QUANTIFICATION OF SOIL MACROPORE NETWORK AND ITS RELATIONSHIP TO PREFERENTIAL FLOW USING COMBINED X-RAY COMPUTED TOMOGRAPHY AND BREAKTHROUGH CURVE ANALYSIS

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by
Lifang Luo

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The dissertation of Lifang Luo was reviewed and approved* by the following:

Hangsheng Lin  
Associate Professor of Hydropedology / Soil Hydrology  
Dissertation Advisor  
Chair of Committee

Daniel D. Fritton  
Professor Emeritus of Soil Physics

Mary Ann Bruns  
Associate Professor of Soil Science / Microbial Ecology

John P. Schmidt  
Adjunct Associate Professor of Soil Science, USDA-ARS

Kamini Singha  
Assistant Professor of Hydrogeology

Phillip Halleck  
Associate Professor of Energy and Mineral Engineering

David M. Sylvia  
Professor of Microbial Ecology  
Head of the Department of Crop and Soil Sciences

*Signatures are on file in the Graduate School
ABSTRACT

One of the unresolved challenges in soil physics/hydrology is to quantify soil structure, especially macropore characteristics, in a manner that can be implemented into current flow and transport models. The goal of this study is to characterize, visualize, and quantify soil macropore characteristics and their relationships to preferential water flow and chemical transport in intact structured soils. Two soils (Hagerstown silt loam and Morrison sand) with contrasting texture/structure and two land uses (cropland and pasture) were investigated through a combined X-ray computed tomography (CT) and solute breakthrough experiments using relatively large intact soil columns (102 mm in diameter and about 350 mm in length).

Five contributions are made in this dissertation. Firstly, an improved protocol is introduced to quantify 3-D macropore networks. Important macropore characteristics were quantified, including macroporosity along soil depth, macropore network density, macropore size distribution, surface area, macropore length density, length distribution, mean hydraulic radius, tortuosity, inclination or angle, and connectivity (i.e., pathway and node density). The approach developed in this study quantified the distinct morphological features of macropore networks in two soil types and two land uses.

The second contribution presented in this dissertation is the understanding of the variation of macropore characteristics in different types of soils and land uses and with soil depth. Within the same soil type, the soils with pasture land use had greater macroporosity, pore length density, and node density, especially in the subsoil. Within the same land use, the Morrison sand displayed fewer macropores and weaker structure than the Hagerstown silt loam. The macropores in the subsurface (i.e., Ap2 and Bt horizons) were less tortuous, more vertically oriented, and less interconnected than the macropores in the Ap1 horizon. The analysis of variance indicated that a
combination of soil type and land use needs to be considered to evaluate the variation of the macropore characteristics. Such results contribute to the enhanced evaluation of preferential flow and transport potential in soils under different land uses.

The third contribution of this dissertation is the development of the quantitative relationships between macropore characteristics and soil hydraulic parameters (i.e., saturated hydraulic conductivity and hydrodynamic dispersion). For the soil columns taken from the Hagerstown silt loam with two types of land uses (i.e., crop and pasture), saturated hydraulic conductivity (Ksat) of each soil horizon and of the whole column were measured and the breakthrough curve (BTC) for CaBr$_2$ was determined. For all the soil columns with two land uses, macroporosity and path (i.e., the number of independent paths between two ends of the soil volume) explained 75% of the variation in Ksat. Within each land use, macroporosity, path, and tortuosity were the most important characteristics to estimate Ksat of the horizon but with different rank of importance. The path, hydraulic radius, and the angle explained 97% of the variation in the dispersion coefficient of all the soil columns. Additionally, the good correlation between the hydrodynamic dispersion and Ksat of the Bt horizon implied that the hydrodynamic dispersion was mainly controlled by the horizon with the lowest conductivity.

The fourth contribution of this dissertation is the examination of the lacunarity to test if macropore networks and flow patterns are fractal and if lacunarity has a diagnostic value in characterizing soil macropore structure and preferential flow pattern where fractal dimension alone could not. Relative lacunarity functions (RLFs) and pore fractal dimensions, both in 2-D and 3-D, were calculated for the macropore networks and tracer distributions at the five positions in the soil column scanned with a micro-CT. The lacunarity function reflected the size distribution of macropores and the spatial pattern of flow and transport. The RLFs indicated that the tracer distributions exhibited more self-similarity than the macropore networks. Lacunarity is
a potentially powerful parameter that may be coupled with the fractal dimension to better describe and model soil structural properties.

The fifth contribution of this dissertation is a simplified method to quantify soil structure (i.e., porosity) and preferential water flow and solute transport (i.e., the velocity, solute mass, and concentration) in the soil macropore domain, matrix domain, and their interface. The voxel-based soil porosity and solute tracer concentration, mass, and velocity were quantified using micro X-ray CT and digital radiograph in an intact soil column (10 cm in diameter and 30 cm in length) of a Hagerstown silt loam. Only part of the macropores, especially the highly continuous biogenetic macropores at the subsurface, were active in transporting the solute. This study illustrates that preferential flow pathways in the intact structured soil consist of a complex network of earthworm burrows, root channels, inter-aggregate macropores, and mesopores or even micropores in the soil matrix. Modeling of this flow network and its dynamics would require a new approach different from the classical continuous-domain approach.
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I dedicate this dissertation to my husband,

Shuangcai Li.
Chapter 1

INTRODUCTION

Preferential flow and transport

It is recognized that preferential flow and transport phenomena caused by macropores are ubiquitous in soils (Clothier et al., 2008). The value of preferential flow and transport to various global ecosystem services is estimated to be about US$ 304 billion per year (Clothier et al., 2008). Among these ecosystem services, the negative effect of preferential flow and transport on water quality has received great attention, because contaminants can bypass a large portion of the soil matrix in the vadose zone and quickly reach water bodies, causing water pollution. In addition, preferential flow also influences the residence time for nitrate, contaminants, and other substances in soils and the availability of soil water for plants.

The classical Darcy’s approach to uniform flow through porous media does not adequately describe preferential flow processes. It is recognized that preferential flow is scale-dependent and its physical basis and mathematical descriptions vary from micro- to macro-scale (Hendrickx and Flury, 2001; Lin et al., 2005). To properly describe preferential flow at the macro-scale, the pore to pedon scale preferential flow mechanisms and their quantitative relationship with soil structure are critically needed.

To accurately predict preferential flow and transport, the physical non-equilibrium processes (i.e., different advective solute transport velocity and concentration in the macropore and matrix domains) have to be considered (Köhne et al., 2005). A variety of models have been developed to describe the physical non-equilibrium processes. However, the parameterization of these models is still challenging. It is generally time-consuming and costly to experimentally measure the hydraulic parameters for various structured soils.
The quantitative relationships between soil structure, especially macropores and preferential flow and solute, have not been firmly established, partially because of the lack of an effective approach to quantify soil structure. Traditional methods such as in situ morphological descriptions by pedologists the quantification of water-stable aggregates by soil physicist cannot provide an adequate surrogate for undisturbed structure (Young et al., 2001). Instead of the solid, pore space (especially the macropores) is believed to be a main control on preferential flow and transport. Lin et al. (2005) have proposed that soil structure should encompass both pedality (i.e., natural aggregation) and pore space. In this study, I have used the macropore characteristics to represent soil structure.

Similarly, destructive methods combined with various dye tracers (Feyen et al., 1998) and indirect methods considering the soil as a “black-box” and collecting leachate (Schmidt and Lin, 2008) have been used to investigate preferential flow. These methods, however, can not offer detailed information regarding flow and transport pathways and patterns, their spatial-temporal organizations, and their direct relationship with soil structural features.

Recent advances in computed tomography (CT) provide a promising tool to non-invasively observe soil structure (Gantzer et al., 2002) and solute transport in real-time (Anderson et al., 1992; Perret et al., 2000). In spite of an impressive body of CT literature, few studies have quantitatively described soil structure, especially macropore geometry and topology, and linked them to the hydraulic properties.

Soil type and land use are among the main factors controlling soil properties and their hydraulic functions (Zhou et al., 2008; Gantzer and Anderson, 2002). Characterization, visualization, and quantification of 3-D macropore networks and preferential flow and transport with different types of soils and land uses are essential to developing quantitative relationships between soil macropore characteristics and soil hydraulic properties, which will improve our ability to predict flow and transport in structured soils.
Goal, objective, and significance

The goal is to characterize, visualize, and quantify soil macropore characteristics and preferential flow and transport and develop quantitative relationships between macropore characteristics and preferential flow and transport in intact large soil columns.

Advanced computed tomography (CT) was coupled with classical breakthrough experiments to determine the impacts of soil types and land uses on macropore characteristics and preferential flow. The specific objectives are:

1) Quantify 3-D macropore network including macroporosity (along depth), macropore network densities, macropore size distribution, surface area, macropore length density, length distribution, mean hydraulic radius, tortuosity, inclination (i.e., angle) and connectivity (i.e., path and node density);

2) Evaluate the effects of soil type, land use, and horizonation on the macropore characteristics;

3) Quantify the parameters of preferential water flow and solute transport and develop quantitative relationships between the macropore characteristics and hydraulic properties;

4) Evaluate the fractal dimension and lacunarity to characterize the macropores and solute distribution;

5) Quantify preferential water flow and solute transport (e.g., velocity, solute mass, and concentration) in real-time in soil macropore domain, matrix domain, and their interface using an industrial CT.

Overall, this thesis research will enhance our understanding of fundamental processes and quantitative descriptions for predicting preferential flow and transport. It also has the potential to shed light on hillslope hydrology and other fields associated with preferential flow phenomena.
Chapter description

This dissertation is divided into the following six chapters in addition to this introductory first chapter:

- Chapter 2 introduces our protocol to quantify soil macropores with X-ray CT images and evaluates the effect of land use and soil types on soil macropore properties.
- Chapter 3 analyzes the variation of macropore characteristics along the depth with different types of soil and land use and develops pedetransfer functions for soil macropore characteristics using other more readily available soil properties such as soil bulk density, organic matter, and soil texture.
- Chapter 4 links the macropore characteristics and other more basic soil properties to Ksat and solute transport parameters and identifies the most important macropore characteristics influencing the structured soil hydraulic functions.
- Chapter 5 characterizes soil macropore network and solute distribution patterns in real-time along soil depth using fractal dimensions and examines if macropore networks and flow patterns are fractal and if lacunarity has a diagnostic value in characterizing soil macropore structure and preferential flow pattern where fractal dimension alone could not. This chapter has been published (Luo L.F. and H. Lin. Fractal and lacunarity analysis on soil macropore and preferential flow using micro X-ray computed tomography. Vadose Zone Journal, In press)
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Chapter 2

QUANTIFICATION OF 3-D SOIL MACROPORE NETWORKS IN DIFFERENT SOIL TYPES AND LAND USES

Abstract

The importance of soil macropores as preferential pathways for water, air, and chemical movement in different soils has been widely recognized. However, quantification of complex macropore structures and their relations to soil types and land uses remains elusive. The objectives of this study were to 1) quantify 3-D macropore networks using an improved method and 2) investigate the effects of soil type and land use on soil macropore characteristics. Two soils with contrasting textures and structures (Hagerstown and Morrison soil series) and two agricultural land uses (crop and pasture) were investigated. Five soil columns, 102 mm in diameter and about 350 mm in length, were taken for each soil type-land use combination. The soil columns were scanned using X-ray computed tomography (CT). After reconstruction, important characteristics of macropore networks were quantified, including macroporosity change with depth, macropore network density, macropore size distribution, and surface area. After skeletonization of macropores, macropore length density, length distribution, mean hydraulic radius, tortuosity, inclination (angle), and connectivity (path and node density) were also calculated. The approach developed in this study provided a means of quantifying soil macropores with different features. The analysis of variance indicated that soil type, land use, and their interaction influenced macroporosity, macropore network density, surface area, length density, node density (interconnectivity), and mean angle. The interaction of soil type and land use also influenced mean tortuosity and hydraulic radius. Within the same soil type, the soils with pasture land use had greater macroporosity, pore length density, and node density, especially in
the subsoil. This was due to greater organic matter content and more biota activity in pasture land use. Within the same land use, the Morrison sand displayed fewer overall macropores and weaker structure than the Hagerstown silt loam because of considerable amount of rock fragments. Such results contribute to the enhanced evaluation of quantitative soil structure and preferential flow potential in different soils and under different land uses.
Introduction

The importance of macropores as preferential pathways of water, air, and chemicals in the soil has been widely recognized (Jarvis, 2007). The macropore conductivity strongly depends on its 3-D geometry and topology. The macroporosity, the number of macropores, pore length, pore size distribution, continuity, tortuosity, and connectivity are considered as the most important characteristics that influence water flow and solute transport (Perret et al., 2000; Pierre et al., 2002; Bastardie et al., 2003; Peth et al., 2008).

Soil type and land use are among the main factors controlling soil properties. The macropore characteristics can be significantly different with different soil types and land uses (Zhou et al., 2008; Gantzer and Anderson, 2002; Udawatta et al., 2008, Mooney and Morris, 2008). The investigation of macropores with different soil type-land use combinations is fundamental to evaluate preferential flow potential (Jarvis, 2007). Generally, there are three main types of macropores: 1) biopores created by burrowing animals (such as earthworms) and root penetration and decay, 2) fissures formed by wetting and drying or freezing and thawing, and 3) irregular inter-aggregate pores. These three types of macropores have distinct geometries and therefore function differently (Luo et al., 2008).

Reconstruction, visualization, and quantification of 3-D macropore networks are essential to correlating macropore characteristics to their physical, chemical, and biological functions and to predicting their dynamics under different land uses. The tradition methods, such as thin-section (Schaap and Lebron, 2001), have limited ability to observe 3-D macropore geometry and topology. With advances in imaging techniques, X-ray CT has become an attractive technology for nondestructively observing soil structure including pore space (Anderson et al., 1990; Perret et al., 1999, 2000; Luo et al., 2008). Gantzer and Anderson (2002) studied the differences in macropore number, area, perimeter, and fractal dimension in 2-D between chisel till and no-till
soils after tillage operation and found that chisel till soil had greater macropore number, area, perimeter, and fractal dimension than no-till soil. Udawatta et al. (2008) showed that 2-D soil pore space, especially macropores, was influenced by different types of land use and management (i.e., crop, grass, agroforestry). These investigations on 2-D macropore characteristics have provided important information for enhanced understanding of soil structures. However, macropores are 3-D in reality. Therefore, it is essential to evaluate macropore features in 3-D.

Although 3-D visualization of macropores has been realized with algorithms that synthesize 2-D CT images (Joschko et al., 1993; Heijs et al., 1995; Mooney and Morris., 2008), the quantification of 3-D macropores is still a challenge. Various approaches have been used to quantify macropore geometry and topology. Mathematical morphology (Serra, 1982) has been used to quantify the characteristics of 3-D earthworm burrows using X-ray CT, including pore size distribution, length of each branch, connectivity, branching intensity (Capowiez et al. 1998; Pierret at al. 2002; Bastardie et al. 2003). Perret et al. (1999) developed a 26-neighbor algorithm to reconstruct the 3-D images of soil macropores and calculated the number of macropore network, length, tortuosity, hydraulic radius, the numerical density of networks, and connectivity of macropore networks in intact soil columns. 3DMA (Lindquist, 2002), a software package, has been used to calculate the pore-size distributions, throat-area distributions, effective throat/pore radii ratios and pore tortuosities of macropores (Peth et al., 2008). Despite these investigations, more reliable approaches are still needed to effectively quantify 3-D macropore characteristics based on clear physical definitions, especially the length distribution (including continuity), tortuosity and connectivity.

The objectives of this study were to 1) introduce a protocol to quantify soil macropores with X-ray CT images and 2) evaluate the effect of land use and soil type on soil macropore features. The results, when combined with hydraulic properties, are important to linking macropore characteristics to their hydraulic functions under different land uses.
Methodology

The site and soil sampling

Two soil types, Hagerstown (fine, mixed, semiactive, mesic Typic Hapludalfs) and Morrison (Fine-loamy, mixed, active, mesic Ultic Hapludalfs), with contrasting soil textures and structures, were selected for this study. Hagerstown and Morrison are typical soils in the Ridge and Valley physiographic region of Pennsylvania. To study the effect of land use, two representative agricultural land uses, cropland and pasture, were selected for each soil type. Thus, there were four combinations: Hagerstown-crop (H-C), Hagerstown-pasture (H-P), Morrison-crop (M-C), and Morrison-pasture (M-P). The sandstone-derived Morrison soils had greater sand content and lower silt and clay contents than the limestone-derived Hagerstown (Table 2-1). Both cropland sites had rotation cropping of corn (*Zea mays* L.) and soybean [*Glycine max* (L.) Merr.]. Both pasture sites were grazed by animals (cows and horses).

Five soil columns, 102 mm in diameter and about 350 mm in length, were randomly taken from each site. A backhoe was used to carefully push polyvinyl chloride (PVC) pipe (with downward edge sharpened) vertically and gradually into the soil. Three soil horizons were contained in each soil column (Table 2-1). Besides the large soil columns, three intact small soil cores, 55 mm in diameter and 60 mm in length, were also taken from each horizon to measure soil bulk density and saturated hydraulic conductivity. Disturbed soil samples were also taken from each horizon to determine soil particle size distribution and organic matter content (Table 2-1).
X-ray CT scanning

A HD250 Medical Scanner (Universal system, Inc., Solon, Ohio), a 4th-generation system, was used to scan all the soil columns at an energy level of 130 kV and 100 mA. The 512×512 images with a voxel size of 0.234 mm ×0.234 mm ×2.000 mm were produced. The soil water content influences the shape of X-ray attenuation value histogram and possibly the threshold value to be used to segment the images. Therefore all soil columns were wetted before scanning to reach a relatively consistent moisture content by allowing several pore volumes of water ponded at surface to flow though columns and left to drain for about 3 days. Therefore, soil water content differences among the soil columns studied were minimized.

Data Analyses

Figure 2-1 shows the procedure of image analysis. The images (512 x 512 pixels) were cut to exclude the area outside the soil column using ImageJ version 1.39 (Rasband, 2002). Furthermore, the edge of each soil column was also cut to eliminate the possible artificial features along the edge. The diameter was cut down to 93.7 mm with about 15% of the original cross-sectional area removed. The images were then resampled to 0.3 mm × 0.3 mm × 0.3 mm to make the voxel cubic to facilitate the computation. The Lanczos filter (Meijering et al., 1999), a widely-used resampling protocol, was used to resample all the CT images. I found that macropore surface became much smoother after resampling. This step may improve the image resolution in the depth direction by interpolating between the original images using Lanczos filter (2-mm slide thickness before resampling). Considering the data size and the computation ability of our computer, the cross-sectional resolution was reduced slightly from 0.234 mm to 0.3 mm after resampling. After that, the medium filter, a commonly used image-processing method to reduce the noise while preserving the edge (Jassogne et al., 2007), was used to minimize noise.
The macropore threshold value determined by the maximum entropy threshold algorithm in ImageJ 1.39 was used to segment the images (Jassogne et al., 2007). The threshold value was selected where the inter-class entropy was maximized. The images were also visually inspected to ensure that a reasonable threshold value was used. After segmentation, all macropores < 0.75 mm in equivalent cylindrical diameter (ECD) were removed (Luo et al, 2008).

After all the soil columns were scanned using CT, the images were used to identify the soil columns with obvious disturbance caused during the sampling (e.g., unnatural macropore morphology), such columns were excluded from the study. Such disturbance was more likely in the Morrison soil because of its high amount of rock fragments. Consequently, only four columns each for H-C and H-P, and two columns each for M-C and M-P were selected in the subsequent analysis.

Quantification of 3-D macropore network

After segmentation, the macropore networks were reconstructed and visualized using Avizo version 5 (Mercury Computer Systems, Chelmsford, MA). The overall macroporosity, macroporosity along the column depth, macropore volume >1000 mm$^3$, macropore number, pore size distribution (sorted by volume), mean pore volume, and total surface area were calculated using Avizo version 5.

Reliable approaches are needed to quantify the continuity, tortuosity and connectivity of macropores. Since soil macropores are not linear features but 3-D, 3-D skeletonization of the macropore is necessary to accurately quantify the length measurements in 3-D (Capowiez et al., 1998) (Fig. 2a). This skeletonization is explained in the following: assuming a fire is ignited simultaneously at the solid-void interface in the entire image domain and that it travels with a constant expansion rate into the pore space perpendicular to the void-grain boundary, the set of voxels where two approaching fire fronts meet (here the fire is considered to be extinguished) is
defined as the skeleton (Palagyi, 2002). Despite a volume of literature on quantification of macropores, there are few studies that calculate the macropore length and tortuosity based on the skeleton. Perriet et al. (2002) obtained ultimate eroded points from the 2-D images and then connected the points from the consecutive images to create 3-D skeletons of macropores. This method is problematic to get the skeleton of the pore horizontally orientied. The skeletonization of highly irregular pores may produce noisy skeletons and cause overestimation of the length (Peth et al., 2008). Lindquist (2002) developed a software package, 3DMA, to obtain the skeleton (i.e., medical axis) of the pore space. However, skeletons with dead ends were deleted to eliminate the noise in that programming. Since most macropores may be isolated in large soil columns (Luo et al., 2008), the actual macropore length is likely to be underestimated by 3DMA (Peth et al., 2008).

