

Advances in Agricultural Systems Modeling 10

Transdisciplinary Research, Synthesis, and Applications: Series Editor, Lajpat R. Ahuja

Modeling Processes and Their Interactions in Cropping Systems

Challenges for the 21st Century



Lajpat R. Ahuja, Kurt C. Kersebaum,
Ole Wendroth, Editors



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Transdisciplinary Research, Synthesis, and Applications

Volume 10

Lajpat R. Ahuja, Series Editor

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Lajpat R. Ahuja
Kurt C. Kersebaum
Ole Wendroth

CONTRIBUTORS

Lajpat R. Ahuja (Retired), Supervisory Research Soil Scientist [retired], USDA-ARS, Agricultural Systems Research, Fort Collins, Colorado; **Saseendran S. Anapalli**, Research Soil Scientist, USDA-ARS, Sustainable Water Management Research Unit, Stoneville, Mississippi; **Gary Feng**, Research Soil Scientist, Genetics and Sustainable Agriculture Research Unit, USDA-ARS, Mississippi State, Mississippi; **Puyu Feng**, College of Land Science and Technology, China Agricultural University, Beijing, China; **Gerald N. Flerchinger**, USDA-ARS, Northwest Watershed Research Center, Boise, Idaho; **Timothy R. Green**, USDA-ARS Water Management and Systems Research Unit, Fort Collins, Colorado; **Gerrit Hoogenboom**, Institute for Sustainable Food Systems, University of Florida, Gainesville, Florida; **Kelin Hu**, College of Land Science and Technology, China Agricultural University, Beijing, China; **Suat Irmak, Ph.D.**; Fellow ASABE; Fellow ASCE-EWRI Professor and Department Head Department of Agricultural and Biological Engineering The Pennsylvania State University, Pennsylvania; **Kurt C. Kersebaum**, Senior Scientist at Leibniz-Centre for Agricultural Landscape Research Müncheberg, Germany; and at Global Change Research Institute, CAS, Brno, Czech Republic; Honorary Professor at Georg-August-University Göttingen, Germany; **Meetpal S. Kukal, Ph.D.**, Assistant Research Professor The Pennsylvania State University Department of Agricultural and Biological Engineering, Pennsylvania; **De Li Liu**, New South Wales Department of Primary Industries, Wagga Wagga Agricultural Institute, Wagga Wagga, New South Wales, Australia and Climate Change Research Centre, University of New South Wales, Sydney, Australia; **Jon I. Lizaso**, CEIGRAM-Universidad Politécnica de Madrid, Madrid, Spain; **Alain Perrier**, Université Paris-Saclay, INRAE, AgroParisTech, UMR EcoSys, Thiverval-Grignon, France; **Mark S. Seyfried**, USDA-ARS, Northwest Watershed Research Center, Boise, Idaho; **Marvin J. Shaffer (Retired)**, Supervisory Research Soil Scientist, USDA-ARS, Great Plains Systems Research, Fort Collins, Colorado; **Vakhtang Shelia**, Institute for Sustainable Food Systems, University of Florida, Gainesville, Florida; **Todd H. Skaggs**, USDA-ARS Salinity Laboratory, Agricultural Water Efficiency and Salinity Research Unit, Riverside, California;

Claudio O. Stöckle, Professor and Chair Biosystems Engineering, Washington State University Pullman, Washington; **Donald L. Suarez**, USDA-ARS Salinity Laboratory, Riverside, California; **Dennis J. Timlin**, USDA-ARS Adaptive Cropping Systems Laboratory Beltsville, Maryland; **Andree J. Tuzet**, Université Paris-Saclay, INRAE, AgroParisTech, UMR EcoSys, Thiverval-Grignon, France; **Bin Wang**, New South Wales Department of Primary Industries, Wagga Wagga Agricultural Institute, Wagga Wagga, New South Wales, Australia; **R. Don Wauchope (Retired)**, USDA-ARS, Tifton, Georgia; **Ole Wendroth**, Professor, Plant and Soil Sciences, University of Kentucky, Lexington, Kentucky; **Qiang Yu**, State Key Laboratory of Soil Erosion and Dryland Farming on the Loess Plateau, Institute of Soil and Water Conservation, Northwest A&F University, Yangling, Shaanxi, China AND School of Life Science, University of Technology, Sydney, Australia, AND College of Resources and Environment, University of Chinese Academy of Science, Beijing China

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Crop Science Society of American
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Overview of Modeling processes and Their Interactions in Cropping Systems

Recently observed environmental trends regarding water and soil quality, climate change with extended drought and heat waves (Trnka et al., 2013, 2019), extreme weather events (Trnka et al., 2014), and irrigation water shortages due to urban use require continual adaptation and optimization of agricultural systems through changes in cropping and management. Moreover, the increasing world population and changing diets will raise global food demand by 100–110% from 2005 to 2050 (Tilman et al. 2011). To double food production by 2050, average annual growth rates in crop production of 2.4% (non-compounding rate) would be required (Ray et al. 2013). Considering the limited land resources and the increasing competition for productive land between food, fodder, and energy production, this increase in crop production must be achieved from the same or less land compared with today (Godfray et al., 2010; Zabel et al. 2014). The advancement of science and technology to achieve these changes requires cutting-edge field research, using a quantitative whole-systems approach.

