Abstract. This paper reviews recent progress in modeling water flow and solute transport in the unsaturated ( vadose) zone. Much progress has been attained in the analytical and numerical description of vadose zone and exchange processes. A variety of deterministic models are currently available for describing and predicting these processes. The most popular ones continue to be the classical Richards equation for unsaturated flow and the phenomenological convection-dispersion equation for solute transport. While deterministic solutions of these equations remain useful tools in research and management, their practical utility for predicting actual field water and solute concentration is increasingly being questioned. Problems caused by preferential flow through soil macropores and by spatial and temporal variability in soil hydraulic properties have caused some disillusionment with the classical models. A number of alternative deterministic and stochastic formulations have been proposed to specifically deal with preferential flow and/or spatial variability. These models have greatly increased our understanding of field scale transport processes, and have in some cases led to better practical tools for management purposes.

Introduction

The importance of the unsaturated ( vadose) zone as an inextricable part of the hydrological cycle has long been understood. Theoretical and experimental studies on water flow and solute transport in this zone have been further motivated by concerns about soil and groundwater pollution, as well as by attempts to optimally manage the root zone of agricultural soils for maximum crop production. These studies have greatly increased our conceptual understanding of the many complex and interactive physical, chemical and microbiological processes occurring in the unsaturated zone. They have also led to a large number of predictive models dealing with various parts of the atmosphere-surface-subsurface transfer problem. Awareness that the flow and transport properties of field soils can be highly variable in time and space has added additional scientific and technological complexities to the modeling venture. In this paper we will briefly review recent progress in modeling unsaturated water flow and solute transport. The main emphasis will be on internal vadose zone transport processes, with little or no discussion of infiltration, evapotranspiration, and of heat or gas transfer.

Classical Modeling Approaches

Traditional descriptions of one-dimensional vertical unsaturated zone transport processes are generally based on the classical Richards equation for unsaturated water flow (Eq. 1), and the phenomenological convection-dispersion equation for solute transport (Eq. 2), or of various simplifications thereof.

\[
\frac{d}{dx} \left( \frac{K(x) \frac{d}{dx} h(x)}{\rho} \right) + \frac{1}{\gamma} \frac{d}{dx} \left( \frac{c(x) \frac{d}{dx} h(x)}{\rho} \right) = 0
\]

(1)

\[
\frac{d}{dx} \left( \frac{K(x) \frac{d}{dx} h(x)}{\rho} \right) + \frac{1}{\gamma} \frac{d}{dx} \left( \frac{c(x) \frac{d}{dx} h(x)}{\rho} \right) = 0
\]

(2)

In these equations, \( h \) represents the pressure head; \( C \) is the soil water capacity or the slope of the soil water retention curve, \( h \); \( K \) is the volumetric water content; \( K \) is the hydraulic conductivity; \( x \) is distance; \( t \) is time; \( c \) is the solute solution concentration; \( R \) is a retardation factor accounting for equilibrium sorption or exchange processes; \( D \) is the dispersion coefficient; and \( q \) is the volumetric fluid flux density. Sources or sinks of water and solute in the system have been continuously ignored in (1) and (2). For conditions of steady-state water flow in homogeneous soils, and linear advection, (2) can be reduced to the much simpler form

\[
k = \frac{d}{dx} \left( \frac{c(x) \frac{d}{dx} h(x)}{\rho} \right) = 0
\]

(3)

where \( v = q/\theta \) is the pore water velocity.

Numerous analytical, quasi-analytical and numerical solutions of (1), (2) and (3), or their two- and three-dimensional equivalents, have been developed over the last 30 years or so. Excellent inventories and discussions of these solutions from varying perspectives are given by Knapik et al. (1964), Knapik and Morrey (1984), van der Heijde et al. (1985) and Nielsen et al. (1986). Here, we shall only summarize review literature contributions made during the last quadrennium.

