FRACTAL ANALYSIS OF SOIL AGGREGATE STRUCTURES AND
ASSOCIATIONS WITH ORGANIC CARBON

A Thesis in
Soil Science
by
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Submitted in Partial Fulfillment
of the Requirements
for the Degree of

Doctor of Philosophy

May 2005
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ABSTRACT

Between 1850 and 1998, the atmospheric carbon stock increased by about 174 Gt C, or 30%. Recent investigations suggest that soils could sequester as much as 30% of this excess carbon. One possible mechanism of soil carbon sequestration is the development of small soil aggregates (microaggregates) within larger aggregates, meaning that hierarchical soil structure may provide clues about the nature of soil organic matter (SOM) dynamics. In this context, fractal theory is useful. Specifically, a soil can be considered a fractal object whose pores obey a number-size power law (solid mass fractal) or whose particles and pores each obey number-size power laws (pore-solid fractal, or PSF). In the first part of this study, soil aggregates (~3 mm in size) from the Hunter Rotation Experiment (HRE) at Rock Springs, PA were analyzed with computed tomography (CT) to obtain images of the undisturbed aggregate structures. Objectives were to 1) compare the PSF and solid mass fractal models in representing aggregate structures, and 2) assess the sensitivity of derived fractal parameters to 2-D or 3-D image analysis. Results showed that the solid mass fractal parameters were most reliable, and that fractal dimensions obtained from 2-D images were comparable to their 3-D counterparts. This analytical approach was extended to aggregates of three different size classes, but no single fractal model could account for the trends observed in either of two soil types from the HRE. In an effort to expand on the potential applications of the PSF model, a modified PSF model was created, accounting for SOM explicitly over time. Out
of many possible formulations, this model was developed because of its compatibility with our understanding of microaggregate formation. Subsequent tests of the modified PSF model were successful, although few constraints exist for the input parameters. If the model is accurate, it underscores the significance of the fractal parameter $b$, low values of which were associated with increased soil carbon storage. This agrees with other findings that low $b$ values are associated with clayey, stable soils.
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PREFACE

A modified version of Chapter 2 will be submitted to Geoderma in May 2005 for consideration in a special issue. In addition, an early version of Chapter 4 was submitted for review to Vadose Zone Journal in August 2004. A revised edition of the manuscript, which is very similar to Chapter 4, was submitted for a second review in February 2005. In all versions of these manuscripts, Jody Gibson has been first author, while Henry Lin and Mary Ann Bruns have been coauthors.
ACKNOWLEDGMENTS

I am grateful to Penn State University for providing me with a free education. Specifically, thanks go to the Department of Geosciences, for supporting my effort to obtain a Master’s degree, and to the Department of Crop and Soil Sciences, for supporting my most recent effort to obtain a Doctoral degree. Also, I would like to thank my advisors, Mary Ann Bruns and Henry Lin, for their general support, but especially for their willingness to tolerate my outer-mainstream ideas. I cannot think of a better environment in which to have developed intellectually. I would like to express gratitude to my remaining committee members—Bill Easterling, Avrami Grader, and Enid Martinez—for providing constructive feedback on this thesis, and for their enlightening discussion. To everyone who has helped me obtain and understand CT scans, including Phil Halleck and Ozgen Karacan, I am much obliged. To my friends in State College, you are a major reason I made it through so many years of post-graduate education, so I thank you for that. Finally, I want to thank my parents and my wife, Amy, for their constant love and their ability to keep my priorities straight.
Chapter 1
INTRODUCTION

Purpose

Global climate stability is desirable for a variety of human endeavors, yet it is widely accepted that human endeavors have led to a significant increase in greenhouse gases in the atmosphere. Between 1850 and 1998, the atmospheric carbon stock increased by approximately 30%, from 586 Gt C to 760 Gt C (1 Gt C is $10^{15}$ g of carbon) (Houghton et al., 1996; Lal, 2004). This increase of approximately 174 Gt C in the atmosphere resulted primarily from a combination of two human activities, fossil fuel combustion and land use conversion (Lal, 2004). Recent estimates suggest that improved land management could allow global soils to sequester 50-66% of the $78 \pm 12$ Gt C they released during historic cultivation (Lal, 2004). This implies that soil carbon sequestration could negate as much as 30% of the human-induced atmospheric carbon increase.

The purpose of this study is to examine the physical associations between soil and soil organic carbon (SOC). Specifically, it is hypothesized that quantitative measures of soil aggregate structure can determine a soil’s organic carbon capacity. Alternatively, it is hypothesized that soil aggregate structure and SOC co-evolve, producing a unique relationship at steady state. The alternate interpretation accounts for the fact that soil
aggregates and SOC interact dynamically, which is precisely why soil aggregate structures should be studied to enhance our understanding of soil carbon sequestration.

In order to quantify soil aggregate structures, a large portion of this study is devoted to the development and testing of new methods and models. Fractal theory was selected as a basis for modeling soil structure, primarily for its ability to describe structures at multiple scales, which many soils exhibit. Therefore, this introductory chapter defines some of the important fractal concepts used in Chapters 2-4. Additionally, it provides the soil science context for fractal analysis necessary in satisfying the ultimate objective of this work—to discover the link between SOC and fractal models of soil aggregate structure. The objective is completely novel, but it takes advantage of recent progress in the understanding of soil aggregate and SOC dynamics.

Fractal Geometry Overview

Fractals are complex geometrical objects that often reveal self-similar patterns over a range in scales (Rieu and Sposito, 1991). In other words, a fractal might exhibit a single pattern, whether viewed at 10X magnification or 100X magnification. This phenomenon results in a complex structure whose properties can be modeled by surprisingly simple equations. As an example, consider a square sheet of paper with a smaller square cut out of its center (Fig. 1-1, Step 1). If we let this sheet of paper serve as a template for patterns at larger scales, then the next step would be to arrange nine such sheets of paper into a square, mimicking the original (smaller) square sheet. Nine sheets
Figure 1-1. Self-similar pattern development at multiple scales for square sheets of paper. A solid mass fractal is the end result of the infinite process.
are used because a central sheet must be removed to mimic the original cut hole (Fig. 1-1, Step 2). This process is continued *ad infinitum* and it results in what is called a solid mass fractal; it is a fractal because of the scale-invariant pattern, and a solid mass fractal because solid mass is removed at each step. By contrast, a pore mass fractal is an object whose template is an empty space filled partially with solid mass.

A solid mass fractal exhibits several interesting properties. Because its mass is not distributed homogeneously—i.e., it contains a large range of pore sizes—it’s size (area or volume) no longer provides a linear estimate of the mass. In contrast, the size of a simple solid object, such as a sphere, retains a linear relationship with its mass. In a solid mass fractal, the positive change in mass relative to the positive change in area is no longer constant; instead, the mass growth slows at a precise rate as the object becomes larger. In our previous example, this phenomenon is explained by the fact that a hole cannot exist in a sheet of equal or smaller size (Fig. 1-1). Thus, as the size of the object increases, larger holes are introduced continually, and mass growth by the object is slowed. In quantitative terms, mass ($M$) scales as a function of linear size ($r$), but according to a reduced exponent (Bird and Perrier, 2003):

$$M(r)=k_mr^D,$$

(1-1)

where $D$ is less than three for 3-D objects, or less than two for 2-D objects. Here, $k_m$ is a constant and $D$ is called the solid mass fractal dimension, smaller values of which correspond generally to increased heterogeneity.

A solid mass fractal exhibits two more properties of interest. The first is density, which is related directly to mass. In the example with square sheets of paper, density of the paper itself is constant. However, examining the original template sheet, its overall
density is reduced upon removal of the central square. The next level in the hierarchy comprises nine of these sheets, yielding an overall density identical to that of the template sheet. Once the central sheet is removed, however, this density decreases, which occurs similarly at all following levels (Fig. 1-1, Step 3). Thus the density of a solid mass fractal decreases as we zoom out, and it increases as we zoom in. Note that this is very different from a simple solid object, whose density is scale-invariant. A simple derivation of the governing equation for solid mass fractal density is presented in Chapter 2. The final property of interest is the pore size distribution. Returning to the paper sheets example, it can be shown that the number of holes \( N \) greater than or equal to a given linear size \( r \) is

\[
N(r) = k_n r^{-D},
\]

where \( k_n \) is a constant and \( D \) is called a number fractal dimension, but equivalent to the solid mass fractal dimension in Eq. (1-1) (Perrier et al., 1999; Bird and Perrier, 2003). The remarkable aspect of a solid mass fractal, then, is that a single parameter, \( D \), relates mass (and density) scaling and the pore size distribution. This is one reason why many refer to \( D \) simply as “the fractal dimension.”

In addition to solid mass fractals and pore mass fractals, there are pore-solid fractals (PSF). The conceptual model of a PSF is identical to that of either mass fractal, except that instead of replacing mass strictly with pores or strictly with solids, it replaces mass with both pores and solids (Perrier et al., 1999). The end result is an object whose mass and density scale quite differently from those of a mass fractal, and whose pores and solids both exhibit number-size distributions with exponent \( D \). In describing soil structure, the PSF model is superior to either of the mass fractal models, simply because
similarly sized pores and solids are allowed to coexist. In fact, in its general form, the PSF model incorporates the mass fractal models as special cases. This will be discussed in greater detail in Chapters 2-4.

Figure 1-2 illustrates the scaling properties of the mass fractal and the PSF. Perrier et al. (1999) showed that, in either model, the fractal dimension can be estimated from the expression:

\[ D = d + \frac{\log(f)}{\log(b)} \]  

Equation (1-3) is identical to Eq. (4-1), but it is introduced here to convey principles of the basic fractal parameters. The first is \( d \), which is simply the embedding dimensionality, or, the theoretical maximum for \( D \). The “fractal phase” is represented by \( f \), which is the proportion of the fractal object that provides heterogeneity at smaller scales. Lastly, the inverse of the similarity ratio, \( b \), is incorporated. The similarity ratio, as named by Rieu and Sposito (1991) and Perrier et al. (1999), describes the number of subunits into which a larger unit of structure can be resolved. For example, in Figs. 1-1 and 1-2, each unit of structure can be resolved into a block of 3X3 subunits. In these examples, the similarity ratio is 1/3 because the linear size of each subunit is 1/3 that of the larger unit. The inverse of the similarity ratio, then, is \( b=3 \), and using Eq. (1-3) we calculate \( D=2+\log(5/9)/\log(3)=1.465 \), for either model in Fig. 1-2. Although the fractal dimension is the same for either model, their masses and pore size distributions are clearly different.
Figure 1-2. Conceptual model for the scaling of a) a solid mass fractal, and b) a pore-solid fractal (PSF). $P$=pore, $S$=solid, $F$=fractal; $i$=hierarchical level, $b$=inverse of similarity ratio. Asterisks (*) indicate $F$ blocks, which reveal heterogeneity at increased resolution.
Fractals and Soil Aggregates

The basic lesson of fractal geometry is that simple equations can govern properties of infinitely complex structures. Natural objects are limited by a minimum and/or maximum scale and, at most, can be defined only as quasi-fractals. Nevertheless, self-similarity can occur over a finite range in scale, and this has been observed in galactic structures, clouds, landscape patterns, fires, mineral surfaces, protein structures, blood vessels, and even DNA sequences, to name a few (Halley et al., 2004). Usually, such structures are analyzed by attempting to simulate their physical appearance, using a type of recursive algorithm, or by attempting to predict one or more of the object’s properties, using fractal equations. Respective examples of these analyses include diffusion-limited aggregation of crystal growth (Halley et al., 2004) and characteristic soil moisture release (Bird et al., 2000).

Soil is an excellent medium for the application of fractal models, primarily because many soils exhibit a self-similar pattern of aggregation over small scales (Rieu and Sposito, 1991). Indeed, fractal models of soil aggregate structures and their relationship to the turnover of SOC are the focus of Chapters 2-4. This study has benefited from the data of Six et al. (2000), which are summarized as a conceptual model linking aggregate hierarchy with potential carbon sequestration. A variation of that model is illustrated in Fig. 4-1, but a short introduction is given here.