The skeletons of macropore networks were generated using an algorithm in Avizo 5. After skeletonization, a program was developed in C to track and quantify each macropore network. One macropore network may be one individual macropore or consist of several branches of connected macropores. A node is defined as where two branches of pores are connected (Fig. 2-2). For each macropore network, the actual length of the longest path (Fig. 2-2) and other branches as well as their position (starting and ending points) and the straight-line distance were calculated. The number of nodes in each macropore network was recorded.

The tortuosity ($\tau$) was calculated as the ratio of the actual macropore length ($L_t$) to the straight-line distance ($L_i$) (Fig. 2b):

$$\tau = \frac{L_t}{L_i}$$  \[1\]

Meanwhile, the mean tortuosity ($\bar{\tau}$) was calculated as ratio of the total actual macropore length ($L_t$) to total straight line distance ($L_i$):
The inclination of a macropore was characterized by the angle $\theta$ to vertical direction (Fig. 2b). The mean angle was calculated as:

$$\bar{\theta} = \frac{\sum_{i=1}^{n} L_i \theta_i}{\sum_{i=1}^{n} L_i}$$

[3]

Macropore network density is the number of macropore networks in a unit volume. The length density ($\text{km.m}^{-3}$) is the total actual length of the macropores ($\sum L_i$) in a unit volume. Likewise, the node density (number.m$^{-3}$) is the number of nodes in a unit volume.

Assuming that the macropore is cylindrical, the mean hydraulic radius was calculated by the total volume $V_i$ and total length $L_i$ of macropores:

$$\bar{r} = \sqrt{\frac{V_i}{L_i \pi}}$$

[4]

The macropore length distribution was analyzed using straight-line length of macropores. Besides the actual length and straight-line length, the vertical length of a macropore was considered because it represents the vertical continuity and is important to vertical flow and solute transport along a soil column. Total vertical length of macropores with vertical length $> 150\text{ mm}$ (as well as their tortuosity and angle) and length distribution were analyzed to investigate the properties of highly continuous macropores.

Connectivity is a measure of the number of independent paths between two points in the pore space (Perret et al, 1999). Two factors need to be defined to link the quantified connectivity to its function: 1) pore size, because connectivity is pore size-dependent (generally, the smaller pores, the greater the connectivity for soils) (Vogel, 1998); 2) scale or distance between the two points
(similarly, the shorter the distance, the higher the possibility of more paths). Vogel (1998, 2002) used the Euler-Poincare characteristic (defined as the number of isolated components minus the total number of redundant connections plus the number of enclosed cavities) to calculate the connectivity function. This method is applicable when the pores are well interconnected, especially at small scale of mm. However, at larger scale (cm or larger), most of larger macropores are isolated (Luo et al., 2008; Noguchi et al., 1999) and thus this method is problematic for obtaining connectivity. Perret et al. (1999) calculated the connectivity of individual macropore networks in a soil column. The connectivity of the individual macropore network did not offer enough information to evaluate its effect on the function of the entire soil column. In order to quantify the paths through the entire soil column and inter-connectivity of macropores, the number of independent paths between two ends of the entire soil column (Fig.2c) and the node density were calculated.

Statistics

All statistical analyses were performed using Minitab (Minitab Inc., State College, 2008). The assumption of homogeneity of variance was made. Since the numbers of replicates were not the same for different soil type-land use combinations, the significance tests for the effects of soil type, land use, and their interaction were performed using the Analysis of Variance (ANOVA) within the General Linear Model (GLM) procedure. The option (TUKEY) was selected for multiple mean comparison of soil macropore characteristics.
Results and discussion

Visualization of macropore networks

Three-dimentional visualizations of macropores in the 12 soil columns studied are showed in Figs. 2-3 and 2-4. Macropore characteristics were distinctly different among the different soil type-land use combinations. Different types of macropores could be observed. The macropores formed by earthworms were highly continuous, relatively large, and tubular. While the macropores formed by roots were also highly continuous and round in shape, they were much smaller and more variable in size. Inter-aggregate macropores, such as those formed by freezing and thawing or wetting and drying, were generally smaller and more randomly and less continuously distributed in the soil columns. The macropores formed by earthworm burrows and roots constituted a significant proportion of the macropore networks of H-C, H-P and M-P (Figs. 2-3 and 2-4). Although the macropores for H-C were not as abundant as those of H-P, the macropores formed by earthworm burrows were more continuous, qualitatively less tortuous and smoother in the surface of H-C. This may be associated with the greater competition among the earthworms in H-P. I observed an earthworm burrow through the whole column in H-C-2 (e.g., the column 2 of cropped Hagerstown). During the soil profile description, I did not observe earthworms at the subsurface of M-C. Thus, the tubular macropores in M-C were likely formed by roots. However, earthworms were observed in M-P during the sampling. Compared with M-C, M-P had greater organic matter content and finer texture (Table 2-1). Many continuous and tubular pores formed by decayed roots of perennial grass were also observed in H-P and M-P. As for M-C, quite a number of macropores at the surface might be cracks caused by the movement of soils and rock fragments during the sampling according to the CT images. The macropores were relatively sparse at the subsurface soil due to the few bio-pores and weak structure.
Quantification of macropore networks

Macroporosity, macropore network density, and total surface area

The macropore characteristics are listed in Table 2-2. The mean macroporosity for H-P was the highest, 0.061, about 2 times of the values of other soil type-land use combinations (0.028 for H-C, 0.024 for M-C, and 0.031 for M-P) (Table 2-2). Figure 2-5 shows the change of the macroporosity with depth. H-P and M-P had a similar pattern in the change of macroporosity with depth (Fig. 2-5). The macroporosity decreased quickly at top 40 mm for H-P and 60 mm for M-P and then increased slowly until about 270-mm depth. The low macroporosity at 40 mm depth for H-P and 60 mm depth for M-P is likely associated with the compaction caused by grazing. The macroporosity with depth were significantly different between H-C and M-C (Fig. 2-5). The finer texture and deep solum of the Hagerstown soil are favorable for earthworms. The organic matter was taken downwards through the earthworm burrows and/or the roots growing along the burrows. Therefore, considerable amount of macroporosity still existed in the subsurface of H-C. On the other hand, Morrison with high sand content, rock fragments, and low organic matter is unfavorable for the growth of earthworms.

The total surface area and macropore network density varied in a similar way as the macroporosity among the different soil type-land use combinations (Table 2-2). The correlation analyses show that the macroporosity, total surface area, and macropore network density, length density, and node density were highly intercorrelated (Table 2-4). The H-P had the greatest total surface area (141,096 mm²) and number of macropore networks (3137) while M-C had the lowest (67,147 mm² for total surface area and 1973 macropore networks).

Pore size distribution and mean macropore size

Figure 2-6 shows the pore size distribution by volume. The pore size distributions with the same soil type-land use were about the same when macropore volume was <100 mm³, and their difference increased with the increase of macropore size (Fig. 2-6). More than 50% of the
macropore volume consisted of macropore volume > 1000 mm$^3$ for all soil columns (55.7% for H-C, 61.7% for H-P, 63.4% for M-C and 55.1% for M-P) (Table 2-2). These large macropores were likely to be biopores. The H-P had the highest macroporosity and largest mean macropore size, 46.3 mm$^3$ on average (Table 2-2). As expected, the greater the macroporosity, the greater chance for macropore to be interconnected and the more macropore networks with larger volume.

Length density and length distribution

The macropore length density was calculated based on the skeleton of macropores (Fig. 2-7). As expected, macropore length density of H-P was the highest, 11.82 km.m$^{-3}$, about twice that of H-C (5.08 km.m$^{-3}$). The macropore length density for M-P and M-C were 4.74 km.m$^{-3}$ and 4.67 km.m$^{-3}$, respectively (Table 2-2). Due to the highly irregular pores at the top of M-C, the skeletons produced might be noisy and cause the overestimation of length density. Generally, length densities of the Hagerstown were greater than those of the Morrison.

The macropores were sorted by the vertical length. The vertical length distributions of the macropores are showed in Fig. 2-8. Although H-C did not have the highest macroporosity, it had the highest total vertical length with macropore vertical length > 90 mm (Fig. 2-8). For example, the mean vertical length with macropore vertical length > 150 mm was the highest for H-C (412 mm), about 1.6 times that of H-P (260 mm) (Table 2-2). On the other hand, M-C had the lowest vertical length with macropore vertical length > 30 mm. No macropore was longer than 150 mm for M-C (Fig. 2-8). The results were consistent with the macropore morphology shown in Figs. 2-3 and 2-4. The highly continuous macropores are potentially active in hydrological processes at near-saturated conditions and critical to preferential flow and transport.

Tortuosity, inclination and connectivity

Mean tortuosity was the lowest for H-C, being 1.53, and gradually increased from M-P (1.62), to H-P (1.75), and to M-C (1.82) (Table 2-2). The highly continuous macropores (i.e., macropore vertical length > 60 mm) of H-C had the mean tortuosity of 1.32-1.34, while that for H-P was 1.50-1.71 and that for M-P was 1.32-1.64. From Figs. 2-3 and 2-4, the highly continuous
macropore could be macropores formed by earthworms, which had relatively low tortuosity. For example, the tortuosity of the earthworm burrow through H-C-2 was about 1.33. Our macropore tortuosity results are greater than that calculated by Perret et al. (1999) (1.12-1.17) and comparable with that of Jassogne et al. (2007) (1.5-2.5).

The macropores of H-C had the smallest mean angle of 33.7°, suggesting the highest degree of vertical inclination due to large proportion of vertically oriented earthworm burrows and roots. The macropores of M-C had much a greater mean angle of 59.7° than any other soil type-land use combination. The mean angles for H-P and M-P were 37.4°and 38.4°, respectively (Table 2-2). Figure 2-10 shows the change of mean angle with macropore vertical length. In general, the macropores with high vertical length tended to have smaller angle.

The node density varied among the soil type-land use combinations in a same way as the macroporosity and macropore length density. The greater macroporosity, the greater node density (i.e., interconnectivity) was. Only H-C-2 had a macropore continuous through the entire column, that is, path = 1. The number of paths for other soil columns was zero.

**The effects of soil type and land use on macropore characteristics**

Within the same soil type, the soils with pasture land use had greater macroporosity, total surface area, macropore network density, pore length density, and node density. Within the same land use, the Morrison sand had lower macroporosity, total surface area, macropore network density, pore length density, and node density. The analysis of variance indicated that the soil type, land use, and their interaction had impacts on macroporosity, total surface area, macropore network density, length density and node density (interconnectivity), and mean angle (inclination), but not on the proportion of macropores with volume > 1000 mm³, path, and the
The greater organic matter content might contribute to the greater abundancy of macropores for the pasture land use. A high positive correlation was found between the organic matter content and the macroporosity of each horizon ($r^2=0.61$). The prennual grass in the pasture land produces abundant living and decayed roots and organic matter in the soils (Table 2-1), which is main resource of food for soil biota. Therefore, there was a high proportion of biopores in the H-P and M-P. The Hagerstown silt loam with finer texture and better soil structure is more favable for plants and soil biota than the Morrison sand. On ther other hand, the Morrison sand displayed fewer overall macropores and weaker structure than the Hagerstown silt loam. The organic matter content for Hagerstown silt loam was also greater than that of Morrison sand (Table 2-1).

The influence of the interaction between soil type and land use on soil macroporosity, surface area, macropore network density, length density and node density (interconnectivity), the mean angle, mean tortuosity and mean hydraulic radius indicated that both soil type and land use need to be considered to investigate the macropore characteristics and their functions (Table 2-3).

**Summary and Conclusion**

Our approach of quantifying macropore structures effectively characterized the distinct macropore morphology shown in 3-D visualizations reconstructed using X-ray computed tomography. The important parameters of macropore networks include macroporosity (along depth), macropore network density, volumetric macropore size distribution, mean hydraulic radius, total surface area, macropore length density, continuity (length >150mm), tortuosity, and connectivity (including path and node density). These were quantified for a total of 12 soil columns with different soil type-land use combinations.
Within the same soil type, the soils with pasture land use had greater macroporosity, pore length density, and pore connectivity, especially the subsurface soil, because of its greater organic matter content and more activity of soil biota. On the other hand, within the same land use, the sandy soils (Morrison) had fewer macropores and weaker structure than the silt loam Hagerstown. Soil type, land use, and their interaction had influences on macroporosity, surface area, macropore network density, length density and node density (interconnectivity), and the mean angle (inclination), but not on proportion of macropore volume >1000 mm³, path, and total vertical length of macropore vertical length > 150 mm. Besides, the interaction of soil type and land use influenced the mean tortuosity and mean hydraulic radius. Consequently, both soil type and land use need to be considered to investigate the macropore characteristics and related functions.

References


Table 2-1 Soil profile description and basic soil properties. The number in parentheses is one standard error.

<table>
<thead>
<tr>
<th>Soil &amp; land use</th>
<th>Horizon</th>
<th>Depth</th>
<th>Pedality (Structure)a</th>
<th>Rootsb</th>
<th>Ksat</th>
<th>Bulk density</th>
<th>sand</th>
<th>silt</th>
<th>clay</th>
<th>OM</th>
<th>Porosityc</th>
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<tbody>
<tr>
<td></td>
<td></td>
<td>cm</td>
<td></td>
<td></td>
<td>cm.min⁻¹</td>
<td>g.cm⁻³</td>
<td>%</td>
<td>%</td>
<td>%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H-C</td>
<td>Ap1</td>
<td>0-15</td>
<td>2 f-m sbk</td>
<td>3 vf-f</td>
<td>0.051 (0.019)</td>
<td>1.34 (0.02)</td>
<td>19</td>
<td>65</td>
<td>16</td>
<td>4.5</td>
<td>0.49</td>
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<tr>
<td></td>
<td>Ap2</td>
<td>15-31</td>
<td>2 m pl parting to 2 m sbk</td>
<td>3 f</td>
<td>0.045 (0.066)</td>
<td>1.35 (0.03)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.49</td>
</tr>
<tr>
<td></td>
<td>Bt1</td>
<td>31-36+</td>
<td>2 m sbk</td>
<td>2 f</td>
<td>0.035 (0.024)</td>
<td>1.46 (0.02)</td>
<td>17</td>
<td>68</td>
<td>15</td>
<td>3.5</td>
<td>0.49</td>
</tr>
<tr>
<td>H-P</td>
<td>A1</td>
<td>0-15</td>
<td>3 f-m gr</td>
<td>3 vf-m</td>
<td>0.206 (0.353)</td>
<td>1.16 (0.01)</td>
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<td>Bt1</td>
<td>32-36+</td>
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<td>2 f</td>
<td>0.074 (0.010)</td>
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<td>1 f</td>
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<td>1.77 (0.04)</td>
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<td>8</td>
<td>9</td>
<td>0.5</td>
<td>0.33</td>
</tr>
<tr>
<td>M-P</td>
<td>A1</td>
<td>0-10</td>
<td>1 f-m sbk</td>
<td>3 vf-m</td>
<td>0.357 (0.104)</td>
<td>1.41 (0.04)</td>
<td>73</td>
<td>18</td>
<td>9</td>
<td>4.3</td>
<td>0.47</td>
</tr>
<tr>
<td></td>
<td>A2</td>
<td>10-20</td>
<td>1 m sbk</td>
<td>2 f</td>
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<td>76</td>
<td>14</td>
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<td>1.2</td>
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<td>Bt1</td>
<td>20-31+</td>
<td>1 m sbk</td>
<td>2 f</td>
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<td>1.69 (0.04)</td>
<td>75</td>
<td>13</td>
<td>12</td>
<td>1.1</td>
<td>0.36</td>
</tr>
</tbody>
</table>

a Pedality is described using ped grade, ped size and ped shape; 1, 2, 3 for weak, moderate, and strong ped grades, respectively; vf, f, m and c for very fine, fine, medium and coarse ped sizes, respectively;

b Roots are described using the quantity and size; 1, 2, 3 for few, common and many, respectively; vf, f, m, c, and vc for very fine, fine, medium, coarse and very coarse root sizes.

c The porosity was calculated from the bulk density (assume particle density to be 2.65 g.cm⁻³).
Table 2-2 The macropore characteristics of all soil columns. The number in parentheses is one standard error.

<table>
<thead>
<tr>
<th>Properties</th>
<th>Macroporosity</th>
<th>Total surface area</th>
<th>POM 1000</th>
<th>Network density</th>
<th>Mean pore size</th>
<th>Length density</th>
<th>Mean Tortuosity</th>
<th>Mean Angle</th>
<th>Path Density</th>
<th>Hydraulic radius</th>
<th>Length 150</th>
<th>Tortuosity 150</th>
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<td>mm²</td>
<td>%</td>
<td>number.m⁻²</td>
<td>mm³</td>
<td>km.m⁻²</td>
<td>degree</td>
<td>degree</td>
<td>number.m⁻²</td>
<td>mm</td>
<td>mm</td>
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<td>5.08</td>
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</table>

* POM1000 was the proportion of macropores with volume > 1000 mm³; † Length 150, tortuosity150, and angle 150 were the total vertical length, mean tortuosity, and mean angle for macropores with vertical length > 150 mm. The lower letters after the parenthesis indicate the significance test of mean difference among the four soil series at p< 0.05.
Table 2-3 The analysis of variance of soil macropore characteristics and the effect of soil type and land use.

<table>
<thead>
<tr>
<th>Effect</th>
<th>Total surface area (mm²)</th>
<th>Macroporosity (m³.m⁻³)</th>
<th>POM1000 £</th>
<th>Network density (number. m⁻³)</th>
<th>Mean pore size (mm³)</th>
<th>Length density (km.m⁻³)</th>
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<tbody>
<tr>
<td></td>
<td>MS</td>
<td>p</td>
<td>MS</td>
<td>p</td>
<td>MS</td>
<td>p</td>
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<td>7.432E-04</td>
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<td>0.000***</td>
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<td>0.008***</td>
<td>134.6</td>
<td>0.235</td>
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<table>
<thead>
<tr>
<th>Effect</th>
<th>Mean tortuosity</th>
<th>Mean Angle (degree)</th>
<th>Path (number)</th>
<th>Node Density (number.m⁻³)</th>
<th>Hydraulic radius (mm)</th>
<th>Length 150 ££ £££</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>MS</td>
<td>p</td>
<td>MS</td>
<td>p</td>
<td>MS</td>
<td>MS</td>
</tr>
<tr>
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<td>0.230</td>
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<td>0.000***</td>
<td>0.042</td>
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<td>0.900</td>
<td>199.8</td>
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<td>0.042</td>
<td>0.524</td>
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<td>Soil*land use</td>
<td>0.114</td>
<td>0.009***</td>
<td>218.4</td>
<td>0.001***</td>
<td>0.042</td>
<td>0.524</td>
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</table>

£POM1000 was the proportion of macropores with volume > 1000 mm³.

£££ Length 150, tortuosity 150, and angle 150 were the total vertical length, mean tortuosity, and mean angle for macropores with vertical length > 150 mm.

MS is the mean square of the effect.

Values of p are indicated using three significance levels (*** p<0.01, ** p<0.05, * p<0.1).
The Pearson correlation coefficients between different macropore characteristics. Values of probability are indicated using three significance levels (** < 0.01, * < 0.05, NS > 0.05).