Agricultural systems are composed of physical, biological, and chemical processes of soil, water, plant, climate, their complex interactions, and their management. The whole-system framework is designed for evaluating the impact of management practices and climate on soil water and nutrient dynamics, biomass production, and environmental quality. In this framework, process-level models integrate interdisciplinary knowledge with field research to evaluate management options and to create well-adapted agricultural management systems. The models help to: (a) integrate field research results in terms of the fundamental theory and concepts that are broadly applicable beyond the site-specific empirical relationships; (b) predict crop and soil process dynamics from knowledge of the fundamental drivers that determine the environment and plant growth under different climates, (c) transfer experimental findings to longer term weather conditions beyond the limited duration of field experiments and to soil types and climates diverging from the experimental plots, and (d) use extended results to develop broad-based precision management decision support tools or simple management guidelines for producers and other users, who may link them to economic and social considerations. The models also promote precision management of spatially variable soils (Kersebaum et al., 2005), help assimilate real-time information about soil and crop conditions obtained with remote or ground-level sensors (Wallor et al. 2019) and allow an in-depth analysis of complex policy or management decisions. As a result, the models are continually improved and serve as an evolving theoretical backbone of complex agricultural system research, decision support, and information transfer.

System modeling has been a vital step in many engineering disciplines. A lot more work is needed to bring agricultural system models to the level of physical and hydraulic system models and to enhance their structure and usability. However, agricultural system models have matured enough that, with some good data to serve as reference, they can be used for many practical applications in research and management (Ahuja et al., 2002; Ewert et al., 2015; Jones et al., 2003; Matthews & Stephens, 2002; Michalczyk

et al., 2014; Stöckle et al., 2014). The effect of management practices regarding tillage or no-till management, different crops and cultivars, crop rotations, organic and mineral fertilizers, water supply, and natural or tile drainage on production and water quality can now be modeled (Anapalli et al., 2005, 2015; Andales et al., 2003; Ma et al., 2000; Malone et al., 2017; Wendroth et al., 2019; Yang et al., 2019). Their integration with field research will expose knowledge and conceptual gaps in the models that will then stimulate new research (Rötter et al., 2018). The International Service for National Agricultural Research (2004) made a case for applying modeling tools and processes in planning and implementation of natural resources research and making sense of the vast amount of data. The CGIAR Science Council (2005) noted in their research priorities:

Modeling and the ability to combine data from different sources, promises to revolutionize understanding of processes affecting management of natural resources. Thanks to strategic accumulation of data, tools, and modeling resources in the coming decade, one can expect the development of a more predictive approach to agriculture.

Integration of field research with system models has the potential to significantly enhance the efficiency of agricultural research and raise agricultural science and technology to a higher level, leading to improved production and protection of the environment. Agricultural system models are also used in hydrological, climate, and ecological research and management.

The National Academies of Sciences, Engineering, and Medicine (2019) have released a new report that identifies the most promising scientific breakthroughs that are possible to be achieved in the next decade to increase the U.S. food and agriculture system's sustainability, competitiveness, and resilience in view of the following key challenges faced by agriculture:

- increasing nutrient use efficiency in crop production systems
- reducing soil loss and degradation
- mobilizing genetic diversity for crop improvement
- optimizing water use in agriculture
- improving food animal genetics
- developing precision livestock production systems
- early and rapid detection and prevention of plant and animal diseases
- early and rapid detection of foodborne pathogens
- reducing food loss and waste throughout the supply chain

The first four challenges involve cropping systems. The five breakthroughs for the next decade identified in the report are:

1. Transdisciplinary research and systems approach
2. Sensing technologies
3. Data science and informatics
4. Genomics and precision breeding
5. Animal, soil, and plant microbiomes

Process-based modeling of cropping systems, updated in this volume, will be an essential component of Breakthroughs 1, 3, and 5 and greatly facilitate Breakthroughs 2 and 4. The models are essential tools for evaluating and mitigating the effect of climate change and the management of increasingly limited water and other resources on the production of food, energy, fiber, and environmental quality (Anapalli et al., 2016; Gillette et al., 2018; Stöckle et al., 2010) and to identify yield gaps and analyze their causes to improve crop production for human nutrition (Schils et al., 2018; van Ittersum et al., 2013; van Wart et al., 2013).

Process-Level Components of Cropping Systems and Their Interactions

System models are composed of algorithms that describe several unique process components and their interactions. The primary components are the transport and dynamic status of soil water, mass, and energy (heat), including evapotranspiration; C/N ratio and nutrient dynamics; soil chemical equilibria; pesticide transport and metabolism dynamics; plant growth; the effects of management practices on the basic soil properties that control these processes; and the effect of weather conditions on all the above. How these processes and their interactions are simulated depends on the purpose of modeling and on the input data availability and uncertainty, which finally determines the performance of a system model at a specific scale. Evaluation and continual advances in knowledge of these processes and their interactions help improve the system models. In addition, certain special features of soil processes, such as the presence of active macropores, surface crusting, residue cover, transport of chemicals in runoff, and spatial variability of soil (see the Root Zone Water Quality Model [RZWQM]: Ahuja et al., 2000; Wallor et al., 2018; Wendroth & Robinson, 2008) need to be simulated well. Adequate estimates of the soil and plant parameters that control the above processes and special features are very important for simulations. However, their robustness must be tested under multiple site conditions to be suitable for extrapolation (Kersebaum et al., 2015). The evolution of system models coincides with basic science in agriculture. These unique process models also enhance applications in hydrology, climate, and ecology.

Modeling of soil–plant–climate–management processes is needed to enhance quantitative teaching of these processes at upper undergraduate and graduate levels and elevates education and the skill set of graduate students. The purpose of this volume in the *Advances in Agricultural Systems Modeling* series is to document the modeling of soil–plant–climate–management processes and their interactions in cropping systems and to serve as a textbook for graduate teaching and research. In 2000, we published a book on modeling processes and management effects in the RZWQM (Ahuja et al., 2000). Here, we update the modeling of processes beyond the RZWQM by introducing new concepts and knowledge of process modeling from other models and from new research in this area conducted during the past 20 years.

This publication will be the first comprehensive and updated state-of-the-art scientific textbook devoted to teaching modeling of the key soil–plant–climate–management processes at upper undergraduate and graduate levels; it also emphasizes new opportunities and paradigms for modern laboratory and field research to improve understanding and quantification of individual processes and their interactions.

