Stochastic model for posttillage soil pore space evolution

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Abstract. Tillage operations disrupt surface layers of agricultural soils, creating a loosened structure with a substantial proportion of interaggregate porosity that enhances liquid and gaseous exchange properties favorable for plant growth. Unfortunately, such desirable soil tilth is structurally unstable and is susceptible to change by subsequent wetting and drying processes and other mechanical stresses that reduce total porosity and modify pore size distribution (PSD). Ability to model posttillage dynamics of soil pore space and concurrent changes in hydraulic properties is important for realistic predictions of transport processes through this surface layer. We propose a stochastic modeling framework that couples the probabilistic nature of pore space distributions with physically based soil deformation models using the Fokker-Planck equation (FPE) formalism. Three important features of soil pore space evolution are addressed: (1) reduction of the total porosity, (2) reduction of mean pore radius, and (3) changes in the variance of the PSD. The proposed framework may be used to provide input to hydrological models concerning temporal variations in near-surface soil hydraulic properties. In a preliminary investigation of this approach we link a previously proposed mechanistic model of soil aggregate coalescence to the stochastic FPE framework to determine the FPE coefficients. An illustrative example is presented which describes changes in interaggregate pore size due to wetting-drying cycles and the resulting effects on dynamics of the soil water characteristic curve and hydraulic conductivity functions.

1. Introduction

The tilled "plow layer" of agricultural soils plays a crucial role in determining crop productivity and transport of gas, water, and chemical fluxes in the environment. A characteristic of this layer is the periodic disruption and destabilization of soil structure by tillage, followed by gradual resettling of the soil into a more stable state. Soil settlement occurs at a rate determined by many factors, such as the nature of the original disturbance, soil type, mechanical compaction, and wetting and drying history [*Stibbe and Hadas*, 1977; *Hadas et al.*, 1990; *Hadas*, 1997]. This "structural cycle" is perpetuated by the next tillage operation. Consequently, important soil properties, such as mechanical strength, water retention capacity, hydraulic and thermal conductivity, and other transport properties are in a constant state of change.

One aspect of this problem, namely, soil surface crust formation due to raindrop impact and ponding-induced slaking, has been extensively researched in the past [*Mualem and Assouline*, 1989; *Sumner and Stewart*, 1992; *Youngs et al.*, 1994]. However, surface crusts represent only a small fraction (albeit an important one) of the tilled layer. Of equal importance to the physical behavior of field soils is the structure of the soil underneath the crust. This soil layer is not subject to direct raindrop impact, and wetting generally occurs more gradually and under greater tensions than in the surface layer [*Hillel*, 1980]. Thus the mechanisms governing soil structural changes are different than for surface crusts, and, in general, the rate of change is likely to be more gradual.

Other than mechanical compaction, the primary events causing structural transformations in tilled soils are the wetting and drying cycles inherent in most irrigated and rain-fed crop production systems. Wetting of structurally unstable soil by irrigation or rainfall results in aggregate disintegration [*Shiel et al.*, 1988] and plastic deformation [*Day and Holmgren*, 1952], resulting in soil settlement, filling of interaggregate pores by microaggregates, reduced porosity, and changes in the distribution of pore sizes [*Collis-George and Greene*, 1979; *Kemper et al.*, 1988].

Realistic modeling of transport processes in the soil plow layer requires better understanding of pore space dynamics and hydrological consequences. Furthermore, because similar values of soil porosity and bulk density may result in very different soil retention and intake properties [*Nimmo and Akstin*, 1988], there is a need for consideration of the dynamics of the entire soil pore size distribution (PSD). The statistical description of soil pore space as a probability density function (PDF) of pore sizes has been instrumental in the development of predictive models for soil hydraulic properties. Recent advances in statistical and parametric methods for expressing soil PSD [*Kosugi*, 1996; *Shcherbakov et al.*, 1995] and progress in physical modeling of dynamic deformation of the solid phase surrounding soil pores during wetting-drying cycles [*Or*, 1996; *Ghezzehei and Or*, 2000] provide the motivation for modeling approaches proposed in this study.

The primary objective of this study was to develop a framework for modeling posttillage evolution of soil PSD based on coupling of stochastic formulation with physically based process models. We propose the use of the forward Kolmogorov

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equation [*Karlin and Taylor*, 1981], also known as the Fokker-Planck equation (FPE) [*Gardiner*, 1985; *Risken*, 1989], for modeling the evolution of soil PSD during posttillage subsoil settlement. This equation has been used for process modeling in different scientific disciplines, for example, dynamics of statistical distributions of plant height and weight [*Hara*, 1984], molecular diffusion and solute transport [*Su*, 1995], and many other processes [*Gardiner*, 1985]. The solution for the FPE problem tracks the evolution of the PDF for the attribute or population of interest. Additional objectives of this study were to (1) use available experimental and theoretical information to establish trends and potential functional relationships between the range of parameters governing the FPE and (2) illustrate the potential usefulness of the proposed framework for predicting temporal changes in soil hydraulic functions.

2. Theoretical Considerations

To develop the underlying theory, we first discuss the probabilistic representation of soil PSDs in section 2.1. Subsequently, the stochastic framework for modeling the evolution of the PSD using the FPE is presented in section 2.2. Physical and experimental considerations regarding the FPE coefficients are discussed in section 2.3. The initial PSD will be presented in section 2.4. The estimation of FPE coefficients derived from a mechanistic model of soil aggregate coalescence [*Ghezzehei and Or*, 2000] is presented in section 2.5. Finally, approaches to solving the FPE numerically and analytically are discussed in section 2.6.

2.1. Soil Pore Size Distributions

On the basis of available evidence we propose to model posttillage pore space evolution as the joint effect of two primary processes: (1) aggregate disintegration during wetting and drying cycles into a distribution of successively smaller aggregates and interaggregate pores [*Shiel et al.*, 1988] and (2) viscoplastic deformation and rejoining of wet aggregates with resulting pore deformation as observed by *Kwaad and Mucher* [1994]. Our preliminary experience [*Snyder et al.*, 1998] indicates that the aggregate disintegration process occurs primarily during water infiltration into relatively dry soil, even under wetting with a fine mist to reduce the possibility of slaking due to air entrapment. Once infiltration is complete and the soil is uniformly wetted, further fragmentation practically ceases until the soil is dried and rewetted. The fragmentation is apparently caused by differential swelling of the solid material associated with moisture gradients during the water absorption process. In view of such behavior, changes in soil PSD caused by aggregate disintegration during wetting and drying cycles should perhaps be modeled as a series of events rather than a time-continuous process.

Aggregate deformation and rejoining, however, is a relatively slow (time dependent) viscoplastic process occurring in wet soils characterized by a low plastic yield stress. The driving force for the rejoining process appears to be negative pore water pressure at menisci connecting adjacent aggregates, causing the aggregate contact points to flatten against each other and gradually rejoin the aggregates into a larger structural unit [*Ghezzehei and Or*, 2000]. During mild wetting and drying cycles (drying only allowed to occur to a limited extent after wetting) we expect viscoplastic deformation, rather than aggregate disintegration, to control PSD evolution [*Silva*, 1995; *Or*, 1996]. For simplicity, our treatment of pore size evolution

in the remainder of this paper will be limited to conditions where capillary-driven viscoplastic deformation is dominant.

Mechanisms and rates of evolution of individual soil pores during aggregate deformation and rejoining processes can be modeled using capillary-driven sintering theory [*Or*, 1996; *Ghezzehei and Or*, 2000]. Information about packs of monodisperse aggregates forming a narrow range of pore sizes or a hierarchical structure of pore sizes [*Scherer*, 1984] may be used to predict changes in mean pore sizes of the soil matrix during aggregate rejoining. For certain narrow PSDs, small-perturbation approximations could be used to estimate evolution of pore sizes. For example, *Scherer* [1977] has shown for glass powder sintering that Gaussian representation of PSD coupled with a mechanistic model enables the estimation of subsequent changes in PSD during the sintering process (for a known initial PSD). The primary limitation of these approaches for describing real field soils lies in the unrealistically narrow range of PSD represented by such models. It is therefore necessary to find methods that combine mechanistic information regarding rates of change and soil deformation with a more flexible representation of soil pore space.