Work by Tisdall and Oades (1982) popularized the notion of hierarchical aggregate structures, and subsequent studies revealed that carbon turnover varied
considerably between aggregate sizes (Puget et al., 2000; Six et al., 2000). Based on the physical and chemical properties of the organic matter in different aggregate size classes, it was apparent that microaggregates (<250 µm) were capable of sequestering carbon on long time scales. Macroaggregates (>250 µm), on the other hand, were associated with healthy, biologically active soils (Gupta and Germida, 1988; Bossuyt et al., 2001). Then Six et al. (2000) proposed that macroaggregates were responsible for the formation of microaggregates, and, ultimately, the sequestration of carbon. Their model underscores the importance of macroaggregate soil residence time in determining how much of its constituent organic matter is passed on to smaller, more recalcitrant, size fractions. It was proposed that no-tillage agriculture was advantageous for increasing the residence times of the larger soil fractions.

Because macroaggregates contribute to the development of microaggregates, and because macroaggregates can, themselves, develop from particulate organic matter (POM) and microaggregates (Bossuyt et al., 2001), there is clearly a feedback between aggregates of different size classes. If a soil exhibits a characteristic steady state aggregate hierarchical structure, then there could be a way to link fractal models of soil aggregate structure with the carbon capacity of the soil. In other words, the long-term SOC fraction should reflect the characteristic steady state. In this context, the ultimate goal of Chapters 2-4 is to allow prediction of SOC dynamics within a relatively simplified framework of fractal geometry.

In the following chapters, we attempt to address these issues using a variety of techniques. In Chapter 2, the foundation is presented for using computed tomography (CT) to analyze quantitatively soil aggregate structures. In Chapter 3, this foundation is
exploited to understand differences in aggregates from three size fractions and from soils of two contrasting organic carbon levels. Additionally, derived fractal parameters are assessed for their potential to characterize SOC. In Chapter 4, a new fractal model is developed that accounts explicitly for organic matter in soil aggregate size classes, and results are used to assess the carbon sequestration potential of different soils.

References Cited


Chapter 2

A COMPARISON OF FRACTAL ANALYTICAL TECHNIQUES ON 2- AND 3-DIMENSIONAL COMPUTED TOMOGRAPHIC SCANS OF SOIL AGGREGATES

Introduction

With continuing advances in computer technology, quantitative analyses of soil structure are increasingly utilized. Fractal analyses, in particular, have become popular because of the wide array of fractal model applications in soil science. These range from gas diffusion, water retention, and hydraulic conductivity (Anderson and McBratney, 2002) to dynamics of the soil microstructure and soil microbiota complex (Young and Crawford, 2004). Such applications require input parameters that predict soil behavior effectively, hence the need to obtain and understand various fractal parameters; these parameters include the mass fractal dimension, the spectral dimension, the surface fractal dimension, and the fragmentation fractal dimension (Anderson and McBratney, 2002), as well as lacunarity and multifractal parameters (Zeng et al., 1996; Posadas et al., 2003). While there are techniques to derive fractal parameter values through indirect methods—e.g., moisture retention curves or particle size distributions—the only approach that can provide direct structural information independent of some pre-existing model is through image analysis (Crawford et al., 1999).
For many years, soil thin sections have provided valuable insights into the complexity of natural soil structure. Using a petrographic microscope, this approach can distinguish between different minerals and is, thus, excellent for qualitative descriptions of the soil matrix (Brewer, 1976). The approach also lends itself to microscopic photography, which can provide quantitative information about the soil structure. Commonly, an image is digitized and partitioned into solid and pore phases, allowing the calculation of porosity, pore size distribution, and many fractal parameters (Anderson and McBratney, 2002). However, these values all correspond to 2-D observations, which, depending on the soil, may or may not be representative of the 3-D structure. Additionally, the thin-sectioning process itself is likely to induce artifacts since the soil is impregnated with a hardening resin and sliced physically to very thin dimensions (Bartoli et al., 1991).

More recently, computed tomography (CT) has provided an alternative for researchers interested in observing undisturbed soil structures (Peyton et al., 1994; Zeng et al., 1996; Rasiah and Aylmore 1998; Tollner et al., 1998; Rogasik et al., 1999; Gantzer and Anderson, 2002; Pierret et al., 2002; Perret et al., 2003). Because the technique is based on the attenuation of X- or gamma-rays by a soil sample, the physical impact is limited primarily to the handling of the sample from field to lab. Second, CT scanning is inherently quantitative since the energy attenuation is a direct result of elemental and bulk densities within the sample. Also, the technique can provide 3-D information, which is especially important for anisotropic media. Finally, CT scanning is often rapid enough to study sample dynamics in real-time, such as with the percolation of a fluid through a porous medium (Rasiah and Aylmore, 1998).
Because of these benefits over traditional methods (e.g., thin-sectioning), CT scanning is being recognized as an excellent technique for acquiring fractal parameters to describe soil structure and model soil properties. In previous studies, the focus has been on the designation of an appropriate pore-solid CT threshold, enabling box-counting estimates of dimensions of solid or pore mass fractals, as well as surface fractals (Peyton et al., 1994; Rogasik et al., 1999; Gantzer and Anderson, 2002; Perret et al., 2003).

While this approach provides useful information on the soil pore system, it imposes two distinct phases on a CT image and eliminates much information on the pattern of density throughout the solid matrix. Alternatively, Zeng et al. (1996) describe how to estimate the lacunarity and surface fractal dimension of CT images without imposing distinct phases. In the present study, we adopt a similar approach in order to preserve structural information within soil images. Since density can be inferred from CT image pixels, we utilized the concept of density scaling to describe the soil as a solid mass fractal (Perfect et al., 2002; Bird and Perrier, 2003).

It is possible to apply density scaling to any type of CT image. In this study, we use CT images of small (approx. 3 mm diameter) aggregates from agricultural soils with two contrasting histories. Factors influencing the decision to analyze individual aggregates include 1) aggregates are natural units in the soil structural hierarchy, 2) future work can incorporate scaling issues between aggregates of different size, 3) total organic carbon (TOC) can be measured on entire aggregates of small size, 4) small aggregates utilize the resolution capability of industrial CT scanners, and 5) preexisting CT literature lacks information on structures of individual soil aggregates. With this context, the objectives are to 1) demonstrate the utility of CT scanning and density scaling for
deriving fractal parameters, 2) contrast and compare several fractal analytical techniques in the process, 3) assess the ability of 2-D scans to represent 3-D structures, and 4) compare fractal parameters and TOC measurements from the two contrasting soils.

Theory

Overview

Fractals all have one common trait—they exhibit at least one type of power law scaling. For surface fractals, the surface length, or area, increases with decreasing scale of observation, as in the classic example of the coastline of Britain (Mandelbrot, 1983). For mass fractals, the mass contained within a unit area, or volume, increases as the unit radius increases; a solid sphere, for example, follows a radius-cubed power law, while a solid with complicated pore structures follows a power law with exponent less than three. Many variations on these power laws have been developed, including the conversion of the mass power law to a density power law. Let $m_r$ be the mass of a fractal enclosed in a space of unit length $r$ and $m_L$ be the mass of the same fractal enclosed in a space of reference unit length $L$. From Bird and Perrier (2003), the mass power law follows as

$$\frac{m_r}{m_L} = \left(\frac{r}{L}\right)^D,$$  \hspace{1cm} (2-1)

where $D$ is the fractal dimension. Since mass is a product of density and volume, we can rewrite Eq. (2-1) as
\[
\frac{V_r \rho_r}{V_L \rho_L} = \left( \frac{r}{L} \right)^D,
\]

which becomes

\[
\frac{r^d \rho_r}{L^d \rho_L} = \left( \frac{r}{L} \right)^D
\]

by using rectilinear shapes to define \(d\)-dimensional enclosures. Solving for \(\rho_r\) gives

\[
\rho_r = \rho_L \left( \frac{r}{L} \right)^{D-d}.
\] (2-2)

Equation (2-2) proves that a mass fractal also exhibits a density power law. As discussed, CT images provide 2-D or 3-D maps of density values, and Eq. (2-2) can be applied to obtain \(D\). To distinguish this approach from that which provides the traditional box-counting fractal dimension, recall that box-counting is performed on discrete-phase images (Anderson and McBratney, 2002). One must first decide on the appropriate density threshold(s) and then partition the image into two (or more) phases. Subsequently, boxes of uniform size cover the image, and mass is estimated by the number of boxes that include at least some of the mass-bearing phase. This is repeated for decreasing box sizes to produce a log-log plot of the number of boxes with mass versus linear box size. As Eq. (2-1) shows, this step can provide an estimate of \(D\) (equal to the absolute value of the slope of the fitted line), but at the expense of information lost in the phase partitioning process. This method is better suited to thin section images, from which quantitative density patterns are not available.
CT density scaling analysis

While soil matrix density patterns are preserved through CT density scaling analysis, it is still necessary to define a pore phase. Before discussing the reasons for this, several important points must be made regarding the interpretation of CT images. First, density information in a CT image is relative unless two or more standards, with known densities, are scanned concurrently. Effectively, the pixels in a CT image have “CT units,” which can be assigned to actual density values by the inclusion of standards. Once actual density values are assigned, pores can be defined, but only with partial objectivity. The selection of a pore-solid threshold is complicated by several factors, including the scanning energy and resolution, the densities of the standards, and the nature of the threshold. Figure 2-1 shows a sample CT scan with pores (black) defined by visual comparison with several unprocessed images. The remainder of the image involves shades that lighten with increasing material density, as determined by the increasing CT units of those pixels.

The reason why pores are separated from the rest of the image is because of the porosity exclusion principle (Perfect et al., 2002). This principle is fundamental to density scaling; essentially, it states that at any given scale of resolution, only pores smaller than the scale of resolution can be included with the solid matrix. This reflects the fact that a classical solid mass fractal reveals ever smaller pores as the scale of resolution decreases. If the scale of resolution were infinitely small, then the fractal would exhibit porosity=1, imposing a physical limitation on the concept. However, the porosity exclusion principle is valid over a finite range in scales, and it actually emulates the effects of soil fragmentation: when a soil clod is broken, there is a high probability
Figure 2-1. Sample CT scan with 512 X 512 resolution (pixels represent 9.46 µm X 9.46 µm, with thickness=10.31 µm); image has been processed to reveal pores. Boxes 1 and 2 capture material that can contribute to the mean density at either scale (equal to the box length) of observation; Boxes 3 and 4 capture material that can contribute to the mean densities, but only if the large pore areas (white arrows) are excluded.
that its largest pores will contribute to the fracture planes, thus resulting in smaller clods that do not contain those large pores. In other words, the combined soil volume shrinks with each step in the fragmentation process, and this is the direct reason why soil aggregate density has been observed to increase with decreasing size (Rieu and Sposito, 1991). Note that scale-invariant density indicates a homogeneous structure without hierarchical arrangement. Equation (2-2) shows that the greater the difference between $D$ and $d$, the more pronounced the density scaling and the more heterogeneous the structure.

When calculating density scaling from a CT image, it is necessary to quantify the sizes of individual pores and exclude the appropriate pores at each scale of resolution. Theoretically, this can be done without knowledge of the spatial pattern of density within the solid matrix. Using soil aggregate fragmentation as an analogy, total soil mass is always conserved, meaning that we need only know the volume of excluded pores to calculate density at each stage in the process. For image analysis, this corresponds to calculating the cumulative volume of pores larger than a given size and subtracting this value from the aggregate volume, which is used to divide the total CT units. While this seemingly justifies the action of phase partitioning, practical considerations suggest otherwise. For example, in many cases the first pore to be excluded is much smaller than the aggregate as a whole, meaning that the range in scales considered will be narrow. Alternatively, one can use the whole aggregate, without any pores excluded, to estimate density at the largest scale. The drawback is the inconsistency in scales considered, so either approach can prevent an accurate estimation of $D$. A more comprehensive technique involves the use of boxes, placed randomly over the image, to sample portions of the solid matrix and obtain a mean density for any given box size. This technique
emulates actual aggregate fragmentation and subsampling, while providing a basis for a consistent and wide range in scales considered. Additionally, the technique provides statistical error, which is a desirable measure for images yielding questionable fits to fractal models.