Lajpat R. Ahuja
Kurt C. Kersebaum
Ole Wendroth

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Lajpat R. Ahuja

Water and Chemical Transport in the Soil Matrix and Macropores

Abstract

In this chapter, we were especially interested in simulating water flow and chemical transport through macropores explicitly, as well as in the soil matrix. For this goal, we divided the water flow process into two phases: (a) infiltration into the soil matrix and macropores and macropore–matrix interaction during a rainfall or an irrigation, modeled by using the semi-analytical, vertical and radial, Green–Ampt approach, which has been theoretically related to Richards’ equation; and (b) redistribution of water in the soil matrix following infiltration, computed by a mass-conservative numerical solution of the one-dimensional Richards equation. The chemical transport during both of these phases is based on the established concept of miscible displacement but is done in a simpler way using partial piston displacement followed by partial mixing in small depth increments. Again, the Green–Ampt approach during infiltration allowed explicit transport of chemicals through macropores and explicit interaction between chemical transport through macropores and the soil matrix.

Introduction

Water flow in soil is the driving force behind all the belowground processes of an agricultural system and significantly affects aboveground plant growth and surface hydrology. It determines how much water is stored in the root zone and how much is taken up by the roots at any given time and how surface-applied fertilizers and heat are transported through this zone. All the vital microbial and biochemical transformations of organic matter and nutrients are highly dependent on soil water content and temperature. Thus, the ability of a plant to grow is also highly dependent on water

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Edited by Lajpat R. Ahuja, Kurt C. Kersebaum, and Ole Wendroth.

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flow. Furthermore, this flow largely determines how applied agricultural chemicals are transferred to surface runoff or leached below the root zone and thus how serious the impacts are on the quality of our surface and groundwater resources. This chapter is an update of Ahuja et al. (2000).

The theories of soil water movement and the related transport of chemicals and heat are now well developed for simple soil systems. One-dimensional vertical movement and retention of water in a partially or variably saturated soil profile is commonly described by a simpler form of the Richards equation that incorporates Darcy's Law and mass conservation and assumes that the role of the soil air or vapor phase and thermal gradients on the liquid flow process is negligible:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[K(h, z) \frac{\partial h}{\partial z} - K(h, z) \right] - S(z, t) \quad (1.1)$$

where θ is volumetric soil water content ($\text{cm}^3 \text{cm}^{-3}$); t is time (h); z is soil depth (cm, assumed positive downward); h is the soil-water pressure head (cm), a function of θ ; K is unsaturated hydraulic conductivity (cm h^{-1}), a function of h and z ; and $S(z, t)$ is a sink term for root water uptake and tile drainage rates (h^{-1}).

Equation 1.1 can be used to described infiltration of water at the soil surface from rain or irrigation, with known rates or surface depths, and subsequent redistribution in the soil profile. For very dry portions of the soil profile, not commonly encountered in agriculture, vapor flow and the effect of soil temperatures on both liquid and vapor flow can be important. Equation 1.1 can then be modified to include these effects (Šimůnek et al., 2013). The modified equation has to be solved in conjunction with the soil heat flow equation.

The theories of chemical and heat transport in soil are based on the concept of miscible displacement of chemicals and heat by the flow of water. This concept is commonly approximated by a convection–dispersion equation. One-dimensional, miscible displacement of an absorptive and degradable chemical species through a soil column of constant water content and flux is simulated by

$$\frac{\partial}{\partial x} \left(D \frac{\partial C}{\partial x} \right) - v \frac{\partial C}{\partial x} - R \frac{\partial C}{\partial t} = \mu C - \gamma \quad (1.2)$$

where $C = C(x, t)$ is the chemical concentration at location x and time t ; $D = \alpha_L |v|$ is the dispersion coefficient; α_L is the dispersivity; $v = q/\theta$ is the pore water velocity; θ is the volumetric water content; q is the flux density of the soil water (or the Darcy velocity); $R = 1 + \rho K_d/\theta$ is the retardation factor; ρ is the soil bulk density; K_d is the partition coefficient between solution and adsorbed phases at equilibrium; μ is the first-order decay constant; and γ is the zero-order production rate constant. For field conditions, this equation is extended to variable water contents and fluxes with space and time by solving in conjunction with the Richards equation. This equation can also be extended to nonlinear partition and nonlinear nonequilibrium or coupled sequential decay reactions (Šimůnek et al., 2013; see also Chapter 7). The heat transport equations are given in Chapter 2.

Generally for field conditions, Equations 1.1 and 1.2 have to be solved by the complex numerical methods. Simpler partially analytical approaches to these equations are available for certain conditions. However, real field soils have several complexities that play important roles which, at this stage, are not completely understood in mechanistic terms. Examples of these complexities are:

- the role of macropores—worm holes, decayed root channels, or structural cracks—in short-circuiting movement of water and chemical from soil surface to deeper layers. Šimůnek et al. (2013) approximately simulated macropore flow implicitly by an interacting dual-permeability (two-soil) system with the one-dimensional Richards equation applied to each soil.
- the role of surface aggregates in retarding downward leaching of surface-applied chemicals but increasing their transfer to runoff or to macropore flow.
- the role of interaggregate immobile pore space and chemical kinetics inside the soil matrix in retarding or enhancing transport of chemicals. This has been simulated by the Richards equation as a dual-porosity (mobile–immobile) system (Šimůnek et al., 2013).
- enormous changes in the basic soil hydraulic properties, macropores, and aggregation brought about by tillage and followed by temporal changes due to reconsolidation.
- the roles of a high water table and an installed drainage system, when incorporated in a one-dimensional model.