In aggregated soils a distinction is often made between textural and structural pore spaces [*Childs*, 1940; *Nimmo*, 1997]. Textural or intra-aggregate pore space is determined by the size distribution of soil primary particles (i.e., sand, silt, and clay fractions) and is relatively stable. Conversely, structural or interaggregate pore space is determined by the position, orientation, and shape of aggregates relative to one another. It is this fraction of soil pore space, corresponding roughly to the 0–33 kPa soil water retention range, that is most affected by tillage and which most affects soil physical characteristics such as transport properties [*Croney and Coleman*, 1954; *Sharma and Uehara*, 1968a, b; *Gupta and Larson*, 1982; *Ahuja et al.*, 1984; *Nimmo*, 1997]. Consequently, our fundamental working hypothesis is that posttillage changes in pore space and hydraulic properties concern primarily the "effective pore space" within the 0–33 kPa water retention range [*Ahuja et al.*, 1998].
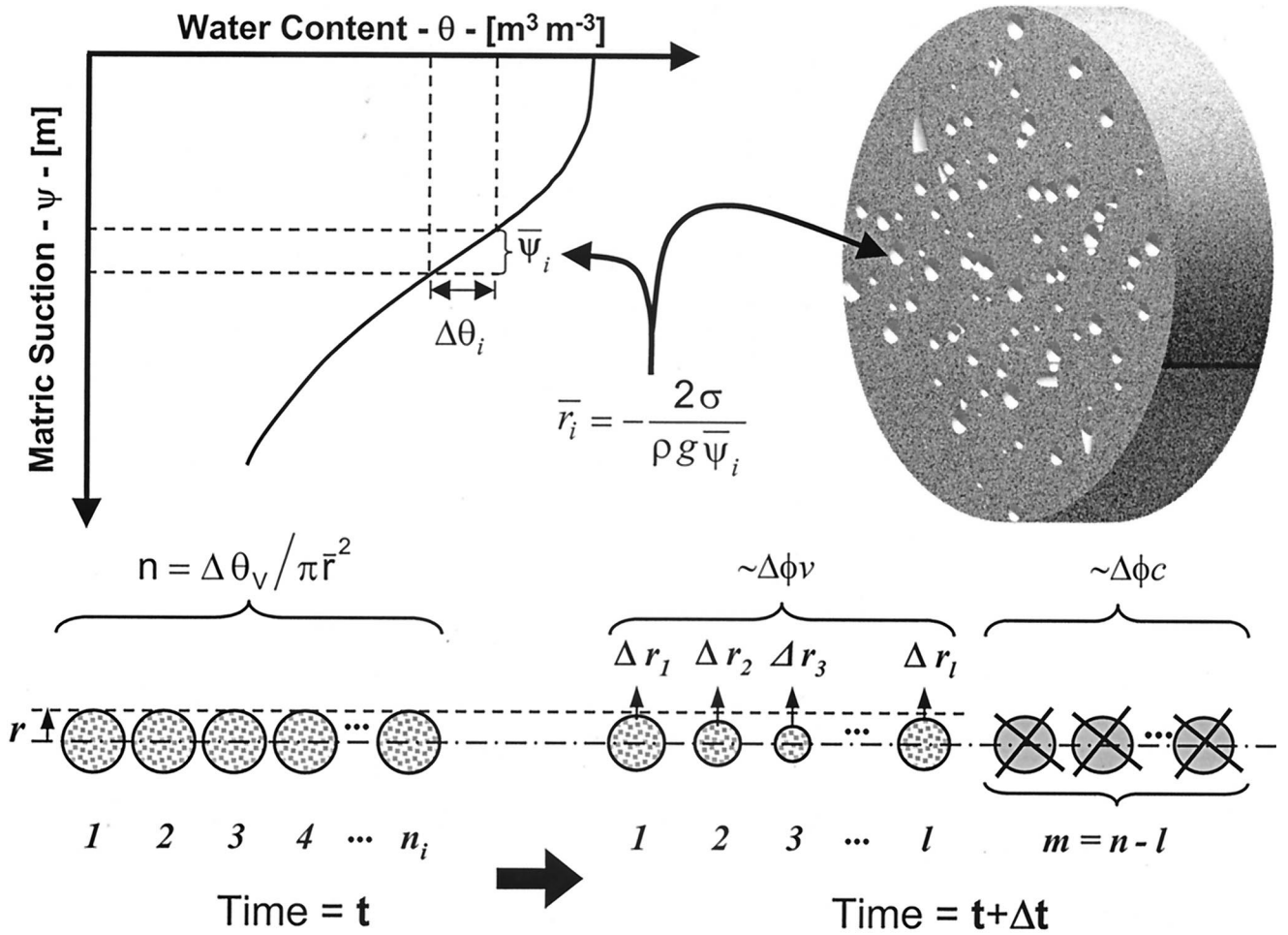
2.2. Fokker-Planck Equation (FPE)

Evidence shows that posttillage changes in soil structure and tilth, as reflected in soil PSD, tend to evolve in rather predictable pathways, which include (1) loss of large pores (or shift to smaller mean pore sizes); (2) reduction in overall porosity; and, possibly, (3) change in the spread of pore sizes (i.e., alteration in variance of PSD). Representing soil PSD in terms of statistical PDF, and considering aggregate deformation and porosity loss in wet soils as a solid diffusion process [*Gessinger et al.*, 1973], enables modeling soil pore space changes as evolution of soil PDF governed by external forcing and soil deformation processes. A well-developed theory already exists for representing stochastic diffusion processes by the Kolmogorov forward equation or the FPE [*Gardiner*, 1985; *Hara*, 1984].

The number of pores with radius $r \in [R, R + dR]$ at initial time $t = 0$ is given by

$$n(r) = n_0 \int_R^{R+dr} f(x)\, dx, \tag{1}$$

where n_0 is the total number of pores at $t = 0$ (i.e., the zeroth moment of the absolute distribution) and $f(r)$ is a (relative) pore size distribution (PSD) with inverse unit of r (L^{-1}). Note

Figure 1. Schematic representation of pore size evolution and physical interpretation of the coefficients of the Fokker-Planck equation.

that $f(r)$ is a PDF with property $\int_0^\infty f(r)\,dr \equiv 1$. The number of pores at an arbitrary time t after soil tillage can be described in a similar manner:

$$n(t, r) = n_0 \int_R^{R+dR} f(t, x)\,dx, \qquad (2)$$

where $f(t, r)$ is a time-dependent PDF to reflect the transient nature of pore size evolution. With the total number of pores varying with time, note that $f(t, r)$ is not the usual PDF, because we express the number of pores with respect to the total number at $t = 0$, n_0, rather than the unknown total number of pores at time t.

The PDF $f(t, r)$ is governed by the following FPE [*Hara*, 1984]:

$$\frac{\partial f(t, r)}{\partial t} = \frac{1}{2}\frac{\partial^2}{\partial r^2}[D(t, r)f(t, r)] - \frac{\partial}{\partial r}[V(t, r)f(t, r)]$$

$$- M(t, r)f(t, r), \qquad (3)$$

where $V(t, r)$ is the drift coefficient ($L\ T^{-1}$) or the infinitesimal mean, $D(t, r)$ is the diffusion coefficient ($L^2\ T^{-1}$) or the infinitesimal variance, and $M(t, r)$ is a first-order pore degradation factor representing instantaneous pore loss (T^{-1}). The application of (3) to modeling pore size evolution was also motivated by its similarity with the advection-dispersion equation and a similar decay term [*van Genuchten*, 1981], which possibly allows the use of existing analytical solutions.