The development of approximate or quasi-analytical solutions of the water flow equation, in many cases geared towards infiltration problems, has remained an active research area (e.g., Baut, 1983a; Boulier et al., 1984; Knight, 1985; Philip, 1985, 1986; Weir, 1986). Bonner and Knapik et al. (1986) also included the effects of water extraction by plant roots, while solutions for
gravity-dominated flows based on kinematic wave theory (as given by Smith (1983) and Charwatous (1984)). While many of these solutions appear to be only of academic interest, some may prove to be useful for predictive purposes per se, for verification of numerical solutions, or for deriving physically-based expressions for the infiltration rate. More flexible one- and multi-

dimensional numerical solutions of the un satu-

rated water flow equation for a variety of specific applications are given by Guiney (1983), Huyakorn et al. (1984, 1986), Nély (1985), Murphy and Allen (1986), and by Narasiah and Brevis (1986), among others. A useful dimen-
sionless numerical solution for infiltration and unsaturated flow was presented by Warrick et al. (1985). Recent progress in one- and multi-
dimensional numerical modeling of combined unsat-

urated water flow and solute transport is exem-
plified by the works of Gureghian (1983), Nélyakorn et al. (1983) and Voss (1984), while improved two-phase str\textit{water} models were discussed by Moret-Seymour and Billica (1985a, b).
In addition, a number of analytical solutions of (3) and its multidimensional forms were added to the literature during the last four years (e.g., Bacu, 1984; Javandel et al., 1984; van Genuchten, 1985a).

While the above classical models based on (1) and (2) have been and will remain indispensable tools, and often the only tools in research and management of unsaturated zone transfer processes (Adickes and Wagener, 1985), growing evidence in the literature suggests that deterministic solutions (such as (1) and (2)) and perhaps the differential equations themselves, may not accur-

dately describe transfer processes in undisturbed (field-scale) soils (e.g., Smith, 1985). Factors contributing to this failure to describe accurately or even accurately or in the complete descriptions of the chemistry affecting transport of reactive solutes, (2) preferential movement (of bypassing) of water and solutes through large, continuous soil macropores, and (3) spatio-temporal variability of field-scale flow and transport properties. These three problems areas are each briefly discussed below.

Reactive Solute Transport

Use of the 

\textit{Darwin} model in (1) assumes equilibrium chemistry and/or a single transport processes in the soil system. If, in addition, simple lixiviation is assumed (when the solution and ad-
sorbed concentrations, then B becomes independent of concentration. Use of a linear equilibrium isotherm greatly simplify the mathematics of a transport problem (Valocchi, 1984). Unfortu-

nately, adsorption and exchange reactions are generally nonlinear and often also depend on the presence of competing species in the solution, thus requiring the consideration of solution chemistry and/or cation exchange principles. Two distinct modeling techniques are currently being pursued in multi-component transport modeling. One technique is to insert the interaction chemistry directly into the transport equations, thereby reducing the multi-component transport problem to a set of coupled nonlinear partial differential equations (Rubin and James, 1973; Rubin, 1983; Kirkner et al., 1984). A somewhat more efficient method, especially when many solute species are involved, appears when some or all of the exchange chemistry is formulated inde-

pendently of the mass transport equation. This method leads to the set of nonlinear algebraic equations for the solution and exchange che-

mistry, and to one or only a few differential equations for the transport part of the model. Examples, in various degrees of complexity, of this second approach are given by Schoell and Heardon (1983), Miller and Benson (1983), Chiew et al. (1985), and Narasiah et al. (1985).

The assumption of instantaneous adsorption itself also continues to be questioned (a number of chemically-controlled kinetic and diffusion-

controlled 'physical' nonequilibrium models have been used to study solute transport (Abrams et al., 1983; Wagener, 1981). Most popular remain the two-site and two-region transport models. Two-site (or partial equilibrium) models assume that sorption sites can be divided into two fractions each exhibiting dif-
f

ferent equilibrium and kinetic adsorption proper-


ties (Fliakler and Jurg, 1984; Parker and Jardine, 1986). Two-region (or multil-immobile) models, on the other hand, assume that the sorption rate is controlled by the rate at which ions diffuse from relatively mobile (flowing) liquid regions to reaction sites in equilibrium with immobile (nonflowing or dead-end) water. Diffusion into and out of the immobile water pockets is general-

ly modeled as an apparent first-order exchange process. Theoretical and experimental applica-


tions of the latter model are given by Brickett et al. (1985), Sierakoff et al. (1986), and Ritter and Baker (1986). The 


two-region models can be put into the same dimen-
sionless model framework, and then used this information to show that the rate of transport can be quite different, and alone cannot be used to differentiate between chemical and physical phenomena that cause an apparent nonequilibrium situation in a soil. This means that independent experiments (such as batch studies or deployments with radioactive tracers) are needed for verification of the two-region model. There also exists the potential problem of contamination between phenomena that occur on a microscopic (poro-ecricle) level. As is the case with many other aspects of dif-


imissible characteristics. Clearly, model
somehow. To this case should be commen-
surate with the specific purpose of the modeling
tacles. For example, Jury et al. (1931, 1966)
developed a useful analytical model to assess
around soil group compounds as to their potential hazard
for groundwater contamination. Such a screening
model can be far less complex than those required
for predicting the temporal and spatial distribu-
tion in the vadose zone (Abriola and Plint, 1985a,b; Faust, 1985). A recent review by Vinder
and Defina (1986) reviews the conceptual and
mathematical complexities that may need to be
considered when linking the unsteady-
saturated transport of nonaqueous phase organic
compounds, even for homogeneous soils.