In Fig. 2-1, four hypothetical boxes are shown. Boxes 1 and 2 contain pore pixels belonging to pores that are smaller than the respective box sizes (i.e., the scales of observation). In those boxes, the CT units of all pixels can contribute to the estimation of density. In Boxes 3 and 4, pixels of pores larger than the respective box sizes are included, and in the case of Box 4 these pixels represent empty space outside of the whole aggregate. The densities in Boxes 3 and 4 are estimated by averaging the CT units in all pixels except those residing in the upper right-hand corner of each box.

Once the density scaling is generated, several fractal models can be fitted. We proceed by discussing two fractal analysis methods that rely on density scaling, in addition to one method that relies solely on the pore-size distribution.

**Fractal analysis method 1: solid mass fractal density scaling**

Solid mass fractals obey Eqs. (2-1) and (2-2). In the case of CT images, Eq. (2-2) can be used directly with the scaling of CT units as a proxy for density scaling. Using either linear (for log-log plots) or nonlinear curve fitting, estimates for $\rho_L$ and $D$ can be obtained.

**Fractal analysis method 2: pore-solid fractal density scaling**

A pore-solid fractal (PSF) is an object that can exhibit both cumulative pore and cumulative solid power law scaling (Perrier et al., 1999). It achieves this by incorporating a third phase whose density is intermediate to that of classical solids and
pores. This intermediate phase approaches zero as resolution approaches infinity, while pores and solids coexist at each level in the hierarchy. In this respect, the PSF model of soil structure is superior to the classical pore or solid mass fractal model. Also, when solids are associated with the intermediate phase, the model simplifies to a classical solid mass fractal; likewise, when pores are associated with the intermediate phase, the model simplifies to a classical pore mass fractal model. Thus, the PSF model is a general form of the mass fractal models.

Because there are three phases in a PSF model, its density scaling is more complex. Only in the theoretical sense, when the structure is developed to infinite resolution and the intermediate phase vanishes, do we find that the PSF exhibits scale-invariant density (Bird and Perrier, 2003). This is true if the density of the solid grains is constant. A more realistic scenario is manifested by a PSF whose structure is developed to some finite resolution. Bird and Perrier (2003) derived the density relation for this scenario:

$$\rho_r = \rho_{PSF} - (\rho_{PSF} - \rho_L) \left(\frac{r}{L}\right)^{D-d}. \quad (2-3)$$

The scale-invariant density of the pores plus solids is given by $\rho_{PSF}$; Eq. (2-3) shows that when this quantity is negligible the relation reduces to Eq. (2-2). The technique for deriving $D$ is therefore identical to the technique applying mass fractal density scaling, except that three parameters—$\rho_{PSF}$, $\rho_L$, and $D$—are determined by nonlinear curve fitting.

**Fractal analysis method 3: cumulative pore number scaling**

While solid mass fractals and pore-solid fractals can be analyzed using density scaling, they can also be analyzed by pore-size distribution. The reason for this is that
either type of fractal produces a power law for the number of pores larger than a given size, which arises because, in theory, the solid or intermediate phase yields an infinite number of pores. Perrier et al. (1999) expressed the cumulative number power law as

$$N_r \propto L^D r^{-D},$$

where \(N_r\) is the number of pores greater than or equal to size \(r\). Thus, a log-log plot of the cumulative number of pores versus the size provides an estimate of \(D\) from the absolute value of the slope of the fitted line. This method is simple but disregards the density information provided by CT images.

**Interpretations**

Once fractal models have been fitted, several steps can be taken to understand further the physical implications of the corresponding soil structures. For example, an estimate of the similarity ratio, which is the ratio of linear size between structural units in adjacent levels in the soil hierarchy, can be obtained by the same CT images. This involves dividing the diameter of the largest pore by the diameter of the whole aggregate (E. Perfect, personal communication). In this study, \(b\) is used to indicate the inverse of the similarity ratio, and it can be used with \(D\) to estimate the proportion of fractal material in the aggregate, \(f\) (Perrier et al., 1999):

$$f = b^{D-d}.$$  \hfill (2-5)

For solid mass fractals, \(f\) is the proportion of solid units and \(1-f\) is the proportion of pore units of any given size. For PSF structures, \(f\) is the proportion of intermediate material and \(1-f\) is the proportion of solid plus pore units of any given size. Thus, \(b\) is the basis for a model of soil composition. More importantly, it provides a measure of hierarchical
signature in the soil: large $b$ values indicate a weak soil hierarchy because there is great disparity in the sizes of structural units. Small $b$ values, on the other hand, indicate the presence of more hierarchical levels over a similar range in scales. Some evidence also suggests that clay-rich soils exhibit smaller $b$ values (Tyler and Wheatcraft, 1992; Perfect et al., 2002), implying that $b$ may be associated with aggregate stability.

Materials and Methods

Soils

As part of the Russell E. Larson agricultural research station in Rock Springs, PA, the Hunter Rotation Experiment (HRE) was established to test the effects of different crop rotations and fertilizer treatments on crop yields, and it provides an excellent opportunity to examine any effects on soil. There are four different crop rotations: 1) continuous corn (CC), 2) one year of corn followed by one year of soybeans (CS), 3) four years of corn followed by four years of alfalfa (CA), and 4) a three-year sequence of corn, oats, and wheat followed by two years of red clover/timothy hay (RO). Rotations CC and CS were initiated in 1969, while rotations CA and RO were initiated in 1990 (Bucher, 2002). These rotations interact with three fertilizer treatments: 1) inorganic fertilizer plus lime to maintain neutral pH (IN), 2) manure to satisfy crop nitrogen requirements and inorganic fertilizer to meet other soil test recommendations (MN), and 3) manure to satisfy crop phosphorus requirements plus inorganic fertilizer to meet other soil test recommendations (MP). Treatment IN was initiated in 1969, treatment MN was
initiated in 1990, and treatment MP was initiated in 1982 (Bucher, 2002). The soil is a typic hapludalf, deep, well-drained, derived from limestone residuum, and is plowed annually with a moldboard plow.

In this study, our goal was to compare the fractal characteristics of soil aggregates from 1) plots of continuous corn receiving only inorganic fertilizer (CC-IN), and 2) plots supporting the five-year crop rotation and fertilized with manure for phosphorus (RO-MP). Of all the treatment combinations at the HRE plots, we expected to see the greatest differences in TOC between soils from these plots. Preliminary tests showed that CC-IN soils averaged $1.37 \pm 0.18\%$ TOC, while the RO-MP soils averaged $1.69 \pm 0.15\%$ TOC. For simplicity, these soils will be referred to as “CC” and “RO,” respectively.

For this study we hypothesized that differences in TOC of these soils would be reflected in their corresponding soil aggregate structures. Specifically, we expected larger values for $D$ and $b$ in aggregates from CC soils. Although preliminary TOC differences were not large, they were significant. Furthermore, other tests of aggregate stability indicated that measurable structural differences existed between the two soils: RO soil aggregates were nearly six times more stable than their CC counterparts (Bucher, 2002; see Appendix A).

**Sampling**

The HRE is divided into 192 plots, each 5.76 m wide by 12.8 m long, and grouped into four replicate blocks. Sampling occurred from all four CC plots and all four RO plots that had grown corn the previous summer. In July 2002, surface soil (upper 10 cm) from 15 random locations within each of the eight plots was sampled using a small garden trowel. Samples were composited by treatment, broken to pass an 8 mm sieve,
and dried for one week in a greenhouse. Aggregates were then refrigerated until ready for scanning.

Prior to scanning, aggregates were shaken gently on a stack of two sieves—4.76 mm and 2 mm—and 10 aggregates on the 2 mm sieve were selected to represent each soil treatment. Selected aggregates were placed by tweezers into the wide openings of disposable plastic pipette tips; prior to this, aggregates were squeezed with the tweezers to ensure they would withstand a modest amount of stress and remain intact inside the pipette tips. The pipette tips served as the housing for aggregates during transport to and from the scanning facility, as well as during the scanning process. Aggregate masses were obtained by weighing the pipette tips before and after aggregate insertion.

**CT scanning**

Aggregate images were acquired via X-ray computed tomography at the Center for Quantitative Imaging (CQI) at Penn State University in February 2003. The facility operates an industrial CT scanner capable of resolving a sample into 1024 X 1024 2-D density maps. The scanner rotates the sample 360° to acquire a single 2-D image. All 20 aggregates were scanned in this way, with care taken to capture the widest portion of each aggregate. The scanner used a current of 200 mA at 100 kV, and CT units ranged from 1 (air) to over 40 000 (mineral matter), reflecting both the scan energy and the inherent density of the samples. Of the 20 aggregates, one of each soil treatment was selected for a full 3-D reconstruction scan, which consisted of several hundred non-overlapping 2-D scans. From these samples, exact volumes and densities were calculated, allowing the creation of a density calibration function. Two data points were used to define this function: the first was obtained by associating CT units for air with a
density of zero, while the second was obtained by associating the mean CT value of a whole aggregate with its known density. For both 3-D scans, this resulted in the function 
\[ y = 1.84 \times 10^{-4} x - 0.690 \]
relating estimated bulk density \((y)\) to CT units \((x)\).

**Carbon and nitrogen analyses**

Using a Carlo Erba analyzer, total carbon and nitrogen contents of the 20 individual aggregates were measured after scanning. The aggregates were small enough so that each could be combusted in entirety to obtain corresponding C and N contents. These were used to help explain variations in fractal parameters, as well as to provide a context for the differences between soil aggregates from the two treatments.

**Image analysis**

MATLAB 6 (The MathWorks Inc., Natick, MA) was used for all computations. CT data were saved as tagged image file format (TIFF) files and converted to numerical text data, from which grayscale images could be plotted. All 2-D images were cropped to 512 X 512 pixels in order to focus on the soil aggregate-bearing areas. The pixel resolution remained 9.46 µm X 9.46 µm, with a scan thickness of 10.31 µm. Figure 2-2 shows the 10 CC aggregate scans and the 10 RO aggregate scans. Also shown are the identifier labels for each aggregate: all CC aggregates are designated with a number (1-10) followed by the letter ‘a,’ while all RO aggregates are designated with a number (1-10) followed by the letter ‘b.’

Because the soil aggregates did not fill the 512 X 512 fields of view, aggregate boundaries had to be defined in common with the pore-solid CT threshold, which was set to 10 000 CT units. This also affected the decision to avoid using traditional box-counting: when a fractal object does not fill the field of view, the box-counting fractal
Figure 2-2 (following page). CT images of 20 aggregates, with 512 X 512 resolution (pixels represent 9.46 μm X 9.46 μm, with thickness=10.31 μm). Shown with label identifiers are the a) 10 continuous corn (CC) aggregates and b) 10 rotation (RO) aggregates.
Continuous Corn Aggregates

Rotation Aggregates
dimension is sensitive to the position and size of the aggregate within the window, as well as to boundary characteristics. Unless the image is cropped further to contain only aggregate pixels, these factors can confound efforts to obtain realistic fractal parameters. Individual pores were identified by using a recursive algorithm that grouped pore pixels based on orthogonal adjacency, and pore sizes were defined as the square roots of their areas (here, area is synonymous with total number of 2-D pixels).