<table>
<thead>
<tr>
<th>Properties</th>
<th>Total surface area</th>
<th>Macroporosity</th>
<th>POM1000</th>
<th>Network density</th>
<th>Mean pore size</th>
<th>Length density</th>
<th>Mean Tortuosity</th>
<th>Mean Angle</th>
<th>Path</th>
<th>Node Density</th>
<th>Hydraulic radius</th>
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<th>Tortuosity150</th>
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<td></td>
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<td>C2</td>
<td>C3</td>
<td>C4</td>
<td>C5</td>
<td>C6</td>
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<td>C8</td>
<td>C9</td>
<td>C10</td>
<td>C11</td>
<td>C12</td>
<td>C13</td>
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</tr>
<tr>
<td>C6</td>
<td>0.99 (0.00) **</td>
<td>0.96 (0.00)</td>
<td>0.38 (0.22)</td>
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<td>0.82 (0.00)</td>
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<td></td>
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<tr>
<td>C7</td>
<td>0.43 (0.17)</td>
<td>0.43 (0.16)</td>
<td>0.66 (0.02)</td>
<td>*</td>
<td>0.27 (0.41)</td>
<td>0.45 (0.14)</td>
<td>0.50 (0.10)</td>
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<tr>
<td>C8</td>
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<td>0.39 (0.21)</td>
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<td>*</td>
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<td>0.96 (0.00) **</td>
<td>0.91 (0.00)</td>
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<tr>
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<td>0.06 (0.87)</td>
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<td>0.02 (0.96)</td>
<td>0.05 (0.88)</td>
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<td>-0.57 (0.05)</td>
<td>0.64 (0.03)</td>
<td>*</td>
<td>0.24 (0.45)</td>
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<td>0.24 (0.54)</td>
<td>0.32 (0.39)</td>
<td>0.25 (0.52)</td>
<td>0.25 (0.52)</td>
<td>0.18 (0.65)</td>
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<tr>
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<td>-0.09 (0.82)</td>
<td>0.12 (0.76)</td>
<td>-0.09 (0.82)</td>
<td>0.08 (0.83)</td>
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<td>-0.12 (0.75)</td>
<td>0.65 (0.06)</td>
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*POM1000 was the proportion of macropores with volume > 1000 mm³; **Length 150, tortuosity 150, and angle 150 were the total vertical length, mean tortuosity, and mean angle for macropores with vertical length > 150 mm; C14 was angle 150.
Figure 2-1 The procedure used in this study for image analysis and quantification of macropore structure.
Figure 2-2  a) An example of skeleton of a macropore, b) a macropore network with three branches and one node (macropore newwork length was the longest distance through a macropore newwork, i.e., branch 1+ branch 2), and c) a path through soil column (path =1).
Figure 2-3 Three-dimensional visualization of soil macropore networks for the soil columns of cropped Hagerstown (H-C) and pastured Hagerstown (H-P).
Figure 2- 4  Three-dimensional visualization of soil macropore networks for the soil columns of cropped Morrison (M-C) and pastured Morrison (M-P).
Figure 2-5 Macroporosity distribution along the soil column depth for each of the soil type-land use combination.
Figure 2-6 Cumulative pore size distribution (by volume) for each of the soil type-land use combination.
Figure 2-7 Representative skeletons of soil macropore networks.
Figure 2-8  Macropore vertical length distribution.
Figure 2-9 The distribution of mean tortuosity vs macropore vertical length.
Figure 2-10  The distribution of mean macropore angle vs macropore vertical length.
Chapter 3

QUANTIFICATION OF MACROPORE NETWORKS ALONG SOIL DEPTHS AND PEDOTRANSFER FUNCTIONS FOR ESTIMATING MACROPORE CHARACTERISTICS

Abstract

The objectives of this study were to 1) analyze the variation of macropore characteristics with soil depth in different types of soils and land uses and 2) develop pedotransfer functions for estimating macropore characteristics using basic soil properties. Two types of soils with contrasting soil textures and structures (i.e., Hagerstown and Morrison soil series) and two types of representative agricultural land uses (i.e., crop and pasture) were selected for this study. Five soil columns, 102 mm in diameter and about 350 mm in length, were taken for each soil type-land use combination. Three soil horizons (i.e., Ap1 and Ap2 horizons and a Bt horizon) were contained in each soil column. For each horizon, macroporosity, length density, mean tortuosity, network density, hydraulic radius, path, node density, mean angle of the macropores, and length density, tortuosity and angle of the macropores with vertical length > 45 mm were quantified using X-ray computed tomography (CT). The macropores at the subsurface (i.e., Ap2 and Bt horizons) were less tortuous, less inter-connected, and more vertically oriented than the macropores at the Ap1 horizon. The macroporosity, length density, network density, node density, mean tortuosity and fractal dimension were inter-correlated and could be reasonably estimated with soil bulk density and organic matter content. Bulk density explained 61% of the variation in macroporosity and organic matter content explained 60% of that variation. Clay content was positively correlated to macropore path ($r^2=-0.32$, p=0.06) and negatively correlated to mean angle ($r^2=-0.37$, p=0.04). A positive correlation was also found between length density >
45 mm and silt content ($r^2=-0.26$ $p=0.09$). The results suggest that soil texture, especially clay and silt content, influences the macropore inclination, continuity and connectivity.
**Introduction**

Soil macropores play an important role in the movement of air, water, and chemicals and the penetration of roots in the soil (Jarvis, 2007). Although the fractional volume of the macropore is usually small (< 5%), it may have a dramatic effect on water flow and solute transport (Perret et al., 2000).

The variation and spatial organization of macropores with soil depth influence the degree of preferential flow and transport in the soil (Haws and Rao, 2004). If macropores decrease along depth, preferential flow pathways will converge into limited macropores in the deeper soil. Generally, an exponential decrease in macroporosity is assumed (Haws and Rao, 2004). However, the depth function of macroporosity may vary with different types of soils and land uses.

There are few studies on the change of 3-D soil macropore characteristics with depth. The traditional methods have limited ability to observe and quantify macropore structure. Indirect methods have been used to estimate the macroporosity, such as water retention curve (Ersahin, 2002) and tension infiltrometer (Zhou, 2007). Thin-sectioning, though a direct method, is destructive and unsophisticated for reconstructing 3-D macropore geometry (Schaap and Lebron, 2001).

Computed tomography is a nondestructive imaging technique to observe and quantify the macropore network. Not only macroporosity, but other characteristics of macropores can also be computed, such as macropore numbers, macropore size distribution, hydraulic radius, surface area, length density, length distribution, tortuosity, inclination and connectivity. Udawatta et al. (2008) studied the macropore number, macroporosity, mesoporosity, pore circularity and fractal dimension in 2-D at about 5-cm, 15-cm, 25-cm, and 35-cm depths. Asare et al. (2001) studied the change of the macroporosity with depth using CT and found that a decreasing macroporosity with
depth was found only in the A horizon but not in the B horizon. Since the macropores are 3-D in reality, it is essential to evaluate their features in 3-D. Various approaches have been used to quantify macropore geometry and topology, including the mathematical morphology (Serra, 1982; Capowiez et al., 1998; Pierret et al., 2002; Bastardie et al., 2003), a 26-neighbor algorithm (Perret et al., 1999) and 3DMA (Lindquist, 2002; Peth et al., 2008). Despite these investigations, the quantification of 3-D macropores still is a challenge (See Chapter 2).

Pedotransfer functions (PFTs), predicting certain soil properties from other more easily measured properties, have been widely used to estimate soil hydraulic properties with basic soil properties (Lin et al., 1999), especially those available in soil survey databases. However, there are few studies using pedotransfer functions for estimating macropore characteristics from more available soil properties. Since it is laborious and expensive to obtain macropore characteristics, it is desirable to develop PFTs for estimating macropore characteristics using widely available basic soil properties. Such PFTs will facilitate the evaluation of soil quality and the potential of preferential flow.

The objectives of this study were to 1) analyze the variation of macropore characteristics with soil depth in different types of soils and land uses and 2) link soil macropore characteristics to more readily-available basic soil properties such as bulk density, organic matter content, and texture.

Methodology

The site and soil sampling

See Chapter 2
X-ray CT scanning

See Chapter 2

Image Analyses and quantification of 3-D macropore network

See Chapter 2. For each horizon, macroporosity, length density, mean tortuosity, network density, hydraulic radius, path, node density, and mean angle of the macropores as well as length density, tortuosity, and angle of the macropores with vertical length > 45 mm were quantified.

Statistics

Stepwise regression was used to link the macropore characteristics to basic soil properties using Minitab (Minitab Inc, State College, PA). The option of standard stepwise regression combining the backward and forward selection was selected. Alpha was set to 0.15 to enter and remove a variable.

Results and Discussion

Macropore characteristics change with soil depth

Macroporosity

The horizon-based macropore characteristics of all the soil columns are listed in Table 3-1. The macroporosity in the Ap1 horizon was always the highest for all the soil columns. For Morrison cropland (M-C), the macroporosity decreased dramatically (Table 3-1 and Fig.3-1). The horizon-averaged macroporosity were 0.054, 0.009, and 0.006 for the Ap1, Ap2, and Bt horizons, respectively for the M-C? (Fig.3-1). But for other soil type-land use combinations, considerable
amount of macropores existed in the Ap2 and Bt horizons. For the Hagerstown cropland (H-C),
the macroporosity changed slightly (though with variation) with depth. The horizon-averaged
macroporosity were 0.032, 0.025, and 0.024 for the Ap1, Ap2, and Bt horizons, respectively. The
Hagerstown pasture (H-P) and Morrison pasture (M-P) had a similar depth function: both became
relatively low around 40 mm depth and increased slowly until about 270 mm (Fig. 3-1). The
decrease in the macroporosity at 40 mm is likely due to the compaction caused by the grazing.
The horizon-averaged macroporosity of H-P (i.e., 0.066, 0.062, and 0.043 for the Ap1, Ap2, and
Bt horizons, respectively) was about the twice of that of H-C (i.e., 0.032, 0.025, and 0.024 for the
Ap1, Ap2, and Bt horizons, respectively.). For M-P, the horizon-averaged macroporosity were
0.045, 0.025, and 0.023 for the Ap1, Ap2, and Bt horizons, respectively.

**Length density and Length > 45 mm**

The change in the macropore length density with depth displayed a similar trend as that of the
macroporosity. The macroporosity and macropore length density were highly positively
correlated ($r^2=0.90$ for Hagerstown and $r^2=0.83$ for Morrison) (Fig. 3-3a). H-P had the highest
length density among the four soil type-land use combinations, being 12.24, 11.87, and 8.27
km.m$^{-3}$ for the Ap1, Ap2, and Bt horizons, respectively. On the other hand, M-C had the lowest
length at the subsurface (i.e., 2.66 and 1.57 km.m$^{-3}$ for the Ap2 and Bt horizons, respectively).

As shown by Fig. 2-8, shot macropores ($< 3$ mm) may mainly contribute to the macropore
length. Since highly continuous macropores are very important to hydraulic functions, I analyzed
the length density, tortuosity and angle of macropores with vertical length $> 45$ mm. Despite the
Ap1 horizon with highest macroporosity and length density, the Ap2 horizon had the greatest
length density $> 45$ mm among the three horizons in three out of the four soil type-land use
combinations (except for M-P) (Fig. 3-2e). The length density $> 45$ mm of M-P increased with
depth.

**Node density and network density**
The mean node density or interconnectivity decreased from the Ap1 to Bt horizons (Fig. 3-2b). Compared to the Hagerstown, the mean node density of the Morrison decreased more rapidly with depth. Figure 3-4 shows the differences in the correlation between the macropore network density and node density for the Ap1, Ap2 and Bt horizons. The slope decreased from the Ap1 to Bt horizon, suggesting a decrease in the inter-connectivity of macropores with depth. The node density and length density were also highly correlated \((r^2=0.92\) for the Hagerstown and \(r^2=0.87\) for the Morrison) (Fig. 3-3b).

**Tortuosity and angle**

In general, mean tortuosity decreased with depth. The mean tortuosity of the Ap1 horizon was greater than that of other two horizons for all the soil type-land use combinations (Fig. 3-2c). For H-P, the mean tortuosity was high, i.e., 1.83, 1.66, and 1.64 for the Ap1, Ap2, and Bt horizons, respectively. For M-P, the mean tortuosity of the Ap2 (i.e., 1.42) and Bt (i.e., 1.34) was much lower than that of H-P. The mean tortuosity for M-C was 1.74, 1.46, and 1.46 for the Ap1, Ap2, and Bt horizons, respectively. The mean tortuosity for H-C was 1.58, 1.47, and 1.49 for the Ap1, Ap2, and Bt horizons, respectively. I found that mean tortuosity and macropore length density were positively correlated \((r^2=0.57\) for the Hagerstown and \(r^2=0.70\) for the Morrison) (Fig. 3-3c), indicating an increase of tortuosity with the amount of macropores. This may be associated with the competition of the roots and soil biota for space and food, especially earthworm burrows.

The variation of mean angle among different horizons was similar to that of tortuosity (Fig. 3-2d). The mean angle and mean tortuosity were positively correlated \((r^2=0.34\) for the Hagerstown and \(r^2=0.58\) for the Morrison) (Fig. 3-3d). As expected, the less tortuous the macropores were, the more vertically oriented they were. Similarly, the mean angle of the Ap1 horizon was much greater those of the Ap2 and Bt horizons. For crop land use (i.e., H-C and M-C), the mean angle of the Ap2 horizon was the lowest and for pasture land use (i.e., H-P and M-
P), the mean angle of the Bt horizon was the lowest. For example, the mean angle for H-C was 43.4, 24.3, and 32.6 degree for the Ap1, Ap2, and Bt horizons, respectively.

The lower mean tortuosity and angle of the subsurface (i.e., the Ap2 and Bt horizons) were associated with a larger proportion of highly continuous and vertically-oriented bio-pores (Figs. 2-3, 2-4, 2-9 and 2-10). The biopores consisted of a considerate proportion of the macropores in H-C, H-P and M-P in the subsurface. These macropores at the Ap2 and Bt horizons are favorable for the occurrence of preferential flow and transport in the soils at near-saturated conditions.

**Fractal dimension**

The fractal dimensions of the macropores varied with depth in a way similar to the changes in the macroporosity (Fig. 3-2f). The 3-D fractal dimensions of the Ap1 horizon were always the highest. The values are within the range of the fractal dimensions reported in the literature for macropore networks (Peyton et al., 1994; Perret et al., 2003) and for tracer distributions (Hatano et al., 1992). The fractal dimensions in 3-D were closely correlated to macroporosity. Positive logarithmic trends were observed ($r^2 = 0.96$) (Fig. 3-5), which is consistent with the results of Peyton et al. (1994) and Perret et al. (2003)

**Pedotransfer functions for macropore characteristics**

Macroporosity, length density, tortuosity, network density, node density, and fractal dimension of the soil horizon were closely correlated to organic matter content and bulk density of the soil horizon (Fig. 3-6 & Table 3-2). In general, macroporosity, length density, network density and node density increased with organic matter content and decreased with bulk density. Macroporosity were best estimated by bulk density and Ksat-core ($R^2=0.86$) using stepwise regression. Bulk density explained 61% of the variation in macroporosity (Fig. 3-6). Organic matter content explained 60% of the variation in macroporosity. Similar relationships presented
between macropore length density and bulk density, Ksat-core and organic matter content. Currently, pedotransfer functions (PFTs) for macropore characteristics are lacking in the literature. The results indicate the feasibility to estimate soil macroporosity from the bulk density or organic matter content. A broader range of soil types and land uses are necessary to develop more generalized relationship pedotransfer functions and test their validation.

Clay content was negatively correlated to mean angle \((r^2=-0.37, p=0.04)\) and positively correlated to path \((r=-0.56, p=0.06)\) (Table 3-2). A positive correlation was found between length density > 45 mm and silt content \((r=-0.51, p=0.09)\). These correlations suggest that soil texture, especially clay and silt content, influences the macropore inclination, continuity and connectivity. Soil texture influences the penetration of roots and animal burrows. For example, the soil with greater silt content is favorable for the growth of plant and soil biota such as earthworms (Brady and Weil, 1999).

- Macroporosity = 0.1328-0.076 Bulk density+0.073 Ksat-core \((R^2=0.86)\)
- Macroporosity = 0.1147-0.075 Bulk density \((r^2=62.79)\)
- Length density = 26.22-15.3 Bulk density+14.4 Ksat-core \((R^2=0.90)\)
- Length density = 28.57-15.0 Bulk density \((r^2=0.66)\)
- Mean Tortuosity = 1.412+0.060 OM% \((r^2=0.51)\)
- Network density = 1232752-613569 Bulk density \((r^2=0.71)\)
- Node density = 4496239-3044819 Bulk density+11681 sand%+80753 OM% \((R^2=0.90)\)
- Node density = 2907488-2041816 Bulk density+9291 sand% \((R^2=0.83)\)
- Path = -0.09538+0.030 clay \((r^2=0.318)\)
- Mean angle=55.19-1.18 clay % \((r^2=0.37)\)
- Fractal dimension = 2.869-0.57 bulk density+0.57 Ksat-core \((R^2=0.81)\)
- Fractal dimension = 2.963-0.56 bulk density \((r^2=0.57)\)
Summary and Conclusion

Three-dimensional macropore characteristics of three soil horizons in the soil columns were quantified and their change with depth in different types of soils and land uses were investigated. The macroporosity, length density, network density, node density, mean tortuosity, mean angle and fractal dimension were inter-correlated. Only macroporosity of M-C decreased dramatically with depth. For H-C, H-P, and M-P, the Ap2, and Bt horizons had relatively high macroporosity due to the existence of biopores formed by biota and roots. The tortuosity decreased with macroporosity and length density. Compared to the Ap1 horizon, the macropores at the subsurface (Ap2 and Bt horizons) were less tortuous, more vertically oriented, less interconnected. The highly continuous, vertically oriented, and low tortuous macropores at the Ap2 and Bt horizons are favorable for the preferential flow and transport at near-saturated conditions at the subsurface (Bouma, 1981; Luo et al., 2008).

Pedotransfer functions for soil macropore characteristics were developed using basic soil properties such as soil bulk density, organic matter and soil texture. Clay and silt content influence the macropore inclination, continuity and connectivity. For each horizon, macroporosity, length density, network density, and node density can be reasonably estimated by soil bulk density, organic matter content and Ksat-core. These PTFs are potentially useful to estimate macropore characteristics using widely available basic soil properties. However, a broader range of soil types and land uses should be used to generate more reliable pedotransfer functions for macropore characteristics.
References


Table 3-1 The variation of macropore characteristics in different soil horizons.

Length density > 45 mm, tortuosity > 45 mm and angle > 45 mm are macropore length density, tortuosity, and angle of the macropores with vertical length > 45 mm.

<table>
<thead>
<tr>
<th>Soil-land use</th>
<th>Horiz.</th>
<th>Macroporosity</th>
<th>length density</th>
<th>Mean Tortuosity</th>
<th>Network density</th>
<th>Hydraulic radius</th>
<th>Node Density</th>
<th>Path</th>
<th>Mean Angle</th>
<th>Length density &gt; 4.5 cm³</th>
<th>Tortuosity &gt; 4.5 cm³</th>
<th>Angle &gt; 4.5 cm³</th>
<th>Fractal dimension</th>
</tr>
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<td>H-C-2</td>
<td>0.037</td>
<td>5.8</td>
<td>1.62</td>
<td>4.0E+05</td>
<td>0.78</td>
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<td>4.81E+05</td>
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Table 3-2 Pearson correlation coefficient (r) between macropore characteristics and soil basic properties. Values of probability (p) are indicated using three significance levels (*** p<0.01, ** p<0.05, * p<0.1).

<table>
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<tr>
<th></th>
<th>Macroporosity</th>
<th>Length density</th>
<th>Mean tortuosity</th>
<th>Network density</th>
<th>Hydraulic radius</th>
<th>Node Density</th>
<th>Path</th>
<th>Mean Angle</th>
<th>Length density&gt;4.5 cm</th>
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Figure 3-1 The depth function of mean macroporosity in different soil types and land uses.
Figure 3-2 The variation of macropore characteristics in different soil horizons: a) macroporosity, b) node density, c) mean tortuosity, d) mean angle, e) length density >45 mm, and f) fractal dimension in 3-D.
Figure 3-3 The correlation between macropore characteristics for the Hagerstown (blue) and the Morrison (red) soils: a) length density and macroporosity, b) length density and node density, c) tortuosity and length density, and d) tortuosity and angle.
Figure 3-4 The relationship between network density and node network density for the Ap1, Ap2, and Bt horizons.
Figure 3-5 The relationship between 3-D fractal dimension and macroporosity.
Figure 3-6 The relationship between macropore characteristics and basic soil basic properties: a) macroporosity and organic matter content, b) length density and organic matter content, c) macroporosity and bulk density, d) mean angle and clay content.
Chapter 4

COMBINING X-RAY COMPUTED TOMOGRAPHY AND BREAKTHROUGH CURVE EXPERIMENTS TO QUANTIFY RELATIONSHIPS BETWEEN SOIL MACROPORE CHARACTERISTICS AND PREFERENTIAL FLOW

Abstract

Developing quantitative relationships between soil structure, especially macropore characteristics, and soil hydraulic properties is essential to improving our ability to predict flow and transport in structured soils. The objectives of this study were to quantitatively relate macropore characteristics to saturated hydraulic conductivities (Ksat) and solute transport parameters and to identify critical macropore characteristics to soil hydraulic functions. Soil columns (100 mm in diameter and about 350 cm in length) were taken from the Hagerstown silt loam with two types of land uses (i.e., crop and pasture). The soil columns were scanned using X-ray computed tomography (CT) to obtain soil structural parameters including macroporosity, length density, mean tortuosity, network density, hydraulic radius, path, node density, and mean angle of the macropores. The Ksat of each soil horizon and the whole column were measured and the breakthrough curve (BTC) of CaBr2 was collected for each soil column. Both the traditional convection-diffusion equation (CDE) (i.e., equilibrium model) and the two-region model (i.e., non-equilibrium model) were used to fit the BTCs and inversely estimate the solute transport parameters. For all the soil columns, macroporosity and macropore path explained 75% of the variation in Ksat of the horizon and 75% of the variation in Ksat of whole soil column. In addition, macropore tortuosity was also one important factor for Ksat. I
also found that the Ksat measured from the large soil columns were 3 to 46 times greater than those measured from the small soil cores. Equilibrium CDE fitted the BTCs well for all soil columns except one with a macropore passing through the entire column (i.e., path = 1). The cropped Hagerstown showed a greater degree of preferential flow compared to its pasture counterpart because the macropores in the pasture Hagerstown were less continuous, more abundant and evenly distributed in the soils. The path, hydraulic radius, and macropore angle explained 97% of the variation in the hydrodynamic dispersion coefficient. The correlation between the hydrodynamic dispersion coefficient and Ksat of the Bt horizon implied that the hydrodynamic dispersion was mainly controlled by the horizon with the lowest conductivity.
Introduction

Preferential flow of water and transport of chemicals continues to receive considerable attention due to its influence on water quality and its significance in hydrological response. To accurately estimate preferential water movement and solute transport, physical non-equilibrium process (i.e., the different advective solute transport velocity and concentration) has to be considered (Köhne et al., 2005). Various models have been developed to describe physical non-equilibrium process, including the dual-porosity model (Van Genuchten et al., 1976), the dual-permeability model (Gerke et al., 1993), the multi-region model (Gwo et al., 1995), and the kinematic wave model (Germann, 1985). Although the above models have sound physical bases, the parameterization of these models is still challenging. Experimental measurements of soil hydraulic parameters are time-consuming and costly. The quantitative relationships between soil structure, especially macropore characteristics, and preferential flow and solute transport have not been well addressed and this prohibits accurate estimation of flow and transport in structured soils using current simulation models (Feyen et al., 1998; Šimunek et al., 2003).