Most of the common cropping system models use simple sequential cascading schemes of water and chemical movement and retention in the root zone, following estimation of infiltration by a simple method such as the SCS Curve Number approach. In modeling water and chemical transport in the Root Zone Water Quality Model (RZWQM) (Ahuja et al., 2000), we utilized the existing theoretical understanding of simple soil systems but also incorporated the role of the above complexities in some simple ways, consistent with our limited knowledge of these complexities at this time. We were especially interested in simulating macropore water flow and chemical transport explicitly. For this goal, we divided the water flow process into two phases: (a) infiltration into the soil matrix and macropores and macropore–matrix interaction during a rainfall or an irrigation, modeled by using the semi-analytical, vertical and radial, Green–Ampt approach (Green & Ampt, 1911), which allows explicit flow through macropores and macropore–soil matrix interactions that the one-dimensional Richards equation does not, and has been theoretically related to the one-dimensional Richards equation (Ahuja, 1983; Morel-Seytoux & Khanji, 1974) and (b) redistribution of water in the soil matrix following infiltration, computed by a mass-conservative numerical solution of the one-dimensional Richards equation (Celia et al., 1990). Chemical transport in the soil matrix during both of these phases is based on the established concept of miscible displacement but is done in a simpler way using partial piston displacement followed by partial mixing in small depth increments. Again, the Green–Ampt approach during infiltration allowed explicit transport of chemicals through macropores and explicit interaction between chemical transport through macropores and the soil matrix.

This chapter describes the components of the model relevant to water flow and chemical transport through the soil matrix and macropores.

Description of the Soil Profile

In order to simulate the transport of water and chemicals, the soil profile must be well defined in its depth, horizon delineation, and physical and hydraulic properties. It can have either homogeneous soil properties with depth or up to a certain number of distinct soil horizons. The RZWQM uses soil horizons to define segments with like soil properties. It then creates two numerical grids, one a nonuniform layering system

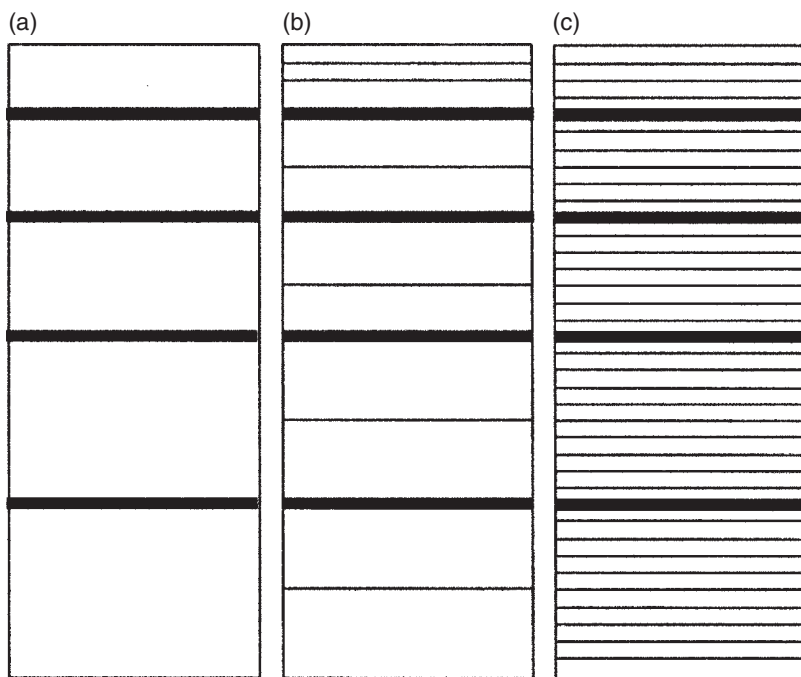


Figure 1.1 The three transport grids used by the Root Zone Water Quality Model: (a) soil profile delineated by horizons for defining hydraulic properties; (b) soil profile delineated by numerical layers for redistribution; and (c) soil profile delineated by 1-cm layers for infiltration.

for redistribution and the other a 1-cm grid used during infiltration (Figure 1.1). These grids are discussed further under Numerical Methods and Space Discretization.

Each soil horizon is characterized by its own soil physical and hydraulic properties. The physical properties are bulk density, particle density, porosity, and texture. Hydraulic properties are defined by the soil water content–matric suction relationship and the unsaturated hydraulic conductivity–matric suction relationship. These relationships are described by functional forms suggested by Brooks and Corey (1964) with slight modifications (Figure 1.2). The Brooks–Corey parameters have been compiled by Rawls et al. (1982) for 11 soil textural classes. These relationships are assumed non-hysteretic.

The soil water content versus the matric suction relationship is represented by

$$\begin{aligned}\theta(\tau) &= \theta_s - A_1 \tau; & \tau \leq \tau_b \\ \theta(\tau) &= \theta_r + B \tau^{-\lambda}; & \tau > \tau_b\end{aligned}\tag{1.3}$$

where θ is volumetric soil water content ($\text{cm}^3 \text{cm}^{-3}$), τ is matric suction head (cm, $\tau = |h|$, where h is the soil water pressure head), θ_s is the saturated soil water content ($\text{cm}^3 \text{cm}^{-3}$), θ_r is the residual water content ($\text{cm}^3 \text{cm}^{-3}$), τ_b is the air-entry or bubbling suction head (cm), λ is the pore size distribution index, and A_1 , B , and λ are constants. The constant B is not an independent parameter; it is determined from other parameters by the condition of continuity at $\tau = \tau_b$. When A_1 is set equal to zero, Equation 1.3 reduces to the Brooks–Corey model.