Aggregates 2a and 7b were selected for 3-D scanning because their survey scans did not reveal any abnormal features. For example, aggregates 8a and 10b were avoided because of the presence of large mineral grains and the lack of obvious porosity (Fig. 2-2). A summary of the two aggregates selected for 3-D scanning is given in Table 2-1; in addition, a comparison of their pore structures is shown in Fig. 2-3. In order to identify individual 3-D pores, 2-D images were analyzed first to identify individual pores in each slice, and these pores were tested subsequently for connectivity in 3-D space. This method—as opposed to testing for orthogonal adjacency in all three dimensions simultaneously—reduced significantly the demands on RAM and virtual memory. Once individual pores were identified, their sizes were calculated as the cube roots of their volumes (here, volume is synonymous with total number of 3-D pixels).

Obtaining the density scaling for each 3-D aggregate also required modification because of computational constraints. Specifically, each aggregate data set was divided into 1/8th fragments (i.e., eight corners of the 3-D enclosure), and one average density was estimated from 1000 randomly located cubes of uniform size. This was repeated five times for each of 13 cube lengths: 63, 51, 41, 33, 27, 21, 17, 13, 11, 9, 7, 5, and 3, all in pixel units. Thus, five density values for eight fragments, yielding a sample size of 40,
Table 2-1. Comparison of two representative aggregates, 2a and 7b. Volumes were determined from CT 3-D reconstruction scans; C and N were determined after scanning through combustion using a Carlo Erba analyzer.

<table>
<thead>
<tr>
<th></th>
<th>Aggregate 2a</th>
<th>Aggregate 7b</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(from CC treatment)</td>
<td>(from RO treatment)</td>
</tr>
<tr>
<td>Mass</td>
<td>0.031 g</td>
<td>0.021 g</td>
</tr>
<tr>
<td>Volume</td>
<td>0.0192 cm$^3$</td>
<td>0.0137 cm$^3$</td>
</tr>
<tr>
<td>Bulk density</td>
<td>1.61 g cm$^{-3}$</td>
<td>1.53 g cm$^{-3}$</td>
</tr>
<tr>
<td>Carbon</td>
<td>1.85%</td>
<td>1.68%</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0.20%</td>
<td>0.15%</td>
</tr>
<tr>
<td>C:N</td>
<td>9.25</td>
<td>11.2</td>
</tr>
<tr>
<td>Number of 2-D scans</td>
<td>410</td>
<td>369</td>
</tr>
</tbody>
</table>
Figure 2-3. Representative 3-D pore structures of a) aggregate 2a (CC treatment) and b) aggregate 7b (RO treatment). Images were produced by using a threshold of 10 000 CT units on each 3-D CT reconstruction; only the innermost 100 X 100 X 100 pixels were used.
were averaged to obtain the aggregate density estimate at each scale of observation. For 2-D images, the densities of 1000 randomly located squares of uniform size were averaged. This was repeated five times, yielding a sample size of five, for each of 13 square lengths (same as before).

**Fractal parameter derivations**

Gauss-Newton nonlinear curve fitting of density scaling was used to derive estimates of $\rho_L$ and $D$ for a solid mass fractal model, and $\rho_L$, $\rho_{PSF}$, and $D$ for a PSF model. Additionally, pore-size distributions were used to derive estimates of $D$. These three methods were applied to each of the full 3-D reconstructions and each of the 20 2-D scans. To test the ability of 2-D slices to represent 3-D aggregate structure, the two density methods were applied to over 200 slices in the middle sections of aggregates 2a and 7b. Finally, $b$ values were derived by using the square root of the ratio of areas, or the cube root of the ratio of volumes, of the aggregate and its largest pore.

**Results and Discussion**

Figure 2-4 shows the 3-D density scaling for aggregates 2a and 7b. Each error bar represents standard deviation on the mean of 40 values. Clearly, the porosity exclusion principle is causing each aggregate to exhibit increasing density at smaller spatial scales, particularly within aggregate 7b. The fitted curves, which represent Eq. (2-2), exhibit pronounced curvature as $D$ deviates from $d$, where $d=3$ is the theoretical maximum for $D$. Thus, in addition to its consistently low bulk density, aggregate 7b appears to have a
Figure 2-4. 3-D density scaling of aggregates 2a (CC) and 7b (RO). Error bars represent standard deviations \( (n=40) \) at each scale of observation; models represent the fitted curves of the solid mass fractal (Eq. (2-2)). Estimated bulk density was determined from CT units using the function: \( y=1.84 \times 10^{-4} x-0.690 \).
smaller fractal dimension. This is in agreement with Fig. 2-3, which suggests that aggregate 7b might be more heterogeneous than aggregate 2a. Equation (2-3) has an additional parameter, $\rho_{PSF}$, that can alter the fitted values of $D$ should the PSF model be the better representation of aggregate structures. To compare the performance of the solid mass fractal and PSF models, Table 2-2 lists the fractal parameter estimates of the 3-D density data, as well as the performances of the two models. The last row in the table shows that $r^2$ values change marginally between the models for either aggregate. This is reflected in the values for $\rho_{PSF}$, which are actually less than zero. While $\rho_{PSF}=0$ reduces a PSF to a mass fractal (Eqs. (2-2)-(2-3)), values less than zero are unrealistic and are returned only to improve the fits. This indicates that positive values would impair the PSF fits, and we can assume that the solid mass fractal is the better model here.

Figure 2-4 reveals two points worth discussing. The first is that measurement errors increase for larger scales of observation, which could reflect a bias in the analytical procedure. Specifically, since aggregates 2a and 7b were analyzed in 1/8th fragments, large box sizes were particularly confined in terms of sampling location. If an aggregate exhibits large-scale heterogeneity, the net effect of such sampling confinement is that the standard deviation of densities will be exaggerated for larger scales of observation. Small-scale observation is less affected because small boxes yield a greater variety of densities within each aggregate corner, causing overlap in values contributing to overall average density. The second point is that the fractal models seem to overestimate density at small scales of observation, which could reflect instrument limitations. Specifically, if many pores are beyond the resolution of the CT scanner, small box sizes might fail to
Table 2-2. Fractal parameters estimated from density scaling of 3-D CT data on aggregates 2a and 7b. $D$ is the fractal dimension, $\rho_L$ is the density at the largest scale of observation (g cm$^{-3}$), $\rho_{PSF}$ is the density of solids plus pores in a PSF structure (g cm$^{-3}$), and $b$ is the inverse of the similarity ratio. Values represent estimates (with 95% confidence intervals in parentheses) from nonlinear curve fitting; initial seeds for $D$, $\rho_L$, and $\rho_{PSF}$ were 2.80, 1.25 g cm$^{-3}$, and 1.50 g cm$^{-3}$, respectively.

<table>
<thead>
<tr>
<th>PSF Parameters#</th>
<th>Mass Fractal Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Aggregate 2a (CC)</td>
</tr>
<tr>
<td>$D$</td>
<td>2.994 (2.328, 3.661)</td>
</tr>
<tr>
<td>$\rho_L$</td>
<td>1.580 (1.566, 1.594)</td>
</tr>
<tr>
<td>$\rho_{PSF}$</td>
<td>-2.108 (-422.5, 418.3)</td>
</tr>
<tr>
<td>$b$</td>
<td>5.328</td>
</tr>
<tr>
<td>$r^2$</td>
<td>0.849</td>
</tr>
</tbody>
</table>

# PSF fits never converged.
exclude low-density (pore) pixels that should not contribute to estimated density. The net effect of this scenario is that the estimated density will be less than it should.

An exploration of the 3-D pore-size distributions and their ability to provide estimates of $D$ proved more challenging. Using both log-log linear and nonlinear fitting procedures with Eq. (2-4), high $r^2$ values were obtained. However, estimates of $D$ ranged from 2.038 to 2.343 for aggregate 2a and 1.726 to 2.135 for aggregate 7b, which are too low given the estimates from density scaling (Table 2-2). Additionally, published 3-D mass fractal dimensions for various soils suggest that values less than two are unrealistic (Crawford et al., 1993; Anderson and McBratney, 2002). Similar problems were encountered while analyzing pore-size distributions of the 20 2-D scans. Because the selection of pore size classes is subjective, it is not surprising that accurate estimates of $D$ using pore-size distributions are difficult to obtain. Therefore, we shall focus on density scaling results throughout the remainder of this study.

The full 3-D reconstructions of aggregates 2a and 7b offered a unique opportunity to test the ability of 2-D slices to represent the structure of an entire aggregate. This ability depends on the level of isotropy within each aggregate, such that 2-D slices are more representative as isotropy increases. The results of this analysis are shown in Table 2-3, which is identical in format to Table 2-2; the values represent medians of the 277 slices from aggregate 2a and the 203 slices from aggregate 7b that provided at least 40,000 pixels (equivalent to a 200 X 200 patch) of aggregate coverage. This constraint was used to avoid analyzing the narrow top or bottom ends of each aggregate. Note that fractal dimensions in Table 2-3 correspond to a theoretical maximum of two, and that in an isotropic medium the values would be precisely one unit less than those in Table 2-2.
Table 2-3. Fractal parameters estimated from density scaling of 2-D CT data on aggregates 2a (n=277) and 7b (n=203). $D$ is the fractal dimension, $\rho_L$ is the density at the largest scale of observation (g cm$^{-3}$), $\rho_{PSF}$ is the density of solids plus pores in a PSF structure (g cm$^{-3}$), and $b$ is the inverse of the similarity ratio. Values represent medians (with percentiles at 2.5% and 97.5% in parentheses) of estimates from nonlinear curve fitting; initial seeds for $D$, $\rho_L$, and $\rho_{PSF}$ were 1.80, 1.25 g cm$^{-3}$, and 1.50 g cm$^{-3}$, respectively.

<table>
<thead>
<tr>
<th>PSF Parameters#</th>
<th>Mass Fractal Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Aggregate 2a (CC)</td>
</tr>
<tr>
<td>$D$</td>
<td>1.993 (1.788, 3.063)</td>
</tr>
<tr>
<td>$\rho_L$</td>
<td>1.576 (1.536, 1.610)</td>
</tr>
<tr>
<td>$\rho_{PSF}$</td>
<td>-0.905 (-4.626, 2.820)</td>
</tr>
<tr>
<td>$r^2$</td>
<td>0.913 (0.474, 0.968)</td>
</tr>
</tbody>
</table>

# Most PSF fits never converged.
(Mandelbrot, 1983; Crawford et al., 1993). Interestingly, this is close to the observed trend for both aggregates. In fact, all parameters in Tables 2-2 and 2-3 are comparable except for the $b$ values, which are noticeably larger when derived from 2-D slices. This phenomenon can be explained by the method used to derive $b$, which is dependent on the shape of a single large pore in each aggregate. Specifically, a pore in 2-D space is defined by connectivity within a plane, which is more limiting than connectivity within a volume. Therefore, large, oddly-shaped pores might be revealed only in 3-D space, effectively reducing the estimated values for $b$. In terms of the practicality of estimated fractal parameters, 2-D slices are advantageous in that they are less affected by an oddly-shaped pore, whose connectedness is highly sensitive to the accuracy of CT data.

The final segment of this study involves single 2-D scans from 10 aggregates selected randomly from each soil treatment. Table 2-4 lists the estimates of $D$ using the density scaling method for both PSF and solid mass fractal models, the estimates of $b$, the percentage of pore pixels, and the TOC measurements, for each aggregate. Nitrogen measurements are not shown because they correlated strongly with TOC. The table reveals a wide range in the PSF fractal dimensions, which is not surprising given the 95% confidence intervals in Tables 2-2 and 2-3 and the fact that most of these values originated from fits that failed to converge. The most likely reason for lack of convergence is the fact that three parameters were being fitted simultaneously. On the other hand, the solid mass fractal values exhibit greater precision. These values indicate that the CC aggregates might have a larger fractal dimension than that of the RO aggregates, which would reflect the greater density of aggregates in the former group. However, the Wilcoxon Rank Sum Test probability that the medians are not different is
Table 2-4. Fractal parameters estimated from density scaling of 2-D CT data on 20 aggregates, with percentage of pore pixels and TOC. $D$ is the fractal dimension and $b$ is the inverse of the similarity ratio; $D$ was estimated from nonlinear curve fitting (initial seed was 1.80). P-values ($p$) indicate the probability that corresponding medians of the two soils are not different, according to the Wilcoxon Rank Sum Test.