2.3. FPE Coefficients: Physical Considerations and Experimental Evidence

The physical processes governing the evolution of the PSD are embodied in the coefficients of the FPE. The coefficients depend on time, reflecting the transient nature of pore size evolution, as well as on pore size. The interpretation of these coefficients and their mathematical definitions are illustrated in Figure 1, considering a group of initially equal-sized pores. Information contained in a soil water characteristic curve can be used to derive PSD by considering discrete pore size classes associated with ranges of matric suction. Let n be the number of pores belonging to a pore size class of radius r at time t. Owing to heterogeneity in conditions experienced by individual pores in the pore size-class r, their respective rates of pore size evolution may be different. We denote the number of pores that are completely closed by m and the number of pores that remain open by l. The changes in pore radii for individual pores during interval Δt are denoted by $\Delta r_1, \Delta r_2, \ldots, \Delta r_l$. The mean ($\overline{\Delta r}$) and variance ($\sigma_{\Delta r}^2$) of the changes in radii of the open pores are given by

$$\overline{\Delta r} = \frac{1}{l} \sum_{i=1}^{l} [r_i(t) - r_i(t + \Delta t)] = \frac{1}{l} \sum_{i=1}^{l} \Delta r_i, \qquad (4)$$

$$\sigma_{\Delta r}^2 = \frac{1}{l} \sum_{i=1}^{l} [\Delta r_i - \overline{\Delta r}]^2. \qquad (5)$$

The coefficients $V(t, r)$, $D(t, r)$, and $M(t, r)$ can be defined as follows [*Hara*, 1984]:

$$V(t, r) = \lim_{\Delta t \to 0} \frac{\overline{\Delta r}}{\Delta t} = \frac{d\bar{r}}{dt}, \qquad (6)$$

$$D(t, r) = \lim_{\Delta t \to 0} \frac{\sigma_{\Delta r}^2}{\Delta t}, \qquad (7)$$

$$M(t, r) = \lim_{\Delta t \to 0} \frac{1}{\Delta t} \frac{m}{n}, \qquad (8)$$

where $l + m = n$. The drift coefficient $V(t, r)$ represents the rate at which the mean change in pore radius ($\overline{\Delta r}$) evolves with time for a given pore size class. Factors that affect the drift coefficient include the pore size, soil rheological properties, and forces that drive the pore size evolution (e.g., capillary forces and external stresses) [*Ghezzehei and Or*, 2000]. The diffusion coefficient (instantaneous variance), $D(t, r)$, denotes the rate at which the variance of changes in pore radii ($\sigma_{\Delta r}^2$) evolves with time. It reflects the tendency of pores in a given pore size class (pores of equal radii) to evolve at different rates. If all pores in a pore size class r evolve at the same rate, then $\sigma_{\Delta r}^2 = 0$; hence $D(t, r) = 0$. The coefficient of instantaneous pore loss, $M(t, r)$, represents the proportion of pores that are closed during Δt interval. The practical challenge in determining $M(t, r)$ lies in the need to separate gradual pore closure due to viscous deformation of soil aggregates (which is not uniform over all pore sizes) from pore closure due to abrupt collapse of voids.

The experimental determination of these coefficients from changes in the soil water characteristic (SWC) measured at different times is a distinct possibility. However, little information is available to estimate these coefficients for field soils, and the physical conditions affecting their behavior are poorly understood. In the following we use available data to offer insights on potential trends in these coefficients.

The value of the instantaneous mean, $V(t, r)$, depends primarily on initial soil structural conditions (loose structure, degree of aggregation, etc.) and external forcing (rates of wetting and drying and other types of loading). The dependence of rate of change of soil PSD on soil type and type of forcing is illustrated in Figure 2. The SWC data shown in Figure 2a show that fast wetting of an expansive and well-aggregated silt loam soil resulted in rapid changes in SWC occurring within a few hours. These SWC data are measurements obtained by *Silva* [1995] on aggregated Millville soil columns subjected to three wetting-drying cycles. Each cycle was composed of 30 min wetting by sprinkling and 30 min drying with sprinkler turned off. For less expansive soils the rate of change in mean pore size can be quite low, as is confirmed by the SWC in Figure 2b, which were taken in the field by *Rivadeneira* [1982] over a period of more than 50 weeks after tillage. Similar rates of change in SWC and PSD of two Hawaiian field soils were reported by *Mapa et al.* [1986]. Soil breakdown by tillage forms
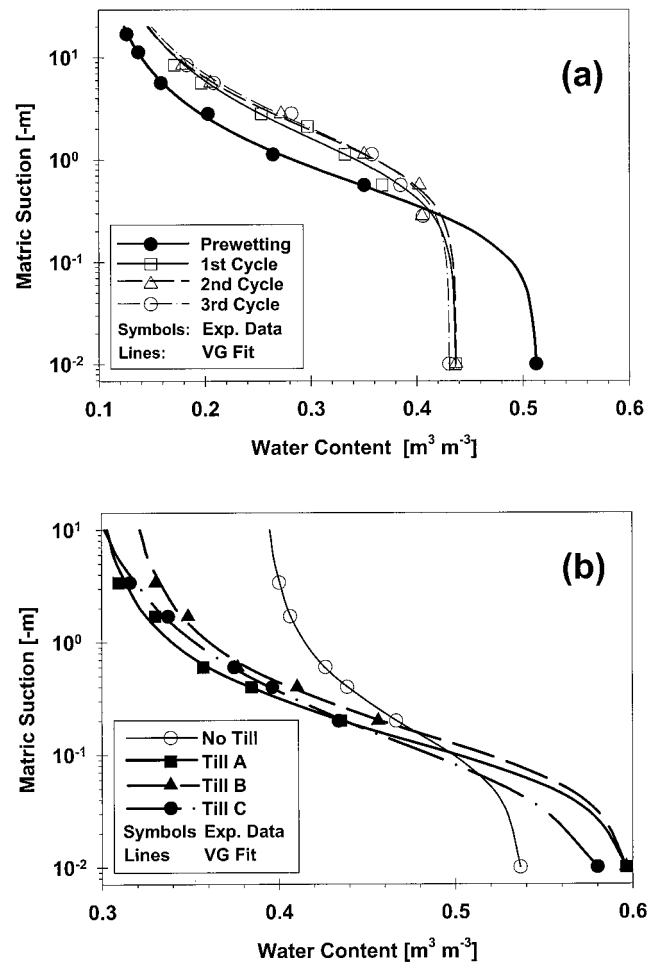
Figure 2. Comparison of evolution rates and shapes of soil water characteristic curves of two different soil types: (a) Millville silt loam soil before and after three cycles of wetting and drying in few hours timescale [*Silva*, 1995] and (b) Cotto clay soil under no till and three different types of tillage practices after 11 weeks of treatment [*Rivadeneira*, 1982]. Note that the tilled treatments in Figure 2b correspond to the prewetting loose state in Figure 2a.