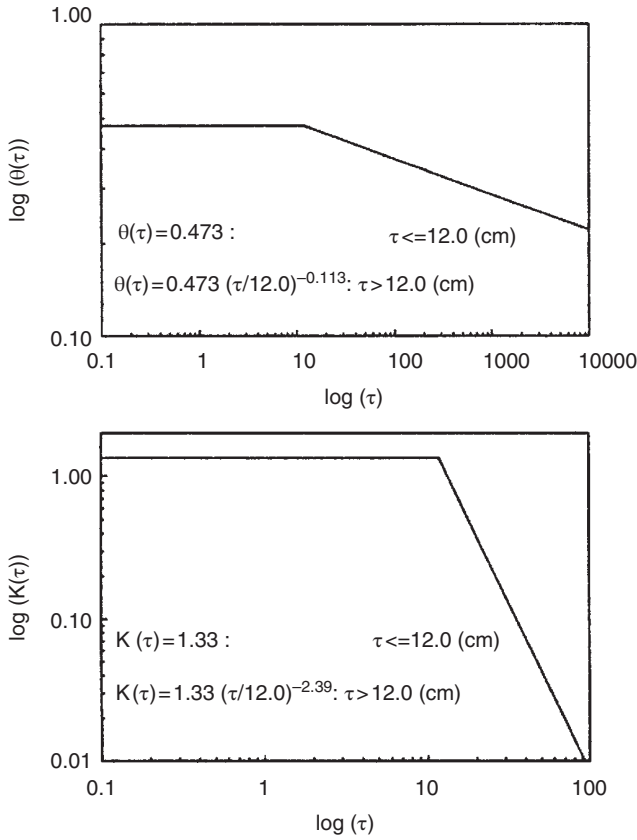


Figure 1.2 An example of the soil hydraulic property functions (soil water content–suction curve $[\theta-\tau]$ and hydraulic conductivity–suction curve $[K-\tau]$) used in the model. The values of the variables used in Equations 1.3–1.4 are $\theta_s = 0.473$, $A_1 = 0.0$, $\theta_r = 0.0$, $B = 0.473/(12^{-0.113})$, $\lambda = 0.113$, $\tau_b = 12.0$, $K_s = 1.33$, $N_1 = 0.0$, $K_2 = 1.33/(12^{-2.39})$, $N_2 = 2.39$, and $\tau_{bK} = 12.0$. *Source:* Based on Brooks and Corey 1964.

The hydraulic conductivity versus matric suction relation is expressed as

$$\begin{aligned} K(\tau) &= K_s \tau^{-N_1}; & \tau \leq \tau_{bK} \\ K(\tau) &= K_2 \tau^{-N_2}; & \tau > \tau_{bK} \end{aligned} \quad (1.4)$$

where K is hydraulic conductivity (cm h^{-1}), K_s is field-saturated hydraulic conductivity (cm h^{-1}), and τ_{bK} is the air-entry or bubbling suction head for this function (cm), which may be equal to τ_b introduced above, and N_1 and N_2 are constants. In the original Brooks–Corey equation, N_1 is zero, $K_2 = K_{sr}$, and $N_2 = 2 + 3\lambda$.

Another commonly used model of soil hydraulic properties was proposed by van Genuchten (1980). This model smooths the water retention curve near saturation:

$$\begin{aligned} \theta(h) &= \frac{\theta_r + (\theta_s - \theta_r)}{(1 + |h|^m)^{1/m}}; & h \leq 0 \\ \theta(h) &= \theta_s; & h \geq 0 \end{aligned} \quad (1.3a)$$

where h is the soil water pressure head ($-\tau$, cm), $\theta(h)$ ($\text{cm}^3 \text{cm}^{-3}$) is the volumetric water content (for $h < 0$), θ_r ($\text{cm}^3 \text{cm}^{-3}$) is the residual water content, θ_s ($\text{cm}^3 \text{cm}^{-3}$) is the saturated water content, m is $1 - (1/n)$ with $n > 1$, and α (cm^{-1}) and n are empirical parameters determining the shape of the curve. Equation 1.3a smooths the water retention curve around the air-entry value.

$$K(h) = K_s S_e^l \left[1 - \left(1 - S_e^{1/m} \right)^m \right]^2 \quad (1.4a)$$

where K_s (cm h^{-1}) is saturated hydraulic conductivity and S_e is the effective saturation, expressed as $S_e = (\theta - \theta_r) / (\theta_s - \theta_r)$. The value of the exponent l in the K function is about 0.5 as an average for many soils.

Vogel and Císlerová (1988) modified the van Genuchten equations to add flexibility in the properties near saturation (higher values). Kosugi (1996) proposed a lognormal distribution model for water retention.

Estimation of Soil Hydraulic Properties

When, as often happens, measured data for these hydraulic properties are not available, they are estimated from regression equations with simpler known properties of soil texture, bulk density, and soil-water content at a 333-cm (1/3-bar) suction head ($\theta_{1/3}$). The technique can also be applied if, instead of the 333-cm value, the soil-water content at 100-cm suction is known. If neither soil-water content value is known, the parameters for the hydraulic property functions are taken from Rawls et al. (1982) based on soil texture class and adjusted based on bulk density alone.

Similar-Media Scaling

If one value of the $\theta(\tau)$ relationship is known, the rest of the function values are estimated by the extended similar-media scaling technique (Ahuja et al., 1985). According to the scaling concept (Simmons et al., 1979; Warrick et al., 1977), the matric suction for a fixed degree of saturation, S [$S = (\theta - \theta_r) / (\theta_s - \theta_r)$], at the i th site, $\tau_i(S)$, is related to the mean τ value for a soil type, $\tau_m(S)$, by

$$\alpha_i \tau_i(S) = \tau_m(S) \quad (1.5)$$

where α_i is a scaling factor for the i th site that applies at all different values of S . Therefore, if $\tau_m(S)$ is known and one value of $\tau_i(S)$ is also known, we can obtain the rest of the unknown $\tau_i(S)$ function. In our model, we utilize the textural-class mean $\theta(\tau)$ or $\tau(S)$ functions of Rawls et al. (1982) as our reference $\tau_m(S)$ functions. We also assume that the soil texture, bulk density, and the 333- or 100-cm water content at the unknown i th site are known. The value of θ_s is assumed equal to porosity, which can be calculated from the soil bulk density. Thus we can estimate the entire $\tau_i(S)$ or $\theta_i(\tau)$ function. This scaling technique is illustrated in Figure 1.3.

