A MEASURE OF SOIL STRUCTURE DERIVED FROM WATER RETENTION PROPERTIES: A KULLBACK-LEIBLER DISTANCE APPROACH

by

SUNG WON YOON

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ABSTRACT OF THE DISSERTATION

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Water retention curves of structured soils reflect the combined effects of pore systems associated to a given distribution of particle sizes (texture) and those that are the result of rearrangement of soil particles into soil structural units. The main hypothesis of this work was that the entropic distance between structural and textural soil pore systems can be a measure of soil structure. It was also hypothesized that such distance can be derived from water retention curves by assuming that both pore systems follow lognormal distributions and that textural pore systems are the result of random arrangements of particles sizes. The entropic difference between the distributions of the two pore systems considered was derived as a Kullback-Leibler Distance or KLD using an explicit equation that uses the geometric means and standard deviations of pores and particle size distributions derived from water retention data and from information on clay, silt and sand content. Data on water retention and texture obtained for this study was supplemented with data from the literature and with data on 1468 soils from the US National Pedon Characterization database. The KLD concept was tested by comparing physically disturbed samples with undisturbed samples over a range of soil structure conditions. Values of KLD from younger soils along two chronosequences, and from compacted and/or degraded soils were smaller than those from older soils and non compacted or degraded soils. Also, KLD values of disturbed samples were lower than those of undisturbed samples. The use of KLD in a large dataset showed that KLD was linearly related to saturated hydraulic conductivity, which is an important hydraulic property. Also, KLD was an important grouping factor in a regression tree analysis for estimation of water content at -33 kPa and in clusters defined from a combination of field and morphological variables. The KLD measure is a promising tool to characterize soil structure. Future studies should consider incorporating KLD into pedotransfer functions or other predictive schemes aimed at improving the estimation of hydraulic properties, which are sensitive to soil structure.

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Chapter 1

Introduction

1.1 General Background

Soil is a mix of mineral particles, nutrients, air, water, and living organisms. Soil structure can be defined as the hierarchical grouping of particles into structural units of various sizes and shapes known as aggregates (Brewer and Sleeman, 1960; Dexter, 1988; Horn et al., 1994; Nikiforoff, 1941; Young and Crawford, 2004). Soil structural units are known as *peds, aggregates* and/or *clods*. Soil peds refer to naturally formed visible soil structure in the field, whereas soil aggregates refer to fragments of the soil matrix resulting from the application of external forces and soil clods to aggregates greater than 10 cm (Kay and Angers, 2000). Soil structure has a profound influence on hydrologic processes due to their distinct relationships to soil pore systems (Holden, 1995; Nimmo, 1997; Pachepsky and Rawls, 2003). Physical, chemical, and biological mechanisms interact to form soil structural units, which is a dynamic rather than a static process affected by soil forming factors and anthropogenic effects (Bronick and Lal, 2005; Diaz-Zorita et al., 2002; Manolis, 2002; Ridolfi et al., 2003; Zonn, 1995). Changes of soil pore systems with structural development, in turn, modify the space of living organisms (microbes and plants) and the pathways of water and nutrients (Wardle et al., 2004; Young and Crawford, 2004).

Soils are highly variable in both space and time with their physical, chemical, and biological properties varying with the scale of observation (Brewer and Sleeman, 1960; Dexter, 1988). Well-structured field soils exhibit non-uniformity in sizes and shapes of soil peds thus resulting in heterogeneity in soil processes that hampers the understanding of soil functions (Bloschl and Sivapalan, 1995; Bouma and Decker, 1978; Dexter, 1988; Elfeki et al., 2002; Lin, 2003; Rao et al., 1980; Sposito, 2004; Starr et al., 1978). In part, this chaos-like heterogeneity results from the hierarchical organization of soil structure where a relatively large number of small structural units are contained in larger and less numerous soil structural units. Soil and soil structure formation result in visible patterns at various scales (Dexter, 1988; Holden, 1995; Horn, 1990; Levine et al., 1996b; Nimmo, 1997; Zonn, 1995). At the horizon scale level, soil aggregates are visually classified based on their type, grade, and size (Nikiforoff, 1941). Understanding the properties of pore systems associated to the various structural units (Fig. 1-1) is a critical issue because hydrologic processes are regulated by soil pore systems (Pachepsky et al., 2008).

Among other methods, fractals, Lyapunov exponents, and Komogorov K-entropy have been applied to soil systems in an attempt to understand chaos-like properties or processes in soils (Culling, 1988; Gimenez et al., 1997; Hugget, 1995; Ibanez et al., 1994; Phillips, 1999). The idea of determinant chaos is that complex behavior in an arbitrary system can be depicted by single parameters of mathematical equations by knowing the initial conditions (Phillips, 2000). Fractal and Lyapunov exponents share similarities in their mathematical formulation, but while fractals depict power law relationships between object properties such as mass or volume, the Lyapunov exponents depict variations of properties in systems over time (Phillips, 2000). The term *entropy* has developed as more or less distinct concepts in statistical mechanics (Boltzmann, 1872) and information theory (Shannon, 1948). Entropy in modern applications uses the formulation of Shannon (1948) and is interpreted as a measure of randomness of a probability distribution. For instance, this concept has been used in ecology to quantify biological diversity (Jost, 2006). The K-entropy is defined as the sum of Lyapunov exponents in the sub-systems and is equal to Shannon entropy, indicating the degree of chaos in the entire system.

Entropy has been used to describe soil structure at various scales. At the landscape scale, entropy has been applied to characterize landscape irregularity due to soil formation (Culling, 1988; Hallet, 1990a; Phillips, 1995; Phillips, 1999; Phillips, 2005). At the pedon scale (Fig. 1-1), Phillips (2000) quantified soil development by calculating entropy from the thickness and number of horizons of soil profiles. At the pore scale (Fig. 1-1), Dexter (1974) characterized the sequence of pores and particles from soil thin section. Since then, entropy has been applied to the characterization of soil particle size distributions and configuration of pore systems from image analysis (Brown, 2000; Caniego et al., 2001; Chun et al., 2008; Khitrov and Chechuyeva, 1995; Martin and Rey, 2000).

The soil water retention characteristic is defined as the relationship between water content and the corresponding pressure potential (Fredlund and Xing, 1994). Soil pore systems can be described as probability distributions of sizes that can be inferred from water retention curves (Brutsaert, 1966; Morel et al., 1991; Nimmo, 1997; Pagliai et al., 2004; Russell, 1941; Wu et al., 1990). Kosugi (1994) proposed the use of a lognormal probability density function to model water retention curves. The parameters of the Kosugi (1994, 1996) lognormal water retention model, geometric mean r_s and standard deviation σ_s, can be used to infer soil pore size distributions from soil water retention curves (Hayashi et al., 2006; Hwang and Powers, 2003; Kosugi, 1996; Kosugi, 1997; Kutilek, 2004). Only a few studies have used parameters of probability density functions from water retention curves to assess soil structure (Hayashi et al., 2006; Kosugi, 1997).

Based on previous studies on the characterization of soil pore systems from images (Caniego et al., 2001; Chun et al., 2008; Dexter, 1976), entropy could be used to characterize soil pore size distributions from water retention curves (Fig. 1-2). Entropy achieves a minimum value when soil pore sizes are contained in a single size class and a maximum value when soil pore sizes are uniformly distributed. However, maximum entropy does not necessarily correspond to the most structured soils because pore size distributions from water retention curves of structured soils contain both soil structural and textural characteristics (Fig. 1-3). Thus, there is need to separate the effect of soil texture when characterizing soil structure from water retention curves. The relative entropy or Kullback-Leibler Distance, KLD, measures the entropic distance between two probability distributions (Kullback, 1951). When the two probability distributions are lognormal, KLD has an explicit equation (El-Baz and Nayak, 2004b). Soil pore size distributions from random arrangement of soil particles can be used as a reference pore size distribution and KLD between the reference distribution and the pore size distribution of structured soils can be considered as measure of soil structure (Fig 1-3).

1.2 Hypotheses

The hypotheses of this dissertation are that 1) the development of visible soil structure units is reflected in the derived soil pore systems, 2) soil pore systems can be inferred from water retention properties and 3) KLD can quantify soil pore systems derived from water retention curves.

1.3 Objectives

- Develop an explicit form of KLD equation for soil pore size distributions inferred from water retention curves assuming that sizes of soil pores and particles are lognormally distributed.

- Identify relationships between KLD from soil water retention curves and visible features of soil structure such as soil structure types and sizes.
- Investigate the effect of soil management on KLD.
- Investigate the relationship between KLD and soil physical and hydraulic properties.

1.4 Dissertation Outline

This dissertation consists of five chapters. Chapter 1 contains a brief background on soil structure, entropy and KLD. In Chapter 2, mathematical expressions of entropic distance between structural and textural pore systems as a Kullback-Leibler Distance, or KLD are introduced and tested with data selected from the literature. Structural pore systems are inferred from water retention curves and textural pore systems are inferred from texture. In Chapter 3, water retention, textural information, and field description of soil structure of various soils with different sample treatment (disturbed/undisturbed), structure types (i.e., shapes) and sizes and management practices are studied using KLD. In Chapter 4, the KLD concept is tested with a large data set with the aid of multivariate statistical approaches (nonlinear categorical PCA, the two-step cluster analysis, and categorical regression tree analysis). Chapter 5 states the major conclusions and proposes future research to extend and generalize the concept proposed in this study.

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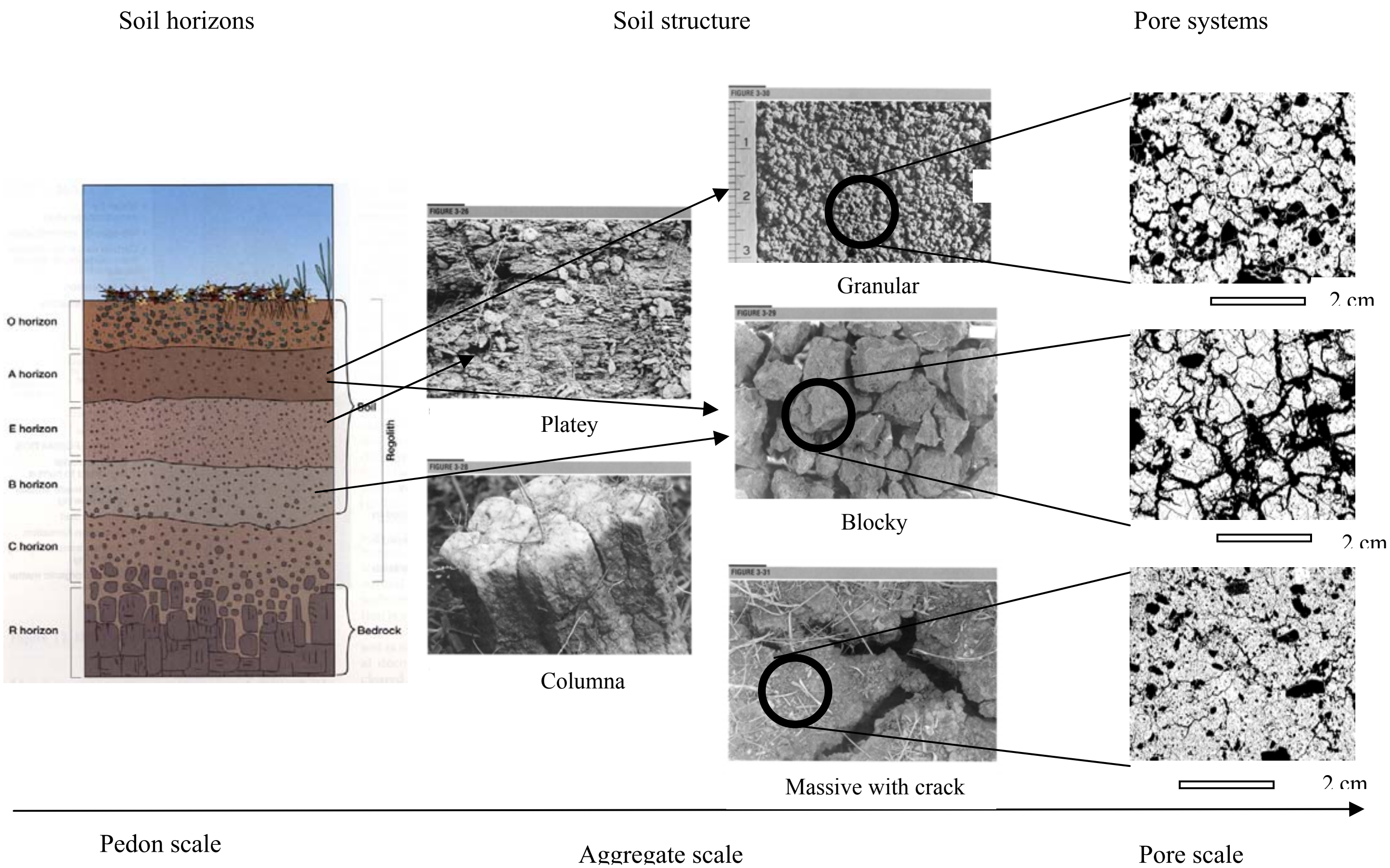

Fig. 1- 1 Illustrations of soil structures at various scales (images were modified from Fitzpatrick, E.A. 2004. Soil Microscopy and Micromorphology, CD, version 2, http://piru.alexandria.ucsb.edu/~tierney/TRS/lab6.htm, and http://soils.usda.gov/technical/manual/contents/chapter3g.html#60).

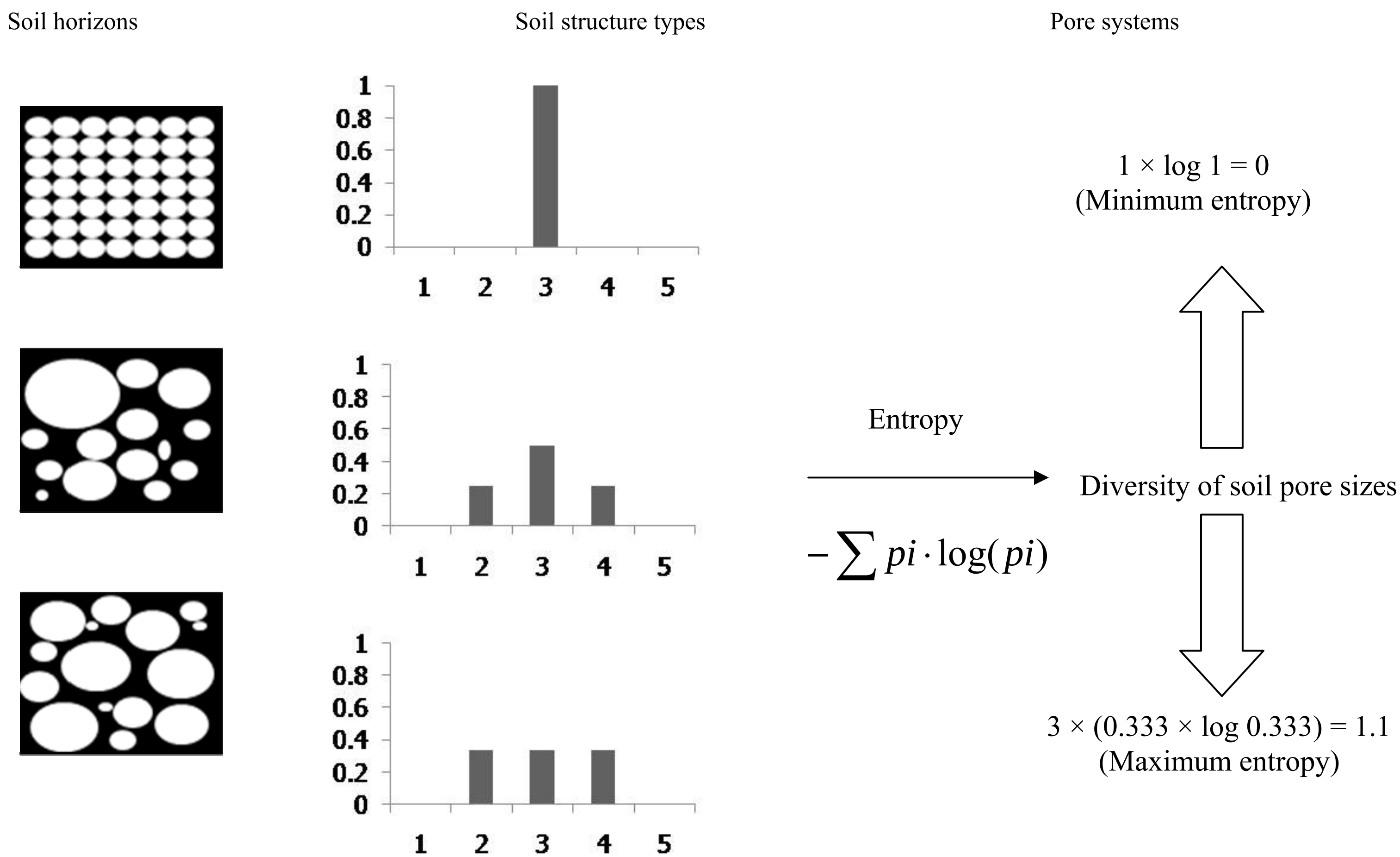

Fig. 1- 2 Examples of entropy from three soil pore size classes, represented by the white areas in the left figures. The corresponding diagrams to the rigth depict the distributions of pore size classes: the top diagram indicates a deterministic case, the middle diagram appears as a normal distribution, and the bottom diagram is a uniform distribution of pore size classes.

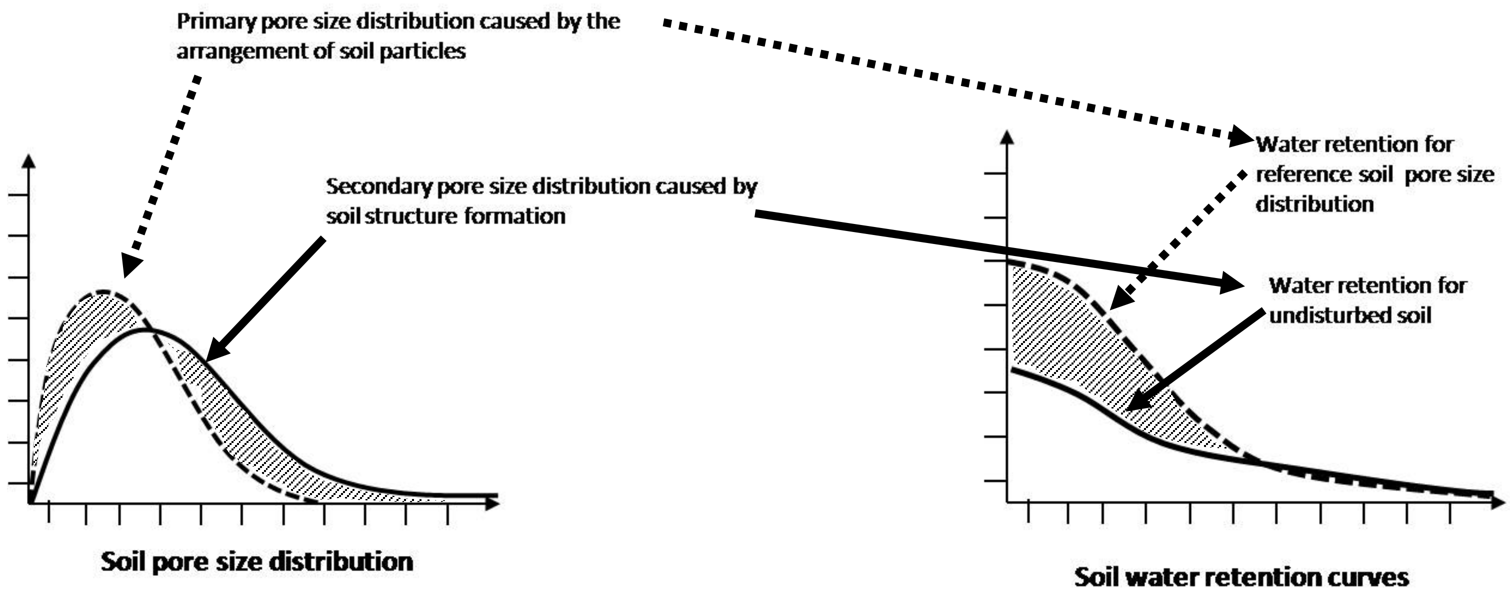

Fig. 1- 3 Illustration for the concept of KLD related to soil pore size distributions and water retention curves. Reference pore size distribution is the result of random arrangement of soil particles. Dashed areas represent KLD of soil structure.

Chapter 2

Soil Structure and the Kullback-Leibler Distance Derived from Water Retention Properties

2.1 Introduction

Pore size distributions of structured soils result from the confluence of the structural and textural characteristics of a soil (Monnier et al., 1973; Nimmo, 1997; Pagliai and Vignozzi, 2002; Wu et al., 1990). An initial pore size distribution resulting from randomly arranged soil particles is modified over time by complex interactions among natural and anthropogenic factors. Hypothetically, repeated packing of a particle size distribution would produce similar pore size distributions (Tamari, 1994). On the other hand, structured soils may develop different pore size distributions from similar particle size distributions or vice versa (Assouline et al., 1997; Tavares-Filho, 1995). Qualitative descriptions of soil structure are well established (Nikiforoff, 1941) but there is a lack of quantitative indices to describe soil structure conditions and or development from changes in soil pore systems.

Pore size distributions can be inferred from soil water retention curves (Crawford et al., 1995; Kutilek, 2004; Russell, 1941). Various functions representing water retention curves have been proposed (Cornelis et al., 2005) and either the parameters of those functions or water contents at equilibrium with specific pressure potentials (e.g., -33 or -1,500 kPa) have been empirically related to descriptions of soil structure (Guber et al., 2003; Hayashi et al., 2006; Kosugi, 1997; Levine et al., 1996b; Rawls and Pachepsky, 2002). Empirical predictions of soil water retention curves are generally based on particle sizes and organic carbon content. Qualitative descriptions of soil structure did not improve predictions from texture and organic carbon (Pachepsky and Rawls, 2003).

Entropy, defined as the expectation of a logarithmically transformed probability distribution, has been recognized as a measure or index of soil structure (Dexter, 1976).

A variety of entropy functions have been proposed to characterize soil particle size distributions (Brown, 2000; Khitrov and Chechuyeva, 1995; Martin and Rey, 2000), soil pore systems from image analysis (Caniego et al., 2001; Chun et al., 2008; Dexter, 1976; Posadas et al., 2003), divergence or convergence of soil horizons (Phillips, 2000), soil cover (Culling, 1988), and landscape relief and evolution (Hallet, 1990a; Hallet, 1990b; Phillips, 1995; Phillips, 1999; Phillips, 2005). The Kullback Leibler Distance (KLD) (Kullback, 1951) is a relative entropy that quantifies the difference between two probability distributions. Therefore, KLD could be used as a measure of soil structure by calculating the relative entropy between the pore size distribution of a structured soil and a reference pore size distribution representing the random packing of particles without any structural development (see Fig. 1-3). While a soil pore size distribution can be inferred by fitting a water retention model to measured data of undisturbed soils, a reference pore size distribution need to be defined in a practical way.

The contrast between entropy and KLD as a measure of soil structure can be illustrated by comparing two structured soils with the same reference pore size distribution (Fig. 2-1). While entropy measures the disorder or randomness of a soil pore size distribution, KLD considers the entropic distance between two probability distributions, in this case between a structured soil and a reference. Soil A with the smaller geometric mean, r_s, and standard deviation, σ_s, and Soil B with greater r_s and σ_s are assumed to have an identical reference pore size distribution (Fig. 2-1a). Considering only the entropy of these distributions, would suggest that Soil A has the most ordered pore size distribution (smallest entropy) followed by the reference pore size distribution and by Soil B (Fig. 2-1b). On the other hand, the KLD values indicate that the pore size distribution of Soil B is more similar to the reference (smallest KLD) than the pore size distribution of Soil A (Fig. 2-1c). According to the proposed interpretation of KLD, the soil structure of Soil A would be more developed than that of Soil B.

The objective of this study was to develop a soil structure index based on the KLD concept. The proposed index of soil structure complexity was evaluated using published experimental data. Pores and particle sizes were assumed to follow lognormal distributions. Pore size distributions of structured soils were estimated by fitting water retention data with the Kosugi (1996) lognormal water retention model, whereas reference pore size distributions were derived combining the models of Shirazi and Boersma (1984) and of Chan and Govindaraju (2004). The concept was tested with data taken along chronosequences (Lohse and Dietrich, 2005; Young et al., 2005), data from rhizosphere and bulk soils (close and away from plant roots, respectively) planted to barley, wheat, and maize (Whalley et al., 2005), and data from soils at various levels of compaction (Reicosky et al., 1981; Zhang et al., 2006), and soil degradation (Omuto et al., 2006).

2.2 The Index of Soil Structure

2.2.1 Estimation of Parameters for the Reference pore size distribution

For this approach, both sizes of soil particles and pores are assumed to be lognormally distributed. It is generally accepted that particle size distributions can be described with lognormal models (Buchan, 1989; Chan and Govindaraju, 2004; Hwang and Choi, 2006; Rouault and Assouline, 1998; Shalizi et al., 2004), and that soils with lognormal particle size distributions tend to show lognormal pore size distributions (Assouline et al., 1997).

Water retention curves from reference pore size distributions were estimated from lognormal particle size distributions as (Chan and Govindaraju, 2004):

$$Se(r_p) = 1 - \frac{(1-n)\exp\{-nS[a_0(\frac{r_p/\alpha}{m_1})^3 + a_1(\frac{r_p/\alpha}{m_1})^2 + a_2(\frac{r_p/\alpha}{m_1})]\}}{\phi} \quad (2\text{-}1)$$

where $Se = \frac{\theta - \theta_r}{\theta_s - \theta_r}$ is the effective saturation, θ_s and θ_r are the saturated and residual volumetric water contents, respectively and r_p is pore radius. The scaling factor, α , is assumed to be equal to 4 (Chan and Govindaraju, 2004) and *n* is a parameter related to porosity, ϕ , as $\phi = n - 1$. The surface area ratio, *S* is given by $S = \frac{m_1 m_2}{m_3}$ and the coefficients a_0, a_1, and a_2 are $a_0 = \frac{(m_1^2/m_2)(1-n)(1-n+3nS)+2n^2S^2}{(1-n)^3}$,

$a_1 = \frac{6(m_1^2/m_2)(1-n)+9nS}{2(1-n)^2}$, and $a_2 = \frac{3}{1-n}$

and m_i the i-*th* moment of lognormal particle size distribution defined as

$$m_i = exp(i\mu_y + \frac{i^2\sigma_y^2}{2})$$

where μ_y is the mean and σ_y is the standard deviation of a lognormal particle size distribution based on the number of particles. The parameters of a lognormal distribution can also be derived from particle mass (more commonly measured in soils). The relationship between the parameters from the two types of measures is:

$$\mu_y = \mu_g - 3\sigma_g \text{ and } \sigma_y = \sigma_g \tag{2-2}$$

where μ_g and σ_g are the mean and standard deviation derived from mass (Chan and Govindaraju, 2004). Furthermore, μ_g can be estimated from the geometric mean d_g as $\mu_g = \ln(d_g)$. Parameters d_g and σ_g were estimated from mass percents of clay, silt, and sand fractions as (Shirazi and Boersma, 1984):

$$d_g = \exp(0.01\sum_{i=1}^{n} f_i \ln M_i),$$

$$\text{and}\ \sigma_g = \sqrt{0.01\sum_{i=1}^{n} f_i \ln^2 M_i - a^2} \tag{2-3}$$

where f_i is the mass percent of the i-*th* component and M_i is the mean of the size interval for each of the i-*th* components.