<table>
<thead>
<tr>
<th>Aggregate Number</th>
<th>PSF $D^b$</th>
<th>Mass Fractal $D$</th>
<th>$b$</th>
<th>Pore Pixels (%)</th>
<th>Total Organic Carbon (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1a</td>
<td>2.004</td>
<td>1.999</td>
<td>20.20</td>
<td>0.81</td>
<td>0.52</td>
</tr>
<tr>
<td>2a</td>
<td>1.989</td>
<td>1.989</td>
<td>15.62</td>
<td>2.73</td>
<td>1.85</td>
</tr>
<tr>
<td>3a</td>
<td>1.994</td>
<td>1.972</td>
<td>6.857</td>
<td>8.32</td>
<td>1.64</td>
</tr>
<tr>
<td>4a</td>
<td>1.994</td>
<td>1.965</td>
<td>5.621</td>
<td>13.1</td>
<td>1.38</td>
</tr>
<tr>
<td>5a</td>
<td>1.984</td>
<td>1.995</td>
<td>13.79</td>
<td>1.51</td>
<td>1.71</td>
</tr>
<tr>
<td>6a</td>
<td>1.993</td>
<td>1.995</td>
<td>10.71</td>
<td>1.66</td>
<td>0.60</td>
</tr>
<tr>
<td>7a</td>
<td>3.791</td>
<td>1.994</td>
<td>7.118</td>
<td>2.83</td>
<td>1.03</td>
</tr>
<tr>
<td>8a</td>
<td>1.995</td>
<td>2.002</td>
<td>31.07</td>
<td>0.20</td>
<td>0.25</td>
</tr>
<tr>
<td>9a</td>
<td>2.734</td>
<td>1.992</td>
<td>8.072</td>
<td>2.71</td>
<td>1.41</td>
</tr>
<tr>
<td>10a</td>
<td>1.994</td>
<td>1.994</td>
<td>10.57</td>
<td>2.02</td>
<td>1.67</td>
</tr>
<tr>
<td>Median (CC)</td>
<td>1.994</td>
<td>1.994</td>
<td>10.64</td>
<td>2.37</td>
<td>1.40</td>
</tr>
<tr>
<td>1b</td>
<td>1.992</td>
<td>1.988</td>
<td>11.14</td>
<td>3.31</td>
<td>1.53</td>
</tr>
<tr>
<td>2b</td>
<td>1.994</td>
<td>1.977</td>
<td>6.024</td>
<td>8.24</td>
<td>1.77</td>
</tr>
<tr>
<td>3b</td>
<td>1.994</td>
<td>1.988</td>
<td>5.173</td>
<td>6.00</td>
<td>1.76</td>
</tr>
<tr>
<td>4b</td>
<td>1.978</td>
<td>1.989</td>
<td>11.04</td>
<td>3.15</td>
<td>1.55</td>
</tr>
<tr>
<td>5b</td>
<td>1.993</td>
<td>1.993</td>
<td>12.23</td>
<td>1.88</td>
<td>1.29</td>
</tr>
<tr>
<td>6b</td>
<td>1.992</td>
<td>1.989</td>
<td>9.732</td>
<td>3.12</td>
<td>1.51</td>
</tr>
<tr>
<td>7b</td>
<td>1.989</td>
<td>1.968</td>
<td>7.659</td>
<td>8.52</td>
<td>1.68</td>
</tr>
<tr>
<td>8b</td>
<td>2.074</td>
<td>1.980</td>
<td>10.52</td>
<td>5.72</td>
<td>1.70</td>
</tr>
<tr>
<td>9b</td>
<td>1.990</td>
<td>1.983</td>
<td>12.11</td>
<td>4.47</td>
<td>1.42</td>
</tr>
<tr>
<td>10b</td>
<td>2.004</td>
<td>1.999</td>
<td>19.55</td>
<td>0.92</td>
<td>0.51</td>
</tr>
<tr>
<td>Median (RO)</td>
<td>1.992</td>
<td>1.988</td>
<td>10.78</td>
<td>3.89</td>
<td>1.54</td>
</tr>
</tbody>
</table>

$p$ | 0.237 | 0.103 | 0.650 | 0.112 | 0.326

# Most PSF fits never converged.
still greater than 10% (Table 2-4). Interestingly, solid mass fractal dimensions from Giménez et al. (1998) are similar to those reported here, but indicate a clear separation between aggregates from soils of continuous corn and soils of either alfalfa or grass.

Plotting TOC versus $D$ fails to distinguish the soils in this study, though there does appear to be a relationship between the two variables (Fig. 2-5). Over large values of $D$, TOC increases with decreasing $D$, but then TOC is relatively constant. This pattern is consistent with our hypothesis, although the TOC plateau is somewhat unexpected. The percentage of pore pixels in each aggregate was highly correlated with $D (r=-0.959)$, suggesting that porosity estimates may be equally efficient as $D$ in predicting TOC. No such relationship was observed for $b$; in addition, there is essentially no difference in the median $b$ between the two sets of aggregates. This finding was inconsistent with the observed differences in aggregate stabilities for the two soils (Bucher, 2002).

Conclusions

The agreement of parameters estimated from 3-D and 2-D analyses of aggregates 2a and 7b is observed in Tables 2-2 and 2-3. However, the true utility of the 2-D analytical technique is supported when a single 2-D scan is compared with its corresponding 3-D structure. Such a test can be performed here, because single 2-D scans were taken of all aggregates prior to the 3-D reconstructions. Thus, the original 2-D scans for aggregates 2a and 7b provide randomized representations of the 3-D aggregate structures. Table 2-4 shows that the single scans of aggregates 2a and 7b
Figure 2-5. Total organic carbon versus solid mass fractal dimension for single 2-D scans from 20 aggregates.
yielded values of $D$ nearly identical to the median values in Table 2-3, which are, in turn, similar to the 3-D values (minus one) in Table 2-2. Again, the $b$ values are less conclusive, but it is interesting to note that in all cases the values for $D$ and $b$ are greater for aggregate 2a than for aggregate 7b. Figure 2-6 summarizes the density scaling results of this study in graphical form. The natural variability between aggregates (black curves) is greater than that within aggregates 2a and 7b (yellow curves). Interestingly, the 3-D density scaling for aggregate 2a is nearly indistinguishable from either its original 2-D scan or its collective 277 2-D scans (Fig. 2-6a). This observation cannot be made for aggregate 7b, though parts of the curve from the original 2-D scan fall within one standard deviation of the 3-D reconstruction curve (Fig. 2-6b). Note that aggregate 10b plots well above the others: this is because of its high density resulting from the inclusion of a large mineral grain (Fig. 2-2b).

The first objective in this study was to demonstrate the utility of CT scanning and density scaling for deriving fractal parameters. This was shown through determinations of consistent values of $D$ and $\rho_L$. Values for $b$ were less consistent, but this could be improved by incorporating some image processing to smooth the boundaries of pores. The second objective was to contrast and compare several fractal analytical techniques. This was performed for the solid mass fractal and PSF models of density scaling, as well as the fractal model of cumulative pore number scaling. Because of the high degree of uncertainty in estimates of $D$ from cumulative pore number scaling, density scaling appears to be the best approach to analyzing CT images. Between the solid mass fractal and PSF models, the latter was found unnecessary in describing the structures of two representative aggregates (2a and 7b). The third objective was to assess the ability of 2-D
Figure 2-6 (following page). 2-D density scaling for a) 10 continuous corn (CC) aggregates (heavy black lines) and 277 slices of aggregate 2a (yellow lines) and b) 10 rotation (RO) aggregates (heavy black lines) and 203 slices of aggregate 7b (yellow lines). Also superimposed are the 3-D observations (with error bars) from Fig. 2-4. Estimated bulk density was determined from CT units using the function: $y=1.84 \times 10^{-4}x-0.690$. 
scans to represent corresponding 3-D structures. This was achieved by examining many 2-D scans from complete 3-D structures. Results indicated that 2-D scans can provide reliable estimates of $D$ and $\rho_L$, and that care must be taken in order to analyze 3-D scans without bias. The final objective was to compare the fractal parameters estimated from aggregates of soils from two contrasting long-term treatments. While there was no statistical difference between aggregates of the two soil types, the 20 single 2-D scans suggested that $D$ was more sensitive to the soil treatment than either $b$ or TOC (Table 2-4).

The novelty of this study is its use of CT to discern the structures of individual soil aggregates. In most previous studies involving CT, undisturbed or packed soil columns have been used. Alternatively, the use of individual aggregates provides a natural approach to addressing scaling issues, as aggregates of different size can be compared. This can lead ultimately to more accurate estimations of fractal (and structural) parameters, which, in turn, can enhance our ability to predict soil behavior in a variety of applications. Besides density scaling, other techniques that are compatible with CT include multifractal and lacunarity analyses, and these need to be explored further to assess the practical offerings of CT. In general, because of physical location and cost, industrial quality CT scanning is not yet available to all interested individuals. However, the procedure is promising in its ability to provide more comprehensive and precise analyses of soil structure and dynamics.
References Cited


Chapter 3
SCALING EFFECTS OF AGGREGATES FROM SOILS OF TWO CONTRASTING ORGANIC CARBON LEVELS

Introduction

Many analyses of soil structure now incorporate fractal theory. The notion of soil as a medium whose structure is scale-invariant, or similar over a wide range in scales, has far-reaching implications. The essential advantage in dealing with a fractal soil is the increased ability to model processes such as water retention, hydraulic conductivity, and chemical transport, to name a few (Rieu and Sposito, 1991; Anderson and McBratney, 2002). The direct reason for this advantage is that a fractal soil can be reduced to a relatively simple geometrical pattern that eliminates our reliance on “black box” modeling approaches. Instead, we can incorporate well-established physical laws in a dynamic, deterministic approach.

Clearly, the confidence to model soil processes deterministically depends on the evidence that a soil is, indeed, fractal. The best way to acquire such evidence is to examine the soil at various spatial scales. Commonly, the scaling exponent, or fractal dimension, $D$, is derived for a soil by fitting a fractal model to a data set that incorporates spatial scale, either directly or indirectly (Anderson and McBratney, 2002). One example of this is the water retention function, which depends on pore size distribution (Bird et al., 2000). Specifically, as the soil dries (or the air pressure increases), the remaining water is
held in increasingly smaller pores. Thus, if the soil exhibits a fractal pore number-size
distribution (Eq. (2-4)), then the water retention function will depend on, and provide an
estimate of, $D$. This example is one of indirect incorporation of scale, since the water
content is plotted against pressure (suction) and soil structure is never observed directly.
An example of a direct method would be particle size analysis, which can provide $D$ for a
pore mass fractal or a pore-solid fractal (PSF) (Perrier and Bird, 2002).

The majority of fractal soil analyses utilize methods that allow the derivation of a
single fractal dimension over a range in scales (Anderson and McBratney, 2002). The
question still remains, however, whether the fractal dimension, or other fractal
parameters, might change as the scale range shifts. An analysis that examines the
robustness of these fractal parameters is essential for a complete understanding of the soil
structure and any models dependent on it. For example, very few studies have reported
the fractal parameters of individual aggregates, but, as Chapter 2 has shown, this is
possible. In fact, the application of computed tomography (CT) to describe the structures
of individual soil aggregates is an ideal choice for testing the scale-dependence of fractal
parameters. This novel approach can be implemented simply by scanning aggregates of
several different sizes. Inherently, image analysis of each aggregate summarizes
information from scales smaller than that of the aggregate itself, but a combination of
different sized aggregates summarizes information from an even larger range in scales.