large interaggregate pore space. These newly formed large pores are structurally unstable, and their sizes tend to evolve to a more stable PSD, primarily determined by soil textural pore space formed by arrangement and bonding of primary particles [*Warkentin*, 1971; *Mapa et al.*, 1986]. There is ample experimental evidence supporting the notion that most PSD changes occur at the interaggregate pore space [*Rivadeneira*, 1982; *Ahuja et al.*, 1998]. Furthermore, theoretical calculations confirm that larger pores deform at faster rates than smaller pores [*Scherer*, 1984; *Ghezzehei and Or*, 2000]. Details of estimation of the drift coefficient $V(t, r)$ from a mechanistic model of aggregate coalescence are discussed in section 2.5.
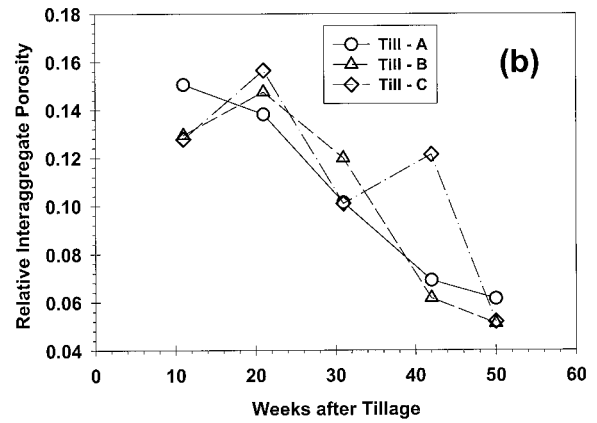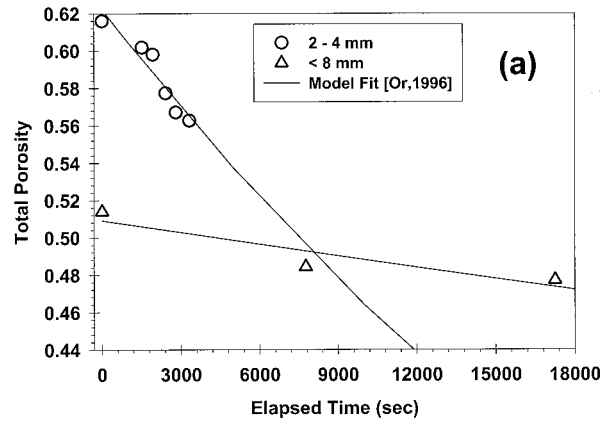
Establishing a functional form for the instantaneous variance $D(t, r)$ poses a challenge. Though some experimental evidence suggests that the variance of the PSD decreases with a reduction in mean pore size [e.g., *Laliberte and Brooks*, 1967] and with loss of porosity, there is virtually no information on the rate of these changes and their dependency on pore size. To illustrate potential trends in $D(t, r)$, we estimated the PSD functions of Columbia sandy loam soil from the experimental
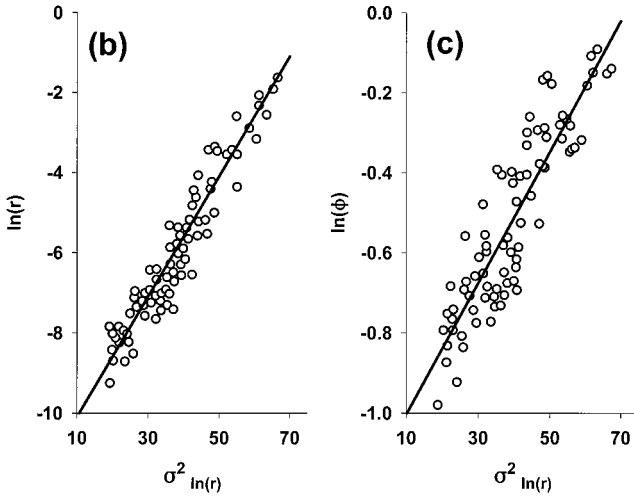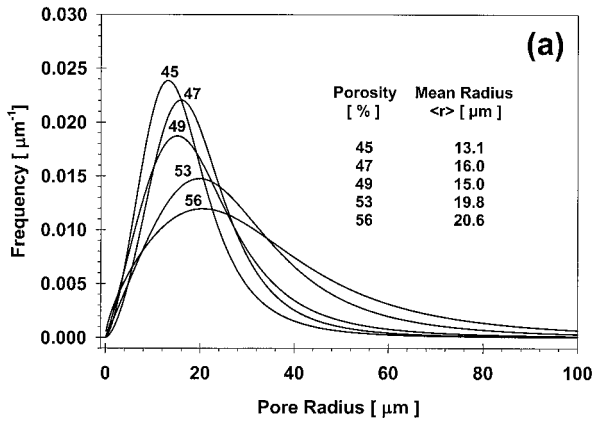
Figure 3. Experimental evidence on the variation of the pore size distribution (PSD) parameters (a) of Columbia sandy loam soil under different packing densities [*Laliberte and Brooks*, 1967] and variations in the logarithm (b) of the mean pore radius and (c) of the logarithm of porosity as a function of logarithmic variance (for a lognormal PSD of Chernozem soil) [*Shcherbakov et al.*, 1995].

Figure 4. Rate of porosity loss, porosity measurements (a) versus elapsed time since initiation of wetting for two aggregate sizes [*Silva*, 1995], and relative interped porosity (b) for three different tillage practices versus weeks after tillage [*Rivadeneira* [1982].

SWC data at five different bulk densities (porosity) [*Laliberte and Brooks*, 1967]. In Figure 3a, it is shown that the reduction in mean pore size ($\langle r \rangle$) and loss of porosity (ϕ) are accompanied by a decrease in variance (or the overall spread) of the PSD. These results imply that if the data in Figure 3a were representing a time sequence of soil densification, the coefficient $D(t, r)$ would indicate a decrease in variance of PSD with time. Additional support for this tendency is offered by correlative relationships developed by *Shcherbakov et al.* [1995] for PSD of Chernozem and Chestnut Brown soils from Ukraine and Russia, respectively. *Shcherbakov et al.* [1995] found linear relationships of the variance of the logarithm of the PSD with the logarithm of the mean pore size and logarithm of the porosity. Results for the Chernozem soil are depicted in Figures 3b and 3c. These and other studies, however, provide insufficient quantitative information regarding the variance of the PSD to formulate an expression for $D(t, r)$.

While measurement of total pore space is relatively simple, the determination of $M(t, r)$ presents a theoretical and experimental challenge. Experimental data on evolution of total porosity and structural porosity are given in Figures 4a and 4b, respectively. The data of *Silva* [1995] (Figure 4a) clearly show

that the rate of change in total porosity is affected primarily by the initial size distribution of soil aggregates. A faster rate was measured for a soil sample containing larger aggregates of the 2–4 mm fraction, and a slower rate was measured for a sample reflecting the more heterogeneous "natural" distribution, with particle sizes of up to 8 mm. *Mapa et al.* [1986] and *Rivadeneira* [1982] measured rates of porosity loss in field experiments. Figure 4b shows an example of the data of *Rivadeneira* [1982]. The interaggregate porosity, determined as the ratio of the total porosity for three tillage treatments to the porosity for zero tillage, is plotted as a function of time after tillage. However, Figure 4 does not provide information on the contribution of complete pore closure to the total porosity loss. Hence a practical option would be to determine $M(t, r)$ as a difference between predicted porosity loss and experimental measurements, such as in Figure 4.

2.4. Initial Pore Size Distribution

The initial PSD of many soils can be fitted by the lognormal probability distribution function [*Brutsaert*, 1966; *Kosugi*, 1999],

$$f_0(r) = \frac{\phi}{\sqrt{2\pi}\sigma r} \exp\left\{ -\frac{[\ln (r/r_m)]^2}{2\sigma^2} \right\}, \qquad (9)$$

where $0 < r < \infty$. The parameter r_m is the geometric mean or median pore radius, and σ is the standard deviation of the log-transformed pore radius. The parameter ϕ is the total
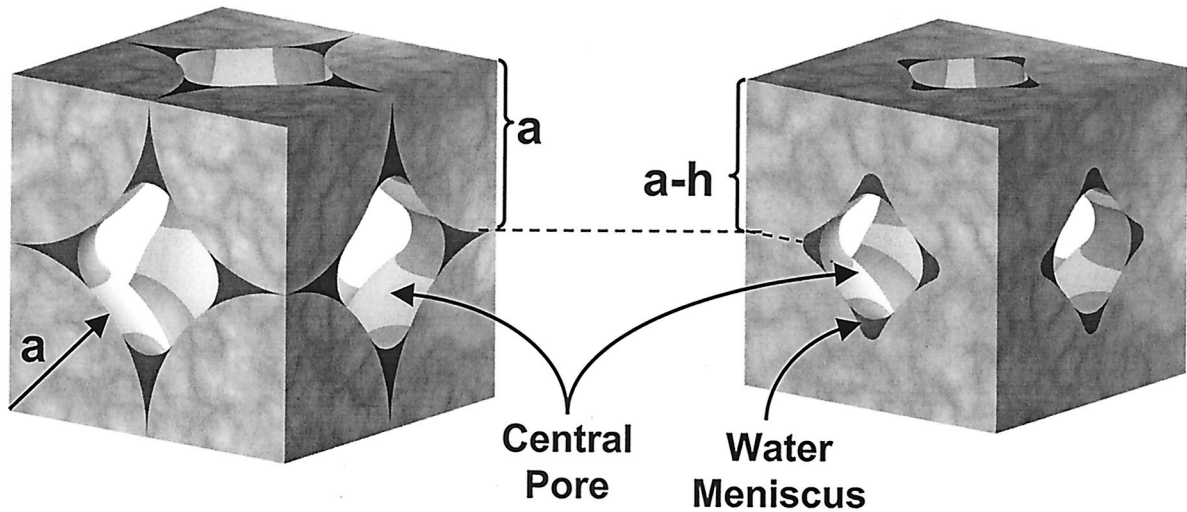
Aggr. Radius (a) [μm]	50	50
Strain (h/a·100) [%]	0	5
Pore Radius (R) [μm]	48.5	43.0
Porosity (φ)	0.48	0.39

