicable to all boundary conditions and soils. And, when infiltration and runoff are considered, the concept is applicable only for mildly heterogeneous soils (Aboujaoude, 1991).

Vauclin and Vachaud (1990) found that the "effective soil" concept is acceptable for small rainfall intensities on a simple, uniform slope. On such a soil, increased soil variability is accompanied by increased runoff. However, for large rainfall intensities, the concept completely collapsed. Binley et al. (1989) found similar results studying runoff on rapidly and slowly permeable soils. Moreover, the results from using the "effective soil" concept disagree with those from the PPHM when the distribution of K_S in the watershed follows the rules of geomorphological formation, the existence of soil catenas and the genesis of secondary crust formation (Smith et al., 1990; Aboujaoude, 1991).

In spite of its restrictions, the simplified model of an "effective soil" with its vertical columns accompanied with the runon concept brought new views of elementary runoff hydrology. For example, considering the sloping surface of a heterogeneous soil, the ponding time concept as derived for the pedon-scale elementary hydrological process is no longer a constant characteristic value for a given rainfall intensity. The value of the ponding time can decrease by an order of magnitude when the coefficient of variation of K_S increases from 0 to 0.8 on a short uniform slope (Smith et al., 1990).

Contemporary model studies still deal with uniform slopes even though each concavity or convexity of the surface together with vertical heterogeneity produces a convergence or divergence of flow paths (Zaslavsky, 1970; Zaslavsky and Sinai, 1981). Because the transition to 2- and 3-dimensional modeling is sorely needed, we present a brief review of initial, incomplete results.

The model of vertical columns of random characteristics of soil properties is a special case of Monte Carlo simulation. In order to allow non-vertical flow of water, the mutual "isolation" of the columns must be removed. Unfortunately, smoothing the local mosaic or variation of unsaturated soil properties does not achieve the large scale behavior of a watershed. Nevertheless, Mantoglou and Gelhar (1987) have demonstrated that local variability of soil properties has important large scale effects on hysteresis and anisotropy.

For runoff characteristics, the 3-dimensional Monte Carlo study of Binley et al. (1989) of a heterogeneous inclined soil surface (150 x 150 m) has shown that peak runoff volumes increase with heterogeneity and with the spatial dependence of soil parameters. Sharma et al. (1987) gave a simple explanation of subsurface lateral flow that occurred in their 3-dimensional study. They concluded that hill slopes with a random distribution of hydraulic characteristics provide greater opportunity for soil units with different water capacities to interact than those hill slopes with spatially correlated distributions. Their results improved our understanding of subsurface lateral flow because they ignored models of 1-dimensional vertical columns.

MODELS OF SOLUTE TRANSPORT

The most frequently used models of solute transport in soils are Richards' equation (5.64) for unsaturated water flow and the convection-diffusion equation (9.42) for solute transport. The equations are solved numerically where the Galerkin linear finite element scheme is appropriate. In order to keep the model realistic, a multicomponent system accounts for other flow processes. In addition to water flow, heat transport is often included in the model inasmuch as the temperature influences thermodynamic constants and reaction rates significantly. Moreover, the concentration of CO_2 in soil air fluctuates between 0.035 and 20% in extreme circumstances. The solubility of many mineral salts strongly depends upon CO_2 concentration. Changes in CO_2 concentration are accompanied by changes of O_2 concentration in the soil air. Both concentrations influence pH and there is a direct link between both pH and redox potential with dissolution constants and rates. Hence, multicomponent transport models are preferred nowadays just to get closer to field reality.

The majority of recent procedures has involved two simultaneous equations. One for equilibrium chemical processes such as precipitation, dissolution and cation exchange and a second for transport. At each numerical time step, the transport equation is interfaced with the equilibrium chemical equation. However, iteration between the two equations is neglected. Yeh and Tripathi (1991) have shown that this simplification can cause serious numerical errors. Another limiting factor is the consideration of equilibrium reactions only. Suarez (1985) demonstrated that the chemical system is frequently controlled by kinetic reactions. Hence, both equilibrium and kinetic reactions are nowadays directly incorporated into multicomponent systems of transport (Šimůnek and Suarez, 1993).

POST-POSTSCRIPT

Models of soil hydrology should be related to the reality of a field or watershed by at least two links. The first is a proper characterization of the physical parameters of the domain including appropriate processes and boundary conditions. The second link is related to the scale of the model. One part of this link is statistical evaluation while the other part is the degree of approximation allowed in the model. It follows that a modeler should work in or at least supervise the experimental activity in the field. And, vice versa, effective field experimentation requires the theoretical knowledge of the modeler. Hence, *without properly taken field data all our effort is futile.*