Chapter 2 also indicated a potential relationship between $D$ and total organic
carbon (TOC). Should such a relationship actually exist, it could arise because of the
structural heterogeneity of organic matter (Rice et al., 1999), which confers heterogeneity
to the soil as a whole (Tisdall and Oades, 1982). However, soil organic matter (SOM)
probably exhibits scale-dependent carbon content, thus complicating any direct relationship between $D$ and TOC. Nevertheless, several such relationships might be established for several distinct ranges in scale. Data of this type are lacking in the literature, yet the significance of SOM to soil structure is well known. In particular, Six et al. (2000) have suggested that soil aggregate hierarchy affects carbon sequestration in the form of SOM. Since SOM enhances aggregate formation (Puget et al., 2000; Six et al., 2000), there is likely a strong feedback between SOM and soil structure. It is possible that certain fractal parameters may indicate the carbon sequestration potential, or steady state carbon level, for a given soil.

In this study, we examined aggregates from agricultural soils of two contrasting management histories, differing in levels of organic carbon. There were several objectives: 1) using CT images, derive fractal parameters for individual aggregates from three distinct ranges in spatial scale, 2) test the dependence of these fractal parameters on changes in scale, as well as on the soil type, 3) among the same aggregates, test for any relationships between fractal parameters and TOC, 4) using secondary samples, derive $D$ from aggregate mass scaling and water retention data, and 5) assess the derived fractal parameters for their potential to characterize SOM dynamically.
Materials and Methods

Soils and sampling

Chapter 2 describes in detail the soil sampling location, the Hunter Rotation Experiment (HRE) at Rock Springs, PA. There, the soil is a typic hapludalf, deep, well-drained, derived from limestone residuum, and plowed annually with a moldboard plow. The two HRE treatment combinations responsible for the largest differences in observed soil organic carbon are 1) continuous corn and inorganic fertilizer (“CC”), and 2) 5-year rotation and manure fertilizer to satisfy crop phosphorus (“RO”). Sampling was performed as described in Chapter 2 from eight plots; however, since soil was collected in June 2003, the four RO plots were planted with wheat (as opposed to oats in 2002).

CT scanning

In September 2003, three aggregate size classes were scanned by CT at the Center for Quantitative Imaging (CQI) at Penn State University. The three size classes represent mean diameters of 3.56 mm (“Small”), 28.4 mm (“Medium”), and 55.0 mm (“Large”), as determined from image analysis. Small aggregates were selected randomly after sieving soil through a 4.76 mm mesh and onto a 2 mm mesh. Tweezers were used to transfer aggregates to disposable plastic pipette tips for transport and scanning. Medium aggregates were chosen based on whether they would fit into the openings of a standard ice-cube tray, for transport. Finally, Large aggregates were chosen from the largest visible peds in each batch of soil, and they were wrapped and transported in newspaper. Ten aggregates from each soil type and scale, totaling 60, were weighed and transported to the scanning facility.
Each of the 60 aggregates was scanned as a single 2-D slice. Resolution was 1024 X 1024 in all cases, resulting in pixel sizes of 5.37 µm (Small), 39.0 µm (Medium), and 70.6 µm (Large). While Small aggregates were scanned in plastic pipette tips, Medium aggregates were scanned in air and Large aggregates were scanned in embedding sand. These differences were, in part, to balance the attenuation of X-rays from different energy settings among the three aggregate size classes. To calibrate the CT units (x) with respect to density (y), a standard silica sample was included with each class of aggregates. This resulted in the following functions: 

\[
y = 4.71 \times 10^{-4} x - 1.83 \quad \text{(Small)}, \\
y = 6.35 \times 10^{-4} x - 0.904 \quad \text{(Medium)}, \\
y = 1.70 \times 10^{-3} x - 0.216 \quad \text{(Large)}. 
\]

In this study, estimated density values were not analyzed directly, but they were used as a guide for interpreting density trends across scales. Any statistical analyses depended only on the choice of two calibration points for each aggregate class; these points corresponded to the maximum CT density of the standard silica and the CT density at the pore-solid aggregate boundary, as described next.

**Image analysis**

MATLAB 6 (The MathWorks Inc., Natick, MA) was used for all computations. CT data were saved as tagged image file format (TIFF) files and converted to numerical text data, from which grayscale images could be plotted. Images were not cropped as in Chapter 2, though all other image analysis procedures were the same. This includes defining the pore-solid aggregate boundary visually by comparing grayscale images to partitioned images. The resulting pore-solid boundary was defined at 6000 CT units for Small aggregates, 3000 CT units for Medium aggregates, and 700 CT units for Large aggregates. An additional processing technique was used to separate sand grains from
the soil matrix in Large aggregate images. This was achieved by inscribing a 10-sided polygon in each of the aggregates (also defined visually) and eliminating CT data outside of the polygon.

Processed images were analyzed using density scaling as described in Chapter 2. However, the enhanced image resolution in this study allowed a greater range in box sizes for density sampling. In addition to the 13 box sizes in Chapter 2, six other box sizes were used; these include 79, 99, 123, 155, 193, and 241 (pixel units). Once density scaling was obtained, the solid mass fractal (Eq. (2-2)) and PSF (Eq. (2-3)) model parameters, including $D$, were derived using Gauss-Newton nonlinear curve fitting. The inverse of the similarity ratio, $b$, was derived using the size of the largest pore as described in Chapter 2. Additional observations included the proportion of pore pixels and the mean CT density, with and without pore pixels, within each aggregate image.

**Carbon analysis**

Using a Carlo Erba analyzer, total carbon contents of the 60 individual aggregates were measured after scanning. Small aggregates were combusted in entirety, as in Chapter 2. Medium and Large aggregates were ground finely by a mortar and pestle, from which subsamples were used for combustion.

**Aggregate mass scaling**

Young and Crawford (1991) documented a technique for acquiring the mass fractal dimension of a soil by measuring the mass and radius of a number of individual aggregates of varying size. It is essentially a log-log fit of Eq. (2-1), requiring the aggregates to be approximately spherical. Young and Crawford (1991) solved this problem by shaving off portions of their aggregates to make them more spherical. In this
study, a similar approach was adopted. Specifically, digital calipers (0.01 mm accuracy) were used to measure three orthogonal axes of an aggregate after shaving it with a razor blade to remove irregular surfaces. The resulting aggregate resembled an ellipsoid, and the measurements corresponded to diameters of the major and minor axes, in addition to the intermediate axis. The volume of an ellipsoid is proportional to the product of the radii in these three directions; therefore, the spherical equivalent radius is represented by the cube root of this product. The spherical equivalent radius was calculated for 60 aggregates, selected randomly, of each soil type. Corresponding masses were then recorded, and $D$ was estimated from Eq. (2-1). Although this provided only one value of $D$ for each soil type, it covered a range in aggregate sizes corresponding to the gap between Small and Medium aggregates, thus serving as an auxiliary observation.

**Water retention**

Using the pressure plate method (Richards, 1947), water retention was measured on small samples of packed 1-2 mm aggregates. Initially air-dry, these aggregates were left to saturate overnight, then allowed to reach equilibrium at each of eight pressures—0.02, 0.04, 0.08, 0.16, 0.32, 1.00, 2.00, and 3.00 bars. Triplicate samples of each soil type were used, and subsamples were removed and oven-dried for each weighing. Gravimetric moisture was converted to volumetric moisture by measuring the bulk density of a second set of packed 1-2 mm aggregates. These densities were 0.916 g cm\(^{-3}\) (CC) and 0.866 g cm\(^{-3}\) (RO) at oven-dry moisture.

Volumetric moisture ($\theta$) plotted against water suction ($h$) can provide an estimate of the fractal dimension (Perrier and Bird, 2003):
\[ \theta = \theta_{\text{max}} - A + A \left( \frac{h_{\text{min}}}{h} \right)^{d-D} \]  

(3-1)

In Eq. (3-1), \( A \) is a fitting parameter, \( d \) is the Euclidean dimension, \( h_{\text{min}} \) is the air entry pressure, and \( \theta_{\text{max}} \) is the corresponding soil moisture content. When \( A=1 \), Eq. (3-1) reduces to a form representative of a solid mass fractal; otherwise, \( A \) represents the porosity of a PSF structure (Perrier and Bird, 2003). In this study, water retention data for the two soil types were fitted to Eq. (3-1), providing estimates of \( A \) and \( D \). A justification of the PSF model can occur if \( A \) is significantly different from one. As with aggregate mass scaling, this method provides an independent estimation of \( D \) for each soil, which can strengthen the interpretation of results.

**Large aggregate porosity**

Prior to carbon analysis, each Large aggregate was also analyzed for total porosity, using 500-850 \( \mu \)m quartz sand as a displacement medium. Other aggregate size classes were not tested in this way due to the method’s precision limitations. With larger aggregates, however, the relatively small sand grains act as a fluid capable of measuring aggregate volumes while preserving the samples for carbon analysis. Also, the particle density within each aggregate was assumed to be 2.65 g cm\(^{-3} \), which is more valid when larger units of soil are considered. The packing density of the sand was 1.58 g cm\(^{-3} \), and a graduated beaker was used to measure the volume of the sand-aggregate mixture. Measuring the mass of the aggregate before immersion, as well as the mass of the sand-aggregate mixture, allowed for the calculation of aggregate porosity. The aggregate masses were corrected for air-dry moisture by oven-drying several Medium-sized...
aggregates of each soil type. The gravimetric moisture contents were determined at 2.30% (CC) and 2.39% (RO).

**Results and Discussion**

Table 3-1 summarizes two-factor ANOVA results for each of six different parameters among the 60 scanned aggregates; these parameters include the solid mass fractal dimension ($D$), the inverse of the similarity ratio ($b$), total organic carbon, the percentage of aggregate pixels classified as pore pixels, the mean CT density for the whole aggregate slice, and the mean CT density for the solid portion of the aggregate slice. Each number in the table represents the statistical probability ($p$) that a parameter is not affected by soil type, scale, or their interaction. For example, Table 3-1 shows that $b$ may be affected by soil type, but not by scale or the interaction between soil type and scale. Using $p=0.100$ as a significance guide, it is clear that no parameter is affected by scale except the CT density measures. This follows from theory: a solid mass fractal should have scale-dependent density, but scale-invariant $D$ and $b$ (Bird and Perrier, 2003). On the other hand, soil type affected $b$, TOC, and the CT density measures. Figure 3-1 shows that RO aggregates exhibit generally smaller $b$ and greater TOC, and these aggregates are also less dense (data not shown). Note that scale-invariance is typified by RO aggregates, while CC aggregates exhibit a certain amount of scale-dependence in $D$ and $b$. 
Table 3-1. Two-factor ANOVA for six parameters from 60 aggregates analyzed by CT. 

\(D\) is the solid mass fractal dimension and \(b\) is the inverse of the similarity ratio; values correspond to levels of statistical significance (\(p\)) for each factor in distinguishing a given parameter.

<table>
<thead>
<tr>
<th></th>
<th>(D)</th>
<th>(b)</th>
<th>Total Organic Carbon</th>
<th>% Pore Pixels</th>
<th>Mean CT Density (whole)</th>
<th>Mean CT Density (solid)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soil Type</td>
<td>0.336</td>
<td>0.057</td>
<td>0.001</td>
<td>0.197</td>
<td>0.048</td>
<td>0.098</td>
</tr>
<tr>
<td>Scale</td>
<td>0.105</td>
<td>0.333</td>
<td>0.185</td>
<td>0.144</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>Interaction</td>
<td>0.423</td>
<td>0.147</td>
<td>0.666</td>
<td>0.166</td>
<td>0.467</td>
<td>0.760</td>
</tr>
</tbody>
</table>
Figure 3-1. Effects of scale and soil type on three parameters from 60 aggregates analyzed by CT: solid mass fractal dimension ($D$), inverse of the similarity ratio ($b$), and total organic carbon. Medians and means are both shown to help discern skewed representations.
A closer inspection of $b$ revealed that it was not statistically different between the soil types ($p=0.544$) without considering Large aggregates. This is important because, otherwise, $b$ is the only fractal parameter distinguishing CC and RO aggregates (Table 3-1). Without Small aggregates, $p=0.098$, and without Medium aggregates, $p=0.021$, so Large aggregates are critical to the distinction of soil type. Despite the fact that Medium CC aggregates appear anomalous in Fig. 3-1, ANOVA suggests that Large CC aggregates are more unusual. Potential reasons for this will be discussed later.