Figure 5. Diagrammatic representation of the unit-cell model at 0 and 5% strains.

porosity. In case of a multimodal distribution the total PSD can be expressed as a weighted sum of all individual component distributions [e.g., *Durner*, 1994],

$$f_0(r) = \sum_{i=1}^{n} \frac{\phi_i}{\sqrt{2\pi}\sigma_i r} \exp\left\{ -\frac{[\ln (r/r_{m_i})]^2}{2\sigma_i^2} \right\}, \qquad (10)$$

where ϕ_i is the porosity occupied by class i (weighting factor) and the total porosity is given by $\Sigma\phi_i$. A bimodal PSD ($n = 2$), consisting of a textural and a structural component, has been used by *Nimmo* [1997].

2.5. Estimation of FPE Coefficients

Theoretically, the coefficients of the FPE should be determined by complete description of the dynamics of the entire pore size distribution. In sections 2.5.1–2.5.3 we present approximation of the drift (V) term from the aggregate coalescence model [*Ghezzehei and Or*, 2000] and conjectures on the estimation of the diffusion (D) and pore loss (M) terms.

2.5.1. Drift term $V(t, r)$. For mathematical simplicity we use a representative unit pore to calculate the drift term pertaining to the entire interaggregate PSD. A unit-cell model formed by cubic packing of spherical aggregates represents an aggregated soil with the central pore radius (R) equal to the geometric-mean radius (r_m) of the initial PSD (Figure 5). If we neglect degradation, the drift term may be estimated from a mechanistic model for soil aggregate coalescence [*Or*, 1996; *Ghezzehei and Or*, 2000]. The model considers a pair of equal-sized soil aggregates (radius equal to a) bridged by liquid meniscus. The objective of the model is to predict rate of axial

strain between the aggregate pair (h/a) as a result of tensile stress induced by the liquid meniscus. The model is based on energy balance between (1) rate of energy dissipation due to viscous coalescence of wet aggregates and (2) rate of energy liberation due to the reconfiguration of the liquid-vapor interface of the meniscus. The rate of aggregate coalescence is governed by the rheological properties of the soil (independently determined coefficient of plastic viscosity η_p and yield stress τ_y) and the wetting and/or drying rate. When only capillary forces are considered, the rate of aggregate coalescence is independent of the spatial orientation of the aggregate pair. Hence the deformation of the unit cell is equal in all directions.

The complex void of the unit cell is represented by a volume-equivalent spherical pore with radius R. The ratio of the pore volume to the total volume of the unit cell defines the porosity of the unit cell (ϕ). The pore radius (R) and porosity (ϕ) of the unit cell are related to the aggregate radius (a) and the time-dependent strain (h/a) by

$$R(t) = a\left\{ \frac{[2(1 - h(t)/a)]^3 - 4\pi/3}{4\pi/3} \right\}^{1/3}, \qquad (11)$$

$$\phi(t) = \frac{\{2[1 - h(t)/a]\}^3 - 4\pi/3}{\{2[1 - h(t)/a]\}^3}. \qquad (12)$$

In the unit-cell representation of the PSD the geometric-mean pore radius of the soil (r_m) in (10) may be equated to the unit-cell pore radius (R). Consequently, drift coefficient (the rate of change of the mean pore radius) given in (6) can be obtained by differentiating the equation of pore radius (11);

$$V(t) = \frac{\partial R(t)}{\partial h} \frac{dh}{dt}. \qquad (13)$$

This representation tacitly assumes that all pore radii drift at the same rate, which circumvents the physically and mathematically more challenging task of formulating a drift term that depends on pore radius.

2.5.2. Pore loss term $M(t, r)$. Reduction of total soil porosity ($\Delta\phi$) such as presented in Figure 4 involves two processes: (1) a decrease in pore radius by viscous deformation of soil aggregates ($\Delta\phi_V$) and (2) complete closure of pores ($\Delta\phi_C$), as shown in Figure 1. The pore loss term (M) refers to the rate of the complete pore closure. Complete pore closure may occur because of gradual closure of smallest interaggregate pores, abrupt collapse of large interaggregate pores due to differential stresses, rearrangement of aggregates, and filling of interaggregate voids by finer aggregates or primary particles.

The rate of total porosity reduction due to decrease in pore radius by viscous coalescence of soil aggregates is obtained by differentiating the equation of unit-cell porosity given by (12), that is, excluding changes in porosity because of complete closure,

$$\frac{\Delta\phi_V}{\Delta t} = \frac{\partial\phi(t)}{\partial h} \frac{dh}{dt}. \qquad (14)$$

For lack of definitive experimental information, such as the complete PSD at different times, we assume that $\Delta\phi_c$ is linearly related to $\Delta\phi_v$ and that the pore loss term can be expressed as

$$M(t) = \frac{\Delta\phi_c}{\Delta t} = \delta \frac{\partial\phi(t)}{\partial h} \frac{dh}{dt}. \qquad (15)$$

The proportionality constant is given by $\delta = \Delta\phi_c/\Delta\phi_V$ (i.e., total reduction in porosity is defined as $\Delta\phi = (1 + \delta)\Delta\phi_V$).

A refinement of the pore loss term (M) involves introduction of a minimum structural pore size, such that pore radii that reach such cutoff size are considered completely closed (from a structural PSD point of view). Note that this refinement of the pore loss term is not implemented in the current study.

2.5.3. Diffusion term $D(t, r)$. Experimental data of *Laliberte and Brooks* [1967] and *Shcherbakov et al.* [1995] shown in Figure 3 suggest existence of direct relationship between mean pore size and the variance of a PSD. Figure 3 represents soil information at different degrees or stages of compaction or coalescence. We postulate that this static relationship between variance of the PSD and mean pore size (a snapshot at a point in time) also reflects the dynamic nature of the relationship between the diffusion and drift terms. As an initial approximation, we suggest a linear relationship between the diffusion and drift terms,

$$\lambda = \frac{D(t)}{V(t)}. \qquad (16)$$

The parameter λ [L] is analogous to the dispersivity used to model solute transport. We assume a positive and constant value for λ in this paper. The potential dependence of λ on pore radius (r) and time (t) and possible negative values for λ will be subjects of future studies. The data of *Shcherbakov et al.* [1995] in Figure 3b show a linear relationship between the logarithm of the mean pore size and the variance of the logarithm of the PSD. It is relatively simple to cast the FPE for the

log-transformed PSD and to derive an expression similar to (16) from the data of *Shcherbakov et al.* [1995].