Various approaches have been developed to estimate soil hydraulic conductivity from soil properties. These models have been based on particle size distribution (shape similarity) (Arya and Paris, 1981), pore size distribution (van Genuchten, 1980; Kosugi 1999), or pedotransfer functions (PTFs) (Lin et al., 1999). However, the particle size distribution approach has difficulties for soils with different grain shapes and aggregations (Hillel, 1998). Most models based on pore size distribution assume a cylindrical shape of the pores. Tortuosity, continuity, and connectivity, which
are considered to be important to the hydraulic functions, have not been adequately considered. As Hillel (1998) addressed, without considering the size, continuity, tortuosity and shape of the pore space in general, the models based on pore size distribution have not been successful in estimating conductivity, especially at near-saturated conditions.

The Kozeny-Carmen equation, based on the definition of hydraulic radius, is one of the most widely applied methods for estimating the saturated hydraulic conductivity (Ksat). Several variants of the Kozeny-Carmen equation are available in the literature (Schaap and Lebron, 2001). Although the hydraulic radius, tortuosity, and specific area have been considered in the equation, hydraulic radius theory may not be applicable to describe structured porous media, such as clay soils with fissures (Hillel, 1998). Additionally, Poiseuille’s equation has been used to estimate Ksat based on pore geometry data (Bastardie et al., 2003), but that also encountered questionable assumptions of pore geometry.

Many experimental efforts have addressed the relationship of soil properties, especially soil structure and macropore, with parameters of flow and solute transport. Due to the difficulty of obtaining macropore data and the complex nature of macropore geometry and topology, artificial macropores in a packed soil column was used to study the effect of macropore characteristics on macropore flow (Kohne et al., 2005; Akay and Fox, 2007). In the field, Bouche et al (1997) found that percolation rates significantly correlated to earthworm burrow length, surface area, volume, and earthworm biomass, but not with the burrow diameter, tortuosity or earthworm number and soil profile depth.

Vervoort et al. (1999) investigated solute transport in two soils with contrasting structures. They found that high variation of Ksat, high dispersivities, low mobile water contents, low exchange
coefficients, and low dyed area indicated a well-developed structure and a high degree of preferential flow. Ersahin et al. (2002) compared the dispersivities, mobile water fractions, and mass exchange coefficients of intact soil columns taken from the A, Bw, and E horizons of a Thatuna silt loam. They found that the Bw horizon had the highest degree of preferential flow and that most of the variability in macropore transport was caused by pores with radii > 0.5 mm. Shaw et al. (2000) found a greater degree of preferential flow with increased clay content and higher level soil structure development. They developed PTFs between soil properties and model parameters for solute transport. Franklin et al. (2007) also found dyed area had less clay content and greater pore area. Jarvis (2007) showed that organic matter content and soil texture could explain 60% of the variation of the mass transfer estimated from the dual-permeability model MACRO. Merdun and Quisenberry (2004) estimated model parameters of flow and transport in soils with contrasting textures and structures and suggested that basic soil properties, such as clay content and structure, may be characteristics from which to differentiate and classify soils based on their flow and solute transport characteristics. Goncalves et al. (2001) developed PTFs to link basic soil properties to parameters of a non-equilibrium convection-diffusion equation (two-region model) using neural network and bootstrap analysis. However, few studies have quantitatively described soil structure, especially macropore geometry and topology, and linked them to hydraulic conductivity and solute transport variables at near-saturated condition.

Traditional methods have limited use in observing and quantifying macropore structure which strongly influences Ksat. Thin-section (Schaap and Lebron, 2001) and dye method (Franklin et al., 2007) are destructive and unsophisticated to reconstruct 3-D macropore geometry. In contrast, computed tomography (CT) is a non-destructive and powerful imaging technique for observing and quantifying macropore networks (Anderson et al., 1992; Luo et al., 2008).
The objectives of this study were to link the macropore characteristics of structured soils to Ksat and solute transport parameters and to identify the most important macropore characteristics influencing soil hydraulic functions in structured soils. I also compared Ksat measured from the large soil columns with the classical small soil cores to evaluate the effect of support volume. Such knowledge will enhance the understanding of how macropores influence soil hydraulic properties and potentially lead to the development of proper management strategies to increase plant available water, reduce soil erosion, and minimize water pollution.

**Methodology**

**The site and soil sampling**

The soil selected was mapped as the Hagerstown silt loam (fine, mixed, semiactive mesic Typic Hapludalfs). To study the effect of land use, two representative agricultural land uses, cropland and pasture, were selected. Thus, there were two combinations: Hagerstown-crop (H-C) and Hagerstown-pasture (H-P). Cropland sites had rotational cropping system with two years of corn (*Zea mays* L.) and one year of soybean (*Glycine max* (L.) Merr.) with conventional tillage. Pasture sites were grazed by animals (cows and horses). Five soil columns, 102 mm in diameter and about 350 mm in length, were taken from each site in July 2007 with corn growing for crop site. Three soil horizons (Ap1, Ap2, and Bt1) were contained in each soil column. Besides the large soil column, three intact small soil cores, 55 mm in diameter and 60 mm in length, were taken from each horizon to measure soil bulk density and Ksat (i.e., Ksat-core) following traditional methods. Soil samples were also taken from each horizon to measure soil particle size distribution and organic matter content (Table 2-1).
All soil columns were scanned using a medical CT (Universal system, Inc., Solon, Ohio). Based on the CT images, columns with obvious structure disturbance inside the column were not used in this study. For each land use, four soil columns were selected for further study with hydraulic properties and BTC measurements.

**Image Analyses and quantification of 3-D macropore network**

See the procedure to quantify the 3-D macropores in Chapter 2.

Macroporosity, length density, mean tortuosity, network density (i.e., the number of macropore networks in a unit volume), hydraulic radius, path, node density, and mean angle of the macropores as well as length density, tortuosity and angle of the macropores with vertical length longer than 150 mm (i.e., length density_150, tortuosity_150, and angle_150) were quantified for each column and horizon contained in the column. The macroporosity of the whole column and each horizon was calculated from image without the edge cut.

**The experimental setup of the flow and solute transport**

Some soil pore spaces may be entrapped with air under natural saturation and ineffective in hydraulic function (Luo et al., 2008). To link the macropore characteristics to the parameters of flow and solute transport, I used a vacuum to improve the saturation ratio (Fig. 4-1a). A PVC cap was placed at the top of the soil column. Grease was used to fill the space between the PVC pipe and cap to prevent air movement during saturation. A pipe fitting and clamp were used at the bottom end to connect the soil column to a flow distributor. I followed the procedure described by Flint and Flint
(2002). Firstly, the vessel was evacuated for about half an hour by a vacuum at a pressure of 10 inches Hg (about 1/3 bar) with the valves on. While maintaining a vacuum, a 0.005 M CaSO₄ solution slowly entered the soil column from the bottom at a rate of 6 ml min⁻¹. A layer of filter paper was placed at the bottom of the soil column to protect the soil from the force of water during saturation and to filter the effluent from the bottom. When solution was observed at the clear tube at the top of the PVC cap, the valve at the bottom was turned off and the soil was left under vacuum for about three days for the soil to saturate. Before and after saturation, the weight of the soil column and all the accessories were measured to estimate the initial soil moisture and the saturated ratio.

After saturation, the Ksat of the whole soil column and each horizon were measured directly using pressure transducers using the same setup (Fig. 4-1b). Pressure transducers (PT) were used to measure the pressure differences between the horizon boundaries (i.e., …). A constant hydraulic head was maintained with a Mariotte siphon. The flux or flow rate was adjusted by the height of outlet tube. At a constant hydraulic head, when the readings of all the PTs were constant, the flow rate was measured and the pressure differences were recorded. The flow rate against the pressure difference was plotted and Ksat was calculated from the slope according to the Darcy’s Law. At least four different flow rates or hydraulic head levels were used to obtain reliable results for each horizon within the soil column. How the Ksat of the whole soil column was obtained? – need to describe it here.

Chemical breakthrough curves (BTCs) of CaBr₂ solution were then collected at a flow rate of 10 ml min⁻¹ for all soil columns. The same flow rate was used to facility the comparison of solute transport variables of different soil columns. When flow rate was constant, a 0.005 M CaBr₂ solution was introduced to replace the 0.005 M CaSO₄ solution. The flow rate was assumed to be constant based on a constant hydraulic head throughout the solute transport process. The effluent was collected
with an automatic fractional collector. A 3-way wye was used to divert the flow and thus only a
fraction of the effluent was collected. The Br concentration was determined by flow injection analysis
using a Lachat autoanalyzer (Quick Chem FIA+ 8000 Series, Lachat Instruments, Loveland, CO),
following the method described by Bogren and Smith (2003).

Modeling

Chemical breakthrough curves were quantitatively evaluated using the computer program
CXTFIT (Toride et al., 1995). Both a traditional convection-diffusion model (i.e., equilibrium model)
and a two-region model (i.e., nonequilibrium model) in CXTFIT were used to inversely estimate the
model parameters. The equilibrium model is written as

\[
\frac{\partial (\theta C)}{\partial t} = \frac{\partial}{\partial x} \left( \theta D \frac{\partial C}{\partial x} - j_w C \right), \tag{1}
\]

where \( \theta \) is the water content, \( t \) is time, \( C \) is the concentration, \( x \) is the vertical coordinate, \( D \) is the
hydrodynamic dispersion coefficient, and \( j_w \) is the flux.

Nonequilibrium model is described as (Toride et al., 1995):

\[
\theta_m \frac{\partial C_m}{\partial t} = \theta_m D_m \frac{\partial^2 C_m}{\partial x^2} - j_w \frac{\partial C_m}{\partial x} - a(C_m - C_{im}), \tag{2}
\]

where \( \theta_m \), \( C_m \) and \( D_m \) are water content, concentration, and hydrodynamic dispersion of the mobile
domain, respectively, \( a \) is the first-order mass transfer coefficient, and \( C_{im} \) is the concentration of
immobile domain. For the traditional convection-diffusion equation, the hydrodynamic dispersion was
inversely estimated by fitting the BTC. For the two-region model, the fraction of mobile water content
to total water content (\( \frac{\theta_m}{\theta} \)), the coefficient of lateral mass exchange (\( a \)), and the coefficient of
hydrodynamic dispersion (\( D_m \)), of the mobile domain were inversely estimated.
Stepwise regression was used to develop quantitative relationships between the macropore characteristics and Ksat and the solute transport variables using Minitab (Minitab Inc, State College, PA). The option of standard stepwise regression combining the backward and forward selection was selected. The alpha was set to 0.15 to enter and remove a variable.

Results and discussion

Saturated hydraulic conductivity and its relationship to macropore characteristics

In general, the measured Ksat for the whole column and each horizon within the column were high (Table 4-1). Due to the existence of a earthworm burrow passing through the entire soil column (Fig. 2-3), H-C-2 had a much greater Ksat (i.e., 43.37, 30.13, and 1.68 cm min⁻¹ for the Ap1, Ap2, and Bt horizons, respectively) than the other columns of H-C (Table 4-1). For example, Ksat for H-C-3 was 0.29, 0.47, and 0.25 cm.min⁻¹ for the Ap1, Ap2, and Bt horizons, respectively. The Ksat for the whole column of H-C-2 (10.26 cm min⁻¹) was more than 20 times of those for H-C-3 (0.26 cm.min⁻¹) and H-C-5 (0.51 cm.min⁻¹). This indicated that this single earthworm burrow dominated the contribution to the high Ksat for H-C-2. Bastardie et al. (2003) also reported high Ksat for soil columns containing earthworm burrows (up to 264 cm min⁻¹).

The saturated hydraulic conductivity of each horizon was positively correlated to the macroporosity of the horizon ($r^2=0.73$ for H-C and $r^2=0.53$ for H-P) (Fig. 4-2). The difference in the slope (i.e., 54.0 for cropped Hagerstown and 37.7 for pasture Hagerstown) at $p<0.1$ reflected the different macropore geometrical features (Fig. 2-3). Compared to H-P, the macropores of H-C were less tortuous, more vertically-oriented and more continuous. For example, the mean tortuosity for H-C
was 1.58, 1.47, and 1.47 for the Ap1, Ap2, and Bt horizons, respectively, and the mean tortuosity for H-P was 1.83, 1.69, and 1.62 for the Ap1, Ap2, and Bt horizons, respectively. The mean angle for H-C was 43.4, 24.3, and 32.6 ° for the Ap1, Ap2, and Bt horizons, respectively and the mean angle for H-P was 45.7, 32.2, and 32.2 ° for the Ap1, Ap2, and Bt horizons, respectively. In addition, H-C had greater proportion of highly continuous macropore (> 45mm) than those of H-P (Table 3-1). Due to the less tortuous, more vertically-oriented and more continuous macropores of H-C, the macropores of H-C were more effective in conducting water flow than those of H-P.

For all the soil columns, the Ksat of each horizon was best predicted by the macroporosity and the path of the horizon (R²=0.75) (Fig. 4-3a) and the Ksat of whole soil column was best predicted by the path and length density (R²=0.78). Since macroporosity and macropore length density are closely correlated (Fig.3-3a), macroporosity and path also well predicted the Ksat of whole soil column (R²=0.75) (Fig.4-4). Compared with length density, macroporosity is more available. Therefore, macroporosity may be a better predictor than length density. Path, i.e., the number of macropores passing through the volume of interest (i.e., entire soil column or horizon), can also be considered as highly continuous macropore. Previous investigations have illustrated the importance of macropore length or continuity to water flow through soils (Smettem,1986; Bastardie et al.,2003).

Within each land use, the path, macroporosity and tortuosity_150 (tortuosity of macropores with vertical length > 150 mm) (listed in the order of the significance) best explained the variation in the Ksat of the horizon (R²=0.90) for H-C (Fig. 4-3b); whereas macroporosity was the most important characteristic, combined with tortuosity and path, to best explain the variation in the Ksat of the horizon (R²=0.88) for H-P (Fig. 4-3c). Therefore, macropore tortuosity could be one of the important factors to the Ksat. The above empirical equations between the Ksat and soil macropore
characteristics are subjected to specific macropore features. The physical relationships between the Ksat and soil macropore geometrical characteristics (i.e., path, macroporosity and tortuosity) should be analyzed and applied to generalize the equations.

Comparison of the Ksat measured from the large soil column and small soil core

I compared mean Ksat measured from the large soil columns and small soil cores to evaluate the effect of sample size. The method using small soil cores is the standard method for laboratory setting (Reynolds et al., 2002). The Ksat measured from the large soil columns were much greater than those measured from the small soil cores (Tables 2-1 and 4-1). For example, for H-C, the Ksat measured from the small soil cores for the Ap1, Ap2 and Bt horizons were 0.051, 0.045 and 0.035 cm.min⁻¹, respectively (Table 2-1), while the Ksat measured from the large soil columns for the Ap1, Ap2 and Bt horizons were 1.65, 2.09 and 0.83 cm.min⁻¹, respectively (Table 4-1). This is likely associated with the compaction along the edge for fine-textured soils (Pires et al., 2004) and/or the support volume. For instance, the small soil core may have a greater proportion of area being compacted during the sampling than the corresponding larger ones. Brooks et al (2004) found that small-scale Ksat measurements underestimate the actual hillslope-scale Ksat. Therefore, caution should be exercised when using the Ksat measured from small soil cores for modeling flow and solute transport at the larger scale.
The solute transport and its relationship to macropore characteristics

All the BTCs showed a quick response and a long tail, indicating the occurrence of preferential flow (Fig. 4-5). At one pore volume, the mean relative concentration was 79.1% (±6.0%) for H-C and 70.0% (±1.9%) for H-P. Except for H-C-2, equilibrium CDE fitted the BTCs well for the other soil columns (Fig. 4-5). Luo et al. (2008) observed preferential flow pathways in real time in the subsurface soils, particularly in the biopores in a soil column with the same soil type and similar soil length. This implies that the equilibrium CDE worked well to model the fluxes of water and solute through soil columns with quite an amount of biopores but without through macropores. The non-equilibrium model (i.e., two-region model) successfully simulated solute transport in H-C-2 (Fig. 4-6). The resultant fraction of mobile water content was 0.07. The coefficient of hydrodynamic dispersion in the macropore domain was 78.9 cm².min⁻¹ and the coefficient of lateral mass exchange was very low (i.e., 5E-06 min⁻¹), indicating a high degree of preferential flow and a low degree of interaction between the mobile (partly the through macropore) and immobile domains.

Although H-C had fewer macropores, the chemical breakthrough was quicker than that of H-P (Fig. 4-5). The higher the hydrodynamic dispersion, the greater degree of preferential flow is. The value of hydrodynamic dispersion estimated from equilibrium model was 212 cm².min⁻¹ for H-C-2 and 18.43 cm².min⁻¹ for H-C-5. This was due to the existence of highly continuous and vertically oriented macropores in the soil column. On the other hand, H-P had a greater number of macropores but they were more homogeneously distributed in the soils (Fig. 2-3) than H-C. Within the same volume, the more abundant the macropores, the less distance there is between macropores. With shorter inter-macropore distance in the soil columns of H-P, solute transport would approach equilibrium with less time of advection and diffusion. Additionally, H-P has better-developed
aggregates (strong fine-medium granular) than H-C (moderate fine-medium subangular) (Table 2-1).

The results of this study support the hypothesis that the degree of preferential flow increases from soils with well-developed structure to soils weak-developed structure (Jarvis, 2007).

The path, hydraulic radius and the angle best explained the variation in the hydrodynamic dispersion coefficient ($R^2=0.97$) (Fig. 4-7). This indicates that the hydrodynamic dispersion coefficient may be more influenced by the macropore size, connectivity and inclination than the Ksat. Figure 4-8 shows that the hydrodynamic dispersion coefficient was much better correlated to the Ksat of the Bt horizon than the Ksat of the whole soil column, or that of Ap2 or Ap1 horizons. This indicated that the hydrodynamic dispersion might be mainly controlled by the Bt horizon with lower conductivity in this study. The BTCs should be measured not only at the end of soil column but also in the middle of the soil column during the process of solute transport to further examine the relationship.

Summary and Conclusion

The results of this study demonstrated that macropores play an important role in water flow and solute transport. The Ksat of whole soil column was up to 10.26 cm.min$^{-1}$ due to the existence of highly conductive biopores. Quantitative relationships have been developed between macropore characteristics, Ksat, and hydrodynamic dispersion. For all the soil columns of the two land uses, macroporosity and path explained 75% of the variation in Ksat for the horizon-based values and for the whole soil columns. Additionally, macropore tortuosity is one of the important factors to Ksat. Thus, the size of the soil column sample had a significant influence on the measured Ksat. The Ksat
measured from the large soil columns were about 10 times greater than those measured from small soil cores. Saturated hydraulic conductivity measured from the large soil columns would better represent actual Ksat in the field.

The equilibrium CDE model described well the BTCs of the soil columns without through macropore (path <1). H-C had a greater degree of preferential flow than H-P because H-P had more macropores that were more evenly distributed throughout the soil. The path, hydraulic radius and the angle150 best explained the variation in the dispersion coefficient (R²=0.97). The dispersion coefficient appears to be mainly controlled by the layer of soils with lower conductivity.

References


Table 4-1 Saturated hydraulic conductivity (cm min⁻¹) for whole soil columns and their component soil horizons. The number in parentheses is one geometric standard error. The lower letters after the parenthesis indicate the significance test of mean difference among the four soil series at p<0.05.

<table>
<thead>
<tr>
<th></th>
<th>H-C-2</th>
<th>H-C-3</th>
<th>H-C-4</th>
<th>H-C-5</th>
<th>Geometric mean (standard error)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ap1</td>
<td>43.37</td>
<td>0.29</td>
<td>1.39</td>
<td>0.36</td>
<td>1.65 (3.71) a</td>
</tr>
<tr>
<td>Ap2</td>
<td>30.13</td>
<td>0.47</td>
<td>0.41</td>
<td>0.64</td>
<td>2.09 (3.11) a</td>
</tr>
<tr>
<td>Bt1</td>
<td>1.68</td>
<td>0.25</td>
<td>No data</td>
<td>1.37</td>
<td>0.83 (1.36) a</td>
</tr>
<tr>
<td>Whole column</td>
<td>10.26</td>
<td>0.26</td>
<td>No data</td>
<td>0.51</td>
<td>1.11 (1.47) a</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>H-P-2</th>
<th>H-P-3</th>
<th>H-P-4</th>
<th>H-P-5</th>
<th>Geometric mean (standard error)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ap1</td>
<td>2.11</td>
<td>7.18</td>
<td>1.75</td>
<td>1.30</td>
<td>1.69 (1.05) a</td>
</tr>
<tr>
<td>Ap2</td>
<td>10.27</td>
<td>5.27</td>
<td>1.20</td>
<td>1.33</td>
<td>2.54 (1.27) a</td>
</tr>
<tr>
<td>Bt1</td>
<td>0.62</td>
<td>1.36</td>
<td>0.42</td>
<td>0.06</td>
<td>0.25 (1.72) a</td>
</tr>
<tr>
<td>Whole column</td>
<td>2.29</td>
<td>4.56</td>
<td>1.19</td>
<td>0.40</td>
<td>1.03 (1.45) a</td>
</tr>
</tbody>
</table>
Figure 4-1 a) The setup to saturate the soil column and b) the experimental setup of flow and transport measurement.
Figure 4-2 The relationship between Ksat and macroporosity of each horizon in the soil columns studied (the open circle represents the outlier).
Figure 4-3 The relationship between macropore characteristics and Ksat of each horizon in the soil columns for: a) crop+ pasure, b) crop, and c) pasture. Ksat was predicted from macropore characteristics using the equation under the figure.

\[
\ln(K\text{sat}) = -2.44 + 0.176 \times \text{path}\ + 44.4 \times \text{macroporosity}
\]

\[
\ln(K\text{sat}) = 3.29 + 0.177 \times \text{path}\ + 56 \times \text{macroporosity} - 4.4 \times \text{tortuosity 150}
\]

\[
\ln(K\text{sat}) = -9.82 + 50.5 \times \text{macroporosity} + 3.8 \times \text{tortuosity} + 0.78 \times \text{path}
\]
\[ y = 0.749x + 0.071 \]
\[ R^2 = 0.75 \]

\[ \ln(K_{sat}) = -2.186 + 3.277 \times \text{path} + 33.90 \times \text{macroporosity} \]

Figure 4-4 The relationship between Ksat and macropore characteristics of whole soil column. Ksat was predicted from macropore characteristics using the equation under the figure.
Figure 4-5 Measured and fitted breakthrough curves (BTCs) using equilibrium convection-diffusion equation (CDE). Hydrodynamic dispersion (D) was inversely estimated.