Water contents at pressure potentials, ψ , of -0.1, -0.2, -0.5, -1, -2, -5, -10, -30, -100, -300, -1,000, -1,500 kPa were calculated with Eq. (2-1) and used to fit the Kosugi (1996) lognormal water retention model to estimate geometric mean, ψ_R and standard deviation, σ_R of water retention curves from the reference pore size distribution.

2.2.2 Determining the Entropy and KLD from Water Retention Curves

The Shannon entropy $H[f(x)]$ of a continuous random variable, *x*, with a probability distribution $f(x)$ is defined as:

$$H[f(x)] = \int_{-\infty}^{\infty} f(x)\ln(1/f(x))dx \tag{2-4}$$

Entropy $h(x)$ is minimized in a deterministic system and maximized in a system that has uniform distribution. A probability density function $f(\psi)$ of pressure potentials, ψ, can be derived from a water retention model as:

$$f(\psi) = dS_e / d\psi \tag{2-5}$$

Pore radius, *r*, can be derived from ψ as (Brutsaert, 1966) r =$149/|\psi|$, where r is size of soil pore expressed in µm and ψ in kPa. The pore size distribution, $f(r)$, can be estimated from soil water retention curves using the (Kosugi, 1996) lognormal water retention model as:

$$f(r) = \frac{1}{r\sigma\sqrt{2\pi}} \exp\left[-\frac{(\ln r - \ln r_s)^2}{2\sigma_s^2}\right] \tag{2-6 }$$

where $\ln r_s$ and σ_s^2 are the mean and variance of log-transformed soil pore sizes, $\ln r$, respectively.

The explicit form of the differential entropy for $f(r)$ can be derived by combining Eq. (2-6) in Eq. (2-4) as (see Appendix A for details):

$$H[f(r)] = \ln r_s + \frac{1}{2} + \frac{1}{2}\ln(2\pi\sigma_s^2) \tag{2-7}$$

Values of $H[f(r)]$ in Eq. (2-7) will tend to a maximum value when all pore sizes have the same probability of occurrence and to be $\ln r_s$ when all pores have the same size.

The Kullback-Leibler Distance (Kullback, 1951) or KLD between two probability density functions $f_s(x)$ and $f_R(x)$ is defined as:

$$KLD = \int f_s(x) \ln\{f_s(x) / f_R(x)\} dx \tag{2-8}$$

If $f_s(x)$ represents the probability density function of the structured soil and $f_R(x)$ the probability density function of the reference pore size distribution. If both distributions are lognormal with parameters (μ_R , $\sigma_R{}^2$) and (μ_s , $\sigma_s{}^2$), KLD can be expressed as (El-Baz and Nayak, 2004a):

$$KLD = \ln \sigma_R - \ln \sigma_s - \frac{1}{2} + \frac{\sigma_s{}^2 + (\mu_s - \mu_R)^2}{2\sigma_R{}^2} \qquad (2\text{-}9)$$

where the parameter values are obtained by fitting with the Kosugi (1996) lognormal water retention model the soil water retention curves of the structured soil and the water retention curve derived from the reference pore size distribution.

2.3 Applications

Entropy and KLD were estimated from soil water retention data from the literature describing soil structure modification caused by 1) time, i.e., changes measured along two chronosequences (Lohse and Dietrich, 2005; Young et al., 2005), 2) plant roots (Whalley et al., 2005), 3) soil compaction (Assouline et al., 1997; Reicosky et al., 1981; Zhang et al., 2006) and 4) soil degradation (Omuto et al., 2006). The literature was selected based on the availability of water retention data (or water retention model parameters) and mass fraction of sand, silt and clay (Table 2-1). When only parameters n and α of the van Genuchten (1980) model of water retention were reported (Table 2-1), the geometric mean of pressure potential, ψ_s , and standard deviation, σ_s , of the Kosugi (1996) lognormal water retention model were obtained as:

$$\psi_s = \psi_0 \exp(\sigma_s^2) \qquad (2\text{-}10)$$

where ψ_0 is the mode of a distribution defined as:

$$\psi_0 = \frac{m^{1-m}}{\alpha} \tag{2-11}$$

and:

$$\sigma_s^2 = (1-m)\ln\left[\frac{2^{1/m}-1}{m}\right] \tag{2-12}$$

where $m = 1 - 1/n$.

2.3.1 Soil Structural Development over Time

The development of soils as a time-dependent system is a classic concern in pedology (Arnold, 1965; Huggett, 1998; Targulian and Krasilnikov, 2007). Most of the studies related to soil development along chronosequences have focused on chemical properties, soil particle composition and weathering, and on soil profile or landscape development (Chorover et al., 1999; Huggett, 1998; McFadden, 1988; Torn et al., 1997).

Young et al. (2005) and Loshe and Detrich (2005) reported soil physical and hydraulic properties along well defined chronosequences in a desert and a tropical environment, respectively (Table 2-2). Young et al. (2005) investigated the effect of soil age (from 50 to10^5 yr) in sites located along the piedmont region of the Providence Mountains in the eastern Mojave Desert. In an earlier study by McDonald et al. (1996), these sites were classified as late Holocene (young soil; Qf7, Qf6) and Pleistocene (old soils: Qf5, Qf4, Qf3) alluvial fans. Young et al. (2005) measured infiltration rates of near surface soil horizons at sites representative of various degrees of pedological development. Infiltration rates were used to infer the parameters of the van Genuchten (1980) water retention model (Table 2-1). Lohse and Dietrich (2005) investigated the variations in hydraulic processes at two sites located on the islands of Hawaii and Kauai, respectively. The sites have similar conditions of vegetation, parent material and climate, but are at different development stages. The soils on the island of Hawaii are 300 year old Andisols, whereas the soils on the island of Kauai are 4.1 million year old Oxisols. Textural information for soil at the Hawaiian site was supplemented with data from Chorover et al. (1999).

The increase in subsurface clay contents with time is a common feature in both soils. However, the two sites exhibited opposite trends in the development of pore size distribution with r_s decreasing and σ_s increasing with time in the Mojave Desert and vice versa in the soils on the Hawaiian Islands (Table 2-2). The source of clay is different in each site. In the case of the Mojave Desert soil, clay and silt contents increased over time because of aeolian deposition and translocation into deeper soil. Concurrently soil structure developed from massive structure to complex blocky structure (Machette, 1986; McDonald et al., 1996; McFadden, 1988; McFadden et al., 1986; Reheis et al., 1989; Young et al., 2005). For the environments on the islands of Hawaii and Kauai, the increase of clay contents and the development of clay rich horizons over time are typical of pedogenetic processes that take place in semiarid and humid environments without significant erosion (Birkeland, 1999; Lohse and Dietrich, 2005).

In the environment of the Mojave Desert, there were no significant differences in KLD values for soils under 4,000 year old, although an increasing trend can be observed during that period (Fig. 2-2). The formation of a pavement in the Mojave Desert due to the deposition and translocation of clay and silt takes between 4,000 to 10,000 years (Young et al., 2005), which seems to correspond to the observed increase in KLD in those periods. Significant increases in KLD values were found for 10,000 and 100,000 year old soils ($p < 0.001$), which matches the described changes in soil structure from massive to blocky. A significant reduction ($p < 0.001$) of KLD in soils 100,000 year old could be interpreted as regressive pedogenetic process. Unidirectional soil formation, defined as a continuous soil forming process that never reaches equilibrium (Rode, 1961) is no longer accepted. Soils are an open system with many possible developmental pathways (Huggett, 1998; Phillips, 1998; Targulian and Krasilnikov, 2007). Stevens and Walker (1970) reported losses of organic/inorganic nutrients from soil degradation after 12,000 years of pedogenesis.

The rate of soil formation is a function of climate, parent material, and also depth (Raeside, 1959; Targulian and Goryachkin, 2004; Targulian and Krasilnikov, 2007). Despite environmental differences, the KLD values of Hawaii/Kauai soils followed the same trend than those from the Mojave Desert (Fig. 2-2). Although statistical tests could not be performed, KLD values of the surface and subsurface of the 300 year old Kauai soil could be greater than those in the Mojave Desert 500 year old soils. In addition, differences of KLD between surface and subsurface soils seem to decrease or vanish over time when comparing KLD values for surface and subsurface soils at 300 and 4.1 million year old. The values of KLD between the Mojave and Hawaii/Kauai soils seems to coincide with the concepts that soil forming potential is higher in tropical than in desert regions and that deep soils require more time for structural development (Targulian and Krasilnikov, 2007).

2.3.2 Plant Roots Effects

Plant roots can alter the soil pore system to promote a favorable environment for their growth (Gregory and Hinsinger, 1999; Hinsinger, 1998; Passioura, 1988). Roots promote soil aggregation and aggregate stability by promoting fungal activity and by exuding gluing agents such as mucilage (Dorioz et al., 1993; Morel et al., 1991; Tisdall and Oades, 1982; Young, 1998).

The soil environment at the root-soil interface also known as rhizosphere exhibits different physical, biological, and chemical properties than the bulk soil, i.e., soil not influenced by roots (Jenny and Grossenbacher, 1963; Young, 1995; Young, 1998). Mucilage excreted by roots changes the wetting angle and surface tension of soil water near roots and may play a role in the transport of water to the root system (Passioura, 1988; Tinker and Nye, 2000; Whalley et al., 2005).

Whalley et al. (2005) measured water retention curves on aggregates of rhizosphere and bulk soil collected six weeks after planting of wheat, maize and barley. In addition, they analyzed images of soil aggregates from both soil regions. They found no significant differences in porosity and bulk density between the bulk and the rhizosphere soils. This is in contradiction with predictions of an exponential increase in bulk density with a decrease in distance to the root-soil interface (Dexter, (1987). On the other hand, water retention properties were significantly different between rhizosphere and bulk soils, especially between -6 and -150 kPa (Whalley et al., 2005). Differences in water retention properties could be caused by the presence of mucilage exudates produced by plant roots in the rhizosphere soil, but this chemical effect would be difficult to separate from a potential difference in pore sizes between the two regions (physical effect).

Pore size distributions derived by fitting the Kosugi (1996) lognormal water retention model showed greater r_s and σ_s in the rhizosphere soils than in the bulk soils

(Table 2-3), which could be the result of both chemical and physical effects. However, the fact the greater numbers of pores and aggregates in the rhizosphere compared to the bulk soil were reported by Whalley et al. (2005) suggests that water retention curves reflect a physical effect. Values of KLD averaged across crops were significantly greater in rhizosphere than in bulk soils (Fig. 2-3). Based on image analysis measurements in Whalley et al. (2005), the greater KLD values of the rhizosphere soils correspond to the increase in the number of pores and aggregates. A plot of number of pores per aggregate *vs.* KLD resulted in a linear relationship with negative slope. The difference of KLD values were statistically significant ($p = 0.015$), although image analysis did not result in statistically significant differences between rhizosphere and bulk soils. Aggregates from the rhizospheres had less pores than aggregates from bulk soils except for soil growing barley (Fig. 2-4). Guide et al. (1988) reported that total porosity of rhizosphere soil aggregates was lower than that of bulk soil aggregates. In this case, however, it could be that compaction reduced the number of large pores (visible in the images) and increased the number of pores smaller than 25 μm (which would account for the increase in water retention in the range between -6 and -150 kPa).

2.3.3 Soil Compaction and Degradation

Compacted soils would typically have greater bulk density values and smaller values of saturated water content, saturated hydraulic conductivity and infiltration (Akram and Kemper, 1979; Dawidowski and Koolen, 1987). The effects of soil compaction are functions of both soil texture and of chemical properties (Assouline et al., 1997; Tavares-Filho, 1995). Soil compaction or improper land use and management practices could decrease organic matter content in the soil, depreciate important soil physical properties, and consequently increase soil erosion (Li et al., 2007; Wu and Tiessen, 2002).

Zhang et al. (2006) reported van Genuchten (1980) water retention parameters and hydraulic properties of compacted soils from two locations in China (Mizhi and Heyang). They sampled undisturbed soil cores from two depths (top soil, 0-5 cm, and bottom soil, 10-15 cm) and compacted the cores to three levels representing 0%, 10%, and 20% increases in bulk density of top soil (1.27 Mg/m^{-3}, 1.37, Mg/m^{-3} , and 1.60 Mg/m^{-3}) and of bottom soil (1.29 Mg/m^{-3}, 1.45 Mg/m^{-3}, and 1.65 Mg/m^{-3}) from Heyang and of top soil (1.3 Mg/m^{-3}, 1.45 Mg/m^{-3}, and 1.61 Mg/m^{-3}) and of bottom soil (1.34 Mg/m^{-3}, 1.47 Mg/m^{-3}, and 1.69 Mg/m^{-3}) from Mizhi. Reicosky et al. (1981) presented water retention curves of compacted soils under laboratory conditions with four different levels of bulk density: 1 Mgm^{-3}, 1.2 Mgm^{-3}, 1.3 Mgm^{-3}, and 1.6 Mgm^{-3}. Assouline et al. (1997) studied compaction of two Oxisols (Palotina and Cascavel) having the same texture but different pH and cation exchange capacity (CEC). Omuto et al. (2006) studied the hydrologic responses at 179 locations of the Upper Athi river watershed in eastern Kenya. According to a visual assessment of the soil physical conditions at each location, data were grouped in three categories; non-degraded, moderately degraded, and severely degraded soils.

Data from the selected literature on soil compaction and degradation showed that r_s decreased as soils were more compacted or degraded but no trend was observed in σ_s (Tables 2-4, 2-5, and 2-6).

Measurements on re-packed soils (Reicosky et al., 1981 and Assouline et al., 1997) exhibited greater KLD values than undisturbed soils (Zhang et al., 2006) (Fig. 2-5).

Probably, soil sieved and repacked at a low bulk density results in a greater contrast between inter- and intra-aggregate pore volumes compared to the corresponding undisturbed (structured) soil; and, therefore, yields greater values of KLD. For each soil, values of KLD and bulk density were linearly correlated with negative slopes. Changes in bulk density due to compaction may affect different types or sizes of soil pores depending on a particular soil condition (Bruand and Cousin, 1995). Undisturbed soils typically exhibited smaller rates of change, suggesting that soil pore size distributions of natural soils are more resistant to external mechanical forces (Fig. 2-5). There were differences of KLD between the general categories of re-packed and undisturbed soils, (Fig. 2-5). The Mizhi soil had greater KLD values than the Heyang soil (Fig. 2-5), although KLD values decreased with compaction at a similar rate. The differences in KLD cannot be explained based on texture because the Heyang soil had greater clay content than the Mizhi soil (Table 2-4). Unfortunately, information on the structural condition of the soils was not included in Zhang et al., (2006); thus preventing further discussion of the possible reasons for the differences. Texture cannot explain the differences between Cascabel and Palotina soils either, but in this case, Assouline et al. (1997) pointed out that the Palotina soil had been subjected to physical damage by 30 years of intensive cultivation and as a result it had low aggregate stability and organic matter content, which translated to a lower bonding capacity of clay particles. In the case of the Palotina soil, low aggregate stability may have created a pore system intermediate between the inter- and intra-aggregate pore systems; thus, increasing KLD values over the levels observed for the Cascabel soil.

Clay content is strongly related to stability of soil structure as a cementing agent of larger particles (Dexter and Czyz, 2007). In the data of Omuto et al. (2006) severely degraded soils, had significantly ($p < 0.001$) lower values of clay content than non degraded or moderately degraded soils (Table 2-6). Significant reduction of infiltration rate and clay content in degraded soils were also reported (Machado et al., 2008; Omuto, 2008; Omuto et al., 2006). Values of KLD decreased as soils were degraded in the study of Omuto et al (2006) (Fig. 2-6).

2.4 Conclusions

The proposed measure of soil structure, KLD, is based on soil pore size distributions derived from water retention curves and soil texture. In addition to its computational simplicity, the main advantage of KLD is that it offers an intuitive picture of the effect of structure formation on soil pore systems as an entropic distance from a reference pore system. A key issue in the development of KLD as a measure of soil structure was to justify the reference pore size distributions and to derive from it theoretical water retention curves using Chan and Govindaraju (2004). Testing of KLD in a range of situations demonstrated that greater values of KLD are typical of structured and for less degraded soils. Although KLD can be an appropriate and robust indicator of soil structure, the concept was evaluated against a limited number of cases from the literature. The next chapter will focus on soils with qualitative descriptions of soil structure and having water retention measurements.

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Table 2- 1 Summary of data selected from the literature and used in this study.

Purpose	Sources	Type of Data	
		Water Retention Curve	Model Parameter
Chronosequence	Young et al. (2005) (4)		n, α (2)
	Loshe and Dietrich (2005) (4)		n , α
Plant Root Effect	Whalley et al. (2004) (5)	X (1)	
Soil Compaction and Degradation	Reicosky et al. (1981)(5)	X	
	Assouline et al. (1997) (5)		λ (3)
	Zhang et al. (2006) (6)		n , α
	Omuto et al. (2006) (4)		n , α

(1) Data obtained from figures in listed publications with ImageJ (Research Services Branch, National Institute of Health, Bethesda, MD). The soil water retention data were fitted with the lognormal water retention model of Kosugi (1996) with a GNU Octave programmed by Seki (2007).
(2) n and α are parameters of the van Genuchten (1980) water retention model $Se = [1 + (\alpha\psi)^n]^{-m}$.
(3) λ and ψ_a are parameters of the Brooks and Corey water retention model $Se = (\psi / \psi_a)^{-\lambda}$, which are related to the van Genuchten (1980) model parameters by $\alpha = \psi_a^{-1}$ and $1/(1-n) = \lambda + 1$ (Assouline et al. 1997).
(4) Data obtained from field measurements.
(5) Water retention curves were measured in disturbed soils.
(6) Water retention curves were measured in undisturbed soils.

Table 2- 2 Texture and pore size distribution parameters of reference size distributions and of structured soils from Young et al. (2005) and Loshe and Detrich (2005).

ID or depth	Age, yr	Texture, %			Pore Size Distribution			
					Reference *		Structured soil**	
		Sand	Silt	Clay	r_R (μm)	σ_R	r_s (μm)	σ_s
Young and et al. (2005)								
Qf8	5×10	94.7±0.9	3.9±0.7	1.4±0.2	65.53±15.68	0.88±0.04	143.62±18.09	0.95±0.15
Qf7	5×10^2	84.4±2.8	13.1±2.1	2.4±0.7	12.55±9.63	0.54±0.17	89.40±16.30	0.99±0.24
Qf6	4×10^3	71.0±3.7	22.7±3.3	6.2±1.7	0.48±0.35	0.44±0.02	70.03±31.12	1.03±0.18
Qf5	1×10^4	47.1±3.3	24.8±3.2	27.9±0.4	2.0E-04±0.00	0.39±0.01	60.39±28.07	1.14±0.20
Qf3	1×10^5	46.0±9.3	29.7±2.0	24.3±7.5	1.3E-03±0.00	0.40±0.02	38.85±21.89	1.15±0.20
Loshe and Detrich (2005)								
0-20cm	3×10^2	54.8	39	6.2	0.40	0.44	15.41	1.80
20-30cm	3×10^2	70.4	27.3	2.3	5.53	0.32	3.69	2.17
0-20cm	4×10^6	9.5	58.1	32.4	0.07	0.38	54.43	1.60
20-50cm	4×10^6	8.8	15.6	75.6	0.01	0.42	12.04	1.29

*: r_R and σ_R are the geometric mean and standard deviation for lognormal density function of the reference.
**: r_s and σ_s are the geometric mean and standard deviation of Kosugi (1996) lognormal water retention model.

Table 2- 3 Texture and pore size distribution parameters of reference and of rhizosphere and bulk soils planted to wheat , maize, and barley from Whalley et al. (2005).

Location	**Texture, %**			**Pore Size Distribution**			
				Reference *		**Structured soil****	
	Sand	**Silt**	**Clay**	**r_R (um)**	**σ_R**	**r_s (um)**	**σ_s**
Rhizosphere	8.0	72.5	19.5	0.23	0.55	9.26	3.01
						18.63	2.62
						45.15	1.62
Bulk						12.21	1.78
						1.62	3.40
						2.47	2.26

*: r_R and σ_R are the geometric mean and standard deviation for lognormal density function of the reference.
**: r_s and σ_s are the geometric mean and standard deviation of Kosugi (1996) lognormal water retention model.

Table 2- 4 Texture and pore size distribution parameters of reference and structured soils Heyang and Mizhi after a series of compactions. Data from Zhang et al. (2006).

Soil & Depth	Compaction level (BD, Mg/m^3)	Texture, %			Pore Size Distribution			
					Reference *		Structured soil **	
		Sand	Silt	Clay	r_R (um)	σ_R	r_s (um)	σ_s
Heyang 0-5cm	C0 (1.27)	2.8	76.5	20.6	0.59	0.73	16.01	2.21
	C1 (1.37)				0.53	0.76	2.67	2.13
	C2 (1.60)				0.41	0.78	1.39	1.96
5-15cm	C0 (1.29)	1.6	73.6	24.8	0.46	0.70	8.16	2.33
	C1 (1.45)				0.43	0.70	4.28	2.25
	C2 (1.65)				0.32	0.73	0.39	2.36
Mizhi 0-5cm	C0 (1.30)	27.7	60.6	11.7	0.07	0.38	8.53	0.85
	C1 (1.45)				0.07	0.38	7.73	0.84
	C2 (1.61)				0.07	0.38	6.64	0.91
5-15cm	C0 (1.34)	29.5	60.3	10.2	0.09	0.38	9.25	0.84
	C1 (1.47)				0.09	0.38	8.00	0.83
	C2 (1.69)				0.08	0.39	6.42	0.90

*: r_R and σ_R are the geometric mean and standard deviation for lognormal density function of the reference.
**: r_s and σ_s are the geometric mean and standard deviation of Kosugi (1996) lognormal water retention model.

Table 2- 5 Texture and pore size distribution parameters of reference and structured soil after a series of compaction. Data from Reicosky et al. (1981) and Assouline et al. (1997).

Soil	Bulk density (g/cm^3)	Texture, %			Pore Size Distribution			
					Reference*		Structured soil**	
		Sand	Silt	Clay	r_R (μm)	σ_R	r_s (μm)	σ_s
Reicosky et al. (1981)								
Barnes loam soil (sieved)	1.6	40	40	20	4.3E-03	0.42	2.83	1.06
	1.3				4.3E-03	0.42	6.75	1.12
	1.2				4.2E-03	0.42	10.18	1.26
	1.0				4.2E-03	0.42	14.59	1.32
Assouline et al. (1997) ***								
Cascavel (NC)	0.96	2	17	81	0.12	0.46	242.36	1.28
Palotina (NC)	1.25	6	11	83	0.02	0.43	138.11	1.51
Cascavel (C)	1.27	2	17	81	0.10	0.48	57.72	1.49
Palotina (C)	1.5	6	11	83	0.02	0.41	52.15	1.64

*: r_R and σ_R are the geometric mean and standard deviation for lognormal density function of the reference.
**: r_s and σ_s are the geometric mean and standard deviation of Kosugi (1996) lognormal water retention model.
***: NC= Non compacted soil and C= Compacted soil.

Table 2- 6 Texture and pore size distribution parameters of references and structured soils with three degree of degradation. Data from Omuto et al. (2006).

Degradation levels[***]	**Texture (average, %)**			**Pore Size Distributions**			
				Reference *		**Structured soil****	
	Sand	**Silt**	**Clay**	r_R **(um)**	σ_R	r_s **(um)**	σ_s
ND	30.8	21.3	47.9	3.6E-05	0.21	104.55	1.19
MD	41.2	29.5	29.3	2.4E-04	0.41	15.18	1.71
SD	43.1	30.2	26.7	3.6E-04	0.36	2.99	2.09

*: r_R and σ_R are the geometric mean and standard deviation for lognormal density function of the reference.
**: r_s and σ_s are the geometric mean and standard deviation of Kosugi (1996) lognormal water retention model.
***: ND= Non-degraded (cases without any sign of degradation), MD= Moderately degraded (case with in situ physical deformation), SD= Severely degraded (case with multiple signs of in situ physical deformation and erosion).

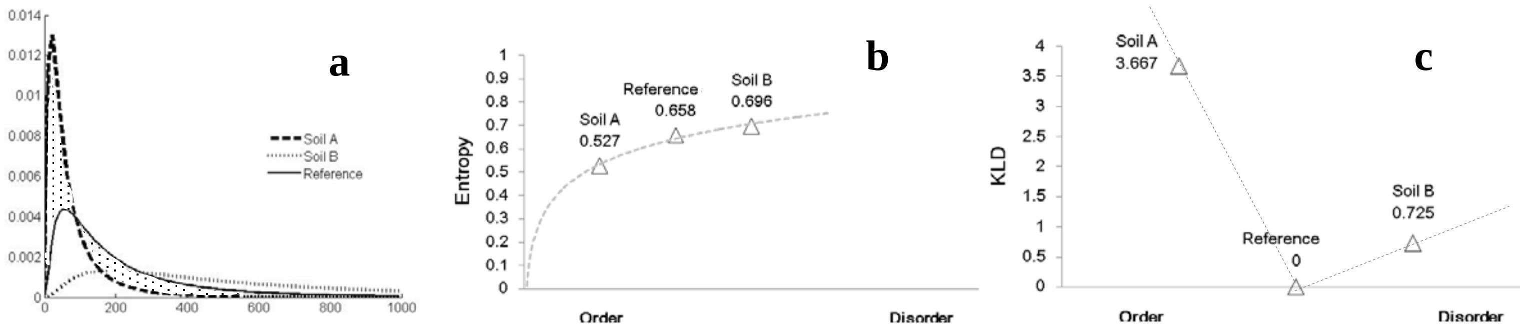

Fig. 2- 1 General sketch of measures of soil structure using entropy and KLD (a) Simulated lognormal pore size distributions of a reference distribution and of Soil A and Soil B, (b) Entropy for the situations shown in (a) , and (c) KLD measures. Dotted area in (a) indicates differences in pore size ditributions between Soil A and the reference. Dashed lines in (b) and (c) describe the conceptual trend of entropy and KLD.