Transfer Processes in Structured Soils

Recently, questions have arisen about the use-
fulness of (1) and (2) to describe unsteady
water flow and solute transport in structured
soils characterized by large, more or less con-
tinuous voids (interaggregate pores, interpedal
voids, earthworm and gopher holes, drying root
channels, drying cracks in clay soils). Infiltration
into and flow of water and solutes through such soils can be substantially different from that in relatively homogeneous materials.
For recent reviews of experimental evidence, see
Attempts to describe water flow in unsteady
structured soils have generally centered on two
domains, two-region, or biocompartmental
approaches. One dissociation rate of the soil matrix in which the water flow is described with the conventional
Darcian-based unsteady water flow equation, while the movement of either single macropores, or of a statistical network of macropores, through which water flows primarily
under the influence of gravity (Yeh and LaMoore,
1982; Davidson, 1985a,b). Closely related approximations to the above models were developed by Germain (1980) and Germahn and
Beyer (1984). The classical Darcian model involving the Green-Ampt infiltration equation was sug-
gested by Bresler and Barnea (1984). A more
simplified numerical model for drainage of
structured soils was developed by Wang and
Harashima (1985). Their formulation not only considers flow along the totally unsat-
tuated rectangular macropores, but also flow
between partially unsteady soil matrix blocks.

While much progress has been made in the last few years, several important implica-
tions in subsurface hydrology in general, and on infiltration and unsteady water flow in
particular, it is clear that the above models are likely to the accelerated movement of surface-applied for-
tillizers or pollutants through the unsteady
zone of structured soils. A large number of
mostly analytical two-region models have been
developed over the years to describe this type of
preferential solute transport. Like the other
previous models, these models also are
written as mobile-immobile equations, these models assume that the chemical is transported using separately well-defined pore
or crack of known geometry, or in the voids bet-
ween well-defined, uniformly-sized aggregates.
Contrary to those previous models, however,
Fickian-based diffusion equations are used to
more rigorously describe the transport of solutes
from the larger pores into micropores of the soil
matrix. Several analytical (Pešnta et al.,
1984; Goltz and Roberts, 1985b) and numerical
(Huyckorn et al., 1985; Ramussen et al., 1982)
transport models have been used to provide
groundwater system models, and these models
have been successfully tested in the
laboratory, their field verification in heterogeneous
saturated systems has only started in the last
quadrantum, both here (Gilliam et al., 1984; Goltz
and Roberts, 1985b, 1986) as well as in
Europe (Hedigkiss and Lever, 1983; Malneswett
and Zuber, 1985).

The above two-region modeling procedures have
thus far been restricted to uniformly-sized and
-shaped aggregates of specific geometry. The natural variability of aggregate geometries in
the vadose zone requires a generalization of the
two-region approach to other aggregate shapes, as
well as to mixtures of aggregates having differ-
ent shapes and sizes. Recently, several attempts
have been made to do so (Kao et al., 1982;
Herstein and Ramussen, 1984; Barker, 1985).

Although two-region models are conceptually
pleasing and have resulted in improved prediction
capabilities, the question remains whether or not
gometry-inspired two-region solute transport
models are too complicated for routine use in
research or management. They require large
numbers of parameters that are not easily measured
independently, especially in the field. In
contrast, the classical Fickian-based transport
equation is much simpler and thus more suited for
practical field applications. Moreover the
classical model also facilitates the introduction of
certain conditions dictated by the spatial scale of
the transport problem. To provide proper distinctions are made between flow-
areas, soil layers, volume-averaged concentrations
(Parker and van Genuchten, 1984a). In
conceptual attempts have been made to define conditions for
which the flow can be treated as the first-order mobile-immobile model may be
valid (Park et al., 1986a). As such, the
the effects of matrix (inter-aggregate) diffusion
can be lumped into an effective dispersion coeffi-
cient for use in equation (3) (Valocchi, 1985;
van Genuchten, 1985b).