Figure 4-6 The measured and fitted breakthrough curves (BTCs) using non-equilibrium two-region model for H-C-2. Hydrodynamic dispersion (D) was inversely estimated.
\[ y = 0.9872x + 0.0157 \]
\[ R^2 = 0.9678 \]

\[ \ln(D) = -6.159 + 2.83 \times \text{path} + 12.2 \times \text{hydraulic radius} - 0.065 \times \text{angle 150} \]

**Figure 4-7** The relationship between macropore characteristics and hydrodynamic dispersion (D).
Figure 4- 8 The relationship between hydrodynamic dispersion ($D$) and saturated hydraulic conductivity ($K_{sat}$) of: a) whole column, b) the Ap1 horizon, c) the Ap2 horizon, and d) the Bt1 horizons. The data of H-C-2 was not used here due to its extremely high value in $K_{sat}$ and $D$. 

\[ y = 0.027x + 1.93 \quad R^2 = 0.007 \] 
\[ y = 0.0286x + 1.86 \quad R^2 = 0.0416 \] 
\[ y = 0.766x + 1.455 \quad R^2 = 0.636 \] 
\[ y = -0.010x + 1.961 \quad R^2 = 0.002 \]
Chapter 5

TWO AND THREE-DIMENSIONAL LACUNARITY AND FRACTAL ANALYSES OF SOIL MACROPORES AND PREFERENTIAL TRANSPORT USING MICRO X-RAY COMPUTED TOMOGRAPHY

Abstract

Quantification of soil macropore networks and solute transport patterns is important to enhance our understanding of preferential flow in structured soils. Computed tomography (CT) provides a nondestructive tool to observe soil macropore structure and to monitor solute transport in real-time. I investigated soil macropore structure and solute transport dynamics in an intact soil column of 76 mm in diameter and 256 mm in length. Five positions (each with a thickness of 10.7 mm) in the Ap1, Ap2, and Bt horizons of the soil column, plus two boundaries between these horizons, were scanned with a voxel resolution of 78.1 µm × 78.1 µm × 86.7 µm. The scanning was done at three stages after the soil column was satiated: 1) before tracer (KI) introduction, 2) after introducing the tracer for 6 min, and 3) after introducing the tracer for 78 min. The macropore network and tracer distribution were reconstructed at the five scanned positions. Relative lacunarity functions (RLFs) and pore fractal dimensions, both in 2-D and 3-D, were calculated. Distinct macropore characteristics and flow patterns were observed at the five positions. The bio-pores (such as earthworm burrows and root channels) were active in solute transport because of their high continuity and low tortuosity. Positive logarithmic trends were found between the pore fractal dimension and the volume percentage of the macropores and tracer distribution. The RLFs of the macropore networks and the tracer distributions over time varied with soil depth. The RLFs indicated that the tracer distributions exhibited more self-
similarity than the macropore networks. The lacunarity function reflected the size distribution of
macropores and the spatial pattern of flow and transport. Lacunarity is a potentially powerful
parameter that may be coupled with the fractal dimension to better describe and model soil structural
properties.
Introduction

Soil macropores play a critical role in preferential water movement and solute transport (Beven and Germann, 1982). Effective techniques for characterizing preferential flow and transport, and their relationship to soil macropore structure, however, remain elusive. New methods to improve the quantification of soil macropore structure and preferential flow pattern are important to enhance our understanding of the processes involved.

Fractal theory is one of the most widely used methods to quantify soil structure and flow patterns (e.g., Baveye et al., 1998; Young et al., 2001). The fractal dimension has been used to describe soil physical properties such as bulk density, pore size distribution, pore surface area, and soil aggregation, as well as soil physical processes such as water retention, percolation, diffusion, and solute transport (e.g., Perfect and Kay, 1995; Zeng et al., 1996; Perret et al., 2003; Anderson et al., 2000; Perrier et al., 1996, 1999; Gimenez et al., 1997; Hatano et al., 1992).

However, even though the fractal dimensions of two objects are the same, their structures can be quite different (Pendleton et al. 2005). As Mandelbrot (1982) pointed out, the fractal dimension alone does not suffice to describe the geometry and properties of ‘lacunar’ fractals; another parameter, which he termed “lacunarity,” is necessary. Lacunarity measures the deviation of a geometric object from the translational invariance or homogeneity and can be considered as a scale-dependent index of heterogeneity (Plotnick et al., 1993). In terms of fractal geometry, the prefactor in the following power-law relationship is associated with the lacunarity while the exponent corresponds to the fractal dimension (Mandelbrot, 1982):

\[
\text{Property} = (\text{prefactor}) \times (\text{scale})^{\text{exponent}} \tag{1}
\]
Lacunarity reflects the fraction of space occupied by the feature of interest, the degree of dispersion and clustering, the presence of self-similarity or randomness, and the existence of hierarchical structure (Plotnick et al., 1993). One of the problems involved with the application of fractal theory is that power-law scaling is not necessarily indicative of a structure exhibiting self-similarity (Baveye and Boast, 1998; Young and Crawford, 1997). The lacunarity curve of a fractal should be a straight line on a double logarithmic scale (Allain and Cloitre, 1991). This property could be a quite useful feature to tell whether self-similarity exists or not.

Despite the promising potential of lacunarity as an index to characterize different structures or spatial patterns, it has received relatively little attention in the soil science and hydrology literature. Lacunarity has been applied to differentiate the structures and spatial patterns of both fractals and non-fractals, such as landscape and land use (Plotnick et al., 1993), temporal changes in sediment transport (Plotnick et al., 1996), and pore space geometry in heterogeneous porous media (Kim et al., 2007). Zeng et al. (1996) calculated the 2-D fractal dimension and lacunarity of soil bulk density using a medical X-ray CT. They found that lacunarity was more sensitive to soil heterogeneity than the fractal dimension, and suggested that the joint distribution of fractal dimension and lacunarity would better discriminate soil structure. Until now, however, lacunarity analysis of soil macropore structure and preferential flow pattern remains unexplored.

With advances in experimental techniques and numerical analyses, CT has become an attractive technology for soil scientists to nondestructively observe soil macropores, solute transport, and their interactions in real-time (Anderson et al., 1990, 1992; Heijs et al., 1995; Perret et al., 1999, 2000; Luo et al., 2008). The intensive information gained from CT images provides a great opportunity to conduct fractal and lacunarity analyses of soil macropores and flow patterns. The CT techniques can
provide 3-D information by synthesizing a series of 2-D CT images using certain algorithms (Perret et al., 1999) and thereby facilitate the comparisons between dimensions – a feature especially important for anisotropic media. Since macropore and tracer distributions are essentially 3-D and apparent anisotropy exists in well-structured soils (Perret et al., 1999; Luo et al., 2008), it seems more sensible to evaluate their properties in 3-D. Perret et al. (2003) calculated 2-D and 3-D pore fractal dimensions of macropore networks using box-counting (2-D) and cube-counting (3-D) techniques. They found positive logarithmic trends between the fractal dimension and macroporosity. However, the relationship between the 2-D and 3-D fractal dimensions was not clear, mainly because of insufficient data. Gibson et al. (2006) compared the 2-D and 3-D fractal co-dimensions of soil aggregates and found that 2-D fractal dimensions could represent 3-D ones reasonably well.

The objectives of this study were to: 1) reconstruct and quantify 3-D macropore structure and preferential tracer transport in real-time in an intact soil column, 2) characterize soil macropore network and solute distribution patterns along soil depth using fractal dimensions and lacunarities, and 3) examine if macropore networks and flow patterns are fractal and if lacunarity has diagnostic value in characterizing soil macropore structure and preferential flow pattern where fractal dimension alone could not.
Materials and Methods

Soil

An intact soil column, 76 mm in diameter and 256 mm in length, was taken from the R.E. Larson Agricultural Research Center of The Pennsylvania State University located at Rock Springs in Centre County, Pennsylvania. The soil series is mapped as a Hagerstown silt loam (fine, mixed, semiactive mesic Typic Hapludalf), which is one of the most important agricultural soils in Pennsylvania. The field has been planted with corn, soybean, and alfalfa in rotation over the past few decades. All plant residues have been left in the field after harvesting. The details of our soil sampling procedures can be found in Luo et al. (2008). Three soil horizons, Ap1 (0-11 cm), Ap2 (11-21 cm), and Bt (21-26 cm), were identified in the soil column collected (Fig. 5-1). Basic soil properties are listed in Table 5-1.

Industrial CT unit

An industrial CT unit (OMNI-X of Bio-Imaging Research, Inc., Lincolnshire, IL) was used in this study. The system has a 225 KV micro-focus X-ray generator and a 225-mm-diameter image intensifier. The X-ray source and detector are fixed and the scanned object rotates (Fig. 5-2a). The sample is rotated 360 degrees to receive the X-ray beam (polychromatic) while the detector provides intensity views to the data acquisition computer. One rotation takes about 10-15 minutes, depending on the number of views taken. In this research, up to 41 slices were acquired in a single rotation with 3600 views. High-resolution images (1,024 x 1,024 pixels) were acquired at the output to the
computer system. I used different kinds of filters/wedges during the tuning-up procedure before our experiment to minimize the noise and to obtain the best image quality. A digital radiography (DR) image was also collected using the same CT unit to monitor the whole column during the experiment. The DR image reproduces a 2-D projection of the whole object exposed to the X-ray beam, and the X-ray attenuation values represent the effect of the object’s density and thickness (see example shown in Fig. 5-1).

**Experimental procedure**

The experimental setup is shown in Fig. 5-2b. The soil column was housed in a PVC pipe and satiated from the bottom by raising the water (0.005 M CaSO₄ solution) table gradually. This satiation process lasted for four days. The soil at satiation was scanned at a resolution of 78.1 µm×78.1 µm×86.7 µm at five positions, namely the Ap1, Ap2, Bt horizons, the boundary between the Ap1 and Ap2 horizons (labeled as Ap1-Ap2), and the boundary between the Ap2 and Bt horizons (labeled as Ap2-Bt) (Fig. 5-2b). For each position, 123 images were obtained (about 10.7 mm-thick in total). After scanning, 0.005 M CaSO₄ solution was supplied to the top end of the soil column at a constant flow rate of 6.7 ml/min using an automatic pump. When the outflow rate became constant, the 0.005 M CaSO₄ solution was replaced with a 60 g/L potassium iodide (KI) solution. An automatic fraction collector was used to collect the center and outer outflows separately (see Fig. 5-2b) at one-minute intervals. After introducing the KI solution for 6 min, the pump and the valve at the outlet tube were turned off to stop the flow. Scanning at the same five positions was repeated to observe the solute distribution. After this scanning, the KI solution leaching was restarted and scanning was repeated
again at the same five locations at 78 min. A total of 528 ml of the KI solution was applied during this experiment, which was about one pore volume of the soil column.

**Data analysis**

The images (1,024 x 1,024 pixels) were cut to exclude the area outside the soil column using ImageJ version 1.39 (Rasband, 2002). The macropore threshold value, determined using the maximum entropy threshold algorithm in ImageJ 1.39, was used to segment the images. The images were also visually inspected to ensure that a reasonable threshold value was used. The tracer distribution was reconstructed by subtracting the images taken when soil was satiated with the 0.005 M CaSO₄ solution from the images taken after the introduction of the 60 g/L KI solution, then dividing it by the difference in X-ray attenuation of the 0.005 M CaSO₄ solution and the 60 g/L KI solution (which is 459). After subtraction, the medium filter, a commonly used image-processing method to reduce the noise while preserving the edge, was used to minimize noise (Jassogne et al., 2007). The binary images were obtained with the following relationship:

\[
\frac{CT(x, y, z, t) - CT(x, y, z, t = 0)}{CT_{KI} - CT_{water}} > 30\%
\]

where \( CT(x, y, z, t) \) is the X-ray attenuation value for a voxel during solute replacement at time \( t \); \( CT(x, y, x, t = 0) \) is the X-ray attenuation value when the soil was satiated with water (0.005 M CaSO₄ solution) at the beginning of the experiment; \( CT_{KI} \) and \( CT_{water} \) are the X-ray attenuation values of the 60 g/L KI solution and the 0.005 M CaSO₄ solution, respectively. The threshold (i.e., 30%) reasonably segmented regions with apparent changes in X-ray attenuation values and excluded noise in the background. I relied on visual inspection, which is very important to ensure that a
reasonable threshold value is used despite the existence of many algorithms. After reconstruction, the macropore networks and tracer distributions were visualized using Amira version 3.1 (TGS Inc., San Diego, CA).

After image segmentation, the macroporosity, tracer volume percentage, average hydraulic radius, pore fractal dimension and lacunarity of macropores, and tracer distribution both in 2-D and 3-D were calculated. Hydraulic radius was calculated as the ratio of the pore volume to the pore surface area. Fractal dimensions were calculated using box-counting (2-D) or cube-counting (3-D) method (Perret et al., 2003). By covering the feature with boxes or cubes with side dimension of \( r \), the fractal dimension \( (D) \) can be estimated from the slope of \( \ln[N(r)] \) against \( \ln r \) with the following relationship:

\[
N(r) = \left( \frac{1}{r} \right)^D
\]

where \( N(r) \) is the number of boxes intersecting the feature of interest. The 3-D third-iteration prefractal Menger sponge with a known fractal dimension of 2.727 was generated to test our algorithm (in this case, the solid phase was counted), which resulted in a fractal dimension of 2.718 (error = 0.3%). The fractal co-dimension \( (H) \) can be used to generalize and compare fractal dimensions in 1, 2 or 3-D. The fractal co-dimension is defined as the difference between the Euclidian dimension \( (E) \) and the fractal dimension (Perret et al., 2003):

\[
H = E - D
\]

Lacunarity was calculated by a method introduced by Allain and Cloitre (1991). The gliding-box algorithm was used, in which a box or cube of size \( r \) moves or “glides” within the image covering all of the pixels or voxels. The lacunarity \( (L) \) was calculated as a function of \( r \):
\[ L(r) = \frac{\sum_m m^2 P(m, r)}{\left[ \sum_m mP(m, r) \right]^2} \]  

where \( P(m, r) \) is the probability that a box or cube of size \( r \) contains \( m \) pixels (in 2-D) or voxels (in 3-D) of the interest. Since the first moment \( \sum_m mP(m, r) \) is equal to the mean \( \langle u \rangle \) of the probability distribution function \( P(m, r) \), and the second moment \( \sum_m m^2 P(m, r) \) is equal to the sum of the variance \( \sigma^2 \) and the square of the mean of \( P(m, r) \), Eq. [5] is easier to understand when rewritten as (Pendleton et al., 2005):

\[ L = \left( \frac{\sigma}{u} \right)^2 + 1 \]  

Lacunarity is a function of three factors: 1) the gliding box or cube size, 2) the fraction \( p \) of the space occupied by the feature, and 3) the spatial distribution or structure of the feature. First, as the box or cube size increases, the variance decreases. Thus, the same image will have lower lacunarities as the box size increases. When lacunarities decrease towards unity (i.e., \( \ln(L(r)) = 0 \)) and remain constant afterwards, this suggests that \( r \) has approached the representative elementary volume (REV) of the material under investigation. For example, in Fig. 5-3, the size of the REV is reached when \( \ln(\text{box size}) \) is greater than 2.5 (i.e., box size = 10) for the “small” image, and at 4 (box size = 63) for the “middle” image. This is consistent with what Grossman and Reinsch (2002) suggested, that is, the REV is 10 to 30 times the largest feature. Second, with the similar spatial patterns, the lower the fraction, the higher the lacunarity. Specifically, when \( r = 1 \), \( L = 1/p \). Finally, with the same fraction level, a higher lacunarity represents a higher degree of clustering or clumping. Figure 5-3 shows the lacunarity curves for images with the same size (216 × 216 pixels), the same fraction (\( p = 0.5 \)), but different patterns. The lacunarities are highest for the image with large-size features and vice versa.
The lacunarities decrease quickly towards zero when approaching the block size (36 × 36 pixels for the “Large”, 6 × 6 pixels for the “Middle”, and 1 × 1 pixels for the “Small” images in Fig. 5-3). The “Hierarchy” image in Fig. 5-3 has equal curdling probabilities at all three levels and therefore its lacunarity curve is nearly linear except near the point where \(\ln(\text{box size})\) is equal to zero (Plotnick et al., 1993). As Allain and Cloitre (1991) pointed out, the lacunarity curve for a fractal should be a straight line.

To calculate the 2-D lacunarities, boxes with side dimension of 1, 2, 3, 4, 6, 10, 16, 25, 40, 63, 100, 123, 158, 251, 398 and 631 pixels were used to “glide” over the 2-D images (820 × 820 pixels). Three images, the 20\(^{th}\), 40\(^{th}\) and 60\(^{th}\) of the 123 images obtained at each scanned position, were selected to calculate the 2-D lacunarities, the mean of which was used to represent the overall 2-D lacunarities for each position. Because of the limited number of images (i.e., 123), a narrower size range of cubes (with side dimension of 1, 2, 3, 4, 6, 10, 16, 25, 40, and 63 voxels) were used to “glide” through the 3-D images (820 × 820 × 123 voxels) and calculate the 3-D lacunarities. The lacunarities of the third-iteration prefractal of Menger sponge and binary image with small randomly-distributed pores were also calculated as references.

Since the overall shapes of the lacunarity curves depend on the degree of clustering or clumping and are independent on the fraction (Plotnick et al., 1993), the relative lacunarity function on a logarithmic scale, \(RLF\), was defined and calculated as:

\[
RLF = -\frac{\ln(L(r))}{\ln(p)} \quad [7]
\]

Therefore, the influence of the fraction on lacunarity was excluded, so that the shape of the lacunarity function and its corresponding spatial pattern could be better evaluated. In addition, integration (i.e., the underlying area) of the relative lacunarity function was also calculated. This
parameter represents the overall lacunarity level and provides a single value to facilitate comparisons among the different features.

To compare the fractal co-dimension and lacunarity in different dimensions (i.e., 2-D and 3-D), the TTEST procedure in MATLAB (MathWorks Inc., Natick, MA) was used with a probability level of 0.01.

**Results and discussion**

**Reconstruction of macropore network and tracer distribution**

Both the macropore network and solute distribution in the soil column varied considerably with depth (Figs. 5-1 and 5-4). This is in part due to the horizonation and different soil structures in this soil (Fig. 5-1). The macropores in the Ap1 horizon were rather evenly distributed compared to the other two subsurface horizons. The macropores formed by earthworm burrows and roots constituted a significant proportion of the Ap2 and Bt horizons and their interface (Ap2-Bt). The macropores formed by earthworms were relatively large, round in shape, and highly continuous. While the macropores formed by roots were also highly continuous and round in shape, they were much smaller and more variable in size. Inter-aggregate macropores, such as those formed by freezing and thawing or wetting and drying, were generally smaller and more randomly and less continuously distributed in the soil column. As expected, the overall macroporosity in this soil column decreased dramatically from about 12% in the Ap1 horizon to less than 4% in the Ap2 horizon and increased slightly to over 4% in the Bt horizon (Table 5-2). The lowest macroporosity in the Ap2 horizon can be related to the platy structure of this plow-pan layer.
Although the entire soil column was satiated from bottom up gradually for four consecutive days, 3.9-17.8% of the macropores contained air bubbles (Table 5-2). Hence, I termed the soil moisture condition “satiated” (<100% pore space filled with water) instead of “saturated” (100% pore space filled with water). After introducing the KI tracer for 6 min, the solute was distributed relatively evenly (but not completely) in the Ap1 horizon (Fig. 5-4b). It then moved preferentially through the underlying horizons via some continuous macropores. The earthworm burrows and root channels were highly active in the flow and transport because of their high continuity and low tortuosity. The solute distribution in the subsurface was clustered along the active macropores (Fig. 5-4b). After 78 min, the solute had moved from the main preferential flow paths to connected local macropores and surrounding matrix (Fig. 5-4c). Again, the solute distribution in the Ap1 horizon was more homogeneous. The effluent breakthrough curve showed a quick increase in relative concentration after the tracer was first introduced. Relative concentrations were ~78% for the central outflow and ~65% for the outer flow at approximately one pore volume, indicating a high degree of preferential flow.