A different technique is used in the model to estimate changes in soil hydraulic properties due to tillage and subsequent reconsolidation. For this purpose, the change in soil bulk density is assumed to be known. The effects of tillage on soil bulk density and hydraulic properties are discussed in Chapter 11.

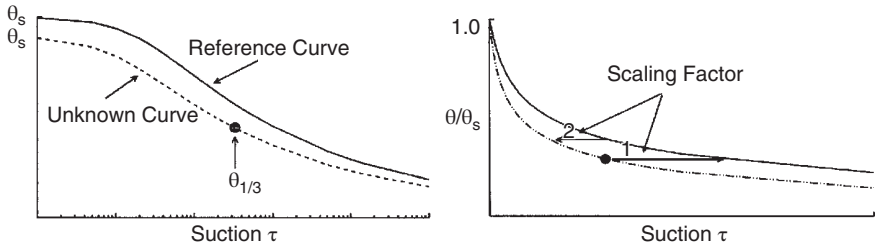


Figure 1.3 Scaling approach used to estimate the soil water content—suction relationship, $\theta(\tau)$, from two known points, θ at saturation (θ_s) and θ at 333-cm suction head ($\theta_{1/3}$), and a reference curve for the soil type or textural class.

One-Parameter Model

A one-parameter model is based on the strong linear correlation ($R^2 = 0.95$) observed between the slope b and intercept a of the log–log linear $h(\theta)$ form of the Brooks–Corey equation below the air-entry value (Ahuja & Williams, 1991; Gregson et al., 1987). Furthermore, the a versus b relationship of a large group of soils merged very nicely into one common relationship $a = p + qb$, with p and q nearly constant for all soils. This allows the determination of the $h(\theta)$ function from one known value, preferably the field capacity 333-cm soil water content. This model gave good results for several soils.

The saturated hydraulic conductivity (K_s) can be user defined or estimated from the effective porosity (ϕ_e), which is defined as

$$\phi_e = \theta_s - \theta_{1/3} \quad (1.6)$$

Recent work by Ahuja et al. (1989) with nine different soils indicated that the K_s of a soil layer is strongly related to ϕ_e as

$$K_s = 764.5\phi_e^{3.29} \quad (1.7a)$$

with $R^2 = 0.67$ and RMSE of $\log K_s = 0.613$

Number of data points for Equation 1.7a = 473

Fitting to the texture mean values of Rawls, et al (1982) also gave good results:

$$K_s = 509.4\phi_e^{3.633} \quad (1.7b)$$

The measurement of saturated hydraulic conductivity is normally subject to a large error (an order of magnitude) because of the unknown effects of air entrapment and the presence of macropores. Considering this limitation, Equations 1.7a and 1.7b provide a good means to estimate K_s where measured data are not available. From knowledge of K_s and $\theta(\tau)$, the complete unsaturated hydraulic conductivity function, $K(\tau)$, is obtained by utilizing the approximate capillary-bundle approach described by Campbell (1974) and others. Once soil properties are defined, modeling of flow and transport processes begins.

Vertical Infiltration of Water into the Soil Matrix

The Green–Ampt equation is used to calculate infiltration rates into a homogeneous or layered profile divided into 1-cm increments (Childs & Bybordi, 1969; Green & Ampt, 1911; Hachum & Alfaro, 1980):

$$V = \bar{K}_s \frac{\tau_c + H_o + Z_{wf}}{Z_{wf}} \quad (1.8)$$

where V is the infiltration rate at any given time (cm h^{-1}), $\bar{K}_s$ is the effective average saturated hydraulic conductivity of the wetting zone (cm h^{-1}), τ_c is the capillary drive or suction head at the wetting front (cm), H_o is the depth of surface ponding (cm), if any, and Z_{wf} is the depth of the wetting front (cm).

If the infiltration rate calculated by Equation 1.8 is greater than the rainfall rate, it is set equal to the rainfall rate (Mein & Larson, 1973). If the converse is true, the excess rainfall is considered overland flow (runoff).

For a homogeneous soil or surface of a layered soil, the effective saturated hydraulic conductivity, $\bar{K}_s$, in Equation 1.8 is set equal to the field-saturated hydraulic conductivity of the soil or horizon. For a layered soil profile with hydraulic conductivity decreasing with depth, $\bar{K}_s$ is set equal to the harmonic mean effective saturated hydraulic conductivity of the wetted zone (Childs & Bybordi, 1969; Hachum & Alfaro, 1980). Thus, for such a layered soil, the effective saturated hydraulic conductivity changes as the wetted depth increases with time. If the saturated hydraulic conductivity of a subsoil layer in a layered soil is greater than that of the layers above, the conductivity of the previous layer continues to govern the flow in this subsoil layer (Hanks & Bowers, 1962).

Based on the work of Bouwer (1969), Morel-Seytoux and Khanji (1974), and Brakensiek and Onstad (1977), it has been found that $\bar{K}_s$ in Equation 1.8 may be reduced by about half due to entrapped air and the resulting viscous resistance. Thus, the actual infiltration rate may be less than that predicted by Equation 1.8. To account for the effects of entrapped air, $\bar{K}_s$ is divided by a viscous resistance correction factor of 2.0, changing Equation 1.8 to

$$V = \frac{\bar{K}_s}{2.0} \frac{\tau_c + H_o + Z_{wf}}{Z_{wf}} \quad (1.9)$$

To account for the effects of a surface crust, an adjustment is made to the saturated hydraulic conductivity, K_s , of the first horizon. Assuming the crust is 0.5 cm thick with a known conductivity, we approximate the value of the suction head at the crust–soil interface under steady-state conditions. Then, the saturated conductivity of the first horizon is assumed to be the conductivity associated with this head value. Because infiltration is governed by the smallest K_s of the wetted soil, this adjusted value can greatly decrease infiltration. Surface crusts are destroyed by tillage and are assumed to reform immediately after rainfall.