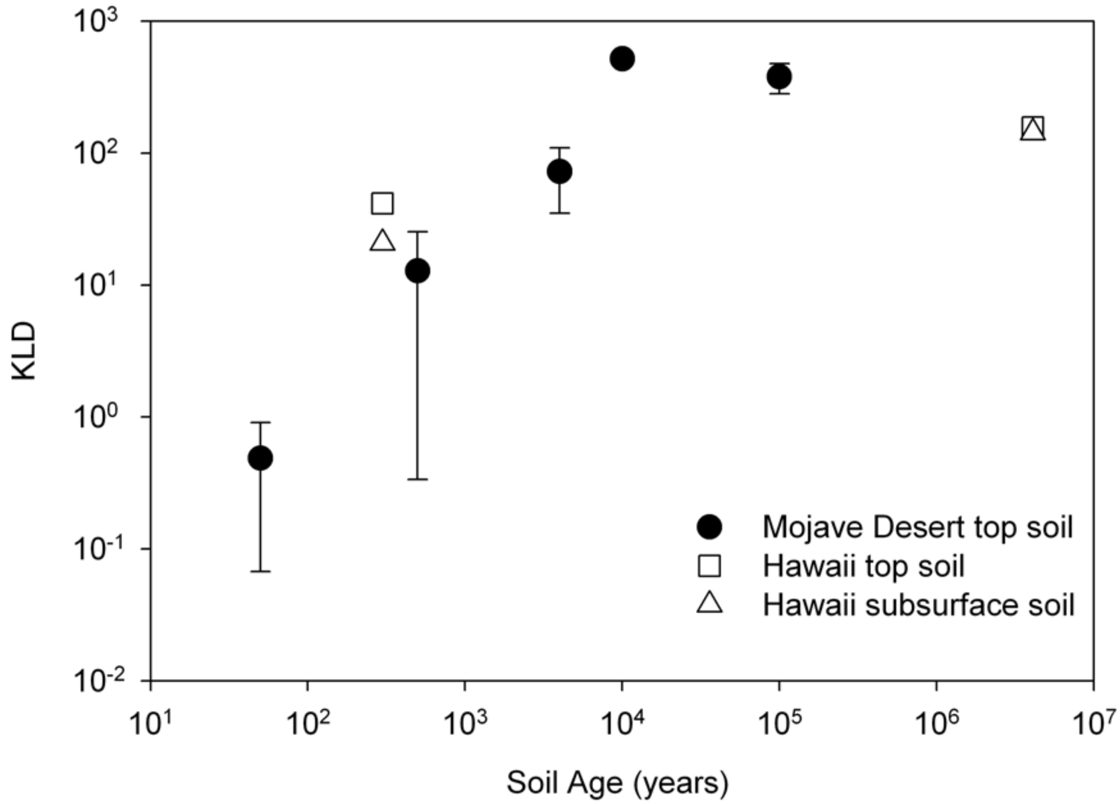

Fig. 2- 2 KLD measures of Mojave Desert soils from Young and et al. (2005) and Hawaiian soils from Loshe and Detrich (2004). Error bars in Mojave Desert soils indicate standard deviations from three replicates.

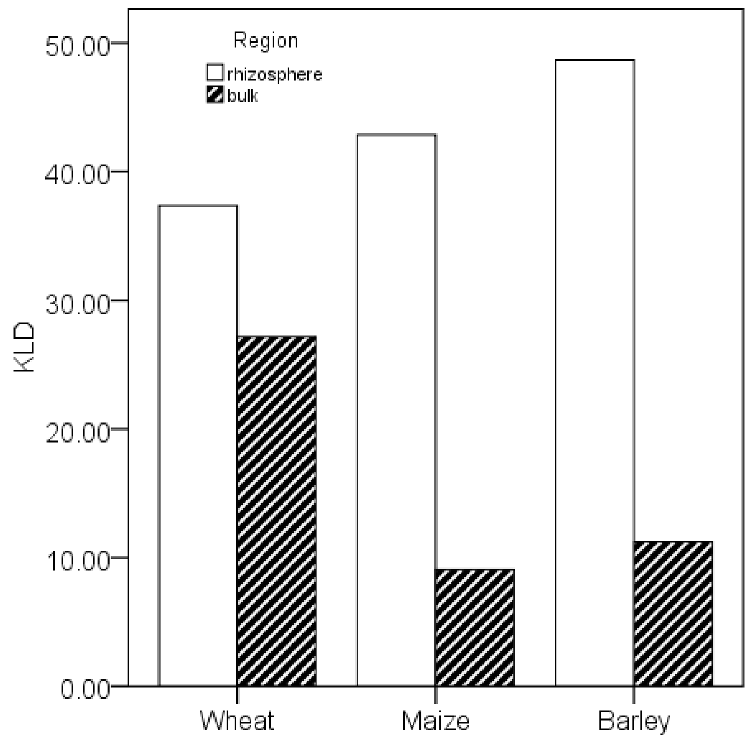

Fig. 2- 3 Average KLD values for rhizosphere and bulk soils planted to wheat, maize and barley. Data from Whalley (2004).

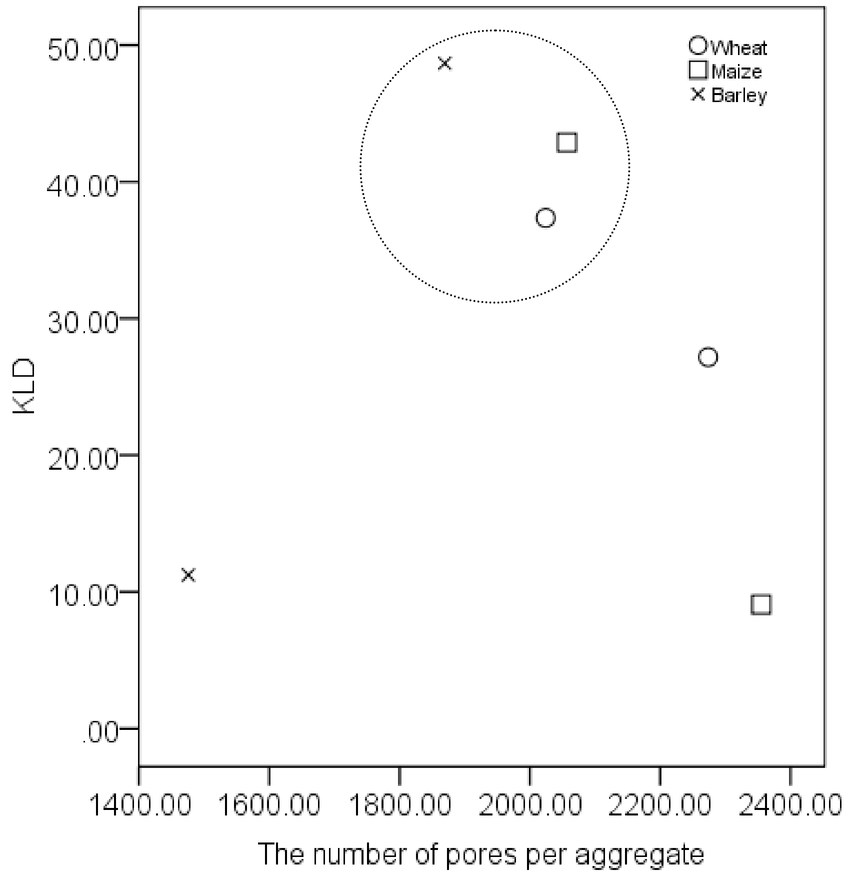

Fig. 2- 4 Relationship between KLD and the number of pores per aggregate from image analysis. Data points in the dotted circle indicates rhizosphere soils; others are bulk soils. Image analysis data from Whalley et al. (2005).

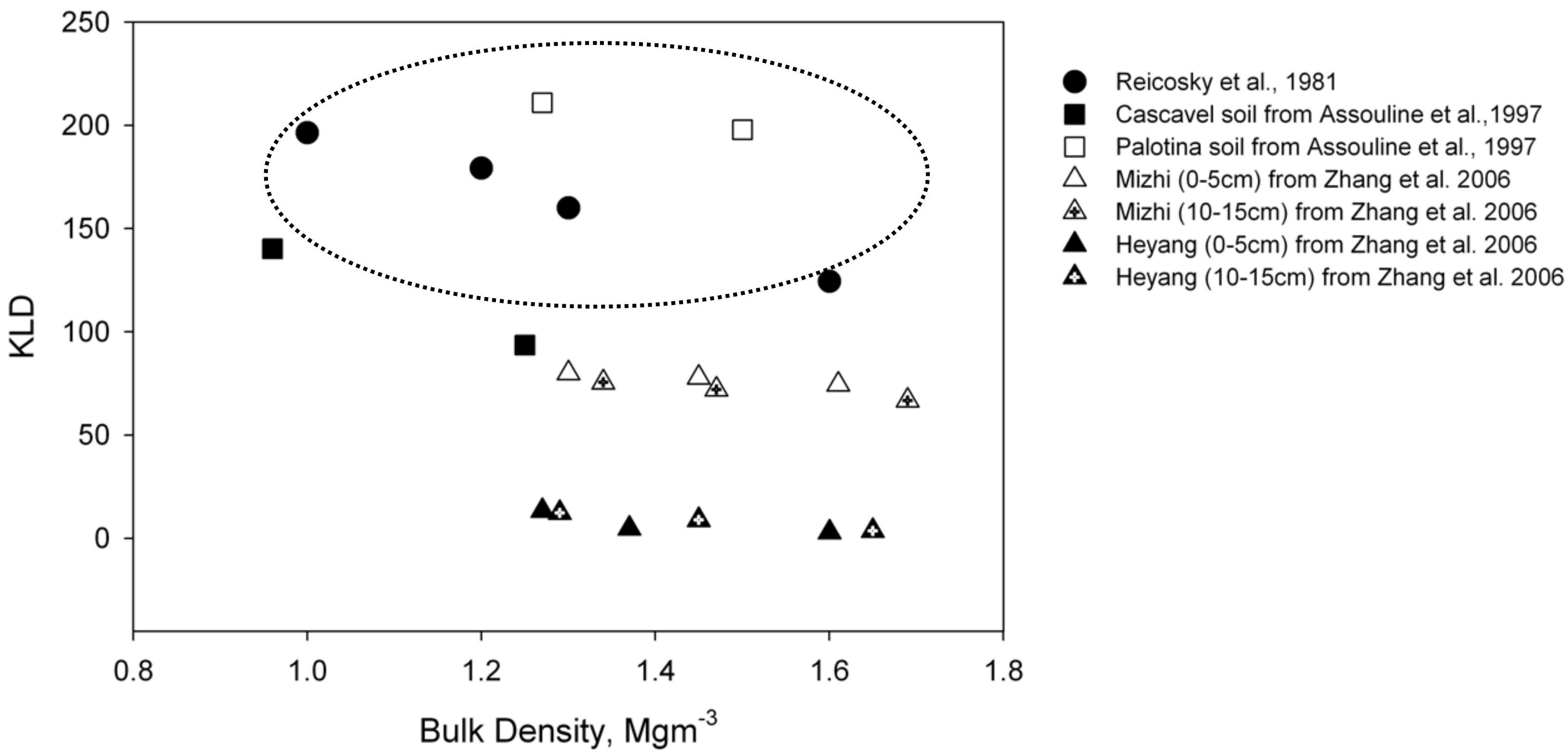

Fig. 2- 5 KLD values as function of bulk density levels caused by compaction. Data inside dotted line are from soils sieved through a 2 mm sieve. Data from Reicosky and et al (1981), Assouline and et al. (1997), and Zhang and et al. (2006).

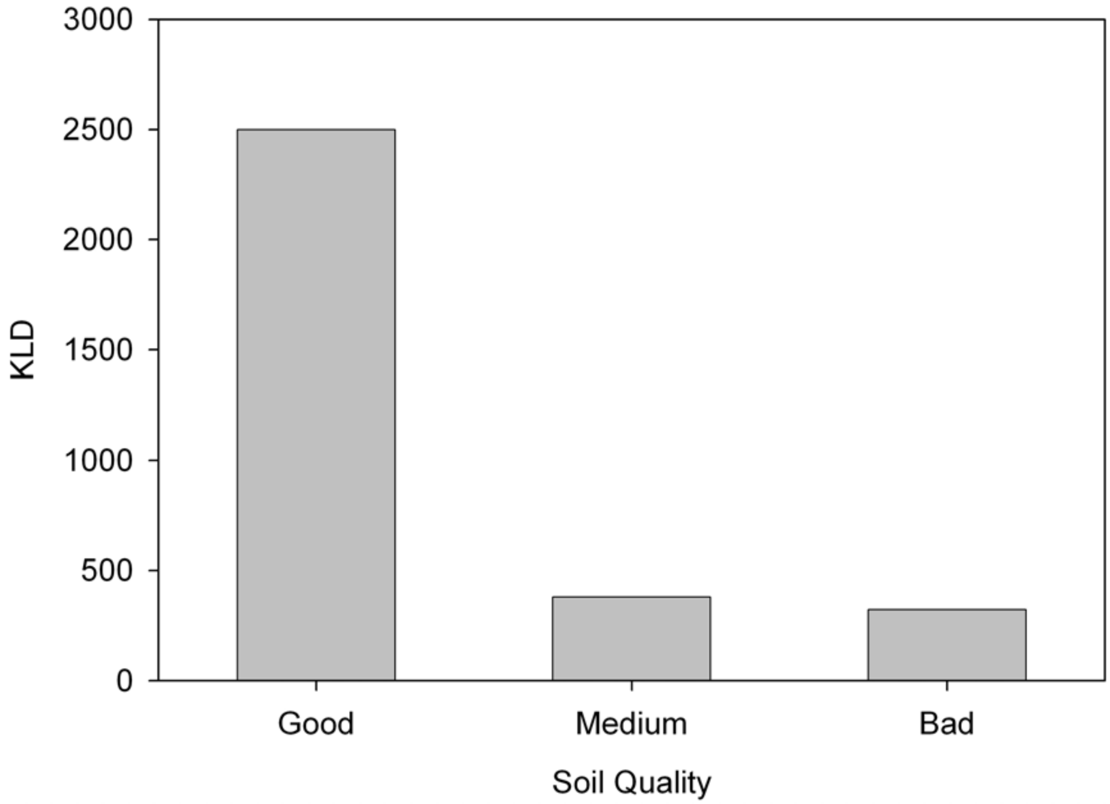

Fig. 2- 6 KLD values for soils under three soil degradation levels. Data from Omuto et al. (2006).

Chapter 3

Using KLD to Assess Soil Structure on Undisturbed and Physically Disturbed Samples from Contrasting Soil Types, Soil Managements, and Depths

3.1 Introduction

Soil pore systems are a measure of the physical quality of soils (Dexter, 2004). Pore systems are dynamic and evolve during the formation of visually identifiable soil structural units. Morphological properties of pore systems such as sizes and shapes are affected by soil management (Leij et al., 2002a; Leij et al., 2002b; Lipiec and Hatano, 2003; Pagliai et al., 2004; Richard et al., 2001; Schwartz et al., 2003). Soil pore systems can be inferred from soil water retention characteristics in the form of probability density functions (Hayashi et al., 2006; Kutilek, 2004; Levine et al., 1996a; Sollins and Radulovich, 1988). Effects of soil structure on soil pore systems have been examined by comparing water retention properties (Crawford et al., 1995; Dexter, 2004; Hayashi et al., 2006; Kosugi, 1997; Kutilek, 2004; Tuli et al., 2005) or by classifying pores by their sizes and shapes (Chun et al., 2008; Hayashi et al., 2006; Pagliai and Vignozzi, 2002; Pagliai et al., 2004; Whalley et al., 2005). Soil pore size distributions directly inferred from water retention, however, contain information on soil texture and soil structure (Nimmo, 1997; Tamari, 1994).

Among the morphological features qualitatively described in the field are the shapes and sizes of soil aggregates (Diaz-Zorita et al., 2002; Levine et al., 1996a; Roger-Estrade et al., 2000; Roger-Estrade et al., 2004). Field morphological descriptions are abundant, but were found to have low predictive power of less available properties such as water retention properties (Holden, 1995; Pachepsky and Rawls, 2003; Pachepsky et al., 2006; Roger-Estrade et al., 2004). Identifying quantitative relationships between morphological descriptions and hydraulic properties would be important because modeling of hydrological processes could be improved using morphological descriptions that are either available or easy to obtain (Lilly et al., 2008).

Methods to assess the effects of soil structure on hydrological processes include disruptive methods aimed at fragmenting a soil mass to isolate individual aggregates (Diaz-Zorita et al., 2002). Although these methods have generally been accepted and typically yield results that are comparable with those from image analysis (Sandri et al., 1998), the incomplete fragmentation of a soil structure may limit our understanding of the relationship between soil structure and soil pore systems. On the other hand, Fernandez-Galvez and Barahona (2005), Hayashi et al. (2006), Kosugi (1997), and Tuli et al. (2005) assessed structural effects on soil hydraulic properties by comparing water retention properties and their parameters between disturbed soil and undisturbed soils. In these cases, the treatment of the disturbed soil was aimed at disrupting as much as possible the original soil structure and to enhance the contrast between the effects of soil texture and soil structure in the property under study.

In Chapter 2, the concept of KLD as an index of soil structure that separates the effect of soil texture from that of soil structure was tested with data from the literature and in some cases by converting parameters from the Brooks and Corey (1964) or van Genuchten (1980) models to the Kosugi (1996) model of water retention. The objective of this study was to investigate trends in the values of KLD using a range of soil structural conditions by comparing KLD values of undisturbed and (physically) disturbed samples. Variation in the soil structural conditions were assured by sampling soil from 3 different depths and management practices, including as many types and sizes of structural units as possible. Water retention data from disturbed and undisturbed soils were obtained from Tuli et al. (2005) and Hayashi et al. (2006) and used to supplement data from this study.

3.2 Materials and Methods

3.2.1 Study Sites

Three data sets were used in this study. The first dataset comprised a total of 24 soil horizons from three New Jersey soil series (Freehold, Quakertown, and Sassafras series), each subjected to at least two soil management types (Table 3-1). The ranges of depths sampled were classified as top, middle, and bottom, covering approximately 2-22, 24-46, and 46-81 cm, respectively. All soil series were classified as Typic Hapludults. Soils under agriculture management (all soil series) and golf courses sites (Freehold and Sassafras series) were considered the most disturbed sites because they are subjected to frequent tillage operations (agriculture sites) or to traffic and alteration of the original texture of the topsoil (golf courses sites). The least disturbed sites were those under forest management (Freehold and Quakertown series). A former agricultural field that was planted with trees about ten years ago (Quakertown) was considered as an intermediate situation and referred as a "restored site". The second and third data sets were from Tuli, et al. (2005) and Hayashi et al. (2006). The data were obtained from Dr. Tuli (University of California, Davis) and Dr. Kosugi (University of Kyoto), respectively, and comprised data from 13 and 56 soil horizons including measurements of water retention on disturbed and undisturbed samples, saturated hydraulic conductivity, K_{sat}, bulk density, and organic matter content.

The field identification of soil structure was based on the USDA system (Soil Survey Staff, 1951) (Table 3-1) and for the New Jersey soils was conducted with support of NRCS personnel. Morphological descriptions of aggregate sizes were converted to actual sizes for this study using the scale shown in Table 3-2. Only three horizons of the New Jersey soils data set had granular structure type and only one had massive structure type. Soils studied by Tuli et al. (2005) had mainly soil structure type massive. Information on soil structure type was not available in the Hayashi et al. (2006) data set, but it was assumed that the soil structure type of the top 5 cm of forest sites was of the type granular (Oades, 1993).

3.2.2 Soil Properties

Bulk soil samples were collected from each of 24 horizons for determination of chemical properties. Determinations of soil texture, organic carbon contents (OC) were done with a combined hydrometer and sieving procedure (Gee and Bauder, 1986), and dichromate oxidation and subsequent titration with ferrous ammonium sulphate (Walkley and Black, 1934) method, respectively. Cation exchange capacity (CEC) was measured by the amount of $NH4^+$ exchanged from soil in 10% NaCl extracted solutions using a Technicon Bran+Luebbe Autoanalyzer 3. Acidity was measured using a pH meter from using distilled water: soil mixture with a 2:1 volume ratio. Five soil cores (5 cm in diameter by 7.5 cm long) for each horizon were sampled carving columns of appropriate size and sliding them in rigid PVC columns or encasing them in soft rubber to facilitate transport to the laboratory. In the laboratory, soil samples were encased with expanding foam to prevent edge-flow. Samples were saturated overnight with a solution of 0.01M $CaCl_2$ to prevent soil dispersion upon saturation. Saturated hydraulic conductivity, K_{sat}

was measured using the constant head method (Klute and Dirksen, 1986). Saturated samples were transferred to the measuring station and a solution of 0.01M $CaCl_2$ was run through them until steady state outflow was reached (typically after 2-3 hours). Outflow was collected for 30 minutes and the solution temperature was recorded.

Typically three to four replicates of undisturbed soil clods from each of the horizons were sampled for bulk density and water retention measurements. The saran-resin coating method (Brasher et al., 1966) was used to measure bulk density of undisturbed soil clods. After bulk density was measured, the opposite ends of the clods were removed, creating flat surfaces. One of the ends was placed in contact with a ceramic plate contained in a cell. Water retained by soil clods was measured by subjecting the bottom of the clods to pressure potential in the range from 0 to -10 kPa and measuring the volume of water released by the clods. Water retained at pressure potentials of -0.1, -0.3, -0.6, -1, -1.5, -3, -6, and -10 kPa were measured with this system. After measuring water retention, clods were air-dried, crushed and placed in a plastic bottle together with 10 glass spheres of 0.5 mm in diameter. Bottles with soil and spheres were shaken for 24 hours to physically disturb the soil. The disturbed soil was packed into cores (5 cm in diameter by 2.5 cm long) and soil water retention was measured again following the same procedure and at the same pressure potentials as before. Water retention at pressure potentials of -100, -300, and -1500 kPa were measured on disturbed (sieved through a 2 mm sieve) samples using pressure plate extractors (Richards, 1949).

3.2.3 Water Retention Model

The lognormal water retention model of Kosugi (1996) was fitted to all water retention data. The Kosugi (1996) water retention model assumes a lognormal distribution of pore radii, *r*, of the form:

$$f(r) = \frac{\theta_s - \theta_r}{r\sigma\sqrt{2\pi}} \exp(-\frac{[\ln(r/r_s)]^2}{2\sigma_s^{\ 2}}) \tag{3-1}$$

where θ_s and θ_r are the saturated and residual water contents, respectively, r_s is the median pore radius and σ_s is the standard deviation of $\ln r$.

The effective saturation, S_e is defined as:

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} = Q[\frac{\ln(\psi/\psi_s)}{\sigma}] \tag{3-2}$$

where the pressure potential, ψ_s (kPa) can be related to pore radius, r_s (μm) using the Young-Laplace equation as (Brutsaert, 1966) $\psi_s = A/r_s$ where A = 149 and Q denotes the complementary normal distribution function defined as:

$$Q(x) = (2\pi)^{-1/2} \int_x^{\infty} \exp(-x^2/2)dx \tag{3-3}$$

The model was fitted to water retention data to estimate θ_r, ψ_s, and σ_s. The saturated water content was assumed to be the water content at equilibrium with ψ = -0.1 kPa. The fitting parameters of the Kosugi (1996) model were used to generate soil pore size distributions from the derivative of Eq. (3-2):

$$dS_e = Q[\frac{\ln(\psi/\psi_s)}{\sigma}]dr \tag{3-4}$$

3.2.4 Kullback-Leibler Distance (KLD)

Details on the calculation of KLD are presented in Chapter 2. Briefly, the explicit form of KLD (see Eq. (2-9) and Appendix A) was used to calculate the entropic distance between the probability density functions of soil pores from the disturbed/undisturbed samples and a reference soil; where r_R, σ_R, r_s and σ_s are the parameters of the Kosugi (1996) water retention model fitted to the probability density functions of the reference $f_R(r)$ and disturbed/undisturbed $f_s(r)$ distributions, respectively. Reference pore size distributions were derived assuming random arrangements of given soil particle distributions before they are modified by environmental and anthropogenic forces.

3.2.5 Statistical Analyses

All statistical analyses were performed with the SPSS software package (SPSS Inc., Chicago, IL, USA), and included the analysis of variance (ANOVA) test, non parametric Kruskal-Wallis H test, and Mann-Whitney U test.

3.3 Results and Discussion

3.3.1 Soil Properties

The soils evaluated in this study were mostly classified as sandy loam, sandy clay loam, loam, and silt clay loam soil texture classes (Fig. 3-1). Soils from Hayashi et al. (2006) were classified mainly in the sand or sandy loam texture classes, whereas soils from Tuli et al. (2005) were mostly in texture classes loam and silt loam. While pH (p = 0.325) and bulk density (p = 0.059) were not significantly different among New Jersey soils, the contents of sand, silt and clay, CEC, OC, and K_{sat} were significantly different among soils ($p < 0.001$). Soils from the Quakertown series had more clay and silt than the other soils. Soils from the Freehold series had greater OC contents, CEC and K_{sat} than the other two soils. All physical properties were significantly ($p < 0.002$) different among management types. Soils in agriculture sites had significantly greater values of bulk density than soils in forest sites ($p < 0.001$), and soils in forest sites had significantly greater values of K_{sat} ($p < 0.001$) and pH ($p < 0.001$) than soils from other management types.

The Kosugi (1996) lognormal distribution model fitted reasonably well the water retention data with r^2 greater than 0.947 for all fits. The parameters of the Kosugi (1996) lognormal water retention model, r_s and σ_s did not show any trend among managements and depths (Fig. 3-2). Soils from the Freehold series had greater r_s and lower σ_s values while soils from the Quakertown had smaller r_s and usually greater σ_s values than other soils (Fig 3-2a and 3-2c). The differences between these two soil series resulted from textural differences (Table 3-3). Values of r_s were greater and σ_s were smaller in soils from forest sites than other management types (Fig. 3-2c). Hayashi et al. (2006) and Kosugi (1997) also reported greater r_s values in forest sites that were attributed to more biological activity in forest soils.

3.3.2 KLD and Soil Structure

Values of KLD of disturbed soils were 60 % lower ($p < 0.001$) than the corresponding KLD values of undisturbed soils (Fig. 3-3a), implying less entropic distance between pore size distributions of disturbed soils and their random counterparts than the corresponding values for structured soils. Although structural features could still be present in the physically disturbed samples, undisturbed soils contain more pores developed from structure formation (Hayashi et al., 2006; Kosugi, 1997; Tuli et al., 2005).

Values of r_s and σ_s decreased significantly ($p < 0.001$) in disturbed soils (Fig 3-3b and 3- 3c), although the data was more scattered. Larger pores are typically associated to structured soils. Therefore, it is expected that r_s from undisturbed samples be greater than r_s from disturbed ones (Hayashi et al., 2006; Hillel, 1998).

Values of KLD were significantly different among texture classes ($p = 0.011$) and tended to increase with clay content (Fig. 3-4). The loamy sand soils showing the lowest KLD values are from Hayashi et al. (2006). Soils of Hayashi et al. (2006) contain more sand than either soils from Tuli et al. (2005) or soils from this study (Fig. 3-1). Soils with high sand content tend to have less structural development (Nimmo, 1997), which would explain the lowest KLD values of the Hayashi et al (2006) soils.

3.3.3 KLD and Soil Management and Soil Depth

Only soils from the New Jersey data set were used to evaluate the effects of management and depth because horizons were not well defined in the data sets of Hayashi et al. (2006) and Tuli et al. (2005). Values of KLD from top soils in forest sites varied over a greater range than soils from either agricultural or golf courses sites (Fig. 3-5). The effects of agriculture management on water retention vary depending on the texture or chemical composition of the soils (Assouline et al., 1997). Except for bulk density ($p < 0.132$) and pH ($p < 0.555$), all other examined soil properties of top soils in agriculture and golf courses sites were significantly different ($p < 0.001$) among soil types. However, KLD values of the top soils in agriculture and golf course sites were not significantly different ($0.886 < p < 0.987$) (Fig 3-5a and 3-5b). Tillage leads to the homogenization of the spatial distribution of mass within aggregates (Chun et al., 2008; Hadas, 1987; Lipiec and Hatano, 2003; Utomo and Dexter, 1981) and this homogenization may explain the convergence of KLD values to a range that is statistically homogeneous.

Except for bulk density ($p < 0.489$) and K_{sat} ($p < 0.932$), all other physical variables, including KLD, were significantly different among soil types from forested sites ($0 < p < 0.007$). This implies that soil structure formation follows different paths and is at different stages at sites where the soil is not disturbed such as soils at forest sites.

Compared to top soils under direct influence of management practices, KLD values for soils at the range of depth defined as middle and bottom were more scattered (Fig. 3-5). Except for the bottom depth of Sassafras soil under golf coarse management, which has fine (5-10 mm) blocky structure, the dominant sizes of the structural units at depth defined as middle and bottom were medium (10-20 mm) and coarse (20-50 mm) blocky structure. Thus, the scatter in KLD values could be the result of samples smaller than a representative value for these structure types (see Fig. 3-9 and explanation below). Another explanation could be the presence of macropores embedded in a more or less compacted matrix. For instance, the relatively large KLD value of the middle depth of Sassafras soil under golf course management (Fig. 3-5) corresponded to a relatively large value of K_{sat} (Table 3-3) and to greatest r_s derived from water retention measurements (Fig. 3-2b).