**Fractal dimensions**

The fractal dimensions of the macropore network and solute distribution (in both 2-D and 3-D) varied with depth in a way similar to the changes in macroporosity and tracer volume percentage (Table 5-2). The fractal dimensions of the Ap1 horizon (1.52 in 2-D and 2.61 in 3-D for macropores, 1.32 in 2-D and 2.41 in 3-D for the tracer distribution at 6 min, and 1.75 in 2-D and 2.86 in 3-D for the tracer distribution at 78 min) were always the highest. The 3-D fractal dimensions of the Ap2 horizon were always the lowest, i.e. 2.23 for macropores, 2.00 for the tracer distribution at 6 min, and
2.35 for the tracer distribution at 78 min. These values are within the range of fractal dimensions reported in the literature for macropore networks (Peyton et al., 1994; Gantzer et al., 2002; Perret et al., 2003) and for tracer distributions (Hatano et al., 1992). They suggest an underlying pore-solid fractal model (Perrier et al., 1999) for the soil structure in this column. The fractal dimensions in 2-D and 3-D were closely correlated to macroporosity and tracer volume percentage over time. Positive logarithmic trends were observed in both 2-D ($R^2 = 0.88$) and 3-D ($R^2 = 0.96$) (Fig. 5-5), which is consistent with the results of Peyton et al. (1994), Perret et al. (2003), and Zeng et al. (1996). Table 5-3 shows significant linear correlations between macroporosity and the tracer volume percentages at 6 and 78 min, and between the 2-D and 3-D fractal dimensions of the macropore network and tracer distribution. These results suggest that macropores were the major control on the flow and transport processes observed in this study.

The difference between the fractal co-dimensions in 2-D and 3-D, was not statistically significant in this study at the 0.01 probability level for both the macropores and the tracer volume percentages at 6 and 78 min. This result is consistent with research reported by Gibson et al. (2006), and indicates that the 3-D fractal co-dimension can be estimated by the 2-D fractal co-dimension.

**Lacunarities**

Relative lacunarity functions (RLF) for the 3-D macropore network and tracer distribution over time are shown in Fig. 5-6. The RLF’s for the third-iteration prefractal Menger sponge (labeled as fractal) and the image with small randomly-distributed pores (labeled as random) are also included in Fig. 5-6 for reference. As expected, the RLF of the third-iteration prefractal Menger sponge was nearly linear except where ln(cube size) was close to zero. The RLF for the image with small
randomly-distributed pores declined very quickly as cube size increased. In contrast, all of the RLFs for the macropore networks were rather convex in shape (Fig. 5-6a), suggesting that middle to large size pores existed and that the pore size distribution was not random. The RLFs for the macropore networks, however, varied with soil depth. The RLF of the macropore network in the Ap1 horizon was the lowest among the five positions investigated, because of its relatively evenly distributed but smaller pores (Fig. 5-4a). On the other hand, the RLFs for the macropore networks in the Ap2 and Bt horizons were higher than those of other horizons, probably due to the large and continuous bio-pores in both horizons (Fig. 5-4). The RLFs for the macropore networks at the two horizon boundaries (i.e., Ap1-Ap2 and Ap2-Bt) fell between the curves for the Ap1 and Ap2 or Bt horizons. The shapes of the lacunarity curves imply that the macropore network may be close to fractal within a given size range, and Euclidean outside of that range.

The relative lacunarity curves for the tracer distribution at 6 min in the Ap1 horizon and the two boundaries were almost linear (Fig. 5-6b), again suggesting the existence of self-similarity over a given size range. In the Ap2 and Bt horizons, the RLF’s for the tracer distribution at 6 min were markedly convex (Fig. 5-6b), reflecting a higher degree of clumping of the tracer in and around the large bio-pores and the occurrence of apparent preferential flow (Fig. 5-4b). The relative lacunarities for the tracer distribution at 78 min generally decreased with more advection and diffusion time (Fig. 5-6c). The RLF of the tracer distribution at 78 min in the Ap1 horizon became concave as more tracer moved into smaller pores (Figs. 5-6c and 5-4c). The relative lacunarity curve for the tracer distribution in the Ap2 and Bt horizons was close to linear with more pores being filled with the tracer. This suggests more similarity to a true fractal in the spatial organization of the solute. Overall,
the RLFs for the tracer distributions at 6 min and 78 min were closer to an ideal fractal than those of
the macropores within the range of cube sizes investigated.

The integrations of the RLFs in 2-D and 3-D are presented in Table 5-2. Interestingly, the
integration of the RLF for the image with small randomly distributed pores was equal to unity. The
integration of the RLF quantifies the overall level of relative lacunarity and is sensitive to the size
distribution of macropores and degree of clustering or clumping of the tracer distribution. The
integrations of the RLFs for the macropores were positively correlated with the mean hydraulic radius
(Table 5-3). Accordingly, the integrations of the RLF for the macropores in the Ap2 horizon were the
highest among the five positions scanned, 2.72 in 2-D and 2.61 in 3-D, which corresponded to the
largest mean hydraulic radius (0.039 mm) among the five positions. The integrations of the RLFs for
the tracer distribution at 6 min were higher than those for the tracer distribution at 78 min,
corresponding to the clustering of the tracer in and around large bio-pores at early times. The
integrated RLF parameter is a helpful index to evaluate the degree of the preferential flow and solute
transport in different soils with similar flow conditions.

Two-dimensional RLFs for the macropore network and tracer distribution were very close to the
3-D values within the same size range (≤ 63) (Fig. 5-6 and 5-7). However, the statistical difference of
the integration of the RLF in 2-D and 3-D was significant at the 0.01 probability level because the 2-D
relative lacunarities were slightly but consistently greater than 3-D values for both the macropore and
the tracer distribution at 6 and 78 min (Table 5-2). According to the lacunarity curves, the REV had
not been reached for the 3-D macropore networks within the size range investigated (cube size ≤ 63)
probably because of their high heterogeneity (Fig. 5-6). However, the REV might have been met for
the 2-D macropore network, especially for the Ap1 horizon since the relative lacunarity decreased
towards zero at the point where ln(box size) was equal to 5.8 (i.e., box-size = 330, or 26 mm) and remained very low afterwards (Fig. 5-7). Table 5-3 also shows a strong negative linear correlation between the fractal dimension and the integration of RLF in both 2-D and 3-D. Armatas et al. (2002) found a similar relationship between the fractal dimension and the lacunarity. More research, however, is needed to investigate whether such a relationship exists for other soils.

**Summary and conclusion**

Soil macropore structure and tracer transport in real-time were reconstructed using an industrial CT at five representative positions of an intact structured soil column (i.e., Ap1, Ap2, Bt horizons, and their boundaries). Each position in the soil column displayed a different macropore characteristic and flow pattern. The earthworm burrows and root channels were highly effective in facilitating water flow and tracer transport because of their high continuity and low resistance. Macropore volume, mean pore hydraulic radius, fractal dimension, and relative lacunarity curves in 2-D and 3-D were computed from the CT images. The results demonstrated the dominant control of macroporosity on flow and transport under the “satiated” experimental conditions used in this study. Positive logarithmic trends were found between the fractal dimensions in either 2-D or 3-D and the volume percentage of macropores and tracer distribution. There was no statistically significant difference between the fractal co-dimensions in 2-D and 3-D. The RLFs of the macropore network and the tracer distribution over time varied with soil depth. The tracer distributions over time were closer to true fractals than the macropore networks based on their RLFs. The 3-D relative lacunarities were slightly lower than the 2-D values.
Overall, the lacunarity has several positive attributes: 1) the lacunarity function is sensitive to structural differences and reflects the size and spatial distribution of the features - it thus has the potential to differentiate one type of structure or pattern from another; 2) the lacunarity function, rather than one single value (e.g., a fractal dimension), can be calculated to obtain size dependent information; 3) the lacunarity parameter can be applied to both fractal and non-fractal features; 4) lacunarity is helpful in determining if self-similarity exists and if a REV for a porous media can be defined; and 5) the algorithm used to calculate the lacunarity is simple to implement. Since the lacunarity is scale-dependent, caution is needed when comparing structures at different image resolutions. The relationship between the fractal dimension and lacunarity is worthy of further study. In particular, the lacunarity functions may be coupled with fractal parameters, as indicated in Eq. 1, to better model heterogeneous soil structural functions.

References


Table 5-1 Basic soil properties of the soil column studied. The number in parentheses is one standard deviation.

<table>
<thead>
<tr>
<th>Horizon</th>
<th>Depth</th>
<th>Organic matter</th>
<th>Sand</th>
<th>Silt</th>
<th>Clay</th>
<th>Ksat-core(^a)</th>
<th>Bulk density</th>
<th>Total porosity</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>cm</td>
<td>%</td>
<td>%</td>
<td>%</td>
<td>%</td>
<td>cm/min</td>
<td>g/cm(^3)</td>
<td>m(^3)/m(^3)</td>
</tr>
<tr>
<td>Ap1</td>
<td>0-11</td>
<td>4.5</td>
<td>19.3</td>
<td>64.8</td>
<td>15.9</td>
<td>0.051 (0.032)</td>
<td>1.43 (0.03)</td>
<td>0.46</td>
</tr>
<tr>
<td>Ap2</td>
<td>11-21</td>
<td>3.5</td>
<td>17.1</td>
<td>68.1</td>
<td>14.8</td>
<td>0.045 (0.114)</td>
<td>1.50 (0.06)</td>
<td>0.43</td>
</tr>
<tr>
<td>Bt</td>
<td>21-26+</td>
<td>1.9</td>
<td>22.9</td>
<td>51.7</td>
<td>25.4</td>
<td>0.035 (0.041)</td>
<td>1.61 (0.04)</td>
<td>0.39</td>
</tr>
</tbody>
</table>

\(^a\)Ksat-core is saturated hydraulic conductivity
Table 5-2 Properties of soil macropore networks and solute distributions in the soil column studied. The number in parentheses is one standard deviation, and $r^2$ is the coefficient of determination (i.e., the goodness of fits associated with the estimation of the fractal dimensions).

<table>
<thead>
<tr>
<th></th>
<th></th>
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<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Macroporosity (%)</td>
<td>12.37</td>
<td>11.61</td>
<td>3.58</td>
<td>4.07</td>
<td>4.11</td>
</tr>
<tr>
<td>Entrapped air (%)</td>
<td>2.20</td>
<td>1.45</td>
<td>0.34</td>
<td>0.16</td>
<td>0.55</td>
</tr>
<tr>
<td>Mean hydraulic radius (mm)</td>
<td>0.026</td>
<td>0.026</td>
<td>0.039</td>
<td>0.033</td>
<td>0.037</td>
</tr>
<tr>
<td>Tracer volume at 6 min (%)</td>
<td>7.79</td>
<td>4.73</td>
<td>1.53</td>
<td>3.37</td>
<td>2.59</td>
</tr>
<tr>
<td>Tracer volume at 78 min (%)</td>
<td>41.43</td>
<td>No data</td>
<td>7.59</td>
<td>11.67</td>
<td>8.04</td>
</tr>
<tr>
<td>Mean fractal dimension in 2-D (macropores)</td>
<td>1.52(0.04) $r^2$=0.99</td>
<td>1.41(0.03) $r^2$=0.99</td>
<td>1.26(0.05) $r^2$=0.98</td>
<td>1.23(0.03) $r^2$=0.99</td>
<td>1.26(0.01) $r^2$=0.98</td>
</tr>
<tr>
<td>Mean fractal dimension in 2-D (tracer at 6 min)</td>
<td>1.32(0.08) $r^2$=0.99</td>
<td>1.20(0.05) $r^2$=0.99</td>
<td>1.17(0.06) $r^2$=0.96</td>
<td>1.12(0.07) $r^2$=0.98</td>
<td>1.15(0.01) $r^2$=0.97</td>
</tr>
<tr>
<td>Mean fractal dimension in 2-D (tracer at 78 min)</td>
<td>1.75(0.04) $r^2$=1</td>
<td>No data</td>
<td>1.35(0.05) $r^2$=0.99</td>
<td>1.40(0.04) $r^2$=0.99</td>
<td>1.33(0.01) $r^2$=0.99</td>
</tr>
<tr>
<td>Fractal dimension in 3-D (macropores)</td>
<td>2.61 $r^2$=0.991</td>
<td>2.47 $r^2$=0.993</td>
<td>2.23 $r^2$=0.990</td>
<td>2.28 $r^2$=0.987</td>
<td>2.26 $r^2$=0.981</td>
</tr>
<tr>
<td>Fractal dimension in 3-D (tracer at 6 min)</td>
<td>2.41 $r^2$=0.987</td>
<td>2.26 $r^2$=0.989</td>
<td>2 $r^2$=0.990</td>
<td>2.14 $r^2$=0.983</td>
<td>2.03 $r^2$=0.988</td>
</tr>
<tr>
<td>Fractal dimension in 3-D (tracer at 78 min)</td>
<td>2.86 $r^2$=0.996</td>
<td>No data</td>
<td>2.35 $r^2$=0.997</td>
<td>2.50 $r^2$=0.996</td>
<td>2.37 $r^2$=0.997</td>
</tr>
<tr>
<td>Integration of RLF in 2-D (macropores)</td>
<td>1.94</td>
<td>2.38</td>
<td>2.72</td>
<td>2.42</td>
<td>2.64</td>
</tr>
<tr>
<td>Integration of RLF in 2-D (tracer at 6 min)</td>
<td>2.10</td>
<td>2.50</td>
<td>3.11</td>
<td>2.62</td>
<td>2.92</td>
</tr>
<tr>
<td>Integration of RLF in 2-D (tracer at 78 min)</td>
<td>1.70</td>
<td>No data</td>
<td>2.77</td>
<td>2.52</td>
<td>2.76</td>
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<tr>
<td>Integration of RLF in 3-D (macropores)</td>
<td>1.69</td>
<td>2.13</td>
<td>2.61</td>
<td>2.19</td>
<td>2.54</td>
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<tr>
<td>Integration of RLF in 3-D (tracer at 6 min)</td>
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<td>2.33</td>
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<td>2.82</td>
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<tr>
<td>Integration of RLF in 3-D (tracer at 78 min)</td>
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<td>No data</td>
<td>2.66</td>
<td>2.36</td>
<td>2.64</td>
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Table 5- 3 The Pearson correlation coefficient between different soil properties investigated in this study. Values of probability are indicated using three significance levels (** < 0.01, * < 0.05, NS > 0.05).

<table>
<thead>
<tr>
<th>Soil Properties</th>
<th>#</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
<th>11</th>
<th>12</th>
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<tr>
<td>Macroporosity (%)</td>
<td>1</td>
<td></td>
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<td></td>
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</tr>
<tr>
<td>Mean hydraulic radius (mm)</td>
<td>2</td>
<td>-0.94*</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td>Tracer volume at 6 min (%)</td>
<td>3</td>
<td>0.89*</td>
<td>-0.89*</td>
<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>Tracer volume at 78 min (%)</td>
<td>4</td>
<td>1.00**</td>
<td>NS</td>
<td>0.98*</td>
<td></td>
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<td></td>
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<td></td>
</tr>
<tr>
<td>Fractal dimension in 3-D (macropores)</td>
<td>5</td>
<td></td>
<td>-0.92*</td>
<td>0.97**</td>
<td>0.98**</td>
<td></td>
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</tr>
<tr>
<td>Fractal dimension in 3-D (tracer at 6 min)</td>
<td>6</td>
<td>0.92*</td>
<td>-0.95*</td>
<td>0.98*</td>
<td>0.98*</td>
<td>0.98**</td>
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<tr>
<td>Fractal dimension in 3-D (tracer at 78 min)</td>
<td>7</td>
<td>0.97*</td>
<td>-0.98*</td>
<td>0.99**</td>
<td>0.99*</td>
<td>0.98*</td>
<td>1.00**</td>
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<tr>
<td>Integration of RLF in 2-D (macropores)</td>
<td>8</td>
<td>NS</td>
<td>NS</td>
<td>-0.99**</td>
<td>-0.97*</td>
<td>-0.93*</td>
<td>-0.97**</td>
<td>-1.00**</td>
<td></td>
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<tr>
<td>Integration of RLF in 2-D (tracer at 6 min)</td>
<td>9</td>
<td>NS</td>
<td>0.92*</td>
<td>-0.98**</td>
<td>NS</td>
<td>-0.93*</td>
<td>-0.98**</td>
<td>-0.98*</td>
<td>0.98**</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Integration of RLF in 2-D (tracer at 78 min)</td>
<td>10</td>
<td>-0.98*</td>
<td>0.97*</td>
<td>-0.99*</td>
<td>-0.99**</td>
<td>-0.99*</td>
<td>-0.99**</td>
<td>-1.00**</td>
<td>0.99*</td>
<td>0.96*</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>Integration of RLF in 3-D (macropores)</td>
<td>11</td>
<td>NS</td>
<td>0.90*</td>
<td>-0.97**</td>
<td>NS</td>
<td>-0.92*</td>
<td>-0.98**</td>
<td>-0.99*</td>
<td>0.99**</td>
<td>0.99**</td>
<td>0.97*</td>
<td></td>
<td></td>
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<tr>
<td>Integration of RLF in 3-D (tracer at 6 min)</td>
<td>12</td>
<td>NS</td>
<td>0.93*</td>
<td>-0.98**</td>
<td>-0.95*</td>
<td>-0.94*</td>
<td>-0.99**</td>
<td>-0.98*</td>
<td>0.98**</td>
<td>1.00**</td>
<td>0.97*</td>
<td>0.99**</td>
<td></td>
</tr>
<tr>
<td>Integration of RLF in 3-D (tracer at 78 min)</td>
<td>13</td>
<td>-0.98*</td>
<td>0.97*</td>
<td>-0.99*</td>
<td>-0.99**</td>
<td>-0.99*</td>
<td>-1.00**</td>
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<td>0.97*</td>
<td>1.00**</td>
<td>0.98*</td>
<td>0.98*</td>
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</table>

* Since the difference between the fractal co-dimensions in 2-D and 3-D was not significant, only fractal dimensions in 3-D were included here. The number in the first row represents the corresponding properties in the first column with the same number.
Figure 5-1 A digital radiograph of the intact soil column investigated in this study.

The higher the soil density, the darker the image. Two earthworm borrows are clearly noticeable that originated in Ap1, passing the plow-pan of Ap2 and into Bt horizon.
Figure 5-2  a) The industrial CT unit used in this study and the position of the soil column used in the experiment. b) The experimental setup used to scan the five positions in the soil column while solute transport experiment was being conducted simultaneously.
Figure 5-3 Lacunarity curves for images with the same size (216 × 216 pixels), the same fraction (p = 0.5), but different patterns (i.e., small-, middle-, and large-size features, hierarchy with three size levels and similar to fractals) (modified from Plotnick et al., 1993).
Figure 5- 4 A 3-D visualization of the five scanned positions in the soil column: a) macropores at satiated condition before tracer experiment (yellow color indicates water-filled pores and blue color indicates air-filled pores), b) tracer distribution (in pink color) at 6 min, and c) tracer distribution (in pink color) at 78 min. Note that the tracer distribution at 6 min in the Ap1 horizon was partly overlapped by the macropores and thus cannot be clearly seen.
Figure 5-5 The relationship between the fractal dimension of the macropores (in the pink color) and tracer distributions (in the blue color) in 2-D or 3-D and the volume percentage of the macropores and tracer distributions.

\[
y = 0.2687 \ln(x) + 1.8488 \\
R^2 = 0.9619 \\
y = 0.1903 \ln(x) + 0.9723 \\
R^2 = 0.8826
\]
Figure 5-6 Log-log plot of 3-D relative lacunarities vs. gliding cube size for a) macropore network, b) tracer distribution at 6 min, and c) tracer distribution at 78 min. Also shown in (a) are the RLFs for the third-iteration prefractal of Menger sponge (labeled as fractal) and for the image with small randomly-distributed pores (labeled as random).
Figure 5-7 Log-log plot of 2-D relative lacunarities vs. gliding box size for a) macropore network, b) tracer distribution at 6 min, and c) tracer distribution at 78 min.
Chapter 6

QUANTIFICATION OF SOIL STRUCTURE AND PREFERENTIAL FLOW IN AN INTACT SOIL COLUMN USING INDUSTRIAL X-RAY CT

Abstract

Quantification of soil structure and its impacts on solute transport is essential to understand complex preferential flow processes. Computed tomography (CT) provides a nondestructive means of observing soil structure and monitoring solute breakthrough in real-time. I investigated an intact soil column 10-cm in diameter and 30-cm in length using an industrial CT with a resolution of 105.5 µm×105.5 µm×125.25 µm. The satiated soil column was scanned to obtain overall soil structure. Then 60 g/L KI solution was injected at 6.6 ml/min for about 23 hours and the solute transport process was monitored in real-time by scanning two critical positions in the column and taking digital radiographs (DRs). At the end of transport process, the whole column was scanned again to obtain the overall solute mass distribution. The voxel-based soil porosity and solute tracer concentration were quantified using a simplified method. The 3-D visualization of the pore network and solute tracer distributions over time showed that both the pore network and the flow pattern varied considerably with soil depth, in part due to the soil horizonation and different macropores involved. Although the total macroporosity below the Ap1 horizon was much lower, macropores were more continuous and less tortuous as a result of limited agricultural disturbance and more natural influence from earthworm burrows. However, only part of the macropores, especially the highly continuous biogenetic macropores (earthworm burrows and
root channels) at the subsurface were effective in transporting the solute. The results from the DRs and the CT images revealed a sequential initialization of the transport process from the macropore domain to the matrix domain and a decreased degree of interaction between the two domains with soil depth. Point-specific breakthrough curves were obtained from real-time point-specific solute concentration and porosity, from which point-specific pore velocity was determined. This study illustrates that preferential flow pathways in the intact structured soil consist of a complex network of earthworm burrows, root channels, inter-aggregate macropores, and mesopores or even micropores in the soil matrix. Modeling of this flow network and its dynamics would require a new approach different from the classical continuous-domain approach.
Soil structure is critical to water movement and solute transport, as bypass flow along soil structural units (such as inter-pedal macropores or wormholes) can move chemicals preferentially to a deeper depth at a faster rate (Beven et al., 1982; Chen et al., 1992; Perret et al., 2000). Although constituting only a small percentage of total soil porosity, macropores may dominate near-saturated flow flux under certain circumstances (Luxmoore et al., 1990). In such cases, traditional models of water movement and solute transport for homogeneous soils do not provide adequate description of the processes involved. Various models for estimating water flow and solute transport in structured soils have been developed. Feyen et al. (1998) reviewed both deterministic and stochastic approaches to quantitatively describe water flow and solute transport in heterogeneous soils. Šimunek et al. (2003) reviewed and compared existing deterministic models to estimate preferential or non-equilibrium flow and transport in the vadose zone. These models include the dual-porosity model (van Genuchten et al., 1976), the dual-permeability model (Gerke et al., 1993), the multi-region model (Gwo et al., 1995), and the kinematic wave model (Germann et al., 1985), and others. However, preferential flow dynamics and their relation to soil structure have not yet been fully understood, prohibiting reliable estimate of water flow and solute movement in structured soils. Beven and Germann (1982) stated that data on the structure of macropore systems, the nature of macropore flow, and the interactions between macropores and matrix were extremely lacking. This lack of detailed and quantitative relationships between soil structure (including macropores) and preferential flow dynamics continues even today (Lin et al., 2005; Šimunek et al., 2003; Köhne and Mohanty, 2005)
It is recognized that experimental measurement and accurate quantification of soil structure and preferential flow pose significant challenges. Traditionally, soil structure has been described by pedologists using *in situ* morphological descriptions or thin sections in the laboratory, and by soil physicists using wet and dry sieving to measure the percentage of water-stable aggregates. However, these methods cannot provide an adequate surrogate for undisturbed structure (Young et al., 2001). On the other hand, the pore network, especially pore size distribution and connectivity are believed to control soil hydraulic properties (Vogel et al., 2000; Perret et al., 2000; Pierret et al., 2002). Research in the linkage between undisturbed soil structure and real-time flow dynamics is needed.