The capillary drive, τ_c , in Equation 1.9 varies from horizon to horizon, corresponding to the location of the wetting front. It is calculated from the unsaturated hydraulic conductivity–suction function, $K(\tau)$, of the wetting horizon as (Ahuja, 1983; Swartzendruber, 1987)

$$\tau_c = \frac{\int_0^{\tau_n} K(\tau) d\tau}{K_s} \quad (1.10)$$

where τ_n is the suction corresponding to the average initial soil water content of the soil horizon. The $K(\tau)$ function can be analytically integrated to solve for τ_c .

A simple and efficient scheme is then used to obtain cumulative infiltration with time. It involves the following steps:

1. An average infiltration rate, V , is calculated by Equation 1.9 using Z_{wf} corresponding to the middle of the 1.0-cm wetting increment.
2. The moisture deficit in this increment is calculated as the difference between the known field-saturated value for the layer (taken as 0.9 or a given fraction of porosity) and the initial moisture (the initial moisture of the wetting increment can change from the original value by lateral absorption below the wetting front from macropores, if present, as described below).
3. The time step in wetting this increment of soil is defined as the deficit divided by the average infiltration rate.
4. These incremental deficits and time steps are summed, thus calculating the cumulative infiltration and time.

The time step for infiltration is thus the time required to wet the last wetting 1-cm increment. The time step increases with time.

Flow into Tile Drains During Infiltration

Movement of water and chemicals below the wetting front during infiltration is assumed to occur according to unit gradient flow except in two cases. In the case of a constant pressure head bottom boundary condition, no transport occurs below the wetting front during infiltration. Unit gradient flow is also not assumed if a water table is present, but it is replaced by a different algorithm, discussed below. In all other cases, however, water contents and chemical concentrations below the current depth of wetting are updated according to the hydraulic conductivity of each 1-cm increment at the end of each time step. This allows for some redistribution to occur during rainfall events and results in a small amount of leakage below the lower boundary of the profile.

When a water table is present in the soil profile above the depth of tile drains, a flux out of the drain will occur. The drainage rate is calculated from soil conditions just prior to infiltration according to the Hooghoudt equation (as outlined below). In addition, if a positive leakage rate out the bottom of the profile exists, seepage from the water table will also occur. The water that flows to the drain and out the bottom of the profile at each infiltration time step is taken from the 1-cm layer at which the water table begins, with the requirement that this layer remain above the water content at 100-cm suction (Figure 1.4). If it should fall below this water content, the water table is moved down 1 cm and the water is taken from the next 1-cm layer. If the water table falls below the tile drain, no more drainage will occur during the infiltration event, although seepage will continue.

On the other hand, if the wetting front should catch up to the water table, completely saturating the profile, the rainfall event continues by taking time steps of five minutes.

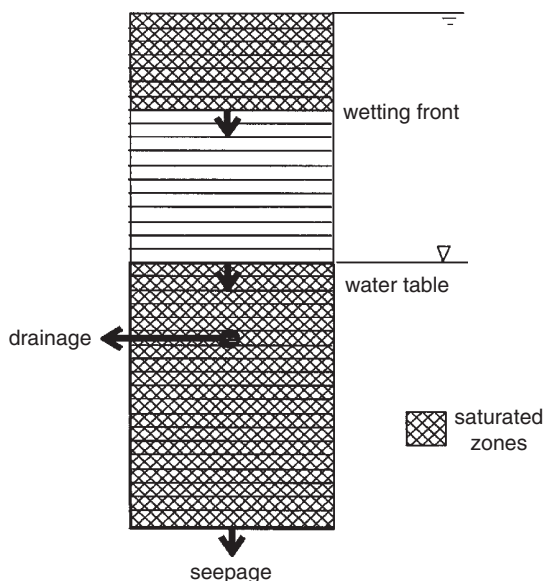


Figure 1.4 Movement of water during infiltration. The wetting front moves down in 1-cm increments as each 1 cm becomes saturated. The water table likewise moves down as water from the top of the water table is moved through the profile into drainage and/or seepage.

A new drainage rate is calculated based on the new depth of the water table, assumed to be at the surface. Then rainfall infiltrates at the drainage plus leakage rates, with any excess going into runoff. If the rainfall rate is such that it cannot satisfy drainage demands, the soil surface layers can become desaturated, and the water table will move back down.

Transport of a Chemical Within the Soil Matrix during Infiltration

We use a sequential partial-displacement and mixing approach in 1-cm increments to transport solutes in the spirit of the established phenomenon of the miscible displacement. However, the soil matrix is subdivided into micropore (immobile) and mesopore (mobile) zones, which introduces a form of preferential chemical transport in the soil matrix (the preferential flow in macropore channels outside the soil matrix is treated separately). The soil matrix porosity is divided into meso- and micropores based on either the user input values of these or the partitioning of the soil water retention curve at an arbitrary suction of 2,000 cm (Addiscott, 1977). Initially and during first wetting of a 1-cm depth increment, the water and chemicals in meso- and micropores are in equilibrium. During successive infiltration steps, the miscible displacement of solution in the saturated soil layers occurs only in the mesopores (mobile regions). This approach is similar to the layer model of Addiscott (1977), but the method of displacement involves only partial piston displacement as described below.