Stochastic Field Scale Models

Two-region type models of preferential move-
ment of water and solutes represent attempts to
deal with pore structure characteristics at field
scales somewhat intermediate between the
usual laboratory measurements and the large field
scale. As such, they seem to be useful predic-
tors of predominantly vertical transport in a
structured but arypeal homogenous field soil.
To evaluate the effects of areal variabilities in
the hydraulic and transport parameters, the
stochastic nature of the flow and/or transport
process must be dealt with. Currently, a number of
widely varying stochastic approaches are being
pursued. For comprehensive reviews of
and Sposito et al. (1986a). Following Jury (1984),
we conveniently group the stochastic approaches
into scaling theories, Monte Carlo methods, and
various stochastic-continuum models. A common
assumption of these stochastic approaches is that
field parameters are random variables.
 scient D in Eq. 3, and developed a formal theore-
 tical approach using the pore water velocity
and the travel time and random variables (van
and Jury et al., 1986) similarly neglected D
in the development of the transfer function model
of solute transport. The latter approach leads to
and transport of

an estimation of the distribution of travel times
from the soil surface down to some reference
depth L. Solute transport is characterized by
a travel time probability density function f(t),
which for many soil transport processes may
be represented as lognormal. The flux concentra-
tion in the profile is represented with a convolution
integral of f(t) and the imposed flux con-
centration at the soil surface. Recent applica-
tions of the transfer function model are given by
White et al. (1986), whereas its relationship to
the classical one-region (Eq. 3) and first-
order (mobility-immobile) region transport
models is discussed by Sposito et al. (1986b).
Yet another continuous formulation, somewhat
resembling the works of Annesi and Yard (1982)
and Bresler and Bagar (1983), was used by
Parker and van Genuchten (1986b). These authors
consider the entire field to be composed of
independent, one-dimensional soil columns, each
having unique flow and transport properties and
subjected to specific local boundary conditions.
The pore-water velocity, while taken to be
constant with time and depth in each column,
is assumed to vary lognormally among the
columns. Finally, transport in each column is
described with the classical transport equation
(equation 3), thus including a dispersion coefficient
which is linearly related to the pore water velocity.
As with any of the stochastic models discussed
above, the formulation does not allow for
any lateral movement between the neighboring
columns, an assumption that likely is not valid
(Sposito et al., 1986a; Schulin et al., 1986).

Concluding Remarks
This review aims to demonstrate an abundance
of models and modeling approaches that are
currently available to describe both laboratory-
and field-scale unsaturated zone flow and
transport processes. Many deterministic and
stochastic models have greatly added to
our understanding of the main physical, chemical
and microbiological mechanisms affecting flow
and transport. While deterministic models have
and likely will continue to be invaluable tools in
research and management, their adequacy for
predicting actual field-scale processes in time
and space is increasingly being questioned. The
stochastic approaches appear especially useful
for estimating solute travel times in the vadose
zone, as well as for predicting areal solute
transport loadings to underlying groundwater
systems. Their evaluation in the field has thus
far been limited to only a handful of data sets.
Hence, a few carefully executed field
experiments are needed to determine their
validity for describing field-scale processes, especially
for relatively deep unsaturated profiles.
The use of computer programs to simulate
water flow and solute transport has become
increasingly popular in research and management, a trend
that is likely to continue as computer power be-
field-scale processes requires considerable effort, in quantifying spatially and temporally varying soil hydraulic and solute transport properties. Thus, the completeness of experimental data may eventually become the critical factor determining the accuracy of site-specific simulations. Many of our current methods for measuring relevant vadose zone water flow and solute transport parameters are largely those that were introduced several decades ago. Thus, new methods and technologies of measurement are needed to keep pace with our ability to simulate increasingly complex laboratory and field systems. A number of potentially powerful methods based on parameter estimation of various unsteady flow (Dane and Hruska, 1983; Knoll et al., 1985, 1986) and solute transport (Farkas and van Genuchten, 1984b; Jury and Spottiswoode, 1985; Wagner and Gorelick, 1986) parameters have recently been introduced. Other papers have contributed significantly to a better technology of measurement (Fasenold et al., 1985; Topp and Davis, 1985; Dasberg and Halvorson, 1985). It is imperative that research in these and related areas continues.