Destructive methods have been used to observe preferential flow, particularly in combination with various dye tracers (Feyen et al., 1999; Flury and Wai, 2003). Indirect methods of collecting leachate through the soil either by gravity (e.g., zero-tension pan lysimeters) or by applying a capillary suction (e.g., wick lysimeters) have also been used to study preferential flow (Boll et al., 1997; Hangen et al., 2005; Schmidt and Lin, 2008), in which breakthrough curve measurements have certain important implications regarding solute transport in the soil. These methods, however, can not offer detailed information regarding flow and transport pathways and patterns, their spatial-temporal organizations, and their direct relationship with soil structural features.

In recent years, CT has provided an attractive tool for soil scientists to non-invasively observe soil structure (Warner et al., 1989; Gantzer and Anderson, 2002; Perret et al., 1999) and solute transport (Anderson et al., 1992; Peyton et al., 1994; Heijs et al., 1995; Perret et al., 2000). Three-dimensional (3-D) visualization and quantification of soil macropores has been realized by synthesizing a series of 2-D CT images using certain algorithms (Capowiez et al. 1998; Pierret et al. 2002; Perret et al. 1999). Although CT was initially intended for viewing still images of scanned objects nondestructively, it can also be used to monitor changes of a process with time if repeated imaging is conducted over certain time intervals.
quantified the solute transport through glass beads using an industrial micro-focus CT at a resolution of 86 µm. Perret et al. (2000) applied medical CT to isolate the soil matrix and macropore domains and monitored solute transport for 13 different locations within an intact soil column (7.7 cm in diameter and 85 cm in length). Anderson et al. (1992, 2003) developed a procedure to determine voxel porosity, breakthrough curve, and pore water velocity with small soil cores (7.6 cm in diameter and 7.6 cm in length) using a medical CT. However, this approach requires a full replacement of water with solute tracer, a difficult process for large soil columns, especially when the soils are fine-textured, have heterogeneous structure, or contain low permeable layers.

Most of the published work has relied on medical CT, which has a limited spatial resolution (typically in the order of 1 mm) and a configuration that may prohibit vertical leaching experiments with large soil columns (Clausnitzer et al., 2000). The industrial CT scanner, on the other hand, has a higher resolution of down to ~5 µm, and can be combined with real-time solute transport experiments using intact soil columns large enough to observe and quantify the dynamics of water, air, and solid interactions.

The objectives of this study were to use high-resolution industrial CT to 1) reconstruct 3-D soil structure in a relatively large intact soil column, and 2) to quantify preferential tracer transport in real-time and its dynamic relationships with soil structure (including various macropores). I used a combination of two techniques to quantify soil structure and real-time solute transport: a high-resolution industrial CT and digital radiograph (DR). The DR is another X-ray imaging technique that allows fast image collection and thus has great potential to observe flow processes effectively. It has been used to examine bulk density profile of soil surface crusts (Bresson et al. 2004) and water movement through the soil (Maruyama et al. 2003). By directly observing and quantifying real-time solute transport in naturally-structured soils with clear horizonation, as demonstrated in this study, I hope to understand better and
quantify the impacts of soil structure and layering on preferential flow and solute transport in an important agricultural soil, leading to new ways of modeling and prediction.

**Methodology**

**The Soil Studied**

Intact soil columns, 10 cm in diameter and 30 cm in height, were taken from The Pennsylvania State University’s R.E. Larson Agricultural Research Center at Rock Springs in Centre County, Pennsylvania. The soil series is mapped as a Hagerstown silt loam (*fine, mixed, semiactive mesic Typic Hapludalf*) and the solum extends to more than 1 m. This is an important agricultural soil in the Ridge and Valley Physiographic region of Pennsylvania. The sampled field has been in no-till since 1995 in a corn, soybean, and alfalfa rotation. All plant residues were left in the field after each harvesting. A backhoe was used to carefully push Polyvinyl chloride (PVC) pipes (10-cm inside diameter, 0.6-cm wall thickness) vertically and gradually into the soil. Five soil columns were collected and the one with the least possible disturbance due to sampling (based on multiple DRs taken at different angles of the columns, see Fig. 6-1) was selected for our experiment. The collected soil columns contained three soil horizons, each with a different structure and bulk density (Fig. 6-1 and Table 6-1). Six small soil cores (5.5-cm diameter and 6.0-cm height) were also taken for each horizon to measure basic soil properties, including bulk density, organic matter content, texture, and saturated hydraulic conductivity (Table 6-1).
Industrial CT

An industrial CT unit (OMNI-X model, Bio-Imaging Research, Inc., Lincolnshire, IL) was used for this experiment. This CT unit is a third generation scanner, where the source and detector are fixed and the scanned object rotates (Fig. 6-2). The system has a 225 KV micro-focus X-ray generator and a 225-mm-diameter image intensifier. The highest resolution that can be obtained by the micro-focus source is about 5 µm. The sample is rotated 360 degrees to receive X-ray beam (polychromatic) while the detector provides intensity views to the data acquisition computer. One rotation takes about 10-15 minutes, depending on the number of views taken. In this experiment, up to 41 slices were acquired in a single rotation with 2400 views. High-resolution images (1,024 x 1,024) were acquired at the output in the computer system. Besides high-resolution cross-sectional CT scans, I also collected DRs using the same industrial CT to monitor the whole column during the experiment. The DRs were taken by collecting data from a single row of detectors while vertically moving the sample (without rotating it). This avoids the vertical geometric distortion that otherwise occurs when collecting a conventional 2-D image. The DRs and cross-sectional CT scans are fundamentally different: Cross-sectional CT scans are used to obtain individual slices across the object, while the DRs reproduce a full two-dimensional projection of the whole object exposed to the X-ray and the X-ray attenuation value represents the effect of the object’s density and thickness.

Experimental Procedure

The experiment setup is shown in Fig. 6-2. The soil column contained in the PVC pipe was housed in an aluminum cylindrical container (0.6-cm wall thickness) with a flow
distributor at both ends of the soil column. A layer of filter paper was placed at the top of the soil column to distribute the solution evenly. A layer of pressure membrane (0.1-mm thick, 600-cm bubbling pressure, and 1.2-µm diameter pore, with a conductivity of 0.2647 cm/min/cm² @ 1-cm hydraulic head, Soil Measurement System, Tucson, AZ) was placed at the bottom of the soil column. A threaded cylinder was tightened at the top of the aluminum container to compress the O-ring between the PVC pipe and flow distributor and create a seal at their interface. Three capped plastic pipette tips (1-cm diameter and 1.5-ml volume) filled with a 0.005 M CaSO₄ water solution, air, and a 60 g/L potassium iodide (KI) solution, respectively, were inserted carefully into the top of the soil column to obtain their standard X-ray attenuation values (as references). The iodide solution is a non-reactive tracer that has been successfully used to observe solute transport when coupling with X-ray CT. A relatively high concentration of iodide (60 g/L) was used in the experiment to enhance the image quality (Perret et al., 2000; Clausnitzer and Hopmans, 2000). However, there may be some possible undesirable effects of introducing 60 g/L KI solution such as the density-driven flow and transport. A pressure transducer was connected to the both ends of the soil column to measure the pressure gradient throughout the experiment. An automatic fractional collector was used to collect the outlet flow at one minute interval within the first hour of the experiment and every two minutes thereafter.

The soil was satiated by pumping 0.005 M CaSO₄ solution slowly (30 ml/h) into the soil column from the bottom. When water started to flow out of the tube at the top of the soil column, the pump rate was decreased to about 6 ml/h for about 24 hours. This satiation process lasted for two days. The pressure difference between the two ends of the soil column and the flow rate were monitored to calculate the hydraulic conductivity of the entire soil column, which was 0.03 cm/min during the experiment. The whole soil column was then scanned at a resolution of 105.5 µm×105.5 µm×125.25 µm, which took 59 rotations and produced a total of 2,419 slices. Two DRs were also taken at orthogonal angles to obtain the
whole column images. After this scanning, a 0.005 M CaSO₄ solution was supplied at a constant flow rate of 6.5 ml/min (i.e., 0.08 cm/min) by pump from the top of the soil column. This flow rate was maintained throughout the experiment. When the outflow rate was constant, the 0.005 M CaSO₄ solution was replaced by a 60 g/L KI solution. After introducing KI solution for 15 minutes, the pump and the valve at the outlet tube were turned off to stop the flow. Two selected critical positions in the soil column were scanned to observe the solute distribution (Figs. 6-1 and 6-2). The first position was located at the boundary between the Ap1 and Ap2 horizons, where preferential flow was expected; the second position was at about 2 cm above the bottom end of the soil column to avoid the possible diffusion from the bottom flow distributor (Perret et al, 2000) but allowing the observation of the solute breakthrough in the Bt horizon and comparing with that measured in the Ap horizons. Each position was scanned for one rotation, with 41 slices representing a vertical thickness of 0.512 cm. In addition, two DRs were taken at orthogonal angles to obtain the whole column images. The above process took about 27 min. It was assumed that all flow processes (diffusion, dispersion, convection, etc.) stopped during this 27-min time period (i.e., the limitation of the scanning speed was overcome by stopping the flow during the scanning). After the above process, KI solution leaching was restarted and stopped again for scans at 30 min, 60 min, 90 min, 150 min, 230 min, 484 min, and 1,374 min of accumulative flow time. At 1,374 min, the whole soil column was scanned again to obtain the overall solute distribution in the column. By the end of the replacement experiment, about 9 pore volumes of the KI solution were entered into the soil. The iodide concentration in the effluent samples was measured using an iodide electrode (Thermo Orion, Waltham, MA).
Data analysis

Image analysis software AMIRA (TGS Inc., San Diego, CA) and ImageJ (Rasband, 2002) were used to analyze the data collected in this experiment.

Image segmentation

There are many but no generally-accepted definitions of a macropore (Beven et al., 1982; Chen et al., 1992; Perret et al., 1999). One main reason is that the definitions of macropores based on equivalent cylindrical diameter (ECD) are ambiguous and lack information about 3D shape and function. Pores with ECD > 1 mm have been commonly considered as macropores (Luxmoore et al., 1990; Perret et al., 1999). Ghezzehei and Or (2005) found a threshold of 0.6 mm in diameter to be a conservative upper limit for the applicability of capillary dominated by Richards’ equation. Schaap et al. (2006) analyzed 235 laboratory data from the UNSODA soil hydraulic database and suggested that pores with 0.075 and 0.75-mm ECD represented break-points of a two-element piecewise linear function between average scaled conductivities and pressure head. Notably, 0.075 mm is also the lower limit of very fine macropores defined by Brewer (1964) and adopted by the Soil Science Society of America (SSSA, 2006). It appears that the definition of macropores should consider both the data availability and the scale in which the problem is to be addressed. In this study, I considered the pores with ECD > 0.75 mm as macropores.

Each voxel (a word combining volume and pixel) may have mixed components of air, water, and solid particles. In this study, macropore network was segmented with voxel porosity large than 65% and ECD > 0.75 mm. The image data were visually inspected to
ensure that a reasonable threshold value was used based on the frequency distribution (histogram) of attenuation coefficient (Peyton et al., 1992; Hopmans et al., 1994).

Calculation of voxel porosity and solute concentration

Spatially-distributed porosity is useful to evaluate soil heterogeneity and quantify solute transport. In soils three phases (solid, water, and air) contribute to the X-ray attenuation.

When solutes in the soil water can be ignored, the X-ray attenuation value for a single voxel $CT(x, y, z)$ is:

$$CT(x, y, z) = CT(x, y, z)_{\text{solid}}[1 - \phi(x, y, z)] + CT_{\text{water}}\phi(x, y, z)S_{\text{water}} + CT_{\text{air}}\phi(x, y, z)S_{\text{air}},$$

[1]

where $CT(x, y, z)_{\text{solid}}$ is the X-ray attenuation value for the solid of a given voxel; $CT_{\text{water}}$ and $CT_{\text{air}}$ are the X-ray attenuation value for water and air, respectively; $\phi(x, y, z)$ is porosity for a given voxel; and $S_{\text{water}}$, $S_{\text{air}}$ are the saturation ratio of water and air in the voxel, respectively. The X-ray attenuation value of air, water, and 60g/L KI solution were 394, 1,271, and 1,860, respectively, based on our standards.

In order to accurately quantify porosity $\phi(x, y, z)$ for a given voxel in the soil, the optimal approach would need to scan the soil at two different conditions, being totally saturated with water and completely dried. Alternatively, the soil can be scanned at either one of the above two conditions using dual energy (Rogasik et al., 1999). However, it is very difficult for the soil to be fully saturated with water or be completely dried (filled with air) under natural conditions. Such a total saturation or dryness may also likely induce swell-shrink for the soil with high clay content (such as the one used in this study). Besides, when the soil sample needs to be scanned twice, time and cost increase.
Since the KI solution displacement starts after the soil column is satiated with water, a linear relationship between average X-ray attenuation value and iodide concentration can be established when water in the soil is substituted by the KI solution. The relative concentration of KI solution $C(x,y,z)_{rel}$ is defined as (Anderson et al., 1992):

$$
C(x,y,z)_{rel} = \frac{CT(x,y,z,t) - CT(x,y,z,t = 0)}{CT(x,y,z,T) - CT(x,y,z,t = 0)} ,
$$

where $CT(x,y,z,t)$ is the X-ray attenuation value for a voxel during breakthrough at time $t$; $CT(x,y,x,t = 0)$ is the X-ray attenuation value when the slice is satiated with water; $CT(x,y,z,T)$ is the X-ray attenuation value when soil is fully replaced by the solution.

Similarly, the porosity can be calculated as (Anderson et al., 2003):

$$
\phi(x,y,z) = \frac{CT(x,y,z,T) - CT(x,y,z,t = 0)}{CT_{KI} - CT_{water}} ,
$$

where $CT_{KI}$ is the X-ray attenuation value of a 60g/L KI solution. The above method requires 1) a full replacement of water with solute, and 2) a non-reactive solute. For a large structured soil (like the one used in this study), it was not easy to fully replace the water by solute, especially in the soil matrix.

Consequently, I used a simplified approximation in this study to determine local porosity and concentration. If I assume that 1) the soil particle is homogeneous, that is, $CT_{solid}$ is constant within a horizon; and 2) when the soil is satiated, the air bubbles are only entrapped in large pores and are big enough to be identified using the images, that is, the voxels within the air bubbles are totally pore space ($\phi = 1$), and those without air bubbles are fully filled with water ($S_{water} = 1$), then the Eq. [1] can be applied to a given horizon (multi-voxels) and written as:

$$
CT_{horizon} = CT_{solid-horizon}(1 - \phi_{horizon}) + CT_{water}(\phi_{horizon} - \phi_{air-horizon}) ,
$$
where $CT_{\text{horizon}}$ is the average X-ray attenuation value for a given horizon; $\phi_{\text{horizon}}$ is the porosity for a given horizon; and $\phi_{\text{air-horizon}}$ is the volume percentage of entrapped air within a given horizon as determined from CT images. The X-ray attenuation value of solid for a given horizon $CT_{\text{solid-horizon}}$ can be obtained by applying Eq. [4] to a region without air bubbles using known $CT_{\text{water}}$, $\phi_{\text{air}}$, and $\phi_{\text{horizon}}$. The value of $\phi_{\text{horizon}}$ can be obtained from the measured soil bulk density data. Then, voxel porosity can be calculated by applying the following equation to each voxel for a given horizon using known $CT_{\text{solid-horizon}}$ and $CT_{\text{water}}$:

$$
\phi(x,y,z) = \frac{CT_{\text{solid-horizon}} - CT(x,y,z)}{CT_{\text{solid-horizon}} - CT_{\text{water}}} \quad [5]
$$

Since a full replacement of water with solute was not obtained in this study, Eq. [2] cannot be used to obtain the relative concentration. Instead, the relative concentration for a given voxel was calculated as:

$$
C(x,y,z)_{rel} = \frac{CT(x,y,z,t) - CT(x,y,z,t = 0)}{(CT_{KI} - CT_{\text{water}})\phi(x,y,z)} \quad [6]
$$

The median filter was used to minimize the noise after subtracting the images taken at different times to quantify the solute concentration.

The first assumption stated above should be reasonable for an agricultural soil with few rock fragments, which is the case in this study. Rogasik et al. (1999) used two energy levels to calculate the phase composition, i.e., solid, water, and air, of each voxel. They implicitly assumed $CT_{\text{solid}}$ as a constant, although they also recognized that when at a micro resolution, the variation in particle density cannot be ignored. For the second assumption, water enters more easily into the smaller pore space driven by capillarity. Likewise, the air tends to be trapped in larger pores. I recognize that some air bubbles may be trapped in smaller pores. For the voxels with trapped air, porosity may be underestimated and the relative concentration may be overestimated. However, I believe our approach will give a reasonable
approximation of the overall picture of the soil structure and preferential movement of water, air, and tracer in this study.

Results and discussion

Reconstruction of soil structure, pore network, and entrapped air

Figure 6-3 shows a 3-D visualization of the spatial distribution of soil porosity determined by our simplified method, depicting macropore network and entrapped air bubbles. Several types of macropores with distinct morphology can be identified, including earthworm burrows, root channels, and inter-aggregate macropores. At the edge of the soil column, a small number of artificial fractures (parallel to the cross-section of the column) were detected. These were probably generated during the field sampling. The macropores formed by earthworm burrows and root channels were round in shape and highly continuous. Root channels were mainly distributed in the Ap1 and Ap2 horizons. Close to the boundary between the Ap1 and Ap2 horizons, root channels were more laterally extended. This is likely due to the dense platy structure of the plow pan (Ap2). Although earthworm burrows appeared in the Ap1 horizon, most of them were distributed in the Ap2 and Bt horizons. Earthworm burrows in the soil studied were vertically-oriented. Some parts of the burrows were refilled with loose soils. In contrast, the inter-aggregate pores were more randomly distributed in the soil and less continuous. It is also clear from Fig. 6-3 that there was no a single continuous macropore running from the top to the bottom of the soil column; instead, there was a complex network of macropores of varying sizes and continuities. Such a macropore network has critical impacts on flow and transport processes (discussed in the next section).
The relative frequency distribution of voxel porosity, that is, the percentage of voxels with the porosity in a certain range, is showed in Fig. 6-4 for each of the three soil horizons. Voxels with the porosity from 35% to 55% dominated all three horizons (Fig. 6-4). The overall macroporosity in this soil column decreased dramatically from about 15% at the surface to about 2% at 4 cm depth, which is about the sowing depth in this soil (Fig. 6-5). Soil macroporosity then changed little (though with variation) with depth until reaching the Bt horizon, where macroporosity increased slightly to over 2% (Fig. 6-5). Although the total macroporosity decreased in the Ap2 and Bt horizons, macropores in these two subsurface horizons were more vertically continuous (Fig. 6-3).