3.3.4 KLD and Field Description of Soil Structure

There were no differences in KLD values ($p = 0.81$) among soil structure types (Fig. 3-6). Other studies also found that soil structure type is not a good predictor of soil physical properties (Holden, 1995; Pachepsky and Rawls, 2003; Rawls and Pachepsky, 2002).

KLD values were statistically different ($p = 0.009$) among sizes of structural units (Fig. 3-7). The increase in KLD values with sizes of the structural units suggests a greater complexity in pore systems of larger aggregates. This result could be explained by the hierarchical nature of soil structure by which larger structural units would contain aggregates from lower organizational levels (Dexter, 1988). In previous studies, water retention was 2-3% greater in fine size aggregate (Pachepsky et al., 2006), which is in agreement with findings in this study of greater θ_s and r_s in the 1-2 mm size class (see Appendix B).

Linear relationships between KLD and clay content were found in blocky soil structural type sampled from agriculture and forest sites and in the granular soil structure type from Hayashi et al. (2006) with different slopes for each case (Fig. 3-8). Clay particles tend to increase soil aggregation and modify the morphology of pores (Fies and Bruand, 1998). This result indicates that the effect of clay content on soil structure and KLD values is a function of soil structure and soil management type and provides further indication that KLD contains information that goes beyond texture.

The dependence of KLD on the size of the soil structural units suggests that the size of the samples used to measure water retention of structured soils should be considered in relation to the prevailing size of the soil structure units. Indeed, KLD values decreased when the ratio of sample diameter to the diameter of the soil structural unit increased (Fig. 3-9). Furthermore, both the average and variance of the measurements decreased linearly with the ratio of sample to structural unit diameters suggesting a possible scaling effect. This result indicate that a representative elementary volume (REV) for KLD is one that is at least three times larger that the volume of the prevailing structural unit.

3.4 Conclusions

Physically disturbed soils had consistently smaller KLD values than the corresponding undisturbed samples, which is consistent with the concept of KLD as an index of soil structure. The analysis of KLD from undisturbed samples revealed that when soil structure was homogenized by management practices KLD values were uniform regardless of soil type and texture. This indicates that effect of management practice can alter not only visible unit of soil structure, but also the soil pore system. There were no unique features in soils of middle and bottom depths while soil management caused distinct variances of KLD in top soils. Values of KLD were correlated to size of the structural units and also to the size of the support with respect to the size of the structural unit. These results suggest the use of KLD to determine a representative elementary volume. Further study considering water retention measurements on various clod sample sizes are needed to explore the full potential of this finding. Future research on KLD should include soil databases with soil structure descriptions.

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Table 3- 1 Soil series, management types, depths, and soil structure descriptions of the New Jersey soils included in this study.

Soil Series	Management / Location	Horizon	Depth, cm	ID	Structure description[4]
Freehold	Golf Course (N 39º 56' 14.69" and W 74 º 47' 59.42")	A2[1]	12.5	FGT	moderate fine granular structure
		Ba[2]	24.0	FGM	massive
		Bt2[3]	51.0	FGB	moderate medium subangular blocky structure
	Forest (N 39º 56' 31.82" and W 74 º 48' 10.78")	A[1]	7.5	FFT	strong medium granular structure
		ABt[2]	38.0	FFM	moderate medium subangular blocky structure
		Bt1[3]	56.0	FFB	moderate medium subangular blocky
	Agriculture (N 39º 56' 31.80" and W 74 º 48' 14.09")	Ap[1]	13.0	FAT	strong coarse subangular blocky structure
		Bt[2]	38.5	FAM	strong coarse subangular blocky structure
		BC1[3]	68.0	FAB	strong coarse subangular blocky structure
Quakertown `	Restored (tree 1 N 40º 33' 42.7" and W 74 º 57' 49.3")	A[1]	10.25	QTT	moderate coarse granular structure
		Bt1[2]	27.0	QTM	moderate medium subangular blocky structure
		Bt2[3]	58.5	QTB	moderate thick platy structure parting to moderate medium subangular blocky structure
	Forest (tree2 N 40º 33' 31.1" and W 74 º 57' 13.7")	Ap[1]	14.0	QFT	moderate fine subangular blocky structure
		Bt1[2]	40.5	QFM	moderate medium subangular blocky structure
		Bt2[3]	66.0	QFB	weak thick platy structure parting to moderate fine and medium subangular blocky structure
	Agriculture (N 40º 33' 38" and W 74 º 57' 42")	Ap[1]	10.0	QAT	moderate medium granular and weak medium subangular blocky structure
		Bt1[2]	34.0	QAM	medium subangular blocky structure;
		Bt2[3]	67.0	QAB	moderate medium and coarse subangular blocky structure.

[1] Top, [2] Middle [3] Bottom. [4] Structure type subangular blocky is referred as blocky.

Table 3-1 Cont'd

Soil Series	Management / Location	Horizon	Depth, cm	ID	Structure description
Sassafras	Golf Course	Ap[1]	10.0	SGT	moderate medium subangular blocky structure
		Bt1[2]	30.0	SGM	moderate medium subangular blocky structure
		Bt2[3]	49.0	SGB	moderate fine subangular blocky structure
	Agriculture	Ap2[1]	20.0	SAT	moderate medium subangular blocky structure, and moderate coarse subangular blocky structure
		Bt[2]	49.5	SAM	moderate medium subangular blocky structure, and moderate coarse subangular blocky structure
		BC1[3]	84.5	SAB	moderate coarse subangular blocky structure, and moderate medium subangular blocky structure

[1] Top, [2] Middle [3] Bottom

Table 3- 2 Symbols and actual sizes of structure types as function of their qualitative (field) description (after Nikiforoff, 1941).

Type	**Fine**	**Medium**	**Coarse**
Blocky	5-10 mm	10-20 mm	20-50 mm
Granular	1-2 mm	2-5 mm	5-10 mm
Massive	No size available		

Table 3- 3 Physical and chemical properties of the New Jersey soils included in this study (see Table 3-1 for a description of the soil horizons).

Soil ID	Texture Class	Sand, %	Silt, %	Clay, %	CEC meq/100 g	OC*, %	pH	K_{sat} $\mu m\ s^{-1}$	BD* $g\ cm^{-3}$
FGT	Sandy loam	68	23	9	18.2	8.63	6.3	55.5±15	1.51±0.09
FGM	Sandy loam	69.5	21	9	17.35	7.69	6.3	12.81±8	1.70±0.04
FGB	Sandy loam	70.5	15.5	14	7	0.71	6.0	8.5±17	1.59±0.04
FFT	Clay	21	36	43	29.7	11.09	5.2	100.5±37	1.28±0.10
FFM	Sandy loam	70	16	14.5	9.7	1.4	4.4	54.2±30	1.55±0.06
FFB	Sandy loam	74	13	13	6.9	0.79	4.5	50.0±22	1.58±0.04
FAT	Sandy loam	71.5	18	11	7.5	0.89	6.8	1.9±2	1.73±0.08
FAM	Clay loam	58	16	25.5	10.35	0.37	6.1	19.2±16	1.69±0.05
FAB	Sandy loam	73	14.5	12.5	6	0.1	5.1	22.8±6	1.59±0.03
QTT	Silty clay loam	14.5	57.5	28	10.25	2.66	5.8	33.3±19	1.54±0.12
QTM	Silty clay loam	16.5	48.5	35.5	7.85	0.82	6.2	21.3	1.74±0.07
QTB	Silty clay loam	17.5	49.5	33	7.3	0.42	6.3	18.5±64	1.72±0.03
QFT	Silt loam	27.5	55.5	16.5	12.15	5.21	4.5	66.2±34	1.11±0.06
QFM	Loam	27	50	23.5	8.25	1.67	4.5		1.35±0.05
QFB	Silt loam	27	50	23.5	8.3	1.95	4.5	34.7±12	1.53±0.09
QAT	Silt loam	27	50.5	22.5	8.25	2.04	6.3	2.9±6	1.52±0.04
QAM	Clay loam	28	44.5	27.5	7.65	0.8	6.5	11.0±8	1.62±0.05
QAB	Clay loam	39	29	32.5	7.25	0.48	6.6	5.5±8	1.73±0.02
SGT	Loam	50	37	13	7.8	3.14	4.4	4.6±1	1.50±0.08
SGM	Sandy clay loam	29	45	26	6.3	0.79	5.0	34.6±13	1.60±0.05
SGB	Loam	43	24	33	8.5	0.26	5.5	7.3±4	1.76±0.06
SAT	Loam	57	31	12	2.5	0.6	7.4	0.7	1.83±0.05
SAM	Sandy clay loam	57	21	22	5.0	0.88	7.2	15.8±8	1.82±0.03
SAB	Sandy loam	55	29	15	3.5	0.71	7.4	20±8	1.64±0.05

*: BD indicates bulk density and OC indicates organic carbon content

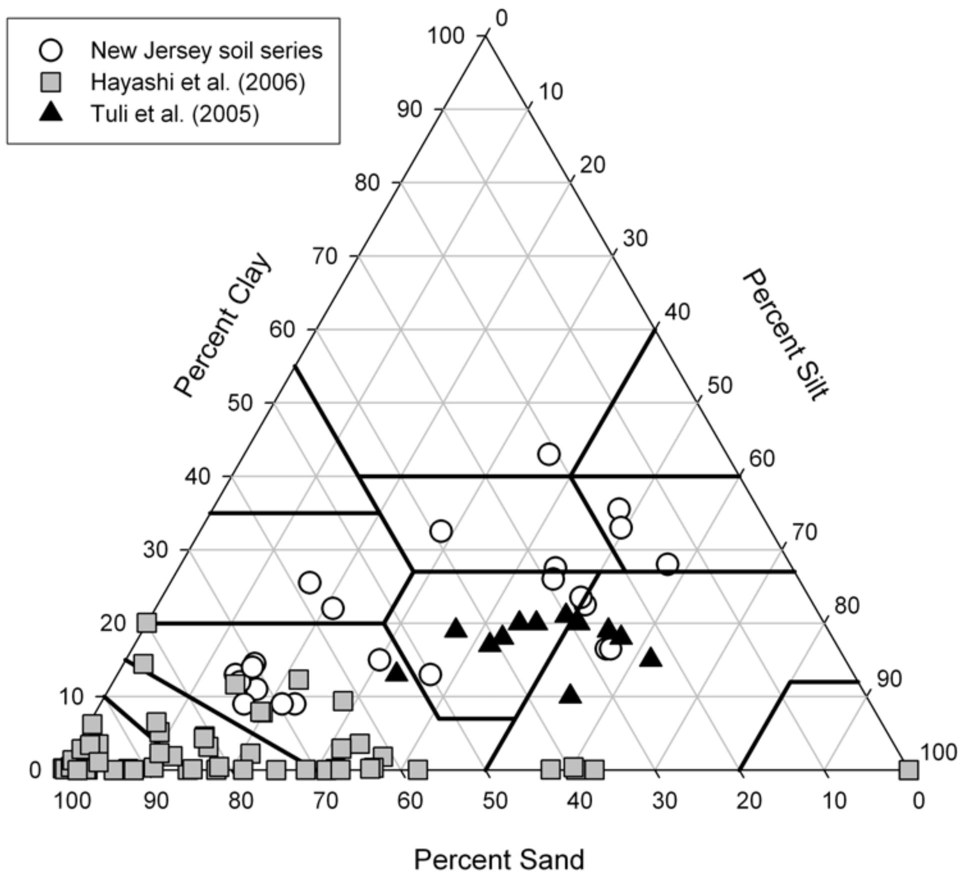

Fig. 3- 1 Texture classes of soils in the New Jersey data set, Hayashi et al. (2006) data set, and Tuli et al. (2005) data set.

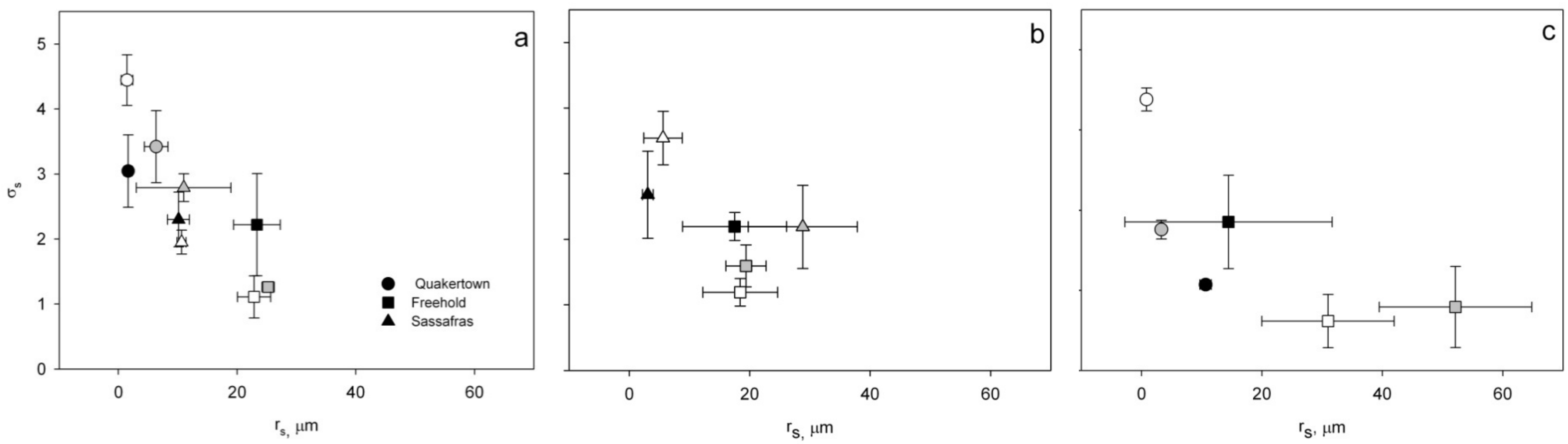

Fig. 3- 2 Fitting parameters r_s and σ_s of the Kosugi (1996) water retention model for: (a) agriculture sites, (b) golf courses sites, and (c) forest sites. Within each management, black, grey, and white indicate top, middle, and bottom depths, respectively. Bars indicate standard deviations of data.

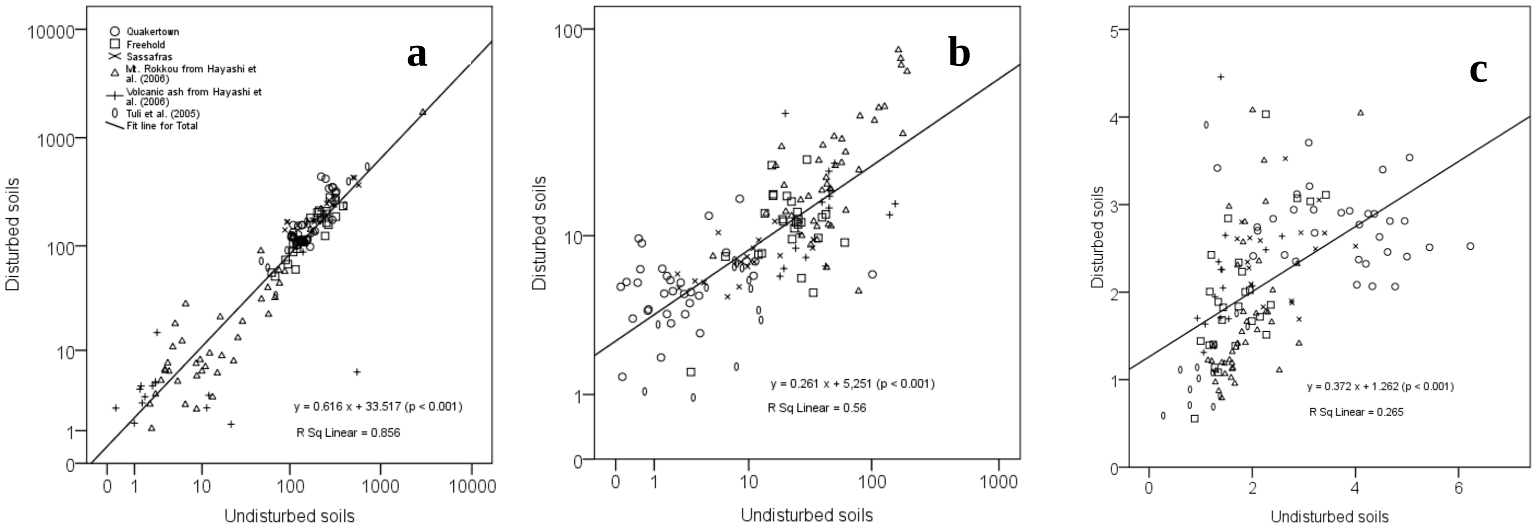

Fig. 3- 3 Plots of parameters obtained from disturbed and undisturbed samples of the New Jersey dataset (Quakertown, Freehold and Sassafras), Tuli et al. (2005) dataset, and Hayashi et al. (2006) dataset: (a) KLD, (b) r_s, and (c) σ_s.

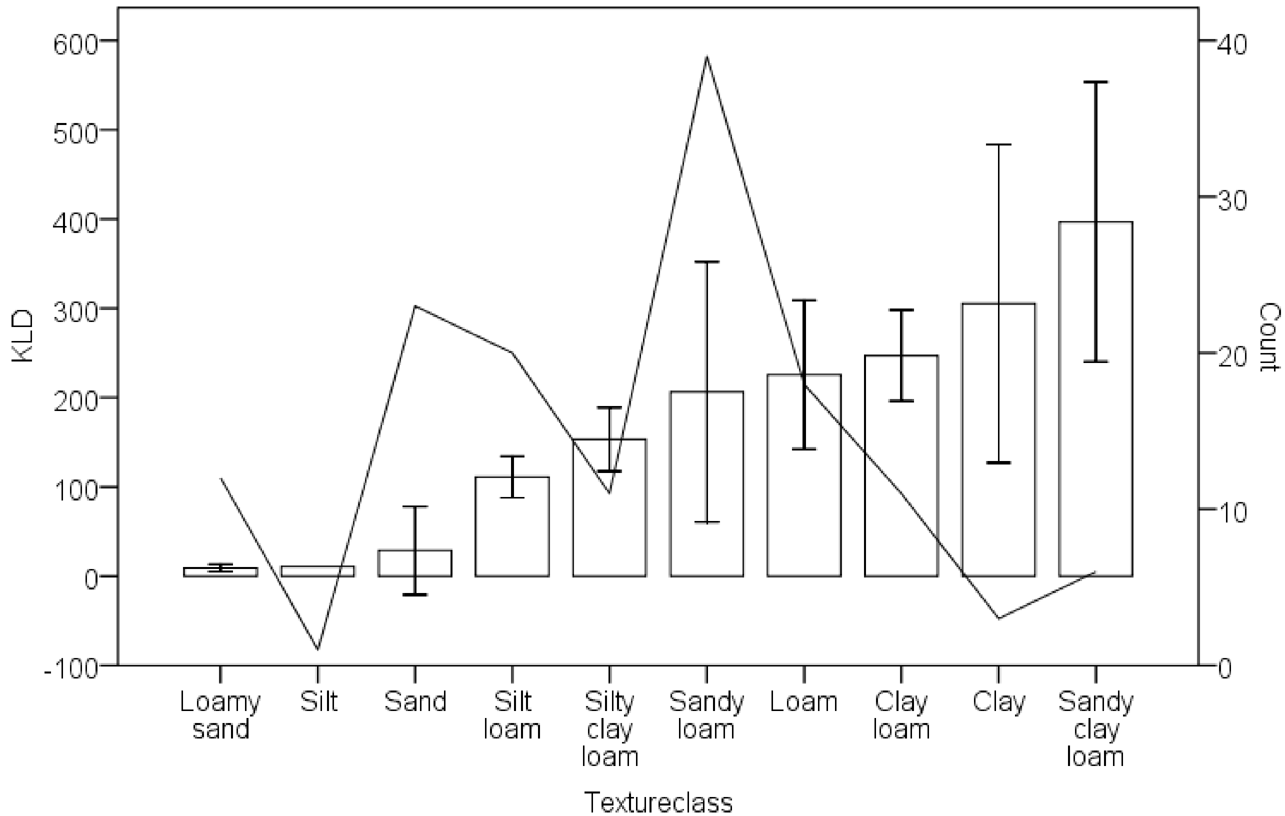

Fig. 3- 4 Mean of KLD values as a function of soil texture class. Bars represent standard deviations of measurements and the solid line represents the number of samples.

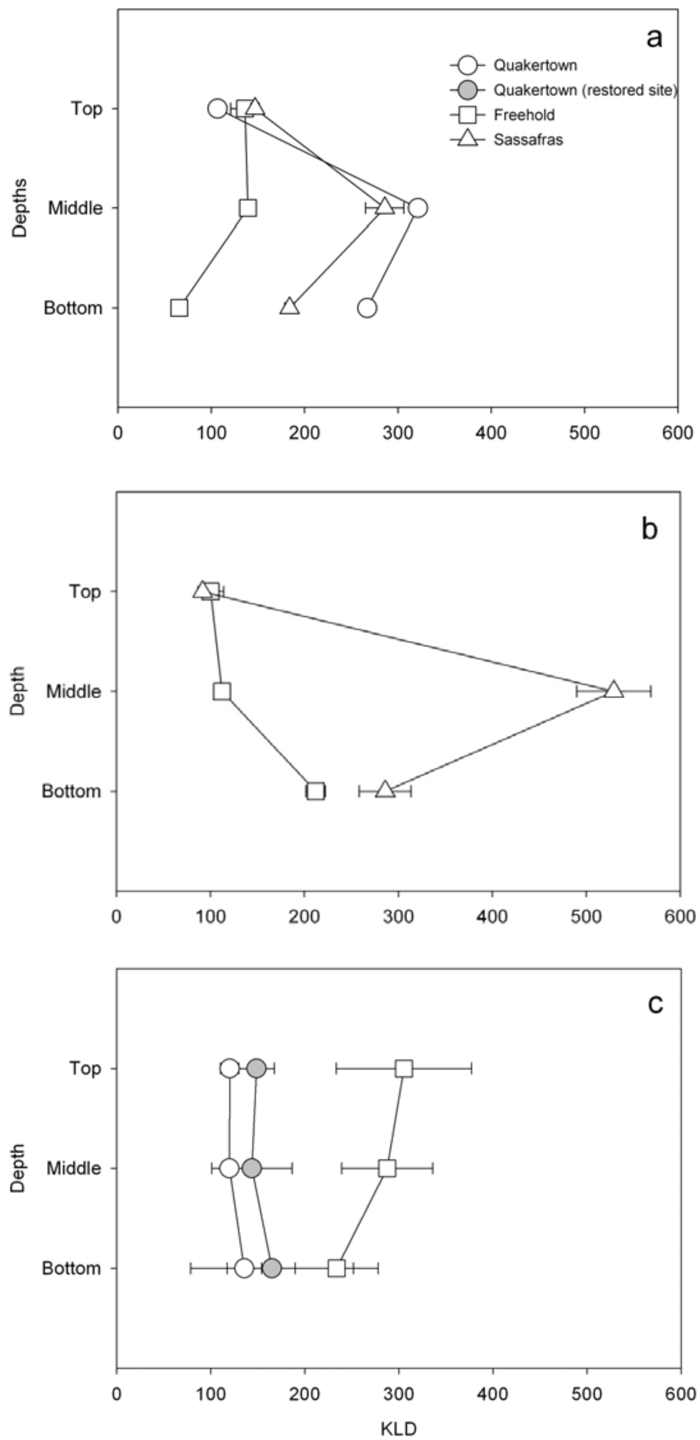

Fig. 3- 5 Values of KLD for New Jersey soils and three range of depths (top, middle, and bottom) for (a) agriculture sites, (b) golf course sites, and (c) forest sites.

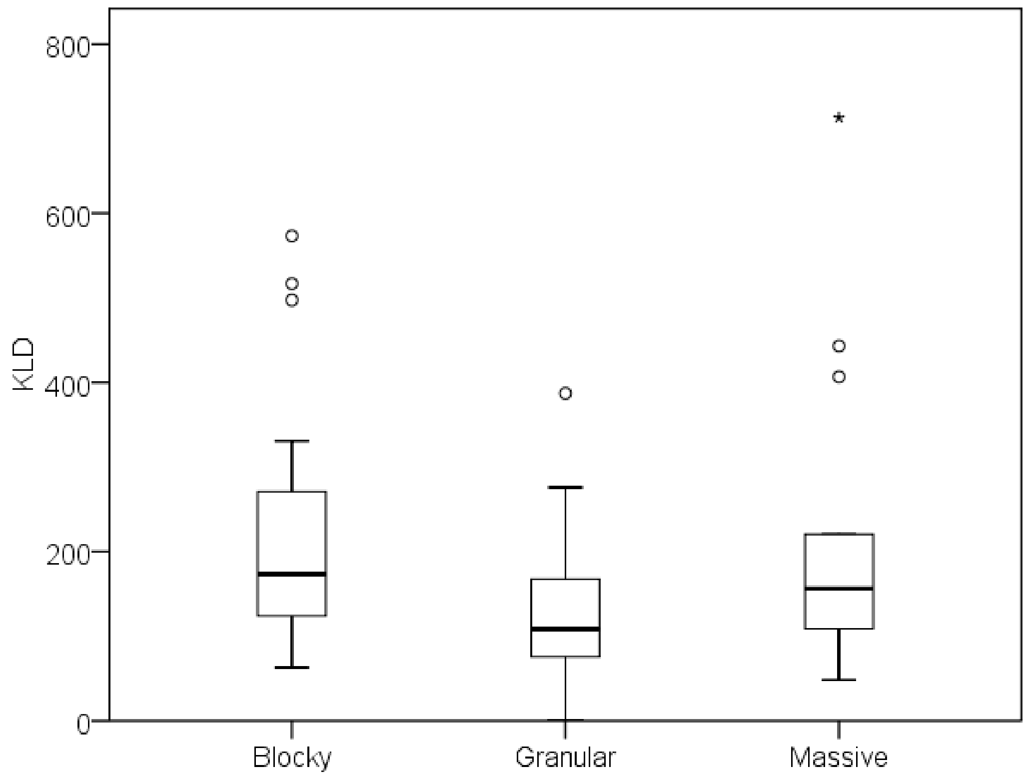

Fig. 3- 6 Box plot of KLD *vs.* soil structure type. Circles and star indicate outliers.