2.6. Solution of FPE

A significant simplification in the problem of quantifying the FPE coefficients may be achieved by considering the coefficients of the FPE to be independent of the pore size. This simplification is further justified if we consider only the structural PSD (see section 2.4). The simplified mathematical problem is given by

$$\frac{\partial f(t, r)}{\partial t} = \frac{1}{2} D(t) \frac{\partial^2 f(t, r)}{\partial r^2} - V(t) \frac{\partial f(t, r)}{\partial r} - M(t) f(t, r). \qquad (17)$$

This problem is subject to the following initial and boundary conditions

$$f(0, r) = f_0(r), \qquad 0 < r < \infty \qquad t = 0, \qquad (18a)$$

$$D(t) \frac{\partial}{\partial r} f(t, 0) - V(t) f(t, 0) = 0, \qquad (18b)$$

$$r = 0 \qquad t > 0,$$

$$\frac{\partial}{\partial r} f(t, \infty) = 0, \qquad r = \infty \qquad t > 0, \qquad (18c)$$

where $f_0(r)$ is the initial structural PSD. The "inlet" condition (18b) stipulates a zero "probability" flux; that is, only positive pore sizes are allowed. While the "outlet" condition (18c) requires the "probability" to be bounded (i.e., zero) for infinitely large pore radii. These homogeneous conditions also imply that any disappearance of pores is accounted for by the coefficient $M(t)$. The "inlet" boundary condition (18b) could be defined at a pore radius greater than zero, reflecting the transition of structural pores to textural pores, as stated in section 2.5.2.

The above problem may be amenable to analytical solution; closed-form solutions can be obtained for simplified expressions for the coefficients. We will solve the FPE numerically to allow flexibility to express the FPE coefficients in terms of soil aggregate size and rheological properties using Millville silt loam soil. The rate of aggregate coalescence and the FPE were solved simultaneously using the mathematical package MATHCAD 7 [*MathSoft, Inc.*, 1997]. The solution to the aggregate coalescence model provides the FPE coefficients at every time step; the FPE is subsequently solved using an explicit finite difference scheme.

3. Illustrative Example

### 3.1. Rate of Soil Aggregate Coalescence and FPE Coefficients

The following illustrative example is based on the rate of aggregate coalescence according to *Ghezzehei and Or* [2000]. Spherical and uniform-sized soil aggregates are subjected to low-amplitude cycles of linear drying and rapid rewetting. Independently determined rheological properties of Millville silt loam soil were used for the simulation. The relevant parameters for the aggregate coalescence simulation are listed in Table 1. The aggregates are wetted under tension to reduce slaking due to air entrapment; the matric suction is shown in Figure 6a as a function of time. The axial strain developed in the unit cell as a function of time (expressed as percent or

Table 1. Parameters Used to Run the Aggregate Coalescence and Pore Size Evolution Models

Variable	Equation	Constants
Aggregate radius a [m]		5×10^{-5}
Coefficient for pore loss term δ [dimensionless]	(15)	0.05
Coefficient for diffusion term λ [m]	(16)	0.50
Soil matric suction ψ [Pa]	$\psi(t) = a + bt$	$a = -5000$ Pa, $b = -25$ Pa s^{-1}
Plastic viscosity of soil η_p [Pa s]	$\eta(\psi) = a \exp(b\psi)$	$a = 58000$ Pa s, $b = -7 \times 10^{-4}$ Pa^{-1}
Yield stress of soil τ_y [Pa]	$\tau(\psi) = a \exp(b\psi)$	$a = 40$ Pa, $b = -7 \times 10^{-4}$ Pa^{-1}

$(h/a)100$) is shown in Figure 6b. The wetting and drying cycle involves subjecting the saturated aggregates to a linear drying rate for 30 min followed by rapid rewetting, after which they are held at a constant head for 30 min, and finally a second drying phase.

Tensile stresses due to capillary menisci exist only when soil is unsaturated. Hence (with the simplified assumption of instantaneous wetting to saturation) aggregate coalescence occurs only during the drying phase [*Ghezzehei and Or*, 2000]. An additional constraint for the onset of coalescence of wet aggregates is imposed by soil yield stress. For aggregate coalescence to take place, the tensile stress of the meniscus must exceed the soil yield stress (strength). As linear drying of the soil progresses, both the tensile stress and yield stress increase concurrently, until the yield stress exceeds tensile stress, leading to cessation of aggregate coalescence.
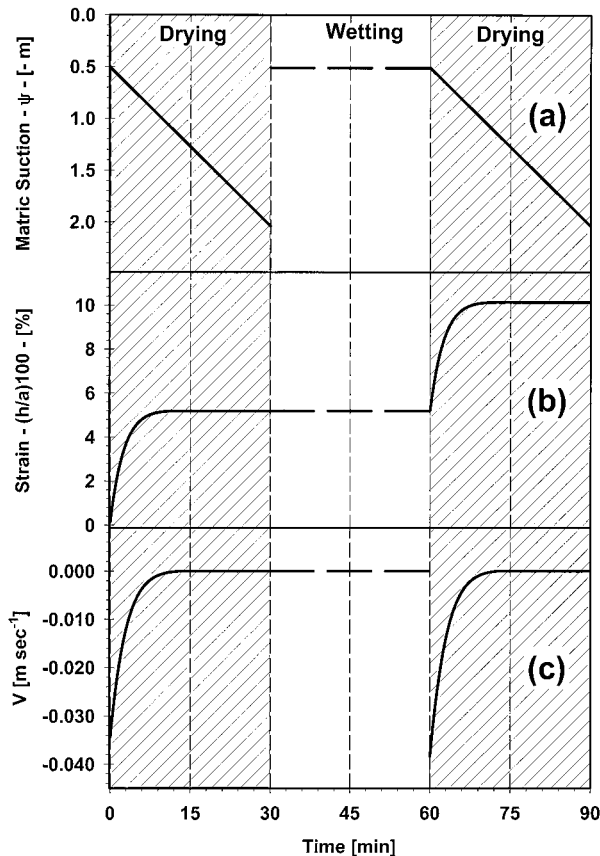
Figure 6. (a) Matric suction during wetting and drying cycles which drive the aggregate coalescence process. (b) The resulting axial strain of a unit cell as a function of time. (c) The drift term (instantaneous mean) for the Fokker-Planck equation calculated using the unit-cell model results.

3.2. Evolution of Pore Size Distribution

The soil pore system is divided into textural and structural components, the latter being far more susceptible to changes due to either wetting and drying processes or external loading [*Ahuja et al.*, 1998]. We illustrate the use of the FPE in evolution of bimodal PSD by considering an evolving interaggregate porosity (structural) and a stationary intra-aggregate porosity (textural). The initial interaggregate porosity is described by a lognormal PSD with a geometric-mean pore radius ($r_m = 48$ μm) equal to the initial pore radius of the unit cell, a prescribed log-transformed variance ($\sigma^2 = 0.2$), and a porosity fraction ($\phi_1 = 0.2$). The intra-aggregate porosity is described by a similar lognormal distribution with prescribed parameters ($r_m = 7$ μm, $\sigma^2 = 0.8$, and $\phi_2 = 0.3$).

For the interaggregate pore size evolution the FPE coefficients were calculated using (13), (15), and (16). The drift coefficient is shown in Figure 6c as a function of time. The evolution of the initial PSD is obtained by numerically solving (17), subject to the initial and boundary conditions given by (18). Figure 7a shows the intra-aggregate, interaggregate, and composite PSD at the beginning and at the ends of the first and second drying cycles (i.e., at 0, 30, and 90 min). The actual mean (α) and variance (β^2) of the PSD (compared to r_m and σ^2 of log-transformed pore radii) are given in Table 2.

All changes in the PSD are attributed to evolution of the structural pore system, while the textural PSD is assumed to be constant. For the "structural" pore space the median pore radius (r_m) diminishes with time, while the variance of the PSD increases (indicated by increased spread of structural PSD in Figure 7a). The PSD is only a measure of relative abundance of pore sizes and does not provide direct information about the porosity. However, the evolution of porosity can be tracked from knowledge of the initial porosity $\phi(0)$ and the evolution of the PSD, as outlined in Appendix A. Any reduction in the total area under the PSD (loss of "probability") is caused by complete pore closure. A reduction in the structural porosity due to both reduction of pore sizes and complete closure of pores is shown in Table 2. As the contribution of structural pore system to total porosity decreases, the relative contribution of the textural pore system increases (although it remains constant in absolute terms), as indicated in Table 2 and Figure 7.