Air was found to be entrapped more frequently at the top end of highly continuous macropores, and in less continuous or isolated macropores in the Ap2 and Bt horizons, as well as in some artificial fractures along the column edge (Figs. 6-3 and 6-6). From Fig. 6-6a, I can see that the ratio of macropores filled with air increased with soil depth. The entrapped air made up 9.8%, 11.5%, and 18.5% of the macropore volume in the Ap1, Ap2, and Bt horizons, respectively. Thus, the hydraulic conductivity measured under this condition is indeed “quasi-saturated” or “saturated” (meaning not 100% of pore space filled with water). Earlier studies by Faybishenko (1995), Chapuis (2004), and Sakaguchi et al. (2005) showed that entrapped air could occupy up to 15% of the bulk soil volume and greatly influenced hydraulic conductivity. Faybishenko (1995) described three stages in temporal behavior of entrapped air and quasi-saturated soil hydraulic conductivity, and proposed a power law and an exponential relationship to describe quasi-saturated hydraulic conductivity as the function of the entrapped air content. However, further research is need on how air is entrapped and changed under different conditions and how to precisely determine the amount of entrapped air in a complex soil pore network.
Quantification of solute transport and entrapped air

The effluent breakthrough curve showed a quick response when the tracer was first introduced and a very long tail, indicating the occurrence of preferential flow and a gradual interaction between the macropore and the matrix domains (Fig. 6-7). The relative concentration of the effluent quickly reached 50% after 60 min but after 200 min the relative concentration increased very slowly. Even after 1,374 min, the water was not completely replaced by the tracer (99.7% relative concentration).

The solute transport over time within the whole soil column can be obtained by subtracting the DRs taken at different times during the experiment (Fig. 6-8). The change of X-ray attenuation value along depth is linearly correlated to the solute mass distribution along the soil column. In the soil column studied, the change of the X-ray attenuation value decreased rapidly in the top 3 cm and decreased more slowly and nearly linearly from 3 cm to the top of the Bt horizon, and then remain relatively constant in the Bt horizon (Fig. 6-8).

An exponential relationship was found between the change of average X-ray attenuation value of the DRs and the relative concentration of effluent solute tracer (Fig. 6-9). This relationship was used to quantify the solute transport processes (Figs. 6-10 and 6-11). As visualized in Figs. 6-10 and 6-11, the solute moved preferentially through cracks at the surface at the beginning, and then quickly reached some macropores in the subsurface. Some earthworm burrows and root channels were highly active in solute transport because of their high continuity and low tortuosity. Once the downward preferential flow had been initiated, lateral expansion of the solute from the preferential flow pathways to the surrounded matrix started. After 230 min, the main preferential flow pathways were almost fully filled the KI solution (Fig. 6-11). The gradual lateral expansion then started to dominate the transport process, even though vertical movement of solute could still be detected (Fig. 6-11). Even after about 23 hours (1,374 min), pores in the soil matrix were still not completely replaced.
by the KI solution, especially in the Bt horizon. Since the DR is a 2-D projection of the soil column exposed to X-ray, the pixel-based concentration was the overlapped effect of solute transport in the soil along a line at a given depth. Thus caution should be exercised when linking the results from the 2-D DR images to the 3-D soil structure and solute distribution. The accuracy of the quantified relative concentration using the DRs is therefore limited. Nevertheless, the DR is still an effective and economical means to nondestructively and quickly observe and quantify the solute transport in real-time along the entire soil column.

Time series data of the two CT scanned key positions (12.0-cm and 27.2-cm depth) provided the details about how macropores and the matrix interacted during the solute transport (Fig. 6-12). At the 12-cm depth, the solute tracer preferentially moved through some root channels and earthworm burrows. However, preferential flow also occurred in some areas without obvious macropores at the 12-cm depth (Fig. 6-12). There were highly continuous and effective macropores below them, suggesting the impact of large continuous macropores on the soil below the 12-cm depth. Because of the higher porosity in the upper portion of the soil column and longer interaction time, there was a higher degree of interaction between the macropore and the matrix domains than that at the lower portion of the soil column. Compared to the upper position, the tracer showed up first in continuous root channels and earthworm burrows at the 27.7-cm depth. Even though some macropores contained trapped air, flow still occurred along these openings. In contrast, even without entrapped air, some macropores in the subsurface horizon were not active in the solute transport (Fig. 6-12). Similarly, Luxmoore et al. (1990) showed that not all macropores were hydrologically active in the forest watershed that they studied.

After dividing the soil into the matrix and the macropore domains, breakthrough curves (BTC) of the macropore and the matrix domains were calculated using the time series of CT images at the two scanned positions (Fig. 6-13). The BTCs for both the macropore and the matrix domains at the two scanned positions were below the measured effluent BTC,
indicating that the flux concentration was greater than the resident concentration and the presence of preferential flow (Zhang et al., 2006). The deviation of these calculated BTCs from the actual effluent BTC implies that the macropore network in itself can not be simply considered as preferential flow pathways. It is the hydrologic connectivity of macropores that is essential. Compared to the scanned position at the 12-cm depth, macropore and matrix BTCs for the 2nd scanned position were further apart (Fig. 6-13), suggesting that more pronounced preferential flow occurred in the deeper soil.

Figure 6-14 shows breakthrough curves at selected specific points (5×5 voxels in the scanned cross-section of the position at the 27.8-cm depth). Point 1 represents a macropore; Point 2 was between a macropore and the matrix (i.e., interface); while Points 3 and 4 represented the soil matrix. Sequential initialization of solute transport at these three types of positions was observed. The concentration decrease occurred at Point 2 and 4 could have resulted from the noise. With the voxel-based BTC, the solute travel time to a voxel could be determined. The solute travel time to a voxel was considered the time when relative concentration was equal to 0.5 (Anderson et al., 1992). A velocity was calculated using the travel time and the vertical distance from the soil surface. The pore velocity differed considerably for different points. For Point 1, 2, and 3 in Fig. 6-14, the pore velocities were 0.68, 0.47, and 0.06 cm/min, respectively. For Point 4, the concentration never reached 50%, so the velocity is < 0.02 cm/min.

The 3-D visualization of the solute mass distribution at 1,374 min displayed a pattern similar to that revealed by the DRs, that is, the solute distribution in the Ap1 was more evenly distributed while that in the Ap2 and Bt horizons were more heterogeneous or preferentially oriented (Fig. 6-15). Such a pattern matches with the conceptualization of preferential flow zones in a soil profile, as suggested by Fluhler et al. (1996) and Kim et al. (2005), that is, there is a distribution or an induction zone near the soil surface and a conveyance or transmission zone below it. The overall match between the DR (Figs. 6-10 and
and the CT images also demonstrated the usefulness of the DR imaging technique as used in this study.

Entrapped air movement was observed during the solute transport process in this study. During the entire experiment, some entrapped air bubbles gradually decreased in size over time, and some disappeared eventually (e.g., comparing Figs. 6-6c and 6-14). There was an obvious relationship between the elapsed time and the reduced air volume in the soil column. The air volume reduction also varied with the soil depth. Air volume percentage decreased 60.3% in the Ap1 horizon, 52.6% in the Ap2 horizon, and 24.6% in the Bt horizon during the 23 hour experiment. Some localized increase in air volume in the subsurface indicated a downward movement of air. With the differential pressure transducer data, I found the pressure difference between the two ends of soil column decreased by about 10% from the beginning to the end of our experiment. Experimentally, vacuum or carbon dioxide (CO₂) could be used to reach a more fully-saturated state and avoid the complexity of flow with trapped air. However, I believe that our experiment reflects the natural flow condition in the field as air is often entrapped by natural rainfall or irrigated water and thus influences flow and transport processes in field soils.

**Summary and Conclusion**

High-resolution industrial CT has allowed reconstruction, visualization, and quantification of soil structure and solute transport in a relatively large intact soil column. Besides cross-sectional scans, DR is also shown to be an effective tool to nondestructively characterize solute transport in real-time when combined with a solute tracer. The potential of DR has been underutilized in the past CT related research.
Different kinds of macropores with distinct morphology (such as earthworm burrows, root channels, and inter-aggregate macropores) and their different functions in solute transport were observed, which varied with soil depth/horizon. Only portions of the macropores, especially the highly continuous biogenetic macropores at the subsurface, were active in transporting the solute, in part because of entrapped air that made up 9.8%, 11.5%, and 18.5% of the macropore volume in the Ap1, Ap2, and Bt horizons, respectively. Air movement was also observed during the flow and transport process in the quasi-saturated flow condition. Voxel-based breakthrough curves determined with real-time solute transport data can be further used to infer local solute dispersion parameters and test current models such as dual-permeability models, and to estimate water flow and solute transport in heterogeneous soils.

This study illustrates the complex nature of preferential flow dynamics in a structured soil. Preferential flow pathways in the intact structured soil consist of a complex network of various macropores, including earthworm burrows, root channels, inter-aggregate macropores, and even mesopores or micropores in the soil matrix. No macropores were continuous from the top to the bottom of the soil column, and some macropores were not effective to flow and transport due to air entrapment and/or hydrologic discontinuity. This result is similar to the in situ finding of Noguchi et al. (1999) who found that about 70% of the macropores (≥ 2 mm) were discontinuous (dead-end) in a 8-cm long section in a forest hillslope and only 1% of all macropores were continued for 40 cm. Therefore, the macropore network by itself can not simply be equated to a preferential flow network. Based on field investigations, including tracer tests, Sidle et al. (2000) considered preferential flow systems in natural soils to consist of more than simply interconnected macropore elements. They proposed the concept of linking individual short macropores via a series of nodes, which may be switched off or on and expand or shrink depending on local soil and antecedent moisture conditions.
conditions. Such a concept may lead to a new way of modeling and predicting preferential flow dynamics in relation to soil structure in the real world.

References


Table 6-1 Basic soil properties of the soil column studied.

<table>
<thead>
<tr>
<th>Horizon</th>
<th>Depth (cm)</th>
<th>Horizon Boundary</th>
<th>Organic matter content (%)</th>
<th>Soil particle size distribution (%)</th>
<th>Root</th>
<th>Soil structure</th>
<th>Ksat (cm/hr)</th>
<th>Bulk density (g/cm³)</th>
<th>Total porosity (m³/m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ap1</td>
<td>0-12</td>
<td>Clear smooth</td>
<td>4.5</td>
<td>19.3 64.8 15.9</td>
<td>many fine and common medium roots</td>
<td>moderate medium subangular blocky</td>
<td>3.1</td>
<td>1.43</td>
<td>0.46</td>
</tr>
<tr>
<td>Ap2</td>
<td>12-23</td>
<td>Abrupt smooth</td>
<td>3.5</td>
<td>17.1 68.1 14.8</td>
<td>common fine and few medium roots</td>
<td>moderate coarse platy</td>
<td>2.7</td>
<td>1.50</td>
<td>0.43</td>
</tr>
<tr>
<td>Bt</td>
<td>23-30+</td>
<td>-</td>
<td>1.9</td>
<td>22.9 51.7 25.4</td>
<td>common fine roots</td>
<td>moderate medium subangular blocky</td>
<td>2.1</td>
<td>1.61</td>
<td>0.39</td>
</tr>
</tbody>
</table>
Figure 6-1 The soil profile (a) and the digital radiograph (DR) (b) of the intact soil column studied. Three soil horizons and their boundaries (black dashed lines), along with two selected scanning positions (red double lines), are indicated. In the DR, earthworm burrows are visible (light color channels).
Figure 6-2 The CT equipment set up showing a) the actual aluminum containment cylinder, inflow tube, and X-ray source and detector, and b) the diagram of the setup used for the solute transport experiment.
Figure 6-3  A 3-D visualization of a) the overall soil column porosity (%) determined by the simplified method, along with entrapped air bubbles (in pink), and b) the segmented macropore network (porosity >65%) in the soil column.
Figure 6-4 The relative frequency distribution (%) of the voxel porosity for the three soil horizons in the soil column studied.
Figure 6-5 Macroporosity distribution along the soil column depth as determined by the segmented macropores with equivalent cylindrical diameter larger than 0.75 mm.
Figure 6-6 The entrapped air distribution in the soil column before KI was introduced: a) volume percentage of air-filled macropores as a function of soil depth, b) a 2-D visualization of the entrapped air in the vertical profile (the dark areas are air pockets), and c) a 3-D visualization of the entrapped air in the soil column (in pink).
Figure 6-7 The measured breakthrough curve of the effluent.
Figure 6-8 The change of the X-ray attenuation value along the soil column over time, representing the change in solute mass distribution along the column depth.
Figure 6-9 The relationship between the change in digital radiograph’s X-ray attenuation value and the effluent relative concentration.
Figure 6-10  The solute transport over time based on the relationship between the change of digital radiograph’s X-ray attenuation value and effluent relative concentration for the entire soil column scanned at two angles: accumulative solute concentration (%) at (a) 0° and (b) 90°.
Figure 6-11 The change of solute concentration (%) during the time interval for the entire soil column scanned at two angles: a) 0°, and b) 90°.
Figure 6-12  The solute distribution (brownish color, in relative concentration [%]) at two scanned positions of 12.0-cm and 27.8-cm depth in the soil column over time. The grey color indicates soil porosity (%) and the pink color indicates the entrapped air bubbles.
Figure 6-13  Breakthrough curves of the macropore and matrix domains at two
scanned positions of 12.0-cm (position 1) and 27.8-cm depth (position 2) in the soil column
studied.
Figure 6-14 Selected points in the cross-section at 27.8-cm depth in the soil column (a) and their CT-measured point-specific breakthrough curves (b). Point 1 is a macropore, point 2 is adjacent to a macropore, and points 3 and 4 are soil matrix. Error bars indicate a variation of ±26 in CT number, corresponding to about ±5% variation in relative concentration.
Figure 6-15 A 3-D reconstruction of the solute mass distribution (in green) and the entrapped air distribution (in pink) at the end of the displacing process. Note that the solute mass was quantified by the ratio of the change of X-ray attenuation value during 1374 min \((CT(x, y, z, t = 1374) - CT(x, y, z, t = 0))\) to the difference between the X-ray attenuation value of the KI solution \((CT_{KI})\) and water \((CT_{water})\).
Chapter 7

SUMMARY AND FUTURE WORK

Summary

Preferential water flow and solute transport related to soil macropores have received great concern because of its importance to water quality and hydrologic response. The physical relationship between soil macropore characteristics and soil hydraulic functions is fundamental to understanding the mechanics and dynamics of flow and transport in structured soils, improving the prediction accuracy with current models, and developing management strategies to increase crop productivity while minimizing environmental pollution. The overall goal of this study is to characterize, visualize, and quantify soil macropore characteristics and their relationships to preferential flow and transport using large intact soil columns. Advanced computed tomography (CT) was coupled with classical breakthrough experiments to determine the impacts of different soil types and land uses on macropore characteristics and preferential flow. Overall main conclusions obtained from this study are summarized below.

In chapter 2, I introduced a new protocol to quantify the macropore networks in large soil columns taken from different soil type (Hagerstown and Morrison soil series) and land uses (crop and pasture) using medical X-ray CT. The following conclusions were drawn:

1) The approach developed in this study effectively quantified soil macropore networks with distinct morphological features reconstructed from CT.

2) Within the same soil type, the soils with pasture land use had higher macroporosity, pore length density, and node density, especially in the subsoil. This was associated with higher organic matter content and more biota activity in pasture land use. Within
the same land use, the Morrison sand displayed less overall macropores and weaker structure than the Hagerstown silt loam.

3) Soil type, land use, and their interaction impacted macroporosity, macropore network density, surface area, length density, node density (interconnectivity), and mean angle. The interaction of soil type and land use also had impact on mean tortuosity and hydraulic radius.

In chapter 3, the same soil columns and CT data as chapter 2 were used to investigate the change of macropore characteristics with the soil horizons (i.e., Ap1, Ap2 and Bt) and pedotransfer functions for estimating macropore characteristics using basic soil properties. The following conclusions were drawn:

4) The macropores at the subsurface (i.e., Ap2 and Bt horizons) were less tortuous, more vertically oriented, less inter-connected than the macropores at the Ap1 horizon.

5) The macroporosity, length density, network density, node density, mean tortuosity and mean angle were inter-correlated.

6) Pedotransfer functions for macropore characteristics were developed using the basic soil properties. For each horizon, the mean macroporosity, length density, tortuosity, network density, node density and fractal dimension could be reasonably estimated by soil bulk density, organic mater content and Ksat-core.

In chapter 4, the saturated hydraulic conductivity (Ksat) of each soil horizon and the whole column were measured and the breakthrough curve (BTC) of CaBr₂ was collected for the soil columns taken from the Hagerstown silt loam with two types of land use (i.e., crop and pasture). The macropore characteristics calculated in the chapter 2 and 3 were linked with the hydraulic functions at saturated conditions. The following conclusions were drawn:

7) For all the soil columns, macroporosity and path explained 75% of the variation in Ksat of the horizon and 75% of the variation in Ksat of whole soil column.
Within each land use, macroporosity, path, and tortuosity were the most important characteristics to estimate Ksat of the horizon but with different order of importance. The Ksat measured from the large soil columns were much higher than those measured from small soil cores.

Equilibrium CDE fitted the BTCs well for all soil columns except one with a macropore continuous through the entire soil column (path =1). Non-equilibrium two-region model well fitted the BTC of the column with one through macropore.

The cropped Hagerstown showed a higher degree of preferential flow than its pasture counterpart because more abundant macropores in the pasture Hagerstown were more evenly distributed in the soils.

The path, hydraulic radius and the angle best explained the variation in the hydrodynamic dispersion (97%).

The hydrodynamic dispersion might be mainly controlled by the Bt horizon with the lowest conductivity in this study.

In chapter 5, In an intact soil column of 76 mm in diameter and 256 mm in length, the soil macropore structure and tracer distribution in real time (0 min, 6 min, and 78 min) were reconstructed using X-ray industrial CT at five positions (each with a thickness of 10.7 mm) in the Ap1, Ap2, and Bt horizons of the soil column, plus two boundaries between these horizons. Soil macropore network and solute distribution patterns along soil depth were characterized using fractal dimensions and lacunarities.

Positive logarithmic trends were found between the pore fractal dimension and the volume percentage of the macropores and tracer distribution.

There was no statistically significant difference between the fractal co-dimensions in 2-D and 3-D. The 3-D relative lacunarities were slightly lower than the 2-D values.
15) The tracer distributions over time were closer to true fractals than the macropore networks based on their relative lacunarity functions (RLFs).

16) The lacunarity function reflected the size distribution of macropores and the spatial pattern of flow and transport. Lacunarity is a potentially powerful parameter that may be coupled with the fractal dimension to better describe and model soil structural properties.

In chapter 6, soil structure and preferential water flow and solute transport (e.g., flow velocity, solute mass, and concentration) in real-time were reconstructed in an intact soil column (10 cm in diameter, and 30 cm in length) using high resolution industrial CT. Another imaging technique, digital radiograph, was also used to quantify the solute distribution.

17) A simplified method effectively quantified the voxel-based soil porosity and solute tracer concentration at the satiated condition.

18) Only part of the macropores, especially the highly continuous biogenetic macropores (earthworm burrows and root channels) at the subsurface were preferential flow pathways, in part because of entrapped air that made up 9.8%, 11.5%, and 18.5% of the macropore volume in the Ap1, Ap2, and Bt horizons, respectively.

19) Flow velocity, solute mass, and concentration of the solute tracer in soil macropore domain, matrix domain, and their interface in real-time were quantified using the CT scanning and DR.

20) DR was also shown to be an effective tool to nondestructively characterize solute transport in real-time when combined with a solute tracer.

Overall, this dissertation research will enhance our understanding of the mechanism and dynamic processed of preferential flow and quantitative descriptions for predicting preferential flow and transport at soil column scales. It also has the potential to shed light on hillslope hydrology and other fields associated with preferential flow phenomena.
Future work

In the light of the main findings of this study and limited time available to further explore related topics, some suggestions are made below for future studies:

1) All the experiments made in this study were conducted under satiated or saturated conditions. Unsaturated flow condition is needed to further investigate the hydraulic effectiveness of macropores and their dynamic influence on preferential water flow and solute transport under varying degrees of saturation.

2) Empirical relationships obtained in this study between soil macropore characteristics and hydraulic parameters should be further coupled with physically-based models to improve the mechanistic understanding of complex preferential flow and transport and their linkages to macropore networks.

3) The effect of soil structure and preferential flow on the transport of reactive or absorptive chemicals would be different from the conservative tracer used in this study, and therefore worth future investigations.

4) An effective quantitative index to describe the degree of preferential flow and transport needs to be developed.

5) Pedotransfer functions for solute transport should be developed using the basic soil properties (especially those in the soil survey) with a broad range of soil types and land uses.

6) A system based the basic soil properties to evaluate the preferential potential and its effect on the water quality is needed.
VITA

Lifang Luo

EDUCATION

Ph.D. Soil Physics / Hydrology, the Pennsylvania State University, University Park, PA, May 2009

M.S. Physical Geography, Beijing Normal University, Beijing, China, 2004

B.S. Resource and Environmental Planning and Management, Beijing Normal University, Beijing, China, 2001

PUBLICATIONS


* In Chinese with English abstract.

MANUSCRIPT REVIEW

• Catena
• Geoderma