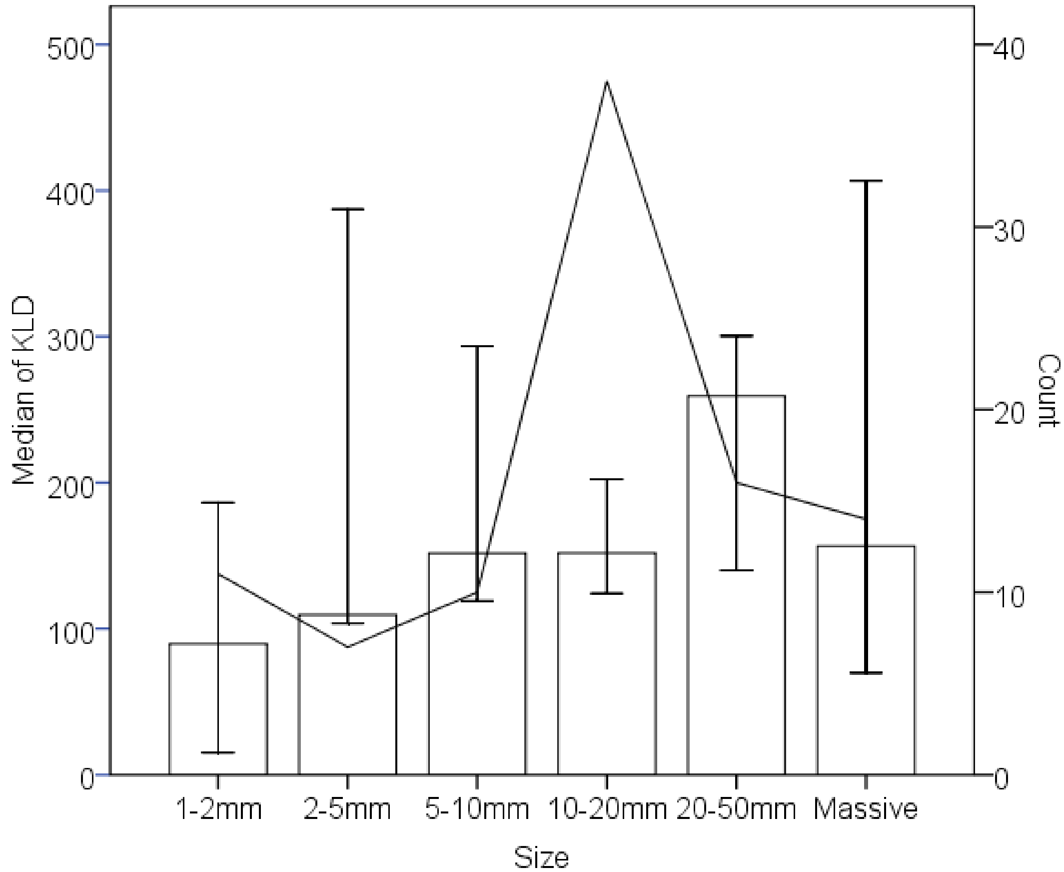

Fig. 3- 7 Median of KLD for each size range of structure type. The bars represent 95% of confidence interval.The solid line represents number of samples.

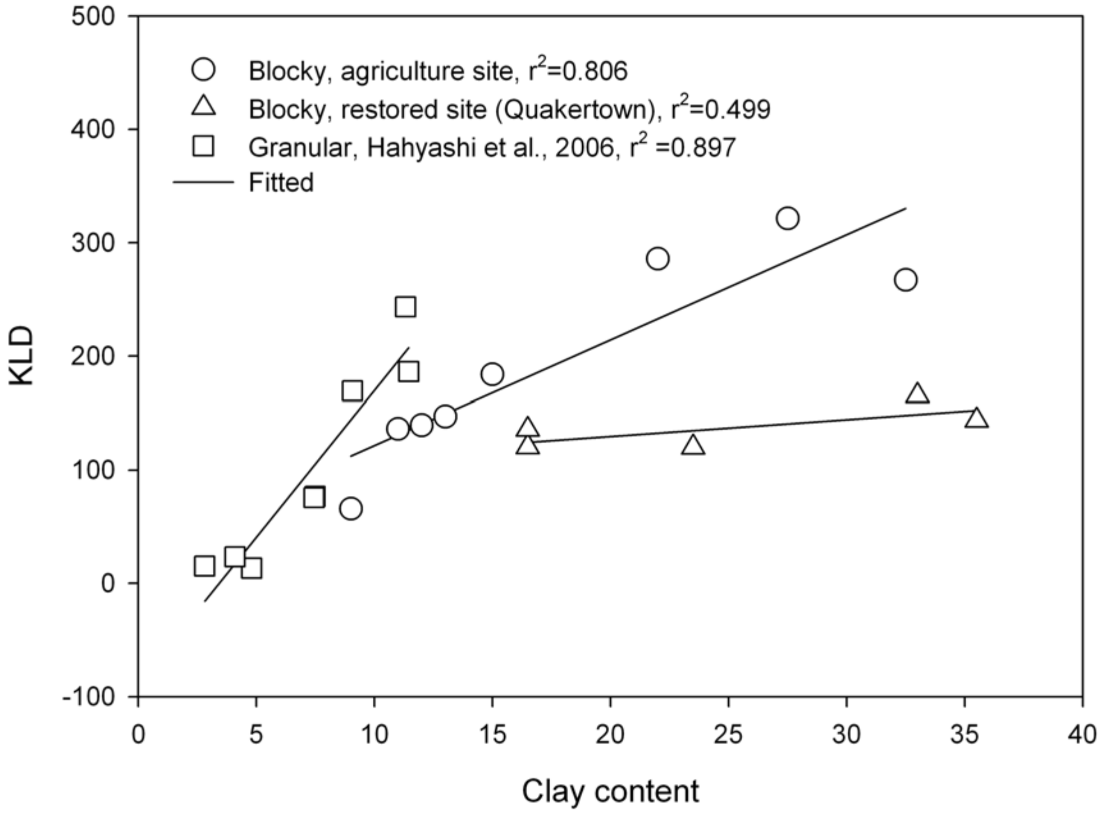

Fig. 3- 8 Relationships between clay content and KLD for soils of blocky and granular structure types of soils from the New Jersey and Hayashi et al. (2006) data sets, respectively.

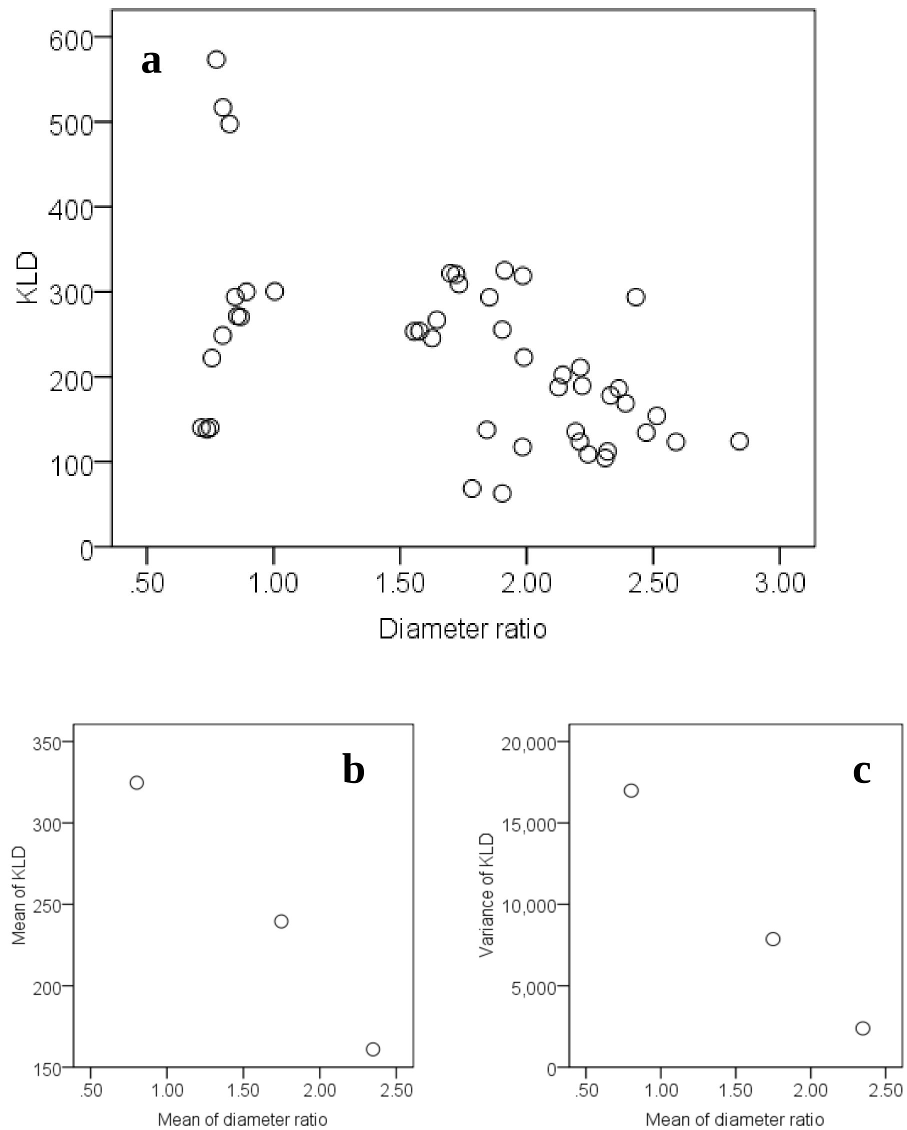

Fig. 3- 9 KLD *vs*. diameter ratio between clod sample and size of structure type: (a) raw data, (b) mean values of KLD, and (c) variance of KLD for the intervals of diameter ratios 0 to 1, 1 to 2, and greater than 2.

Chapter 4

Assessing KLD with the US National Pedon Characterization Database

4.1 Introduction

The performance of hydrological models relies, among others, on the selection of hydraulic input parameters such as soil water retention and hydraulic conductivity. It is difficult to measure these properties because their measurements are time consuming and costly, especially for the characterization of large areas of land (Nemes et al., 2006; Pachepsky and Rawls, 2003). An alternative is to predict these properties from more readily available soil data (e.g., particle sizes, bulk density and/or organic matter content) using pedo-transfer functions, PTFs (Nemes et al., 2006; Pachepsky et al., 2006; Rawls et al., 1998), which are defined as relationships between soil properties or characteristics (Wosten et al., 1990).

Soil structure is characterized in the field by describing visible units of soil peds or inferred by soil physical properties such as bulk density or water retention (Rawls and Pachepsky, 2002). Shape, size, and grade (i.e., relative distinctness of soil structural units) of soil clods are considered to regulate many of the hydrological processes related to soil water, solute transport, and runoff from tilled landscapes (Holden, 1995; Levine et al., 1996b; Lin et al., 1999; McKenzie et al., 1991; Pachepsky and Rawls, 2003). Previous studies confirmed that there is potential in using qualitative descriptions to assess the change of soil structure along a chronosequence (Calero et al., 2008; Schaetzl and Anderson, 2005), and for estimation of water retention and hydraulic properties (Levine et al., 1996b; Lilly et al., 2008; Lin et al., 1999; Pachepsky and Rawls, 2003). Due to the non-numerical characteristics of soil structural descriptions, however, it is difficult to evaluate relationships among soil structural descriptions and other soil properties or hydraulic processes using most traditional PT methods (Pachepsky and

Rawls, 2003). A few studies identified relationships between soil structure and physical properties from soil databases using artificial neural networks (Levine et al., 1996b) or regression trees techniques (Guber et al., 2003; Lilly et al., 2008; Pachepsky and Rawls, 2003; Pachepsky et al., 2006). Pachepsky and Rawls (2003) utilized a regression tree technique to estimate water retention at -33 kPa and -1500 kPa from the US National Pedon Characterization database. Lilly et al. (2008) investigated the significance of soil horizons, structure unit sizes, and soil textures in the estimation of saturated hydraulic conductivity by assigning dummy variables to qualitative soil structure descriptions.

In previous chapters, the significance of KLD was successfully established on soils under a range of conditions. In order to further test the validity of the KLD concept, KLD values should be related to structural features and to physical and hydraulic properties in a large dataset, such as the US National Pedon Characterization database containing qualitative descriptions of soil structure.

The objectives of this study were to investigate how qualitative soil morphological features such as aggregate size, shape and grade, dry/moist consistence, stickiness and plasticity from the US National Pedon Characterization database are related to soil physical properties such as clay content, bulk density, organic matter, water content at -33 (W33) and at -1500 kPa (W1500), hydraulic properties (water retention curves and saturated hydraulic conductivity), and to the proposed structural index, KLD. The relative significance of KLD and of soil physical properties in the estimation of W33 and bulk density was investigated with transformed morphological variables using regression tree analyses.

4.2. Materials and Methods

4.2.1 Data selection from the US National Pedon Characterization database

A total of 1486 soil horizons were selected from the US National Pedon Characterization database (Soil Survey Staff, 1997) (Table 4-1). Each sample contained field morphological descriptions of aggregates shapes (granular, wedge, blocky, platy, and prismatic), sizes (fine, medium, and coarse) and grades (weak, moderate, and strong), dry (soft and hard) and moist (loose and friable) consistency, plasticity (non, slightly, moderately, and very), stickiness (non, slightly, and very), field texture class, bulk density (BD), organic matter (OM), particle size distribution (at least five data points) and volumetric water contents at pressure potentials of -33 (W33) and of -1500 kPa (W1500). Over 64% of soils were classified as blocky shape and around 76% of soils were in the texture classes sandy loam, loam, and silty loam (Table 4-1). It should also be noted that there were few samples classified as clay (C), silt clay (siC), clay loam (cL) and silt (Si).

In this study, data having soil particle size distributions with a minimum of five data points were fitted with the lognormal density function defined as:

$$F(\ln d) = F_n\left(\frac{\ln d - \ln d_m}{\sigma_d}\right) \tag{4-1}$$

where ln d is the log-converted particle diameter, $F_n(x)$ is the cumulative normal distribution function of x, ln d_m is the mean and σ_d is the standard deviation of ln d. This constitutes a departure from the methodology used in previous chapters in that before only sand, silt, and clay fractions were used to estimate the parameters of a lognormal distribution of particle sizes. In the dataset, the size of each structural shape considered was classified into three size classes: fine, medium, coarse. The original classification was converted to actual size using the classification of Nikiforoff (1941) shown in Table 4-2.

4.2.2 Pedo-Transfer Functions (PTFs) for the Estimation of Water Retention Curves

The van Genuchten (1980) water retention model parameters were estimated with the software ROSETTA (Schaap et al., 2001) from information on soil texture (sand, silt, and clay fractions), bulk density, and measured water content at -33 and at -1500 kPa. The van Genuchten (1980) model parameters were converted to the Kosugi (1996) lognormal water retention model parameters using Eq. (2-11) and Eq. (2-12). The parameters of the Kosugi (1996) model were used to estimate KLD with Eq. (2-9).

4.2.2 Pedo-Transfer Functions (PTFs) for the Estimation of K_{sat}

A total of 1359 data points from the original 1468 data points were used to estimate saturated hydraulic conductivity (K_{sat}, cm/day) using seven different PTFs (Table 4-3), including a prediction with the computer program ROSETTA (Schaap et al., 2001) with the same options selected for the estimation of the van Genuchten (1980) water retention model parameters. The van Genuchten (1980) model parameters required by the K_{sat} model of Han et al. (2008) were estimated with the Wosten et al. (1999) and ROSETTA (Schaap, 2001) models. The two procedures are identified in Fig. 4-1 as Han, 2008 (Wosten) and Han, 2008 (ROSETTA), respectively and are considered as two independent predictions. The PTFs of Han et al. (2008), ROSETTA and Wösten et al.

(1999) showed less variance in their estimation than others (Fig 4-1). Rawls et al. (1998) estimated the lowest K_{sat} with a large variance.

There may be intrinsic correlations between KLD and K_{sat} values because the PTFs used to estimate water retention curves for KLD estimations use the same physical properties to estimate K_{sat}. In this study, K_{sat} estimations using seven different methods were averaged to simulate the natural variability of K_{sat} and to diminish the correlation problem between KLD and K_{sat}. Guber et al. (2006) called this approach *multi model ensemble prediction* and showed that it is an effective tool to predict hydrological variables.

4.2.3 A Categorical Principal Component Analysis (CATPCA)

A Categorical Principal Component Analysis (CATPCA) as implemented in the statistical software package SPSS (SPSS Inc., Chicago, IL, USA) was utilized to transform field soil morphological descriptions into quantitative variables. A CATPCA explores relationships among descriptors having various measurement types (e.g., numerical, ordinal, or nominal) as an optimization problem using an alternating least squares algorithm (Ellis et al., 2006). The optimal scaling is a transformed quantity from the descriptors by the algorithm searching for the optimal mean squared correlation between optimal scaling and the components. It does so by changing the component loadings and their quantifications. Combining categorical variables with optimal scaling into the principal components maximizes the variance explained by the principal components for the data set (Calero et al., 2008; Ellis et al., 2006; Gifi, 1990; Meulman and Heiser, 1999). As an additional useful outcome, the optimal scaling can describe non linear relationships among those categorical variables and can also be useful for other analyses such as cluster analyses (Calero et al., 2008). In this study, texture and shape classes were assigned as multiple nominal types whereas the rest of the field morphological descriptions including size (Table 4-2) were assigned as ordinal type. Details on the criteria used for the selection of measurement type can be found in Carlero et al. (2008).

4.2.4 The Two Step Clustering Technique

The quantitatively transformed categorical variables from CATPCA were used in the two-step clustering procedure to identify homogeneous groups within a dataset. Among the advantages of the technique are an automatic selection of the number of clusters, the ability to handle both categorical and continuous variables, and the ability to handle large data sets. The procedures are summarized as follows: 1) pre-clustering the cases into many small clusters, and 2) re-cluster the small clusters into the appropriate number of clusters. The appropriate numbers of clusters were found with the Schwarz's Bayesian Criterion (BIC) or the Akaike Information Criterion (AIC) for each number of clusters within a specified range. Then, hierarchical clustering is performed on the initial estimate and the final clusters are defined by finding the largest increase in Log-Likelihood distance between the closest clusters in each stage (SPSS Inc., 2007).

4.2.5 Statistical Approaches

The stepwise linear regression technique was conducted to estimate K_{sat} using KLD and the quantitatively transformed field morphological descriptions using CATPCA. ANOVA and non-parametric approaches such as the Kruskal-Wallice H and Mann-Whitney U tests were used to test significance of differences in measured soil properties, of parameters of estimated water retention curves (θ_s, θ_r, ψ_m, σ), of averaged K_{sat}, and of KLD related to texture classes, structure types, and size classes. The Kruskal-Wallis H test is a useful nonparametric alternative to one-way analysis of variance for multiple samples in case that the variance and sample sizes are not equal. If the H test confirms differences among groups, then pairwise comparisons using the Mann-Whitney test or Post-Hoc analysis with Tamahnes's T2 were used to identify details among variables. Data resulting from the CATPCA and the two-step clustering were subject to a classification and regression tree with a Chi-square Automatic Interaction Detector (CHAID) (Kass, 1980) to infer potential relationships among KLD and soil physical properties (clay content, W33, and bulk density), and newly classified clusters using the two-step cluster analysis.

According to visual evaluations of histograms of all variables, OM and KLD were log-transformed for statistical tests requiring normal distributions (e.g., ANOVA).

4.3 Results and Discussions

4.3.1 General Characterization of the Dataset

Values of log OM, of water contents at -33 kPa (W33), and at -1500 kPa (W1500), and bulk density (BD) were significantly different ($p < 0.001$) across texture classes (Table 4-4, Appendix C). In agreement with results by Olness and Archer (2005) and Petersen et al., (1996), average texture class OM followed a linear relationship with clay. However, the linear relationship was not as strong when individual points were considered (Pearson correlation coefficient of 0.114, $p < 0.001$). There were positive correlations between W33 and clay content (Pearson correlation coefficient of 0.514, p <

0.001), between log OM and W1500 (Pearson correlation coefficient of 0.787, $p < 0.001$), and between OM and BD (Pearson correlation coefficient of -492, $p < 0.001$). Petersen et al. (1996) reported strong correlation among clay and OM, CEC, and W1500. The literature report contradictory results on the effects of OM on water retention values such as W33 and W1500 (Rawls et al., 2003). Recently, Olness and Archer (2005) analyzed more than 100,000 points and showed that both W33 and W1500 were correlated to clay contents, which is in agreement with results in this study.

Clay content, log OM, W33, W1500, and BD were significantly different ($p <$ 0.013) among structure type classes (Table 4-4). Differences in clay content were mainly due to soils with a prismatic soil structure type ($p < 0.005$). Bulk density (BD) and log OM were significantly different among all shape classes ($p < 0.03$). Prismatic soils have the highest clay content, W33, W1500, and BD but the lowest OM. Rawls and Pachepsky (2002) used a regression tree approach to estimate W33 and found that the blocky and prismatic structure types had smaller averaged water content at -33 kPa. Their results are different than those in this study, but results in Rawls and Pachepsky (2002) comprised a subset of the data (weak grade and soft (dry) consistency class).

Soils with structural units of estimated sizes between 2 and 5 cm (S5, Table 4-2) had the highest values of W33 and W1500 (Table 4-4). Except W33 ($p = 0.283$), other variables were significantly different ($p < 0.005$) among size classes. Except W33 and OM, values of clay content, W1500, and bulk density increased with aggregate size. Kay and Dexter (1990) also found that clay content increased as aggregate size increased. On the other hand, results in this study are different than in previous ones that reported a positive correlation between aggregate sizes and water retention (Tamboli et al. 1964), and a negative correlation between aggregate size and bulk density (Wittmuss and Mazurak, 1958). However, the cited studies considered aggregates smaller than 2 cm, whereas in this study aggregates were as large as 10 cm. Organic matter content decreased significantly with aggregate size ($p < 0.001$). Tamboli et al. (1964) pointed out that OM is mainly placed on the external surface of aggregates and, therefore, it is negatively correlated to aggregate size. It is worth noting that no clear trend or significant difference in W33 was found among size classes. These results differ from the finding of Pachepsky et al. (2006), who reported 2-5% smaller values of W33 in large soil aggregates. However, they used a qualitative scale of aggregate sizes (small, medium and large), each of which would contain a mix of actual sizes (see Table 4-2)

Estimated K_{sat} and parameters of the Kosugi (1994) model were significantly different across texture classes. Clay content had positive correlation with θ_r (Pearson correlation coefficient of 0.551, $p < 0.001$) and negative correlation with K_{sat} (Pearson correlation coefficient of -0.718, $p < 0.001$). These results were expected because PTFs used in their estimation utilized soil texture as main inputs. The relationship between water retention and soil texture are well know and constitute the bases for PTFs development (Pachepsky et al., 2006).

Among shape classes, significant differences were found in saturated hydraulic conductivity, K_{sat} ($p < 0.001$), saturated water content, θ_s ($p < 0.001$), and the standard deviation of the mean soil pore size, σ ($p = 0.014$), but no significant differences in residual water content, θ_r ($p = 0.739$), and geometric mean of soil pore size, ψ_m ($p = 0.061$) were found (Table 4-5). Values of K_{sat} were significantly lower in soils with prismatic soil structure type ($p < 0.003$) and higher in soils with granular soil structure type ($p < 0.005$). These results may be driven by the negative correlation between BD and K_{sat} (Pearson coefficient of -0.475, $p < 0.001$). Lin et al. (1999) also reported that soil structure type granular had greater values of K_{sat} than any other soil structure type due to a greater amount of inter-aggregate porosity in the granular soil structure type. On the other hand, Bouma and Anderson (1997) compared K_{sat} values from prismatic and blocky structures and found greater values of K_{sat} in the former that in the latter soil structure type. The discrepancy could be caused by the influence of texture within each soil structure type (Lin et al., 1999). Soils with fine texture and with structure type prismatic often present greater K_{sat} because of the development of macropores between aggregates (prisms), but soils with medium texture and prismatic structure type often have smaller K_{sat} than soils of blocky type.

The saturated water content, θ_s ($p < 0.001$), and K_{sat} ($p < 0.001$) were statistically different among aggregate size groups. Within each texture class, K_{sat} and θ_s decreased as aggregate size increased (Fig. 4-2). This is related to the increase of clay content with aggregate size (Table 4-4). Greater K_{sat} in smaller aggregates may also correspond to results of Kosugi (1997) who found that smaller structural units had smaller ψ_m. Horn (1994) pointed out that K_{sat} through single aggregates are lower than K_{sat} between aggregates (intra-aggregate flow), which would imply smaller K_{sat} values in larger aggregates due to a predominance of inter-aggregate flow over intra-aggregate flow.

Values of KLD were highly correlated to clay content (Pearson correlation coefficient of 0.526, $p < 0.001$) (Fig. 4-3). Clay was an important grouping parameter in the estimation of W33 in regression trees (Pachepsky et al., 2006). There were significant differences ($p < 0.001$) in KLD among texture classes. Sandy soils had the lowest KLD values, which reflect the relationship between KLD and clay content. According to an ANOVA test, there were no statistical differences in KLD ($p = 0.051$) among size classes but size S5 had significantly greater KLD values than other size classes (Fig. 4-4). The overall trend was different than the results of Chapter 2, but prismatic and platy soil structure types were not considered in that chapter.

4.3.2 Field Morphological Descriptions using CATPCA

The two-dimensional solution with eigenvalues greater than 1 accounted for 49.2% of the variance from CATPCA using variables derived from morphological field descriptions (Table 4-6). This variance is lower than those in Calero et al. (2008) and Scalenghe et al. (2000) who utilized similar procedures. Their model accounted for around 80% of the variance but used 17 variables as opposed to only 8 variables (texture, shape, grade, moisture, dryness, stickiness, plasticity, and size class) used in this study. Indeed the purpose of CATPCA in this study was to quantify field morphological variables. A different approach was used by Lilly et al. (2008), who assigned dummy values to different levels of qualitative variables.

Non linear characteristics of morphological properties were found in the transformation (Fig. 4-5). Mean values of optimal scaling were assigned to each category of the variables. The optimal scaling of multiple nominal variables such as texture and shape class were their centroid coordinate values. Soils in very coarse texture classes had negative scores (Fig. 4-5a). The approximate linear characteristics of shape classes (Fig. 4-5b) are in agreement with results in Calero et al. (2008). Increases of optimal scales from granular soil structure type to others such as blocky and prismatic were related to the clay content that was shown to be correlated to those classes (Calero et al., 2008). For aggregate sizes, soils can be grouped in two groups based on the sign of the optimal scaling values (Fig 4-5c). The first group showing negative optimal scaling values contains smaller size classes (s1, s2, s3) than the second group, which shows positive optimal scaling values (s4, s5, s6). Shape classes in the joint plot were closely located to size classes indicating high correlation because shape class information was already implicitly included in the size class category (Fig. 4-6a). The coordinates of the end point of vectors for stickiness and plasticity given by object scores were close together indicating high correlation between them. The cosines of the vector angles for variables indicated no correlation between shape class and other variables, and strong correlations among plasticity, stickiness, and moisture classes. On the first dimension, all variables have positive component loadings and, with the exception of size class, all variables are negative in the second dimension (Fig. 4-6b). As size decreases, the grade of soil structural elements tends to become stronger. Therefore, the second dimension will define a contrast between these two variables. Quantification of field morphological descriptions obtained from optimal scaling would be useful for other statistical analysis requiring variables in numerical type.

Using transformed values from categorical morphological variables, stepwise linear regression analysis was performed to estimate K_{sat}. In addition to the transformed morphological variables, KLD was included as a predictor. The selected final model resulted in K_{sat} (cm/day) = 1.291- 0.345 Texture – 0.109 Stickiness – 0.094 Dryness – 0.057 Log (KLD) - 0.059 Plasticity – 0.029 Size – 0.031 Grade with an $r^2 = 0.484$ and $p = 0.018$ (Fig. 4-7). Interestingly, size class and KLD were selected in the final model, whereas structure type and moisture classes were excluded. All selected variables in the final model were statistically significant and no collinearity problem was detected. KLD and size class were considered important in the final model.