The median pore radius (r_m) and total porosity (ϕ) of the composite PSD decreases with time due to drift of the "structural" median to smaller values. The variance of the composite PSD decreases as the structural pore system converges toward the textural pore system. This is reflected in the reduction of the separation between the structural and the textural components (Figure 7a).

The most obvious consequence of pore size evolution in any porous medium is the reduction in total porosity (ϕ). Furthermore, the evolution of the PSD and total porosity can be used
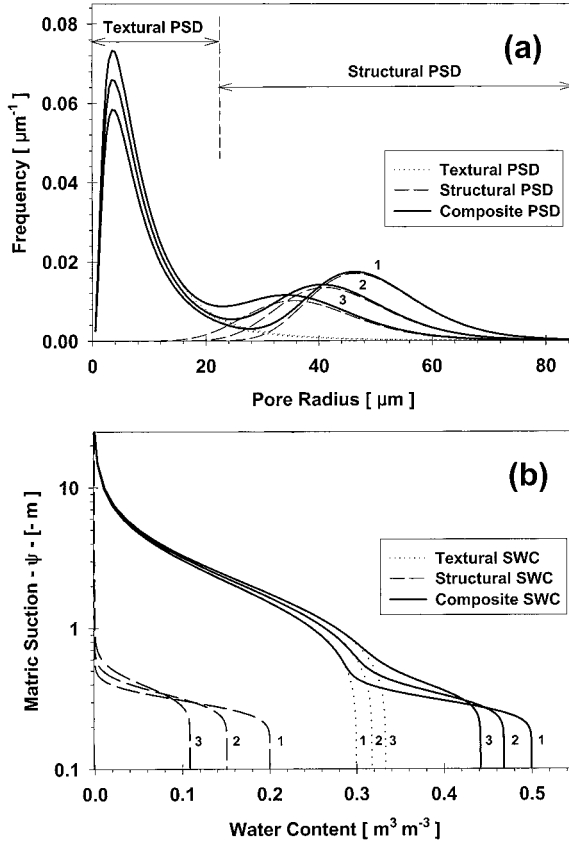
Figure 7. Evolution of (a) soil pore size distributions and (b) soil water characteristic curves resulting from two cycles of wetting and drying (see Figure 6). Numbers represent the wetting-drying cycles (1 is initial; 2 is the end of first cycle; and 3 is the end of second cycle). Dashed curves represent the evolving structural (interaggregate) pore system.

to quantify the transient behavior of soil hydraulic properties, as will be illustrated in sections 3.3 and 3.4.

3.3. Soil Water Characteristic (SWC)

Evolution of the PSD is readily reflected in the soil water characteristic (SWC) or $\theta(\psi)$ function, where θ is the volumetric water content and ψ is matric suction. The slope of the SWC, water capacity function $C(\psi)$, is obtained from the PSD function $f(r)$ by variable transformation assuming a one-to-one correspondence between pore radius (r) and matric suction (capillary pressure ψ). The pore radius can be related to matric potential by the capillary equation

$$\psi(t, r) = \frac{-2\gamma \cos(\beta)}{\rho_w g r(t)}, \quad (19)$$

where β is the contact angle, ρ_w is the density of water, and g is the acceleration due to gravity. The water capacity function ($C(\psi)$) is defined with the PSD ($f(r)$) according to

$$C(\psi) = \frac{d\theta}{d\psi} = f(r)\frac{dr}{d\psi}. \quad (20)$$

Integration of (20) leads to

$$\theta(\psi) = \int_{-\infty}^{\psi} C(\psi)\, d\psi + \theta_r, \quad (21)$$

where $\theta_r = \lim_{\psi \to -\infty} \theta(\psi)$ is the residual water content.

The resultant SWC evolution calculated using (21) is shown in Figure 7b. The dotted curves represent the textural pore space portion of the SWC with its proportion modified by the changes in the structural pore space. Similar to the PSD, the strong bimodality exhibited immediately after tillage diminishes with each wetting and drying cycle. Total porosity loss is reflected by reduction in soil θ_S with time.

3.4. Hydraulic Conductivity

One of the potential applications of the stochastic pore size evolution model is for prediction of temporal changes in the saturated and unsaturated hydraulic conductivity, K_s and $K(\psi)$, respectively. For illustrative purposes we selected the Kozeny-Carman relationships to estimate changes in the saturated hydraulic conductivity from changes in total porosity [Hillel, 1980]. When the estimated saturated hydraulic conductivity ($K_s(t)$) is written with respect to the initial saturated conductivity ($K_s(0)$), the Kozeny-Carman equation yields the following expression for the relative saturated conductivity in terms of porosity:

$$\frac{K_s(t)}{K_s(0)} = \left(\frac{\phi(t)}{\phi(0)}\right)^3 \left(\frac{1 - \phi(0)}{1 - \phi(t)}\right)^2. \quad (22)$$

The relative saturated hydraulic conductivity for the previously used example (compare Figures 6 and 7) is shown in Figure 8a; the numbers indicate the beginning and the ends of the first and second drying cycles (i.e., 0, 30, and 60 min).

The behavior of the relative unsaturated hydraulic conductivity (K_r) can be obtained from the SWC, according to the predictive equation given by Mualem [1976]:

$$K_r = \frac{K(t, \psi)}{K_s(0)} = S_e^{1/2} \left\{ \int_0^{S_e} \frac{dx}{|\psi(x)|} \middle/ \int_0^1 \frac{dx}{|\psi(x)|} \right\}^2, \quad (23)$$

where the relative saturation (S_e) is given by $S_e(\psi) = (\theta(\psi) - \theta_r)/(\theta_s - \theta_r)$. Figure 8b shows the relative unsaturated hydraulic conductivity with respect to the initial saturated hydraulic conductivity. As expected, the effect of com-

Table 2. Statistics of Pore Size Distributions at Different Time Stages

	Textural Component			Structural Component			Composite		
	α	β^2	ϕ_t	α	β^2	ϕ_s	α	β^2	ϕ
Time = 0 (initial)	9.62	79.82	0.30	49.33	99.28	0.20	25.50	466.03	0.50
Time = 30 min (first cycle)	9.62	79.82	0.32	43.77	101.91	0.15	20.72	342.86	0.46
Time = 90 min (second cycle)	9.62	79.82	0.33	38.21	104.54	0.11	16.72	238.63	0.44

α is Mean, β^2 is Variance, and ϕ is Porosity.
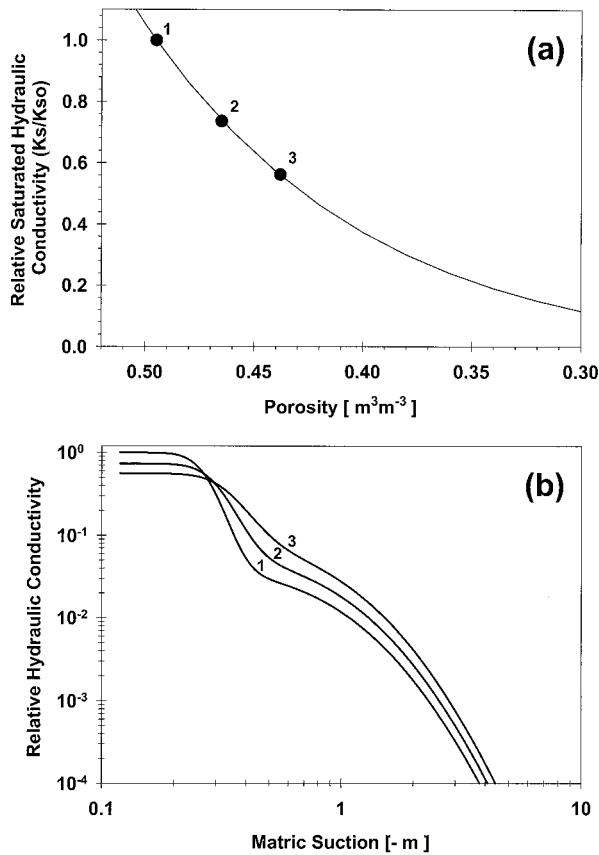
Figure 8. Effect of pore size evolution on soil hydraulic conductivity. (a) Effect of changes in total porosity on saturated hydraulic conductivity predicted by the Kozeny-Carman equation. (b) Effect of evolution of pore size distribution on the relative unsaturated hydraulic conductivity estimated by the van Genuchten-Mualem model. Numbers represent wetting-drying cycles (see Figure 7).

paction (coalescence) is reflected mostly in the wet range ($0 > \psi > -2$ m) [*Mapa et al.*, 1986; *Silva*, 1995; *Ahuja et al.*, 1998]. The saturated conductivity decreases after tillage, while bimodality of unsaturated conductivity diminishes with time (with number of wetting-drying cycles). The theoretical results shown in Figure 8 are in qualitative agreement with data reported by *Silva* [1995] for K_s and field measurements reported by *Hadas* [1997] for K_r.