Table 3-2 is a correlation matrix among the six parameters from Table 3-1. Table 3-2, however, considers all scales and soil types together in the calculation of each linear correlation statistic ($r$). From the table, it is clear that $D$ and $b$ provide some redundant information. Even more redundant is $D$ and the pore pixel percentage, which is somewhat surprising since it indicates that $D$ is determined more from the amount of pore space than the actual spatial distribution of this pore space. It follows that the correlation between $D$ and TOC is poor, as illustrated by Fig. 3-2. The figure shows TOC versus $D$, and there is clearly no linear relationship, even when examining the data one scale at a time. Furthermore, the scatter in Fig. 3-2 is so great that even nonlinear models would be difficult to develop. Because of the larger data set here, the potential relationship between TOC and $D$ in Chapter 2 is contraindicated. In fact, Table 3-2 does not provide evidence of a single significant relationship with TOC.

In order to supplement the fractal results from image analysis, we conducted tests with aggregate mass scaling and water retention. Figure 3-3 shows the results of aggregate mass scaling, using a log-log plot to derive slope, and solid mass fractal dimension, for each soil type. Note that values for $D$ are reported according to the
Table 3-2. Correlation ($\rho$) matrix amongst six parameters from 60 aggregates analyzed by CT. $D$ is the solid mass fractal dimension and $b$ is the inverse of the similarity ratio; see text for details.

<table>
<thead>
<tr>
<th></th>
<th>$D$</th>
<th>$b$</th>
<th>Total Organic Carbon</th>
<th>% Pore Pixels</th>
<th>Mean CT Density (whole)</th>
<th>Mean CT Density (solid)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D$</td>
<td>0.737</td>
<td>-0.123</td>
<td>-0.955</td>
<td>0.571</td>
<td>0.412</td>
<td></td>
</tr>
<tr>
<td>$b$</td>
<td>-0.254</td>
<td>-0.761</td>
<td>0.487</td>
<td>0.339</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total Organic Carbon</td>
<td>0.123</td>
<td>-0.138</td>
<td>-0.092</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>% Pore Pixels</td>
<td>-0.548</td>
<td>-0.370</td>
<td>0.976</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>


Figure 3-2. Total organic carbon versus solid mass fractal dimension for single 2-D scans from 60 aggregates, distinguished by size class.
Figure 3-3. Aggregate mass scaling relationship for aggregates from CC and RO soils. Solid mass fractal dimensions were derived by linear regression; regression lines are not shown due to their extreme proximity to one another.
embedding Euclidean dimension, so that 2-D images have a theoretical maximum $D=2$
and secondary sets of aggregates have a theoretical maximum $D=3$. Linear regression on
a second set of aggregates yielded $D=2.955 \pm 0.065$ for CC aggregates and
$D=2.999 \pm 0.058$ for RO aggregates (95% confidence interval for each), suggesting that
neither soil exhibits significant heterogeneous distribution of mass. It is especially
counterintuitive that the RO aggregates revealed a greater degree of homogeneity.
However, at least two reasons could be responsible for this trend: 1) the RO aggregates
require the use of a PSF mass scaling model, or 2) the caliper technique is not reliable for
heterogeneous soils. The second reason seems more plausible, particularly since most
aggregate images were characterized best by solid mass fractal models. The fact that the
caliper technique requires the use of a razor blade to shave off portions of aggregate
material means that the technique is biased toward producing homogeneous structures.
Specifically, a heterogeneous aggregate has portions of dense and light material, and
significant shaving will likely select for the measurement of one of the dense regions.
This bias would affect heterogeneous structures the most and could explain why $D$ is
greater for RO than CC, despite the contrary evidence in Fig. 3-1.

A second independent source for $D$ was explored through water retention. Figure
3-4 shows the water retention data for packed 1-2 mm aggregates from the CC and RO
soils. Models fitted to each soil type include a solid mass fractal model (Eq. (3-1), with
$A=1$) and a PSF model (Eq. (3-1), with $A$ estimated from the fitting process). The
difference in model performance was minimal, but, because $A$ is an additional free
parameter in the PSF model, by default this version will outperform the solid mass fractal
version. The solid mass fractal dimensions were $D=2.949 \pm 0.012$ (CC) and
Figure 3-4. Water retention of 1-2 mm packed aggregates from a) CC and b) RO soils. Dashed lines represent the fitted solid mass fractal models; solid lines represent the fitted PSF models. Error bars represent standard deviations ($n=3$) at each scale of observation.
$D = 2.951 \pm 0.019$ (RO), while the PSF dimensions were $D = 2.838 \pm 0.198$ (CC) and $D = 2.726 \pm 0.325$ (RO) (all with 95% confidence intervals). Note that the uncertainty in the PSF values is much greater, and that the values themselves are significantly lower, than for corresponding solid mass fractal values. From a practical standpoint, the solid mass fractal models are more attractive, especially since they tend to outperform the PSF models at the highest suctions—i.e., at the smallest scales (Fig. 3-4). Interestingly, the solid mass fractal dimensions of the aggregate mass scaling and water retention data are very similar for CC soil. However, these values, minus one for dimensionality, are slightly low compared to $D$ from image analysis (Fig. 3-1). While both aggregate mass scaling and water retention suggest that RO soil has a solid mass fractal dimension less than that of CC soil, it is not significantly less. This is especially true when considering the reliability of the caliper technique, which is minimal. Table 3-1 corroborates the findings that the two soils exhibit relatively similar values for $D$.

Only 14 of the 60 aggregates analyzed by image analysis were suitable for characterization by the PSF model of soil structure. When fitting models to CT density scaling data, the PSF model was deemed appropriate if its $r^2$ value was at least 0.001 greater than that for the solid mass fractal model. Figure 3-4 suggests that the PSF model does not outperform the solid mass fractal model at small scales, and this is in agreement with the fact that only two Small and two Medium aggregates were characterized best by the PSF model. On the other hand, 10 Large aggregates were characterized best by the PSF model, and they are shown in Fig. 3-5, along with the other 10 Large aggregates. In each panel is the grayscale CT representation of the 2-D slice from one aggregate, where increasing brightness corresponds to increasing density. The solid mass fractal
Figure 3-5 (following page). CT images of 20 Large aggregates, with 1024 X 1024 resolution (pixels represent 70.6 µm X 70.6 µm, with thickness=76.4 µm). Corresponding solid mass fractal dimensions are located below each panel; where appropriate, PSF fractal dimensions are shown in parentheses.
Continuous Corn Aggregates

(b) 72.3 mm

Rotation Aggregates
dimension is shown below each panel, and, where appropriate, the PSF dimension is shown in parentheses. Note that the PSF dimensions are typically low compared to the solid mass fractal dimensions; similar trends were observed in Fig. 3-4 and in Bird and Perrier (2003). Figure 3-5 also shows a striking feature of the PSF aggregates: they are devoid of relatively large pores. The reason for this is that a PSF model is warranted only when pores and mineral grains are comparable in size (Perrier et al., 1999). Since most aggregates in Fig. 3-5 show small mineral grains (bright regions), those aggregates cannot be characterized by PSF models unless the pores are also small.

An analysis of Large aggregate $b$ values, using Wilcoxon Rank Sum Tests, showed that $b$ was highly significant in distinguishing CC versus RO and PSF versus non-PSF aggregates (Table 3-3). As stated earlier, the $b$ values of CC aggregates deviate most from those of RO aggregates at the largest scale. Figure 3-5 provides visual evidence that this is because the Large CC aggregates have very few significant pores. However, prevalence of the PSF model is not much greater for CC aggregates ($n=6$) than for RO aggregates ($n=4$), so it is difficult to explain differences in soil type according to a particular fractal model (Fig. 3-5). Nevertheless, differences between the two sets of Large aggregates remain. An additional significant distinction was made through the measured porosity of these aggregates (Table 3-3). Combined with TOC, this information indicates differences between the two soils at a fundamental level, but without implications for specific fractal models.

One possible explanation for these observations is that Large aggregates were affected during sampling. Specifically, many of the largest pores may have collapsed under the pressure of the sampling device. In fact, the mean densities of Medium and
Table 3-3. Comparison of Large aggregate porosity and $b$ value medians. ‘PSF’ refers to aggregates modeled best by a PSF structure; ‘Non-PSF’ refers to aggregates modeled best by a mass fractal model. For CC PSF aggregates, $n=6$ (out of 10); for RO PSF aggregates, $n=4$ (out of 10). Superscript designations correspond to Wilcoxon Rank Sum Test for differences (at $p=0.05$) in medians. Different letters in a column indicate a soil type significance, while different letters in a row indicate a model type significance.

<table>
<thead>
<tr>
<th></th>
<th>Porosity</th>
<th></th>
<th>$b$</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>PSF</td>
<td>Non-PSF</td>
<td>Total</td>
<td>PSF</td>
<td>Non-PSF</td>
</tr>
<tr>
<td>CC Aggs.</td>
<td>0.422</td>
<td>0.333</td>
<td>0.375&lt;sup&gt;a&lt;/sup&gt;</td>
<td>14.52</td>
<td>9.658</td>
</tr>
<tr>
<td>RO Aggs.</td>
<td>0.462</td>
<td>0.443</td>
<td>0.455&lt;sup&gt;b&lt;/sup&gt;</td>
<td>11.86</td>
<td>7.147</td>
</tr>
<tr>
<td>Total</td>
<td>0.427&lt;sup&gt;a&lt;/sup&gt;</td>
<td>0.377&lt;sup&gt;a&lt;/sup&gt;</td>
<td>0.424</td>
<td>13.31&lt;sup&gt;a&lt;/sup&gt;</td>
<td>8.662&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
</tbody>
</table>
Large aggregates, estimated from CT analysis, were $\rho_{\text{Medium}} = 1.457 \pm 0.087 \text{ g cm}^{-3}$ and $\rho_{\text{Large}} = 1.590 \pm 0.126 \text{ g cm}^{-3}$, respectively (± standard deviation for each). This represents a trend opposite that which is expected for a heterogeneous medium, but could be explained by a sampling bias. Aggregate collapse could have been facilitated by moist conditions: data from the Penn State University Automated Weather Observation System at Rock Springs, PA show that May 2003 was 27% wetter than normal, and that these conditions persisted into June (see Appendix A). However, if the preceding interpretations are accurate, then there was a differential rate of collapse, such that Large CC aggregates were more susceptible to sampling than Large RO aggregates. Such a phenomenon would explain the measured porosity and $b$ differences between Large CC and RO aggregates, while also accounting for the increased densities at the largest scale. This may reflect a fundamental aggregate stability difference between the two soils, which is corroborated by data from Bucher (2002).

**Conclusions**

This study addressed scaling issues in two soils with statistically different levels of TOC. The ultimate objective was to derive fractal parameters that might help model the structure of each soil, explain their TOC difference, and lead to a greater understanding of factors involved in carbon sequestration. Analysis of aggregates through CT, as well as aggregate mass scaling and water retention, led to statistically similar values of $D$ for both soils. The other important fractal parameter, $b$, proved to be
highly significant in distinguishing soil type at the largest scale. This parameter was also linked to the PSF model, in that greater \( b \) values correlated with PSF structures and smaller \( b \) values were correlated with solid mass fractal structures. While this was a significant discovery, PSF prevalence was similar in either soil. More evidence from Large aggregate porosity indicated that there were significant differences between soils at this scale. It was conjectured that soil sampling may have amplified these differences, but that the differences reflect some fundamental factor, such as aggregate stability.