Clay was an important variable, followed by aggregate size and shape class when KLD was estimated by regression tree analysis (Fig. 4-8). It should be noted that size class ($F = 12.51$) is more informative than shape class ($F = 6.63$), which agrees with the results in Chapter 2. Transformed field morphological variables presented significant correlations to many physical properties (Table 4-7). Values of KLD were correlated to texture. Although Pachepsky and Rawls (2003) considered grade class as the most important variable for the estimation of W33 or water content at -10 kPa, in this study stickiness and plasticity class were more related to W33. Stickiness and plasticity were also highly correlated to clay content and to K_{sat}. Although nonlinear transformation of field morphological descriptions helped to identify quantitative relationship to other measured soil properties, quantified field morphological variables were not strongly correlated to physical properties that are related to soil structure, such as bulk density, W33, ψ_m, and KLD.

4.3.3 Characteristics of Clustered Groups using Field Morphological Descriptions

The reduction of data into a smaller number of homogeneous groups is helpful for the identification of the effect of soil structure. Three groups were identified by the two-step clustering analysis and approximately half of the data was assigned to cluster 3 (Table 4-8). The number of groups was determined based on the maximized ratio of distance measures using Bayesian Information Criteria. Within each group, transformed field morphological variables were lined up vertically in descending order of importance (Fig. 4-9). For a variable to be significant, the absolute value of the *t*-statistic should exceed the boundaries defined by the vertical dashed lines representing the critical value. In cluster 1, shape class was most significant with negative *t*-statistics, followed by size classes. In cluster 3 size and shape classes were most significant, but with positive *t*-statistics. Dryness and size class with positive and significant *t*-statistics followed. The separation of variables into clusters can be confirmed by their centroids (Table 4-9). Mean value of cluster 1 for quantified texture class is between mean values of cluster 2 and cluster 3, indicating texture between coarse (cluster 3) and fine (cluster 2). Cluster 1 contained mostly small size of granular and platy structural types. It should be noted that cluster 2 consisted of lower values for all variables except shape and size classes.

The selection of the clusters were based only on field morphological descriptions and can, therefore, be considered independent of the physical properties of soils and of the KLD values associated to the morphological properties. Regression tree analysis was performed to identify the significance of physical properties in the estimation of these clusters (Fig. 4-10). Bulk density, clay, W33, and KLD, considered important variables for soil structure characterization, were used as dependant variables for the estimation of the three clusters. The best predictor for the estimation of the three clusters was W33 (Fig. 4-10a). Node 1 for water content less than 15.40% and it was composed mainly by samples in cluster 2. The main predictor of Node 2 (W33 between 15.40 and 20.50%) was KLD. Node 2 contained about 10% of the total data equally distributed among the three clusters. KLD values less than 0.91 was assigned to cluster 2 samples, whereas cluster 3 that contained the largest number of data points. Samples from cluster 3 containing the largest number of data points defined the group with W33 greater than 24.40% that was related to clay content.

Grade class is considered an important grouping parameter in the estimation of W33 or W10 (Pachepsky and Rawls, 2003; Bouma, 1992). In this study, texture and KLD were the most important predictors and were superior to grade class in the estimation of W33 (Fig. 4-10b). Without KLD and texture, grade class was the most important variable, which validates the result by Pachepsky and Rawls (2003). Size classification was also an important grouping parameter in the tree. The differences between results in Pachepsky and Rawls (2003) and the results in this study may have been caused by the optimal scaling introduced by CATPCA. When considering categorical variables directly in a regression tree, results were similar to Pachepsky and Rawls (2003) except for plasticity class appearing superior to grade class. Indeed, plasticity was better correlated with water retention properties that grade in this data set (Table 4-7). While the relationship between conventional descriptors of soil structure such as shape classes and KLD was unclear, differences in KLD among clusters were significant ($p < 0.001$), which suggests that KLD is an important variable for the description of soil structure.

4.4 Conclusions

Despite being widely available, soil structural descriptions use mostly categorical variables, limiting their use in PTFs or other modeling scenarios. In this study, categorical morphological descriptions were transformed to quantitative scores. In a regression tree analysis, KLD turned out to be an important factor for explaining clusters selected by a two-step clustering procedure using morphological variables. Although this study provides an advanced method relating soil structure description to KLD, the same approach should be tested using a datasets containing measured hydraulic properties.

More insight on the predictive power of KLD to estimate hydraulic properties would be achieved by considering measured K_{sat} and water retention.

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Table 4- 1 Number of samples as functions of shape and texture classes. Numbers in parenthesis are samples used in the prediction of K_{sat}.

Texture	**Shape**				
	Crumble & Granular	**Platy**	**Blocky**	**Prismatic**	**Total**
S	11	7	45	4	67
lS	10	4	48	2	64
Sl	49(48)	18	221(216)	27 (25)	315 (307)
L	34	22(20)	149 (145)	19 (17)	224 (216)
siL	51	72(69)	293 (279)	82 (74)	498 (473)
Si	0	1	3	2	6
scL	7	2	47 (45)	7	63 (61)
cL	2	1	20 (18)	6 (5)	29 (26)
sicL	22(19)	11(10)	94 (74)	27 (20)	154 (123)
siC	2(1)	4	30 (8)	1(0)	37 (13)
C	1	1	5 (0)	4(1)	11 (3)
Total	189 (184)	143 (137)	955 (881)	181 (157)	1468 (1359)

Table 4- 2 Symbols and actual sizes of structure types as function of their qualitative (field) description (after Nikiforoff, 1941).

Structure type	**Size**		
	Fine	**Medium**	**Coarse**
Platy	S1 (1-2mm)	S2 (2-5mm)	S3 (5-10mm)
Prismatic	S4 (1-2cm)	S5 (2-5cm)	S6 (5-10cm)
Blocky	S3 (5-10mm)	S4 (1-2cm)	S5 (2-5cm)
Granular	S1 (1-2mm)	S2 (2-5mm)	S3 (5-10mm)

Table 4- 3 Selected PTFs for the estimation of K_{sat} (cm/day) and water retention parameters of the van Genuchten (1980) model.

Model	Equation
	For K_{sat} estimation
Wosten et al. 1999	$K_{sat} = 1.15741 \cdot 10^{-7} \exp[7.755 + 0.0352\,silt + 0.93\,topsoil - 0.967\,D^2 - 0.000484\,clay^2 - 0.000322\,silt^2 + 0.01/silt - 0.0748/om - 0.643\ln(silt) - 0.01398\,D\,clay - 0.1673\,D\,om + 0.02986\,topsoil\,clay - 0.03305\,topsoil\,silt]$
Brakensiek et al. 1984	$K_{sat} = 2.78 \cdot 10^{-6} \exp(19.52348\,\theta_s - 8.96847 - 0.028212\,clay + 1.8107 \cdot 10^{-4}\,sand^2 - 9.4125 \cdot 10^{-3}\,clay^2 – 8.395215\,\theta_s^2 + 0.077718\,sand\,\theta_s - 0.00298\,sand^2\,\theta_s^2 - 0.019492\,clay^2\,\theta_s^2 + 1.73 \cdot 10^{-5}\,sand^2\,clay + 0.02733\,clay^2\,\theta_s + 0.001434\,sand^2\,\theta_s - 3.5 \cdot 10^{-6}\,clay^2\,sand)$
Saxton et al. 1986	$K_{sat} = 2.778 \cdot 10^{-6} \exp[12.012 - 7.55 \cdot 10^{-2}\,sand + (-3.895 + 3.671 \cdot 10^{-2}\,sand - 0.1103\,clay + 8.7546 \cdot 10^{-4}\,clay^2)/\theta_s]$
Rawls et al. 1998	$5.361 \cdot 10^{-4}\,\theta_{eff}^{m}$, where m=3.-(1./b), θ_{eff}^{m} is saturated water content minus water content at field capacity and b is the Campbell parameter
Han et al. 2008	$K_{sat} = 20\phi_{\inf}^{3-\frac{5}{\theta_s}}$, where $\phi_{\inf} = \theta_s - \theta_{\inf}$
Schaap 2001	No equation available, neural network approach using software ROSETTA to estimate K_{sat}.
	For water retention
Wosten et al. 1999	$\alpha = \exp[-14.96 + 0.03135\,clay + 0.0351\,silt + 0.646\,om + 15.29\,D - 0.192\,topsoil - 4.671D^2 – 0.000781\,clay_2 - 0.00687\,om_2 + 0.0449/om + 0.0663\ln(silt) + 0.1482\ln(om) – 0.04546\,D\,silt – 0.4852\,D\,om + 0.00673\,topsoil\,clay]$ $n = \exp[-25.23 – 0.02195\,clay + 0.0074\,silt – 0.194\,om + 45.5\,D – 7.24\,D_2 + 0.0003658\,clay^2 + 0.002885\,om^2 – 12.81/D – 0.1524/silt – 0.01958/om – 0.2876\ln(silt) – 0.0709\ln(om) – 44.6\ln(D) – 0.02264\,D\,clay + 0.0896\,D\,om + 0.00718\,topsoil\,clay]$
Schaap 2001	No equation available, neural network approach using software ROSETTA to estimate α and n.

Table 4- 4 Summary of soil physical properties of soils in the US National Pedon Characterization database.

	N	Mean					Std. Deviation				
		Clay, %	OM, %	W33, %	W1500, %	BD, Mg/m^{-3}	Clay	OM	W33	W1500	BD
Texture class											
S	67	4.89	0.49	12.06	3.89	1.59	2.65	0.54	5.76	2.06	0.13
lS	64	6.93	1.31	16.45	6.60	1.56	2.96	1.93	8.40	2.53	0.19
Sl	315	12.45	1.44	22.39	9.92	1.53	4.40	2.65	8.21	4.04	0.23
L	224	19.15	1.85	28.73	14.05	1.47	4.79	2.51	6.55	4.75	0.20
siL	498	16.69	1.91	33.12	13.69	1.40	6.59	2.37	6.25	4.45	0.18
Si	6	6.75	0.54	34.32	9.13	1.46	3.85	0.56	5.19	5.24	0.13
scL	63	23.75	1.15	26.81	15.90	1.57	2.73	1.24	5.52	4.34	0.20
cL	29	28.37	1.94	32.99	18.47	1.51	1.12	3.06	6.23	3.87	0.20
sicL	154	31.89	2.77	36.80	20.21	1.47	3.38	4.03	5.84	3.75	0.21
siC	37	48.45	2.22	40.75	26.31	1.59	5.10	2.71	4.25	5.20	0.20
C	11	61.61	3.69	42.51	28.90	1.57	2.59	4.43	7.55	4.61	0.45
Soil structure type											
Crumble & Granular	189	17.34	4.05	27.38	12.31	1.37	9.54	4.26	8.83	5.44	0.23
Platy	143	17.19	2.01	29.45	13.03	1.44	10.23	2.38	8.57	5.37	0.18
Blocky	955	18.38	1.49	28.71	13.46	1.50	10.50	2.24	10.13	6.50	0.21
Prismatic	181	20.73	0.81	30.53	15.03	1.53	10.38	0.81	7.89	5.39	0.19

Table 4-4 Cont'd

	N	Mean					Std. Deviation				
		Clay, %	OM, %	W33, %	W1500%	BD, Mg/m^{-3}	Clay	OM	W33	W1500	BD
Size class											
s1	196	16.94	3.64	28.22	12.58	1.38	9.81	4.31	8.62	5.45	0.22
s2	122	18.22	2.54	28.76	13.00	1.43	9.99	2.36	9.19	5.48	0.19
s3	300	17.67	1.64	28.43	13.30	1.49	10.80	2.29	10.31	6.82	0.21
s4	744	18.68	1.36	28.96	13.57	1.50	10.31	2.16	9.75	6.21	0.21
s5	79	21.65	0.82	31.17	15.76	1.51	8.49	0.72	7.83	4.90	0.17
s6	27	21.53	0.89	28.23	14.24	1.61	15.03	0.78	10.12	7.32	0.19
Total	1468	18.42	1.78	28.84	13.46	1.48	10.38	2.66	9.60	6.17	0.21

Table 4- 5 Water retention properties of soils in the US National Pedon Characterization database estimated with ROSETTA (Schaap et al., 2001).

	N	Mean					Std. Deviation				
		θ_s, g/g	**θ_r, g/g**	**ψ_m, kPa**	**σ**	**K_{sat}, cm/day**	**θ_s**	**θ_r**	**ψ_m**	**σ**	**K_{sat}**
Texture class											
S	67	0.36	0.03	2.52	1.33	2.21	0.03	0.01	53.40	0.29	0.22
lS	64	0.37	0.04	4.59	1.40	1.96	0.05	0.02	108.37	0.34	0.30
Sl	315	0.38	0.04	6.42	1.57	1.53	0.06	0.01	132.24	0.26	0.45
L	224	0.40	0.05	9.07	1.60	1.06	0.05	0.02	150.73	0.30	0.46
siL	498	0.42	0.06	20.68	1.36	1.18	0.04	0.02	250.34	0.33	0.56
Si	6	0.42	0.06	48.83	1.05	1.48	0.04	0.02	451.36	0.47	0.48
scL	63	0.39	0.06	2.52	1.81	1.13	0.05	0.02	24.61	0.21	0.47
cL	29	0.42	0.07	8.08	1.70	0.73	0.05	0.01	87.59	0.28	0.40
sicL	154	0.45	0.08	15.71	1.66	0.59	0.05	0.02	251.58	0.45	0.45
siC	37	0.45	0.08	8.54	2.06	0.44	0.05	0.02	115.24	0.48	0.43
C	11	0.46	0.08	6.55	2.27	1.22	0.10	0.03	112.96	0.65	0.92
Soil structure type											
Crumble & Granular	189	0.43	0.05	9.55	1.50	1.44	0.06	0.03	164.06	0.31	0.64
Platy	143	0.41	0.06	15.50	1.46	1.25	0.05	0.02	245.44	0.36	0.61
Blocky	955	0.40	0.05	12.74	1.52	1.26	0.06	0.02	208.81	0.38	0.61
Prismatic	181	0.40	0.06	11.74	1.59	1.04	0.05	0.02	186.08	0.38	0.54

Table 4-5 Cont'd

	N	Mean					Std. Deviation				
		θ_s	θ_r	ψ_m, kPa	σ	K_{sat}, cm/day	θ_s	θ_r	ψ_m	σ	K_{sat}
Size class											
s1	196	0.42	0.05	10.72	1.51	1.43	0.06	0.03	197.58	0.32	0.61
s2	122	0.42	0.06	14.50	1.45	1.23	0.05	0.04	217.04	0.35	0.65
s3	300	0.40	0.05	12.11	1.52	1.31	0.06	0.02	206.40	0.38	0.62
s4	744	0.40	0.05	13.02	1.53	1.23	0.05	0.02	209.10	0.39	0.60
s5	79	0.41	0.06	10.88	1.59	1.01	0.04	0.02	181.48	0.33	0.55
s6	27	0.38	0.05	9.67	1.61	1.07	0.04	0.02	134.75	0.43	0.49
Total	1468	0.41	0.05	12.47	1.52	1.26	0.06	0.02	205.17	0.37	0.61

Table 4- 6 Variance Accounted For (VAF) of texture class and morphological variables considered in CATPCA.

	Centroid Coordinates			**Vector Coordinates**			**Total**		
	Dimension		**Mean**	**Dimension**		**Total**	**Dimension**		**Total**
	1	**2**		**1**	**2**		**1**	**2**	
Texture*	0.467	0.128	0.298				0.467	0.128	0.298
Shape class*	0.235	0.786	0.51				0.235	0.786	0.51
Grade class	0.218	0.097	0.158	0.217	0.093	0.31	0.217	0.093	0.31
Moisture class	0.065	0.007	0.036	0.065	0.007	0.072	0.065	0.007	0.072
Dry class	0.319	0.011	0.165	0.319	0.011	0.33	0.319	0.011	0.33
Sticky class	0.655	0.062	0.359	0.655	0.061	0.716	0.655	0.061	0.716
Plasticity class	0.713	0.053	0.383	0.713	0.052	0.765	0.713	0.052	0.765
Size class	0.203	0.781	0.492	0.192	0.746	0.937	0.192	0.746	0.937
Total eigenvalue	2.874	1.925	2.4	2.159	0.97	3.129	2.861	1.884	3.937
Variance Accounted For**	35.93	24.06	29.995	35.987	16.165	52.151	35.757	23.55	49.210

* indicates multiple nominal variable. ** VAF indicates variance explained by variable considered in principal component.

Table 4- 7 Correlation coefficients among transformed morphological descriptors and physical and hydraulic variables in the US National Pedon Characterization database.

	Texture	**Structure type**	**Grade**	**Moisture**	**Dryness**	**Stickiness**	**Plasticity**	**Size**
BD	-.132**	.190**	.071**	-0.01	.190**	.104**	.089**	.212**
Clay	.739**	.056*	.253**	.135**	.279**	.547**	.549**	.069**
Log OM	.294**	-.313**	.076**	.097**	-.127**	.052*	.060*	-.350**
W33	.666**	0.025	.287**	.135**	.262**	.432**	.492**	0.033
W1500	.695**	.068**	.299**	.152**	.307**	.528**	.535**	.073**
K_{sat}	-.607**	-.081**	-.279**	-.155**	-.379**	-.537**	-.536**	-.115**
Qs	.410**	-.123**	.081**	0.049	-0.011	.167**	.174**	-.139**
Qr	.531**	-0.007	.197**	.100**	.210**	.344**	.328**	0.001
hm	.159**	0.005	.086**	0.002	.068**	0.032	.087**	0.015
sigma	.217**	.052*	.113**	.066*	.114**	.251**	.232**	0.047
Log KLD	.439**	-0.021	.137**	.081**	.154**	.379**	.352**	-0.015

** : Statistically significant at $\alpha = 0.05$.

Table 4- 8 Number of samples assigned to each of 3 clusters by the two-step clustering technique.

Cluster	**N**	**% of Total**
1	325	22.1
2	336	22.9
3	807	55.0
Total	1468	100%

Table 4- 9 Means and standard deviations of quantitatively transformed variable for each cluster.

	Cluster 1		**Cluster 2**		**Cluster 3**	
	Mean	**Std. deviation**	**Mean**	**Std. deviation**	**Mean**	**Std. deviation**
Texture	-0.004	0.648	-0.630	0.739	0.264	0.468
Shape	-1.634	0.146	0.441	0.300	0.474	0.046
Grade	0.105	1.086	-0.533	0.669	0.180	1.003
Moisture	0.105	0.000	-0.354	2.054	0.105	0.000
Dryness	-0.439	1.244	-0.643	1.291	0.445	0.242
Stickiness	-0.170	0.976	-1.009	0.752	0.489	0.727
Plasticity	-0.236	0.980	-1.149	0.693	0.573	0.578
Size	-1.717	0.446	0.423	0.477	0.516	0.342

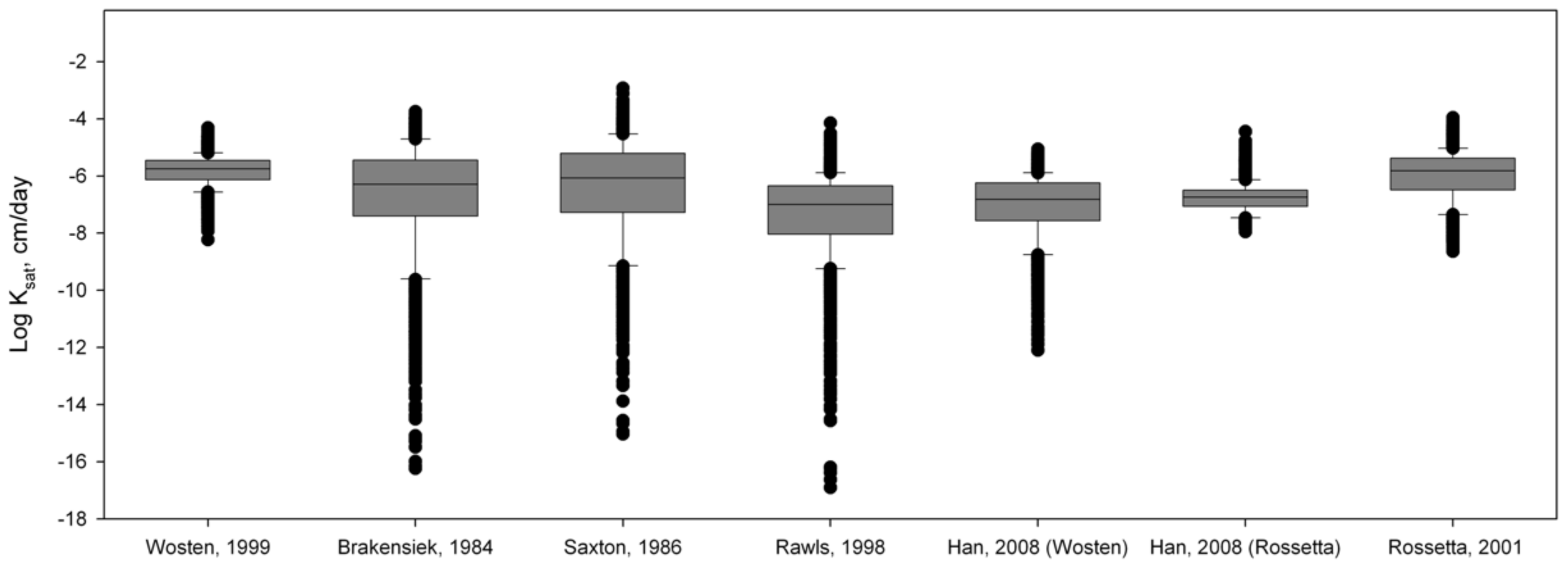


Fig. 4- 1 Box-plot of the estimated saturated hydraulic conductivities from multiple PTFs. Bars are the 5 and 95 percentiles and the black circles are outliers.

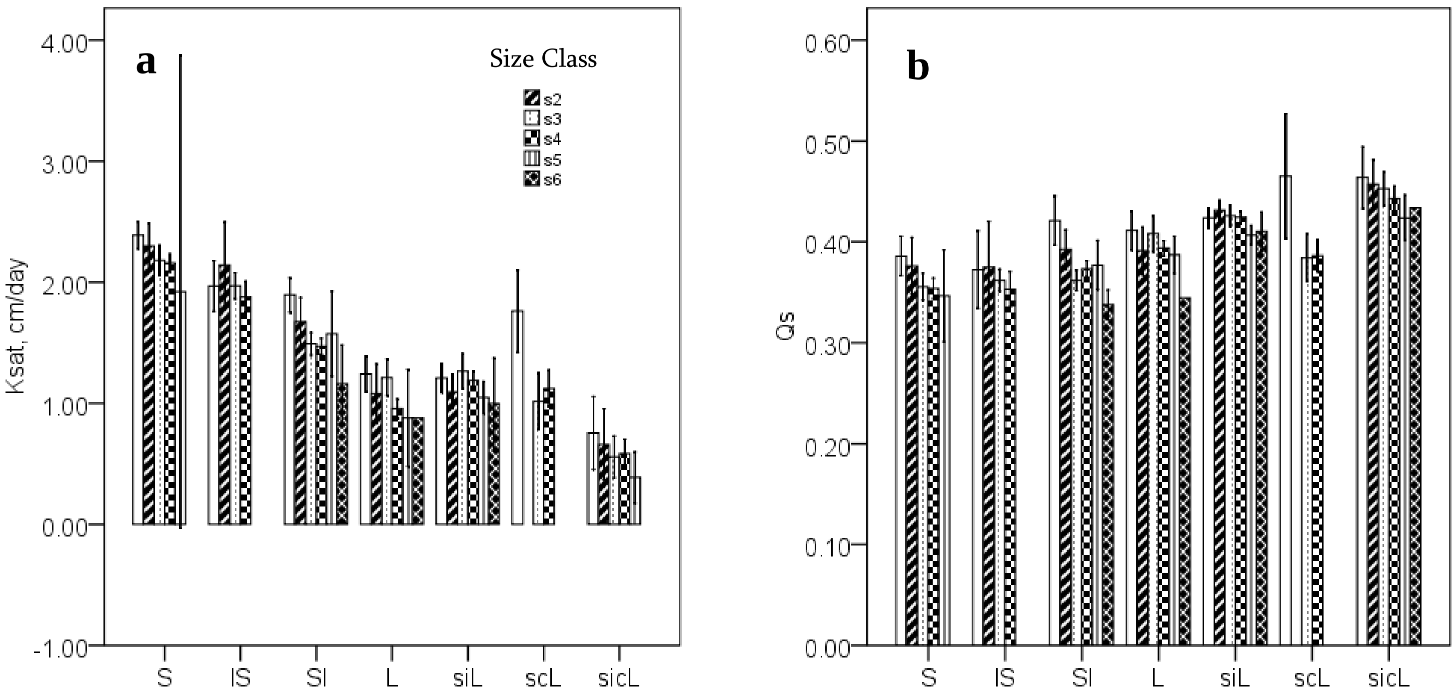


Fig. 4- 2 Estimated values of a) saturated hydraulic conductivity and b) saturated water content plotted as functions of soil texture and size classes. See text for details in the estimation procedures.

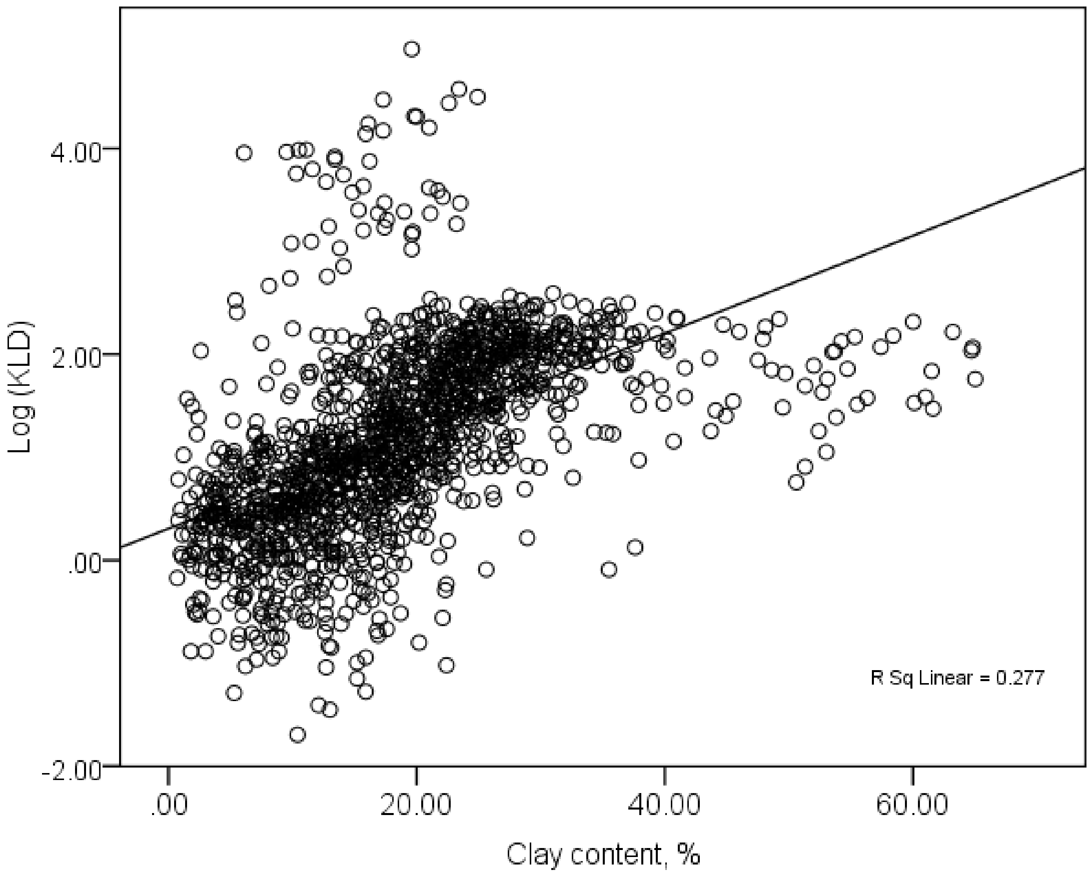


Fig. 4- 3 Relationship between log converted KLD *vs.* clay content for 1359 samples.