4. Summary and Conclusions

The constant state of change in surface soil layers of agricultural fields presents a challenge to hydraulic characterization and modeling. Key variables affecting soil hydraulic properties are porosity and pore size distribution (PSD). A stochastic framework using the Fokker-Planck equation (FPE) for modeling pore size evolution is proposed. The model accounts for the dynamics of the mean pore radius, total porosity, and variance of PSD. The stochastic nature of pore size evolution, using the PSD as dependent variable in the FPE, has been linked with the physical process model of soil structural change. The FPE coefficients were quantified by using previously developed mechanistic models of soil aggregate coalescence [*Or*, 1996; *Ghezzehei and Or*, 2000]. This approach is probably most realistic for the drift term $V(t, r)$. The lack of

information on the behavior of the instantaneous variance $D(t, r)$ required conjecture that a constant of proportionality exists between $V(t, r)$ and $D(t, r)$ similar to that of solute transport, although rather limited experimental data seem to support such a "dispersivity" for pore size evolution.

The FPE can be used to model any arbitrary PSD function. A lognormal function was selected in this study for the initial PSD. Structural changes due to wetting-drying cycles occurred in the interaggregate pore space only (structural porosity), whereas intra-aggregate pore space (textural porosity) was assumed stable with time (constant pore volume, although its relative contribution to entire pore space changes). Model results of pore space evolution have been used along with existing soil hydraulic models to predict the dynamics of water retention and hydraulic conductivity functions. The ability to model changes in the PSD and the resulting effects on soil hydraulic properties at a particular time can be useful. Furthermore, the modeling framework is capable of providing estimates of rates of change over time, which may be equally important. The proposed modeling approach relies on information not readily available. More work is underway to provide further experimental validation and to improve the estimation of the diffusion and degradation terms.

Appendix A: Estimation of Evolution of Porosity From Expected Pore Volumes

In this appendix we present a method for calculating the evolution of soil porosity ($\phi(t)$) from knowledge of initial porosity ($\phi(0)$) and PSD evolution. We can consider pore radii (r) representing cylindrical pores (two dimensions) or spherical voids (three dimensions) to determine the areal (cross-sectional) or volumetric porosity, respectively. The derivation presented here considers volumetric porosity.

We consider a dual soil pore system comprising textural and structural components. The total porosity (ϕ) at any given time is represented as the sum of the textural (ϕ_t) and structural (ϕ_s) porosity

$$\phi(t) = \phi_t(t) + \phi_s(t). \qquad (A1)$$

The expected (ensemble average) textural and structural pore volumes (VP_t and VP_s, respectively) for a unit mass of soil at an arbitrary time can be expressed as

$$VP_t = \frac{4}{3}\pi \int_0^{r_{max}} r^3 f_t(r)\, dr, \qquad (A2)$$

$$VP_s(t) = \frac{4}{3}\pi \int_0^{r_{max}} r^3 f_s(r)\, dr, \qquad (A3)$$

where $0 < r < r_{max}$ denotes the pore radius and $f_t(r)$ and $f_s(r)$ are textural and structural PDFs. The overall average pore volume (VP) of the unit mass is given by

$$VP(t) = \zeta VP_t + (1 - \zeta)VP_s(t), \qquad (A4)$$

where $0 \leq \zeta \leq 1$ is a mixing proportion. The void ratios with respect to the initial total porosity $\phi(0)$ and textural porosity $\phi_t(0)$ are given by

$$\frac{\phi(0)}{1 - \phi(0)} = \frac{VP(0)}{VS}, \qquad (A5)$$

$$\frac{\phi_t(0)}{1 - \phi_t(0)} = \frac{\zeta VP_t(0)}{VS + (1 - \zeta)VP_s(0)}, \quad (A6)$$

where the initial expected pore volumes $VP_t(0)$ and $VP_s(0)$ are calculated with (A2) and (A3) using the textural PSD and initial structural PSD, f_0, given by (10). Because pore size evolution (densification) involves the change of only the structural void volume (VP_s), the expected volumes of soil solid mass (VS) and textural voids (VP_t) remain constant throughout the PSD evolution. The mixing proportion ζ that satisfies the initial conditions can be obtained by solving (A5) and (A6) simultaneously,

$$\zeta = \frac{VP_s(0)\phi_t(0)}{VP_s(0)\phi_t(0) - VP_t[\phi_t(0) - \phi(0)]}. \quad (A7)$$

The porosity at a later time (t) can be given by

$$\phi(t) = \frac{VP(t)}{VP(t) + VS}. \quad (A8)$$

where VS is obtained from (A5) and $VP(t)$ is calculated from (A7) and (A4). Note that although the expected textural pore volume (VP_t) remains constant during the evolution of the PSD, the textural porosity (ϕ_t) increases with time because of the reduction in the total soil volume.

Appendix B: An Approximate Analytical Expression for Porosity Evolution

Analytical expressions for porosity evolution were derived with the assumption that the PSD preserves its "lognormal shape" during its evolution and use of formulae of mean, variance, and skewness of the lognormal PDF. These expressions can be used to predict evolution of total porosity without actually solving the full FPE.

The mean (α), variance (β^2), and skewness (κ) of the lognormal density function are related to the geometric mean (r_m) and log-transformed variance (σ^2) of the PSD by [*Aitchison and Brown*, 1976]

$$\alpha = E(r) = r_m \exp(\sigma^2/2), \quad (A9)$$

$$\beta^2 = E[(r - \alpha)^2] = \alpha^2[\exp(\sigma^2) - 1], \quad (A10)$$

$$\kappa = E[(r - \alpha)^3] = \alpha^3\{[\exp(\sigma^2) - 1]^3 + 3[\exp(\sigma^2) - 1]^2\}, \quad (A11)$$

where $E(x) = \int_0^\infty x f(x)\, dx$ denotes the expectation operator (ensemble average). The mean (α) of the PSD at any time (t) can be obtained by integrating the FPE drift coefficient $V(t)$ (equations (4) or (11)),

$$\alpha(t) = \int_0^t V(\tau)\, d\tau + \alpha(0), \quad (A12)$$

where $\alpha(0)$ is the mean of the initial lognormal PSD for the structural pore space.

By using the definitions of the mean (α), variance (β^2), and skewness (κ) of the lognormal distribution, given in (A9), (A10), and (A11), respectively, the expected structural pore volume at any given time $VP_s(t)$ can be expressed as

$$VP_s(t) = \frac{4}{3}\pi E(r^3) = \frac{4}{3}\pi\alpha(t)^3(\eta(t)^6 + 3\eta(t)^4 + 3\eta(t)^2 + 1), \quad (A13)$$

where $\eta^2 = [\exp(\sigma^2) - 1]$. Similar derivations for the expected structural void area (AP_s) to calculate areal (i.e., cross-sectional) porosity lead to

$$AP_s(t) = \pi E(r^2) = \pi\alpha(t)^2(1 + \eta(t)^2). \quad (A14)$$

It should be noted that the calculation of the volumetric porosity relies on the third moment of the PSD (skewness) that requires an assumption that the lognormal shape of the PSD is retained at all times. However, this assumption is not necessary for areal porosity calculation, because it depends only on the first and second moments (mean and variance).

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