For each infiltration step, the soil solution is partially displaced sequentially across the 1-cm soil increments in the manner of piston displacement, followed by mixing in

each increment. To simulate this partial displacement, we assume a two-stage process. In the first stage, half of the volumetric air space of the wetting increment is filled. Soil solution is displaced through the mesopores of the wetted increments by this amount and mixed before the second displacement step is taken. The second step then moves the remaining water and its solution through the mesopores of the wetted profile in the same manner. This two-stage process simulates miscible displacement and dispersion in the mesopores. In soils that are initially very dry and in which the dispersion is low, we have obtained better results with a one-stage displacement, but the two-stage process works well in most cases and no changes are needed in the program.

The model allows diffusion between meso- and micropore solutions for certain chemicals applied by the user, such as pesticides or tracers. The equation for this process is

$$\frac{\Delta C_{\text{sol}}}{\Delta t} = D_a (C_{\text{micr}} - C_{\text{sol}}) \quad (1.11)$$

where C_{sol} is the concentration of chemical in solution (mg L^{-1}) in the mesopores, C_{micr} is the concentration in solution of the micropores (mg L^{-1}), and D_a is the apparent diffusion coefficient or diffusion distance factor (user defined or calculated from a default database).

At the end of each time step, the exchange of chemical is calculated and the concentrations in each 1-cm increment appropriately adjusted.

For a soil-adsorbed chemical, such as some pesticides, a linear relationship and an instantaneous equilibrium are assumed to occur between the soil solution and adsorbed phases in both meso- and micropore regions. We also have an option in the model to allow a portion of a reactive chemical in the soil matrix to be subject to a first-order kinetic absorption-desorption between solid and solution phases. The equations for these processes are (Cameron & Klute, 1977)

$$C_{\text{ad}} = f K_d C_{\text{sol}} \quad (1.12)$$

$$\frac{\Delta C_{\text{ab}}}{\Delta t} = R_{Kz} [(1-f) K_d C_{\text{sol}} - C_{\text{ab}}] \quad (1.13)$$

where C_{ad} is the concentration of chemical on the soil surface (g g^{-1}) in equilibrium with the solution phase, C_{sol} is the concentration in the soil solution (mg L^{-1}), f is the fraction of sorption sites of soil in equilibrium, K_d is the partition coefficient between C_{sol} and C_{ad} , C_{ab} is the concentration in the solid phase (g g^{-1}) not in instantaneous equilibrium (kinetic pool), t is time, and R_{Kz} is a kinetic rate constant.

The parameters needed for the processes are either user supplied for each chemical or obtained from a default empirical database.

At the end of an infiltration event, when the water movement slows down, the meso- and micropore regions are allowed to equilibrate and the overall solute concentration is calculated. However, instantaneous equilibrium and kinetic pools are kept separate for redistribution.

If the water table is present, the flux within the water table will carry chemicals with it that may go out through the drain and into seepage. The transport of chemicals in this saturated zone is calculated using piston displacement in only the mesopores, similar to the method described below. After the initial infiltration and chemical transport into the soil matrix has occurred within a time step, the flux of water from the top of the water table to the bottom of the profile is displaced sequentially across the 1-cm increments, mixing with the chemical concentration in the mesopores of each increment. At the depth of the tile drain, the new mesopore chemical concentration is the

concentration in the drainage water. Similarly, the concentration of chemicals in the seepage water is equal to the concentration in the mesopores in the bottom layer of the profile. To simplify the processes in the water table, two-stage displacement, diffusion between micro- and mesopores, and kinetic absorption-desorption processes are not simulated. The meso- and micropore regions below the water table are allowed to equilibrate at the end of the infiltration event.

Transfer of the Chemical to Overland Flow during Rainfall

Overland flow (also referred to as runoff) is calculated as the difference between the rainfall and infiltration in each time step. The model does not currently simulate the storage of runoff, but instead, in the absence of macropores, considers this water and its chemical solution as a loss to the system. The chemical in overland flow is extracted from the soil surface layers by raindrop impact. The extraction occurs from depths as great as 2 cm, but the contribution decreases exponentially with depth (Ahuja, 1986). This process can be modeled as an accelerated diffusion (Ahuja, 1990), but here we use a simpler approximation. We model this extraction process with a nonuniform mixing model (Ahuja, 1986; Heathman et al., 1986). The degree of mixing (M) between rainwater and soil solution in the micro- and mesopores is assumed to be complete (equal to unity) at the soil surface ($z = 0$ cm) and to decrease with depth as

$$M = \exp(-bz) \quad (1.14)$$

where b is a parameter that depends somewhat on the soil type, surface roughness, and cover conditions. Equation 1.14 can be integrated over a 1-cm increment and an average value of mixing, M_{ave} , calculated. This value may then be expressed in the same functional manner as Equation 1.14 as

$$M_{ave} = \exp(-Bz) \quad (1.15)$$

where B is a new exponent, different from b , and z is the depth of the midpoint of the increment. The value of B is kept constant for both of the top two soil compartments, which, with the experimentally determined value of B as 4.4 cm^{-1} (Ahuja, 1986), gives a degree-of-mixing value in the 1–2-cm layer of approximately 1/100 of that in the top 1-cm increment. We compute chemical transfer to overland flow (then available to move into the macropores or run off the site) from micro- and mesopores by Equation 1.15 at the midpoint of the top two 1-cm intervals. During each infiltration step in which overland flow occurs, the chemical is first transferred to the rainfall solution, part of which then infiltrates into the soil. Thus, the water that infiltrates during the time interval has the same chemical concentration as the overland flow.

Transport of Overland Water and Chemical in Solution through Macropores

Two domains of flow, the soil matrix and macropore channels, interact through the walls of the macropores, which act as a common boundary condition or a source-sink term. Thus, in concept, our model is similar to the transient water flow models of Hoogmoed and Bouma (1980), Beven and Germann (1981) and Hetrick et al. (1982). However, the methods used here are different. The only source of water and chemicals transported through the macropores is the overland flow (rainfall excess) generated at

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