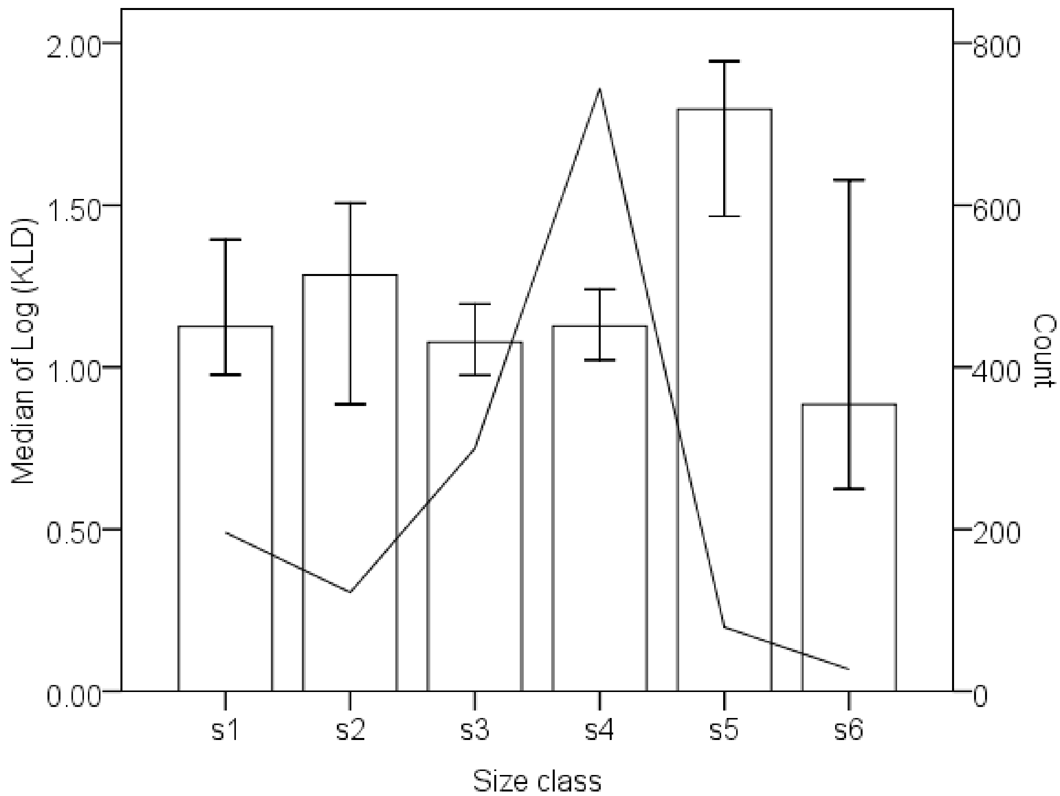


Fig. 4- 4 Median of log converted KLD *vs*. size class. Bars represent the standard deviations of measurements within a class. The solid line is the number of samples.

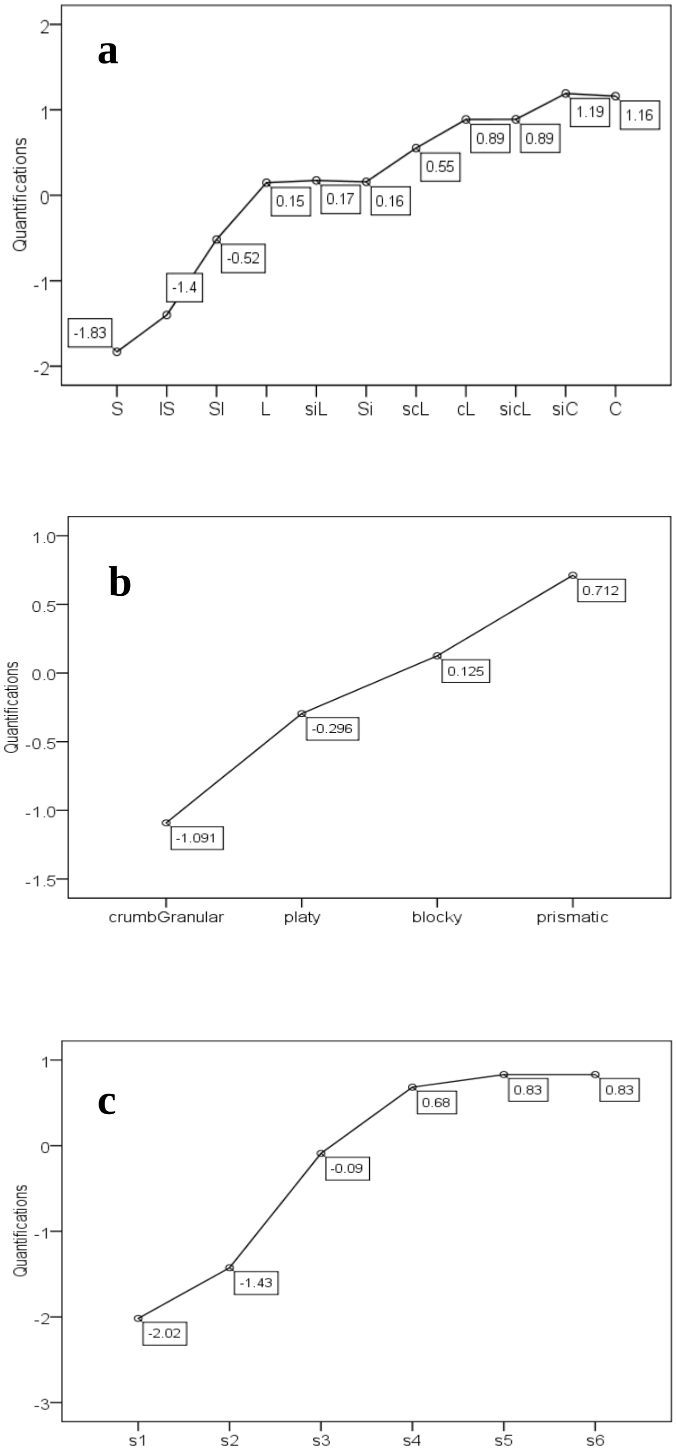


Fig. 4- 5 Optimal scaling values for (a) texture classes, (b) shape classes, and (c) size classes obtained from a Categorical Principal Component Analysis (CATPCA).

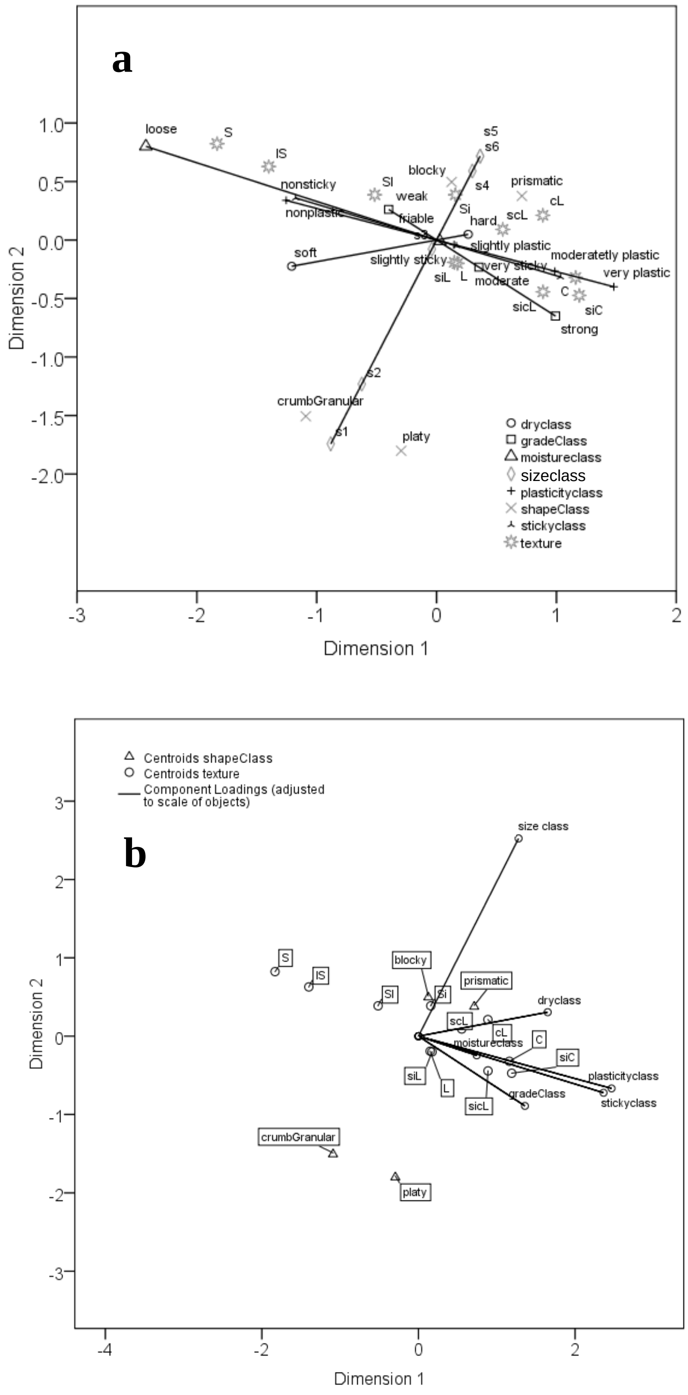


Fig. 4- 6 (a) Quantifications in joint plot of the category points of each of the morphological variables, and (b) plot of component loadings for ordinal variables with vector and multiple nominals for centroid coordinates.

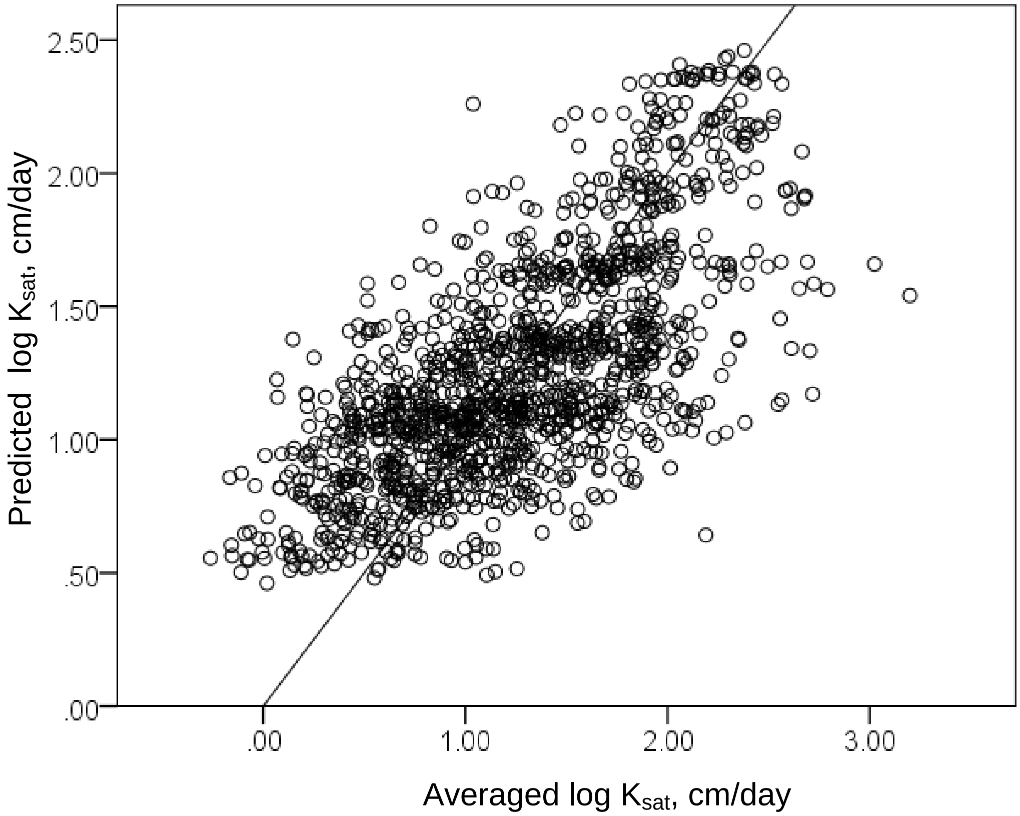


Fig. 4- 7 Averaged K_{sat} from estimation with seven models (see Table 4-3) *vs.* K_{sat} estimated with stepwise linear regression from morphological variables and KLD (the line indicates a 1:1 relationship).

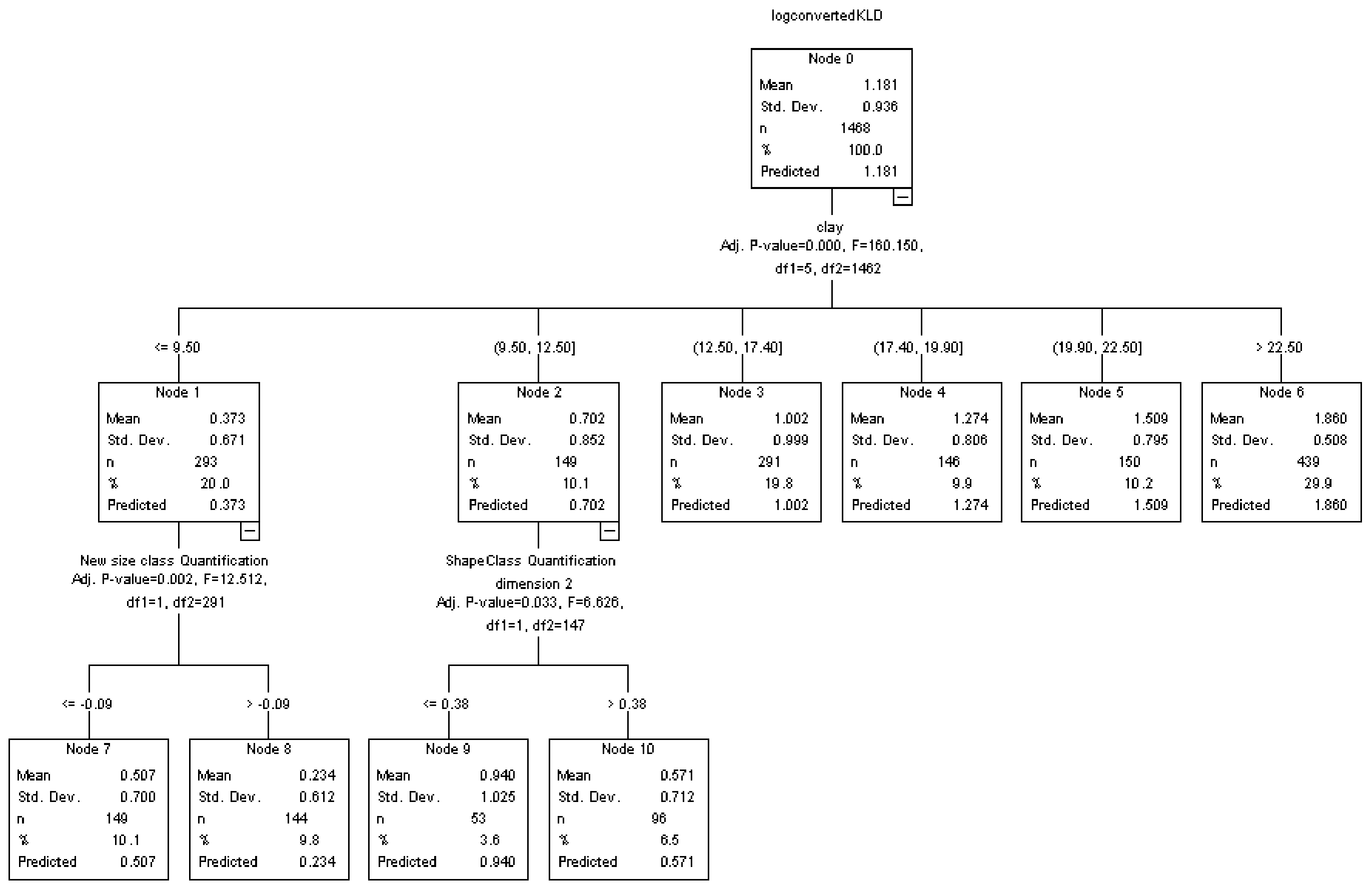


Fig. 4- 8 Regression tree to estimate KLD using clay content, structure type, grade and size classes. Partitioning range of variable is shown above the box and the *F* statistics to test significance of the variables is shown beneath each variable name.

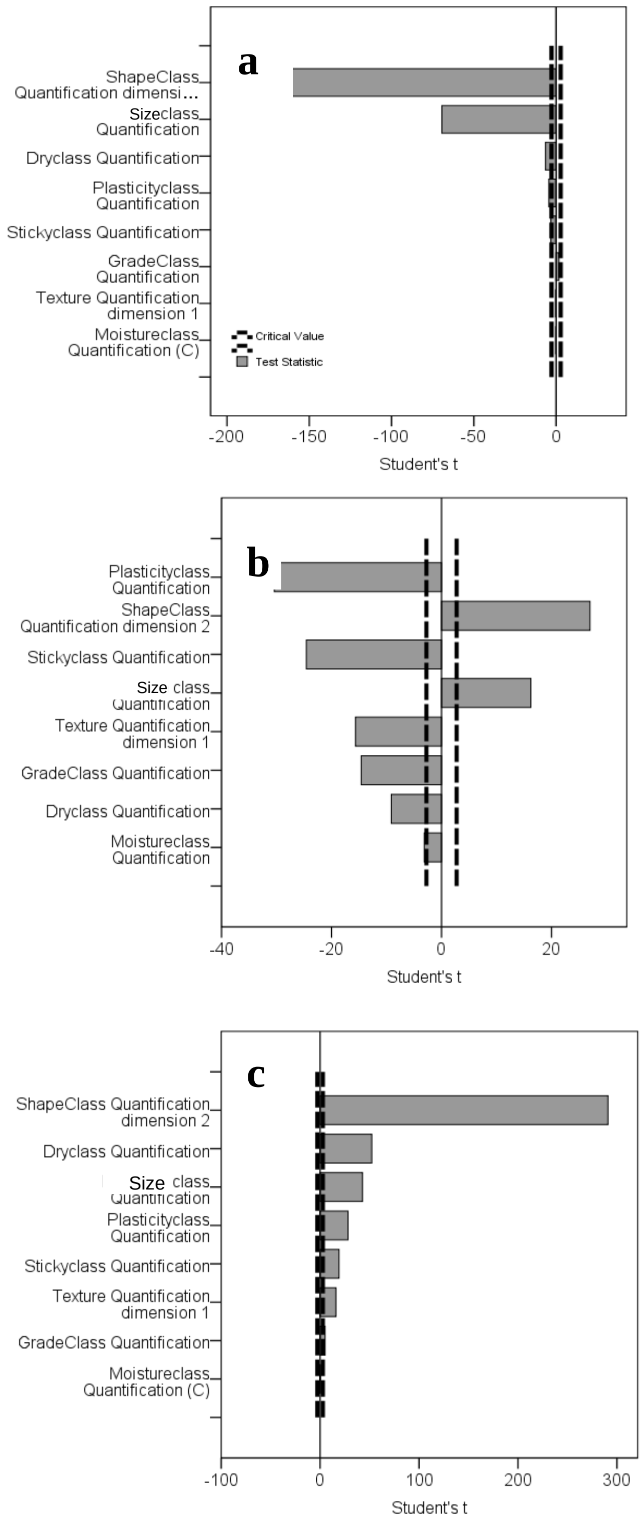
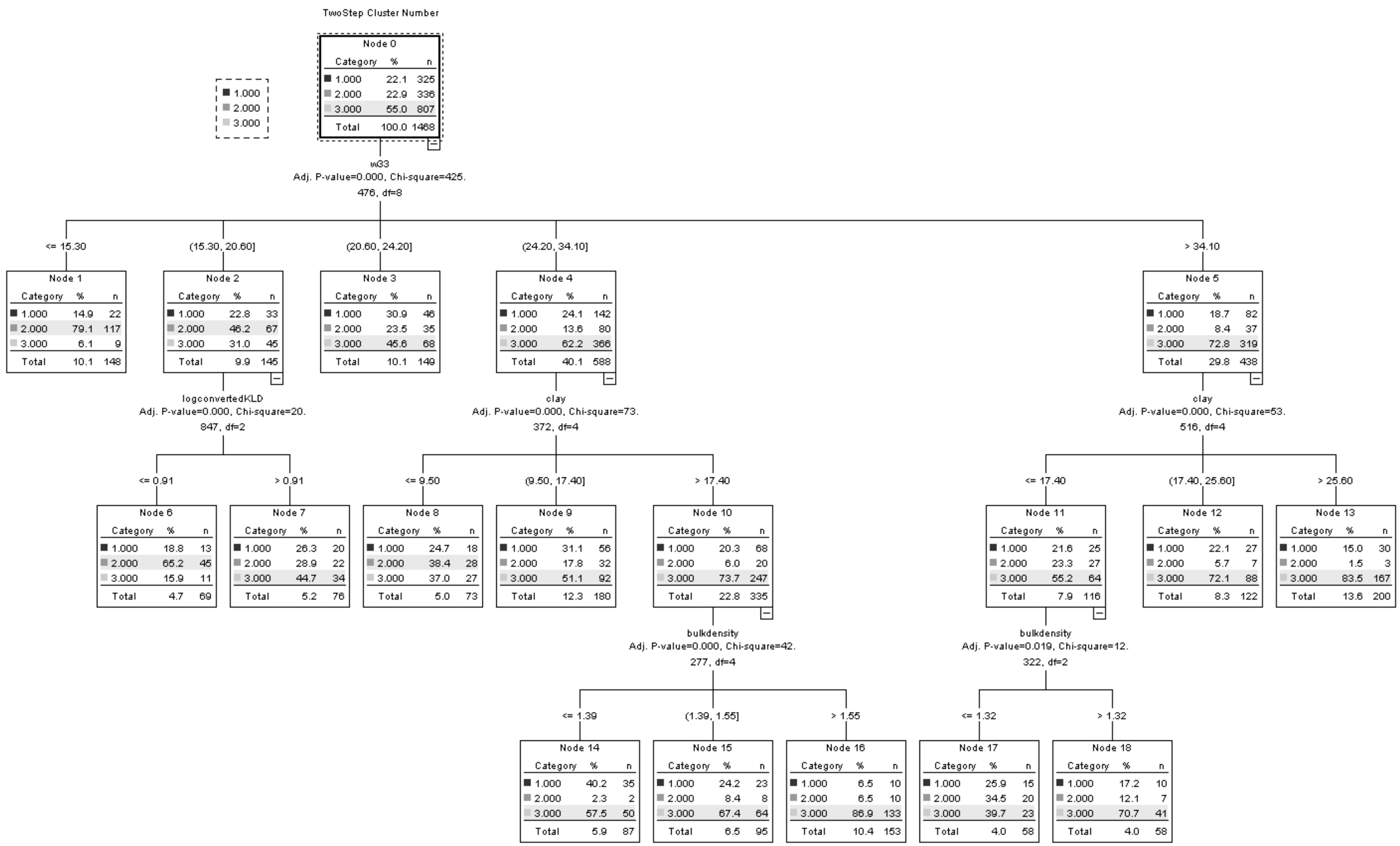


Fig. 4- 9 Significance chart for variables in (a) cluster 1, (b) cluster 2, and (c) cluster 3.

a


TwoStep Cluster Number
1.000
2.000
3.000
Node 0
Category % n
1.000 22.1 325
2.000 22.9 336
3.000 55.0 807
Total 100.0 1468
w33
Adj. P-value=0.000, Chi-square=425.
476, df=8
<= 15.30
(15.30, 20.60]
(20.60, 24.20]
(24.20, 34.10]
> 34.10
Node 1
Category % n
1.000 14.9 22
2.000 79.1 117
3.000 6.1 9
Total 10.1 148
Node 2
Category % n
1.000 22.8 33
2.000 46.2 67
3.000 31.0 45
Total 9.9 145
Node 3
Category % n
1.000 30.9 46
2.000 23.5 35
3.000 45.6 68
Total 10.1 149
Node 4
Category % n
1.000 24.1 142
2.000 13.6 80
3.000 62.2 366
Total 40.1 588
Node 5
Category % n
1.000 18.7 82
2.000 8.4 37
3.000 72.8 319
Total 29.8 438
logconvertedKLD
Adj. P-value=0.000, Chi-square=20.
847, df=2
clay
Adj. P-value=0.000, Chi-square=73.
372, df=4
clay
Adj. P-value=0.000, Chi-square=53.
516, df=4
<= 0.91
> 0.91
<= 9.50
(9.50, 17.40]
> 17.40
<= 17.40
(17.40, 25.60]
> 25.60
Node 6
Category % n
1.000 18.8 13
2.000 65.2 45
3.000 15.9 11
Total 4.7 69
Node 7
Category % n
1.000 26.3 20
2.000 28.9 22
3.000 44.7 34
Total 5.2 76
Node 8
Category % n
1.000 24.7 18
2.000 38.4 28
3.000 37.0 27
Total 5.0 73
Node 9
Category % n
1.000 31.1 56
2.000 17.8 32
3.000 51.1 92
Total 12.3 180
Node 10
Category % n
1.000 20.3 68
2.000 6.0 20
3.000 73.7 247
Total 22.8 335
Node 11
Category % n
1.000 21.6 25
2.000 23.3 27
3.000 55.2 64
Total 7.9 116
Node 12
Category % n
1.000 22.1 27
2.000 5.7 7
3.000 72.1 88
Total 8.3 122
Node 13
Category % n
1.000 15.0 30
2.000 1.5 3
3.000 83.5 167
Total 13.6 200
bulkdensity
Adj. P-value=0.000, Chi-square=42.
277, df=4
bulkdensity
Adj. P-value=0.019, Chi-square=12.
322, df=2
<= 1.39
(1.39, 1.55]
> 1.55
<= 1.32
> 1.32
Node 14
Category % n
1.000 40.2 35
2.000 2.3 2
3.000 57.5 50
Total 5.9 87
Node 15
Category % n
1.000 24.2 23
2.000 8.4 8
3.000 67.4 64
Total 6.5 95
Node 16
Category % n
1.000 6.5 10
2.000 6.5 10
3.000 86.9 133
Total 10.4 153
Node 17
Category % n
1.000 25.9 15
2.000 34.5 20
3.000 39.7 23
Total 4.0 58
Node 18
Category % n
1.000 17.2 10
2.000 12.1 7
3.000 70.7 41
Total 4.0 58

b

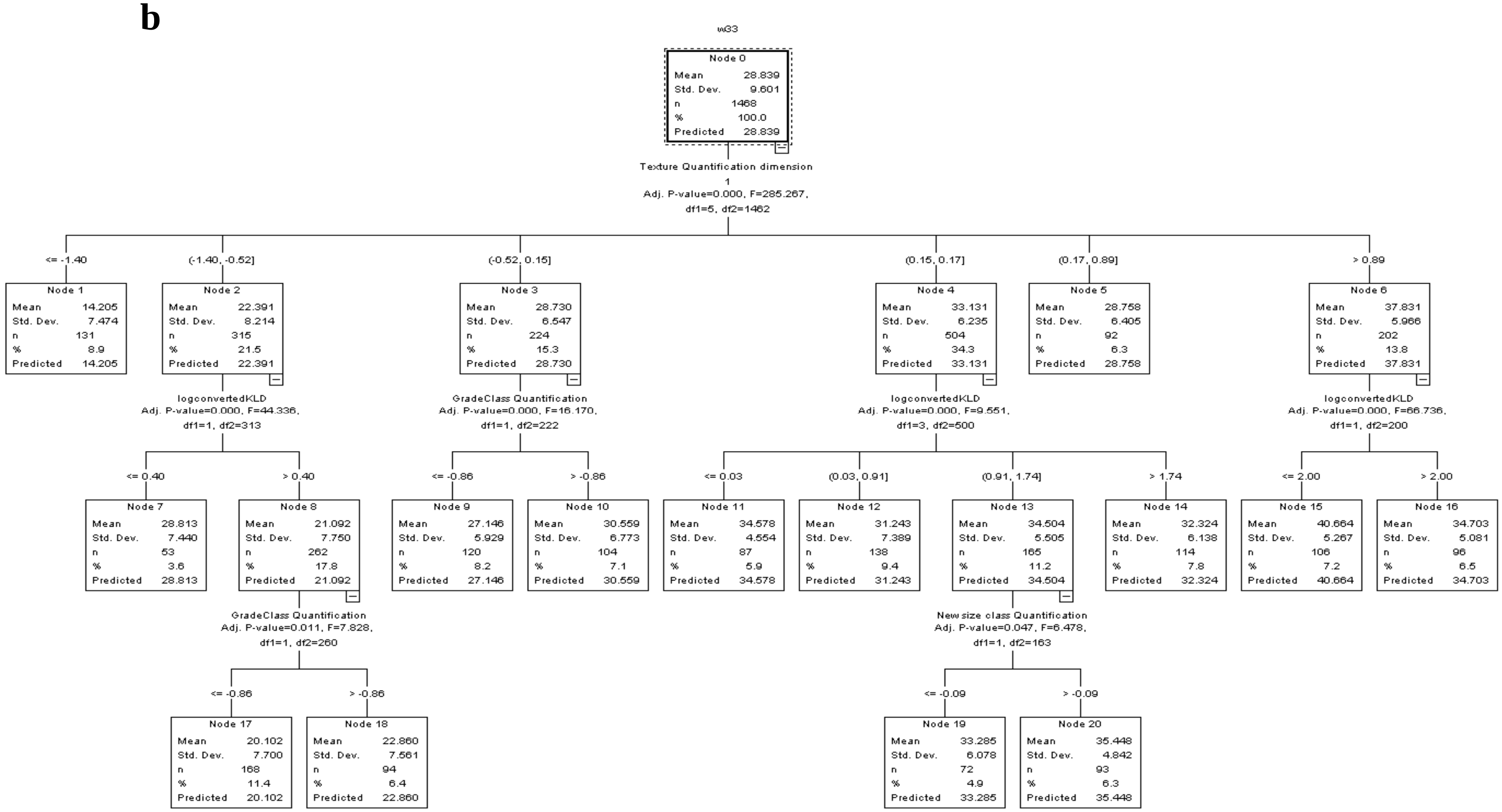


Fig. 4- 10 Regression tree to estimate; (a) three clusters from the two-step clustering and (b) W33 from texture classes, field morphological variables, and KLD. Partitioning range of variables is shown above the box and the *F* statistics to test for significance of the variables is shown beneath each variable name.

Chapter 5 Conclusions and Future Research

The proposed KLD measure is based on soil pore size distributions derived from water retention curves and soil texture. It quantifies soil pore systems relative to a reference pore system derived from information on texture. The effect of soil structure development on soil pore systems appeared as distinct entropic distances from a reference pore system. The greater KLD values found in more structured and less degraded soil suggest that KLD could be a useful indicator of soil structural development. One of the main advantages of using KLD is its conceptual and computational simplicity.

While KLD showed consistent descriptions of structured soils under various conditions, some limitations in the research approach should be pointed out. Since KLD is based on water retention curves, any hydraulic process influenced by more or less spatially isolated or rare features will be difficult to quantify, unless those features are accounted for in the water retention measurements. One example of such process is preferential flow that takes place in large and more or less sparse macropores (cm scale). Another problem related to the measurement of water retention curves is that current methods do not accurately depict the distribution on pores very close to saturation. Therefore, those pores will not be typically represented in KLD values. The proposed method to estimate water retention from the reference pore size distribution using Chan and Govindaraju (2004) produces unrealistically small estimates of r_r for fine texture soils. This problem could potentially be solved by selecting the appropriate value α in Eq. (2-1). In fact, a future research line would be to refine Chan and Govindaraju's (2004) model to produce realistic parameters from different particle size distributions..

One of the most interesting findings in Chapter 3 was the scaling effect on the soil pore system (Fig. 3-7), because KLD would contribute to indentify the representative elementary volume related to soil structure and water retention. Future research should consider a range of soil volumes when measuring water retention for improved justification. Results for the relationship between KLD and hydraulic and physical properties in Chapter 4 suggest that KLD could be used to improve current PTFs. It would be of interest to investigate using KLD for prediction of saturated and unsaturated hydraulic conductivities. Use of database containing measured water retentions and hydraulic conductivities would contribute to develop improved PTFs considering soil structural effects.

Appendix A

Entropy and KLD Derived from Water Retention Curves

A-1 Entropy derived from water retention curves

Let x be a random variable with a probability density function f whose support is a set X. The differential entropy is defined as:

$$H[f(x)] = -\int_X f(x)\ln f(x)dx \qquad \text{A-1-1}$$

An effective pore size distribution of random variable, r, can be derived from the Kosugi (1996) lognormal water retention as:

$$f(r) = \frac{1}{r\sigma\sqrt{2\pi}}\exp[-\frac{(\ln r-\mu)^2}{2\sigma^2}] \qquad \text{A-1-2}$$

where $\mu = \ln r_m$ and r_m is the geometric mean of $f(r)$

Substitute f(x) in Eq. (A-1-1) with $f(r)$ from Eq. (A-1-2), then

$$H[f(r)] = -\int_0^R f(r)\ln\{\frac{\exp[-(\ln r-\mu)^2/2\sigma^2]}{r\sigma\sqrt{2\pi}}\}dr$$

$$= -\int_0^R f(r)[-(\ln r-\mu)^2/2\sigma^2]dr + \int_0^R f(r)(\ln r + \ln\sigma\sqrt{2\pi})dr$$

$$= \frac{1}{2\sigma^2}\int_0^R f(r)(\ln r-\mu)^2 dr + \int_0^R f(r)\ln r dr + \ln\sigma\sqrt{2\pi}\int_0^R f(r)dr$$

$$H[f(r)] = \frac{1}{2\sigma^2}\int_0^R f(r)(\ln r-\mu)^2 dr + \int_0^R f(r)\ln r dr + \ln\sigma\sqrt{2\pi}\int_0^R f(r)dr \qquad \text{A-1-3}$$

Each term in Eq. (A-1-3) are subject to the constraints:

$$\int_0^R f(r)dr = 1,\ E(\ln r) = \int_0^R f(r)\ln r dr = \mu,$$

$$E[(\ln r-\mu)^2] = \int_0^R f(r)(\ln r-\mu)^2 = \sigma^2$$

Therefore, it is simplified as:

$$H[f(r)] = \ln r_m + \frac{1}{2} + \frac{1}{2}\ln 2\pi\sigma^2$$

A-2 KLD derived from water retention curves

Let x be a random variable with a probability density functions f and g whose support is a set X. The KLD is defined as:

$$KLD = \int_X f(x) \ln \frac{f(x)}{g(x)} dx$$

$$KLD = \int_X f(x) ln\, f(x) dx - \int_X f(x) ln\, g(x) dx \quad \text{A-2-1}$$

The first term in the right hand side is equal to $-H[f(x)]$

Effective pore size distributions *f(r)* and *g(r)*, representing the pore size distribution of a structured soil and a reference pore size distribution, respectively, can be derived from the Kosugi (1996) lognormal water retention as:

$$f(r) = \frac{1}{r\sigma_f \sqrt{2\pi}} \exp[-\frac{(\ln r - \mu_f)^2}{2\sigma_f^2}] \quad \text{A-2-2}$$

$$g(r) = \frac{1}{r\sigma_g \sqrt{2\pi}} \exp[-\frac{(\ln r - \mu_g)^2}{2\sigma_g^2}] \quad \text{A-2-3}$$

By introducing Eq. (A-2-2) and Eq. (A-2-3) into the second term of the right hand side of Eq. (A-2-1),

$$-\int_R f(r) \ln\{\frac{1}{r\sigma_g \sqrt{2\pi}} \exp[-\frac{(\ln r - \mu_g)^2}{2\sigma_g^2}]\} dr \quad \text{A-2-4}$$

$$= -\int_R f(r)[-\frac{(\ln r - \mu_g)^2}{2\sigma_g^2}] dr + \int_R f(r) \ln r\sigma_g \sqrt{2\pi} dr$$

$$= \frac{1}{2\sigma_g^2} \int_R f(r)(\ln r - \mu_g)^2 dr + \int_R f(r)(\ln r + \ln \sigma_g \sqrt{2\pi}) dr$$

$$= \frac{1}{2\sigma_g^2}\int_R f(r)(\ln r - \mu_f + \mu_f - \mu_g)^2 dr + \int_R f(r)\ln r dr + \ln\sigma_g\sqrt{2\pi}\int_R f(r)dr$$

The first term of the above equation can be expanded to:

$$= \frac{1}{2\sigma_g^2}\int_R f(r)[(\ln r - \mu_f)^2 + 2(\ln r - \mu_f)(\mu_f - \mu_g) + (\mu_f - \mu_g)^2]dr$$

$$= \frac{1}{2\sigma_g^2}[\int_R f(r)(\ln r - \mu_f)^2 + 2(\mu_f - \mu_g)\int_R f(r)(\ln r - \mu_f) + (\mu_f - \mu_g)^2\int_R f(r)]dr$$

Due to the constraints $\int_R f(r)dr = 1$ and $\int_R f(r)\ln r dr = E(\ln r) = \mu$,

the second term in the above equation is equal to zero and the remaining terms can be simplified considering that $E[(\ln r - \mu)^2] = \int_0^R f(r)(\ln r - \mu)^2 = \sigma^2$ to:

$$= \frac{1}{2\sigma_g^2}[\sigma_f^2 + (\mu_f - \mu_g)^2]$$

Then, Eq. (A-2-4) becomes

$$\frac{1}{2\sigma_g^2}[\sigma_f^2 + (\mu_f - \mu_g)^2] + \mu_f + \ln\sigma_g\sqrt{2\pi}$$

Finally, KLD can be expressed as

$$KLD = -H[f(r)] + \frac{1}{2\sigma_g^2}[\sigma_f^2 + (\mu_f - \mu_g)^2] + \ln\sigma_g\sqrt{2\pi}$$

$$KLD = -\mu_f - \frac{1}{2} - \frac{1}{2}ln\,2\pi\sigma_f^2 + \frac{1}{2\sigma_g^2}[\sigma_f^2 + (\mu_f - \mu_g)^2] + ln\,\sigma_g\sqrt{2\pi}$$

$$KLD = ln\,\sigma_g - ln\,\sigma_f - \frac{1}{2} + \frac{1}{2\sigma_g^2}[\sigma_f^2 + (\mu_f - \mu_g)^2] \qquad \text{A-2-5}$$

where Eq. (A-2-5) is Eq. (2-9) in the body of the Dissertation, except for symbols *g* and *f* which are replaced by the symbols R and s, respectively.

Appendix B

Details on Statistical Results on New Jersey Data Set

B-1 Kosugi (1996) lognormal water retention curves fitting parameters for soil of New Jersey set, Hayashi et al. (2006), and Tuli et al. (2005).

		For undisturbed soils					For disturbed soils				
		θ_s, g/g	θ_r, g/g	ψ_m, - kPa	σ	r^2	θ_s, g/g	θ_r, g/g	ψ_m, - kPa	σ	r^2
Freehold	Golf course	0.344	0.063	9.210	1.693	0.996	0.362	0.057	15.701	1.651	0.991
	Forest	0.330	0.054	11.715	2.087	0.981	0.418	0.028	24.126	2.499	0.984
	Agriculture	0.333	0.041	6.331	1.532	0.989	0.331	0.032	12.569	1.622	0.982
Quakertown	Restored site	0.293	0.040	449.311	4.466	0.947	0.457	0.082	36.616	2.766	0.995
	Forest	0.440	0.059	99.711	3.070	0.978	0.524	0.059	37.480	2.751	0.988
	Agriculture	0.292	0.044	96.836	3.637	0.981	0.450	0.060	24.436	2.795	0.992
Sassafras	Golf course	0.322	0.054	31.751	2.804	0.984	0.414	0.051	23.932	2.403	0.989
	Agriculture	0.223	0.046	15.836	2.348	0.979	0.311	0.030	17.227	2.561	0.987
Hayashi et al. (2006)	R1 site	0.497	0.145	1.736	1.789	0.990	0.475	0.137	3.824	1.254	0.990
	R2 site	0.510	0.215	5.474	1.509	0.976	0.503	0.155	8.457	1.863	0.986
	R3 site	0.474	0.203	6.672	2.444	0.981	0.504	0.123	14.620	2.245	0.983
	R4 site	0.568	0.200	2.964	1.702	0.980	0.491	0.144	9.607	1.528	0.995
Tuli et al. (2005)	25cm depth	0.402	0.229	50.505	1.117	0.998	0.446	0.193	59.135	1.071	0.988
	50cm depth	0.419	0.202	52.054	1.022	0.998	0.456	0.179	49.724	1.139	0.984

B-2 Physical, chemical, and hydraulic properties by size class on soils of New Jersey set.

	Size class	N	Mean	Std. Error	95% Confidence Interval for Mean		Minimum	Maximum
					Lower Bound	Upper Bound		
Sand	1-2mm	11.00	72.62	2.22	67.68	77.57	62.10	85.91
	2-5mm	7.00	24.43	1.21	21.46	27.39	21.00	27.00
	5-10mm	10.00	22.75	2.25	17.65	27.85	14.50	29.00
	10-20mm	38.00	44.45	3.50	37.36	51.54	16.50	74.00
	20-50mm	16.00	57.28	3.55	49.72	64.84	39.00	73.00
	6.00	14.00	41.89	4.45	32.29	51.50	25.00	69.50
	Total	96.00	45.72	2.19	41.38	50.07	14.50	85.91
Silt	1-2mm	11.00	19.31	1.64	15.65	22.97	8.92	28.51
	2-5mm	7.00	44.29	2.93	37.12	51.45	36.00	50.50
	5-10mm	10.00	53.15	1.80	49.08	57.22	45.00	57.50
	10-20mm	38.00	35.95	2.51	30.86	41.04	13.00	62.00
	20-50mm	16.00	20.88	1.49	17.71	24.04	15.00	29.00
	6.00	14.00	42.07	3.48	34.56	49.58	21.00	57.00
	Total	96.00	34.82	1.59	31.66	37.98	8.92	62.00
Clay	1-2mm	11.00	8.07	0.86	6.14	9.99	3.12	12.30
	2-5mm	7.00	31.29	4.14	21.15	41.42	22.50	43.00
	5-10mm	10.00	23.95	1.65	20.22	27.68	16.50	28.00
	10-20mm	38.00	19.45	1.37	16.68	22.22	9.00	35.50
	20-50mm	16.00	22.00	2.28	17.13	26.87	11.00	32.50
	6.00	14.00	15.93	1.28	13.16	18.70	9.00	21.00
	Total	96.00	19.39	0.94	17.52	21.26	3.12	43.00
θs	1-2mm	11.00	0.54	0.04	0.46	0.62	0.31	0.66
	2-5mm	7.00	0.36	0.03	0.28	0.43	0.28	0.51
	5-10mm	10.00	0.39	0.04	0.30	0.48	0.26	0.63
	10-20mm	38.00	0.30	0.01	0.28	0.33	0.17	0.50
	20-50mm	16.00	0.30	0.01	0.27	0.33	0.21	0.40
	6.00	14.00	0.37	0.02	0.32	0.42	0.22	0.45
	Total	96.00	0.35	0.01	0.33	0.37	0.17	0.66
θr	1-2mm	11.00	0.18	0.02	0.13	0.23	0.06	0.28
	2-5mm	7.00	0.03	0.01	0.01	0.05	0.00	0.06
	5-10mm	10.00	0.06	0.01	0.03	0.09	0.00	0.12
	10-20mm	38.00	0.06	0.01	0.04	0.08	0.00	0.31
	20-50mm	16.00	0.05	0.01	0.04	0.07	0.00	0.11
	6.00	14.00	0.19	0.03	0.12	0.25	0.00	0.34
	Total	96.00	0.09	0.01	0.07	0.11	0.00	0.34
r_m	1-2mm	11.00	78.20	17.82	38.49	117.92	12.11	190.10
	2-5mm	7.00	7.11	4.57	-4.06	18.29	0.78	34.21

	5-10mm	10.00	5.45	1.37	2.34	8.55	0.49	11.34
	10-20mm	38.00	14.82	3.27	8.19	21.45	0.09	101.39
	20-50mm	16.00	16.33	3.08	9.76	22.90	0.51	34.26
	6.00	14.00	9.07	1.73	5.33	12.81	0.69	22.79
	Total	96.00	19.96	3.27	13.47	26.44	0.09	190.10
	1-2mm	11.00	1.82	0.13	1.53	2.10	1.28	2.52
	2-5mm	7.00	2.96	0.20	2.48	3.45	2.26	3.73
	5-10mm	10.00	3.40	0.32	2.67	4.14	2.02	4.77
σ	10-20mm	38.00	2.67	0.23	2.21	3.14	0.88	6.23
	20-50mm	16.00	2.80	0.33	2.11	3.50	1.18	5.00
	6.00	14.00	1.19	0.13	0.90	1.47	0.28	1.91
	Total	96.00	2.48	0.13	2.22	2.74	0.28	6.23
KLD	1-2mm	11.00	100.39	22.34	50.62	150.16	13.37	243.34
	2-5mm	7.00	191.87	43.08	86.46	297.27	103.79	387.16
	5-10mm	10.00	181.34	23.83	127.43	235.25	110.85	309.08
	10-20mm	38.00	178.73	13.00	152.38	205.08	62.86	331.03
	20-50mm	16.00	270.09	36.24	192.85	347.33	121.29	573.32
	6.00	14.00	214.17	49.78	106.64	321.70	48.08	713.08
	Total	96.00	191.38	12.36	166.85	215.91	13.37	713.08
K_{sat}	1-2mm	11.00	4033.82	1479.27	737.80	7329.85	479.52	14312.00
	2-5mm	7.00	386.45	170.37	-30.41	803.32	25.06	868.32
	5-10mm	10.00	305.60	65.88	156.57	454.62	63.07	571.97
	10-20mm	35.00	185.03	24.17	135.90	234.15	6.05	468.29
	20-50mm	16.00	125.12	25.52	70.72	179.52	16.42	298.94
	6.00	14.00	44.64	11.03	20.80	68.48	1.88	110.68
	Total	93.00	636.95	212.93	214.06	1059.83	1.88	14312.00
OM	1-2mm	10.00	3.06	1.22	0.29	5.82	0.00	9.00
	2-5mm	7.00	5.92	1.83	1.44	10.39	2.00	11.00
	5-10mm	10.00	2.70	0.64	1.26	4.15	0.00	5.00
	10-20mm	38.00	1.07	0.13	0.82	1.33	0.00	3.00
	20-50mm	16.00	0.66	0.06	0.55	0.78	0.00	1.00
	6.00	14.00	2.40	0.77	0.73	4.06	1.00	8.00
	Total	95.00	1.94	0.27	1.41	2.46	0.00	11.00
CEC	1-2mm	3.00	18.20	0.00	18.20	18.20	18.00	18.00
	2-5mm	7.00	17.44	4.33	6.84	28.05	8.00	30.00
	5-10mm	10.00	10.30	0.47	9.23	11.36	8.00	12.00
	10-20mm	36.00	6.85	0.32	6.21	7.50	2.00	10.00
	20-50mm	16.00	7.44	0.42	6.56	8.33	5.00	10.00
	6.00	3.00	17.35	0.00	17.35	17.35	17.00	17.00
	Total	75.00	9.30	0.62	8.06	10.54	2.00	30.00
pH	1-2mm	3.00	6.28	0.00	6.28	6.28	6.00	6.00
	2-5mm	7.00	5.82	0.24	5.24	6.40	5.00	6.00
	5-10mm	10.00	5.28	0.19	4.86	5.70	4.00	6.00

10-20mm	36.00	5.62	0.19	5.24	6.00	4.00	7.00
20-50mm	16.00	6.30	0.18	5.92	6.68	5.00	7.00
6.00	3.00	6.28	0.00	6.28	6.28	6.00	6.00
Total	75.00	5.79	0.11	5.57	6.01	4.00	7.00

Appendix C

Statistical Summary of the US National Pedon Characterization Database by Texture, Structure Type, and Size Class

C-1 Correlation coefficients among physical properties, estimated parameters of water retention curve, and KLD of the US National Pedon Characterization database.

	BD	Clay	log OM	W33	W1500	K_{sat}	θs	θr	r_s	σ_s	log KLD
BD	1	.113**	-.492**	-.287**	-0.016	-.475**	-.823**	-.274**	-.156**	.284**	-0.037
Clay		1	.192**	.514**	.787**	-.718**	.320**	.551**	-0.045	.418**	.526**
Log OM			1	.298**	.207**	0.012	.495**	.255**	.082**	-0.048	.177**
W 33				1	.701**	-.391**	.651**	.615**	.556**	-.093**	.200**
W 1500					1	-.567**	.476**	.709**	-0.005	.462**	.538**
Averaged K_{sat}						1	.147**	-.300**	-0.03	-.279**	-.371**
θs							1	.633**	.321**	-.172**	.214**
θr								1	.342**	-.095**	.347**
r_s									1	-.672**	-.287**
σ_s										1	.480**
Log KLD											1

** Significant at the 0.01 probability level.

C-2 Kruskal Wallis test of physical, chemical, and hydraulic properties on soil texture as grouping variable

	BD	Clay	Silt	Sand	Log KLD	Averaged K_{sat}	W33	W1500	Log OM	θ_s	θ_r	ψ_m	σ
Chi-Square	206.563	937.036	1274	1300	481.674	516.412	747.041	780.94	158.172	456.144	632.315	402.888	298.618
df	10	10	10	10	10	10	10	10	10	10	10	10	10
Asymp. Sig.	0	0	0	0	0	0	0	0	0	0	0	0	0

C-3 ANOVA statistical test of physical, chemical, and hydraulic properties by shape class

		Sum of Squares	df	Mean Square	F	Sig.
Clay	Between Groups	1405.97	3	468.657	4.382	0.004
	Within Groups	156573.544	1464	106.949		
	Total	157979.514	1467			
Silt	Between Groups	22465.777	3	7488.592	16.085	0
	Within Groups	681579.187	1464	465.56		
	Total	704044.964	1467			
Sand	Between Groups	28947.118	3	9649.039	13.858	0
	Within Groups	1019385.129	1464	696.301		
	Total	1048332.247	1467			
Log OM	Between Groups	52.559	3	17.52	97.39	0
	Within Groups	262.463	1459	0.18		
	Total	315.022	1462			
BD	Between Groups	3.24	3	1.08	25.406	0
	Within Groups	62.23	1464	0.043		
	Total	65.47	1467			
Averaged K_{sat}	Between Groups	13.713	3	4.571	12.469	0
	Within Groups	496.723	1355	0.367		
	Total	510.435	1358			
W33	Between Groups	987.83	3	329.277	3.591	0.013
	Within Groups	134228.607	1464	91.686		
	Total	135216.438	1467			
W1500	Between Groups	721.528	3	240.509	6.383	0
	Within Groups	55160.308	1464	37.678		
	Total	55881.835	1467			
θ_s	Between Groups	0.089	3	0.03	9.867	0
	Within Groups	4.424	1464	0.003		
	Total	4.513	1467			
θ_r	Between Groups	0.001	3	0	0.419	0.739
	Within Groups	0.854	1464	0.001		
	Total	0.854	1467			
ψ_m	Between Groups	309306.397	3	103102.132	2.457	0.061
	Within Groups	61440000	1464	41970.042		
	Total	61750000	1467			
σ	Between Groups	1.484	3	0.495	3.564	0.014
	Within Groups	203.202	1464	0.139		
	Total	204.686	1467			
Log KLD	Between Groups	1.505	2	0.753	0.86	0.424
	Within Groups	1282.738	1465	0.876		
	Total	1284.243	1467			

C-4 ANOVA statistical test of physical, chemical, and hydraulic properties by shape class Size

		Sum of Squares	df	Mean Square	F	Sig.
Clay	Between Groups	345.915	2	172.957	1.607	0.201
	Within Groups	157633.6	1465	107.6		
	Total	157979.514	1467			
Silt	Between Groups	39.983	2	19.992	0.042	0.959
	Within Groups	704004.981	1465	480.549		
	Total	704044.964	1467			
Sand	Between Groups	543.903	2	271.952	0.38	0.684
	Within Groups	1047788.344	1465	715.214		
	Total	1048332.247	1467			
Log OM	Between Groups	4.127	2	2.064	9.692	0
	Within Groups	310.895	1460	0.213		
	Total	315.022	1462			
BD	Between Groups	0.821	2	0.41	9.297	0
	Within Groups	64.649	1465	0.044		
	Total	65.47	1467			
Averaged K_{sat}	Between Groups	2.853	2	1.427	3.811	0.022
	Within Groups	507.582	1356	0.374		
	Total	510.435	1358			
W33	Between Groups	134.054	2	67.027	0.727	0.484
	Within Groups	135082.383	1465	92.206		
	Total	135216.438	1467			
W1500	Between Groups	25.061	2	12.53	0.329	0.72
	Within Groups	55856.775	1465	38.127		
	Total	55881.835	1467			
θ_s	Between Groups	0.039	2	0.019	6.381	0.002
	Within Groups	4.474	1465	0.003		
	Total	4.513	1467			
θ_r	Between Groups	0.003	2	0.002	2.845	0.058
	Within Groups	0.851	1465	0.001		
	Total	0.854	1467			
ψ_m	Between Groups	109603.115	2	54801.558	1.302	0.272
	Within Groups	61640000	1465	42077.71		
	Total	61750000	1467			
σ	Between Groups	0.146	2	0.073	0.523	0.593
	Within Groups	204.54	1465	0.14		
	Total	204.686	1467			
Log KLD	Between Groups	1.505	2	0.753	0.86	0.424
	Within Groups	1282.738	1465	0.876		
	Total	1284.243	1467			

Curriculum Vita

Sung Won Yoon

Education

2009 Rutgers, the State University of New Jersey, New Brunswick, New Jersey
Ph.D. in Environmental Sciences
2001 Illinois Institute of Technology, Chicago, Illinois
M.E in Environmental Engineering
1997 Hanyang University, Seoul, Korea
M.S. in Environmental Sciences
1995 Soonchunghyang University, Asan, Korea
BS in Environmental Health Science

Principal Occupations and Positions

Jan 2003 to December 2008 Graduate assistant, The Graduate School-New Brunswick, Rutgers University
Jun 2005 to August 2007 soil testing laboratory, New Jersey Agricultural Experiment Station, Rutgers, The state University of New Jersey
August 2004 to May 2005 Environmental and Occupational Health Sciences Institute, A Joint Institute of Rutgers and University of Medicine and Dentistry of New Jerse

Publication

Kim, Y., T. Lee, S.W. Yoon, 1996. "Developing of Emergency Medical Transportation System using GIS", J. Korean Public Health Assoc. 22: 193-203.
Chun, H.C., D. Gimenez, and S.W. Yoon (2008), "Properties of Intraggregate Pores: Aggregate Size and Soil Management Effects", Geoderma 142:83-93.
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