Because of ambiguous results, we cannot prescribe exact fractal parameter values to either soil, and it is difficult to explain their TOC difference in terms of soil structure, as observed through CT image analysis. However, if the stability of RO aggregates is significantly greater than that of CC aggregates, there is a high probability that RO aggregate lifetime exceeds CC aggregate lifetime. According to Six et al. (2000), the lifetime of macroaggregates is critical in determining the production of microaggregates that protect carbon on long time scales. Thus, we can assume that RO soil has a higher organic carbon capacity, but whether or not this capacity has been utilized is unanswered. Quite possibly, the increased additions of organic matter to RO soil has, in itself, altered the aggregate stability enough to retain even more organic matter. This potential positive feedback would be an important mechanism for carbon sequestration on a global scale, and it should be investigated thoroughly.
References Cited


Chapter 4

A MODIFIED PORE-SOLID FRACTAL MODEL OF SOIL STRUCTURE
INCORPORATING AGGREGATE AND ORGANIC MATTER DYNAMICS

Introduction

Fractal geometry has found diverse applications in soil science, including the description of soil variation across a landscape (Burrough, 1983), estimation of soil water retention curves (Tyler and Wheatcraft, 1989; Perfect et al., 1996), and characterization of soil structure (Bartoli et al., 1991; Rieu and Spositio, 1991a, 1991b; Peyton et al., 1994). Because soil porosity is a particularly critical determinant of permeability and moisture-holding capacity, many fractal models of soil structure have been based on pore-solid boundaries (Rieu and Spositio, 1991a; Crawford and Matsui, 1996), taking advantage of the fact that soil pores are often visibly distinguishable from the matrix. Consequently, most fractal models of soil structure have two phases: they describe soil as a mass fractal embedded in 2-D or 3-D space with a non-fractal complementary phase. Research by Crawford and Matsui (1996) indicates that the fractal phase is associated commonly with the ‘solid’ matrix, while the complement is usually the pore space. In this case, a solid mass fractal can be used to model the soil structure. Such a model has limited applicability, however, as the fractal phase tends toward zero as resolution approaches infinity. In other words, the only true phase in a solid mass fractal is the pore phase.
The pore-solid fractal (PSF) model of soil structure is a newer fractal approach developed by Perrier et al. (1999). This approach enables a more realistic depiction of soil structure, wherein both pores and solids coexist as true phases through the introduction of a third, virtual phase (i.e., the “fractal” phase). In the PSF model, neither the pore nor solid phase is a mass fractal, although pore and solid units share symmetrical power law number-size distributions. The third phase consists of unresolved pores and solids, and it can be used to represent soil aggregates (Perrier and Bird, 2002), which have intermediate density between that of pores and solids.

The inclusion of a third phase in the PSF model has practical advantages. Specifically, in a two-phase solid mass fractal model, the extent of the solid phase is predicted to approach zero as resolution approaches infinity (the same is true for pores in a pore mass fractal). This can lead to unrealistic properties, such as abnormally dense soil aggregates at modestly small length scales (Bird and Perrier, 2003). The PSF model can avoid these conditions because it is the intermediate phase that approaches zero as resolution approaches infinity. In other words, pores and solids coexist at each level in the soil hierarchy, independent of scale (Perrier et al., 1999). Even though pore and solid number-size distributions must follow power laws over the range in scale considered by the PSF model, the presence of a third phase provides flexibility in practical situations. This flexibility is observed in two special cases of the PSF model. The first case is when the solid phase is set to zero, so that pores are the only complement and the model becomes a solid mass fractal. The second case is when the pore phase is set to zero, so that solids are the only complement, and the PSF model becomes a pore mass fractal (Perrier et al., 1999). Thus, the PSF model is useful for soils whose solids and pores both
exhibit fractal number-size distributions, or for soils that exhibit only one type of fractal number-size distribution.

While the PSF approach has improved our ability to model soil structure quantitatively, it does not account explicitly for soil organic matter (SOM). Like porosity, SOM is an important factor in soil permeability, moisture-holding capacity, and reactivity, partly because of its highly porous nature. However, SOM also confers biochemical properties to the soil as a matrix both for proton and cation exchange and for C and N storage and transformations; microorganisms use SOM as sources of energy and sites of attachment (Ladd et al., 1993; Oades, 1993). Since the density of SOM is known to vary from $<1.0$ to over $2.2 \text{ g cm}^{-3}$ (Baisden et al., 2002), it is reasonable to propose that the unresolved PSF aggregates are associated with SOM. However, any associations are complicated by the fact that such aggregates also contain pores and mineral matter. Therefore, SOM is only an implicit component of the PSF intermediate phase. In this study, we work towards a modification of the PSF model in which SOM is accounted for explicitly as a distinct and dynamic soil phase that behaves as a mass fractal. The objectives are to 1) develop the mathematical foundation for modifying the original PSF model in order to link soil aggregate hierarchy to SOM, 2) test the modified model against soil aggregate density and SOM data, and 3) assess the utility of the modified model in describing time-dependent dynamics of soil aggregates and SOM.
Theory

Aggregate hierarchy and SOM dynamics

For context, we describe the current understanding of soil aggregate hierarchy and the dynamics of aggregate and SOM cycling. Figure 4-1 illustrates the basic principles, adapted from Six et al. (2000a). In this figure, a soil macroaggregate (>250 µm) is shown at various stages of internal development. The focus is on internal development of the aggregate, rather than on its formation, because evidence indicates that macroaggregate formation is quite rapid (Bossuyt et al., 2001). Specifically, it is thought that fungal hyphae are the dominant aggregating agent at this scale, binding minerals (silt/sand and clay flocculates) together with particulate organic matter (POM), which can be broken down for nutrients (Wright and Upadhyaya, 1998; Bossuyt et al., 2001). Relatively rapid microbial growth and metabolism, then, define and stabilize the aggregate, creating a discrete microenvironment in which microorganisms are protected physically from larger grazers (Crawford et al., 1993). Internal development of the aggregate proceeds as protected organisms decompose the organic matter into smaller units, which then react with metabolic byproducts such as exopolysaccharides (Tisdall and Oades, 1982).

Within the developing macroaggregate, large organic particles are degraded into smaller organic fragments, which undergo biogeochemical interactions with mineral colloids, microbes, and microbial binding agents. These processes result in the formation of secondary aggregates inside the larger ones, which, theoretically, can occur \textit{ad infinitum} to produce a nested hierarchical aggregate structure with a variety of pore sizes. Because it has been shown that organic matter associated with the smallest aggregate size
Figure 4-1. Schematic of soil aggregate and SOM dynamics, adapted from Six et al. (2000a). See text for details.
fractions is most resistant to decomposition, the physical protection of microaggregates (<250 µm) is important for long-term soil carbon retention. When a critical level of organic matter degradation has occurred, the original macroaggregate loses stability, causing a release of any internal aggregates. In the presence of fresh POM, new macroaggregates can form from smaller aggregates, thus affording protection for the organic matter contained within them (Fig. 4-1). If fresh POM is not replenished, smaller aggregates remain exposed and their associated organic matter is less protected. Six et al. (2000a) proposed that macroaggregate turnover controls microaggregate formation, which ultimately controls carbon sequestration and the carbon saturation level in soil. Macroaggregate turnover should not be too rapid, or secondary aggregates will not form; alternatively, macroaggregate turnover should not be too slow, or fresh POM will not be incorporated for carbon sequestration.

The apparent relationship between soil structure and soil carbon cycling is that an aggregate hierarchy is necessary for the sequestration of carbon in soil. Because fractal theory is based on the hierarchical arrangement of particles, we hypothesize a relationship between fractal parameters of a soil and its ability to sequester carbon. In the following section, we describe the PSF model for soil structure, which provides the basis for our modified model that incorporates SOM.

**Original PSF model**

A structural unit of soil is depicted in Fig. 4-2 as a PSF, illustrating the concepts of the PSF model of Perrier et al. (1999). In the example shown, two pore blocks (labeled \( P \)) and two solid blocks (labeled \( S \)) occur at each scale. The other five intermediate blocks (labeled \( F \)) behave as fractals; here, the term “fractal” indicates an
Figure 4-2. Original PSF conceptual model. In this example, $d=2$ and $f=5/9$, for a fractal dimension, $D$, of 1.465. Asterisks (*) indicate fractal blocks ($F=5$). The hierarchy level is designated by $i$, which increases as size decreases.
object whose coverage decreases, via replacement by pore or solid material, as resolution
increases. In this context, the intermediate blocks are considered as nested soil
aggregates of decreasing size (Perrier and Bird, 2002). Because these aggregate blocks
are fractals, we can obtain their fractal dimension, \( D \). Perrier et al. (1999) used the
equation

\[
D = d + \frac{\log(f)}{\log(b)},
\]

where \( d \) is the embedding Euclidean dimension, \( f \) is the portion of soil that is in the
intermediate phase (range is \( >0 \) to \( 1 \)), and \( b \) is the inverse of the similarity ratio (range is
\( >1 \) to \( \infty \)). The similarity ratio is simply the ratio of linear size, or diameter, of blocks at
adjacent scales. Note that as \( f \) or \( b \) increases, \( D \) also increases.

The three phases in a PSF structure are fractals, solids, and pores, referred to here
as ‘F,’ ‘S,’ and ‘P’ phases, respectively. For each phase, the number of blocks forming a
structural unit of any size can be written as

\[
F = f \cdot b^d \tag{4-2}
\]

\[
S = s \cdot b^d \tag{4-3}
\]

\[
P = p \cdot b^d \tag{4-4}
\]

where the lower case variables sum to unity:

\[
f + s + p = 1. \tag{4-5}
\]

Note that Eqs. (4-2)-(4-5) require that

\[
F + S + P = b^d. \tag{4-6}
\]
In summary, a PSF can be described as a three-phase model for soil structure in which the F phase is interpreted as soil aggregates, while physical analogs of the S and P phases are mineral grains and pore spaces, respectively (Perrier and Bird, 2002). PSF aggregates exhibit nested self-similar structure and a fractal dimension given by Eq. (4-1). In the next section, we work towards a model that distinguishes between pore spaces, mineral grains, and organic matter.

**Modified PSF model**

Using the geometry of the PSF model of Perrier et al. (1999), Fig. 4-3 illustrates the concepts of our modified PSF model, which incorporates organic matter as a distinct phase. In the example shown, two pore blocks (labeled $P'$) and two mineral matter blocks (labeled $S'$) remain at each scale, just as in Fig. 4-2; the difference is that the other five blocks, which represented secondary aggregates in Fig. 4-2, now comprise distinct organic matter blocks (labeled $F'$) and mineral matter blocks. Here, organic matter is a classical mass fractal that contains pores, unlike the intermediate phase of the original PSF model, which contains both pores and solids. In other words, secondary aggregates are implied as preexisting in the original PSF model, which is not the case in our modified version. Instead, the modified PSF model requires a portion of mineral matter blocks to subdivide in order to combine with decomposing organic matter blocks, and this process leads to secondary aggregate formation ($i=1$ in Fig. 4-3). Thus, the modified PSF model depends implicitly on time, such that the “initial” state for soil is one with large organic matter fragments and no secondary aggregates; the “advanced” state for soil is one with small organic matter fragments and several layers of nested aggregates. The modified PSF structure is constrained by two rules: 1) when organic matter is entirely
Figure 4-3. Modified PSF conceptual model. As in Fig. 4-2, the fractal dimension, $D$, is 1.465. Asterisks (*) indicate blocks that subdivide, corresponding to the F blocks in Fig. 4-2. The particular example requires a 1:1 recombination ratio of initial solid and organic matter blocks, but this varies depending on PSF phase composition. The hierarchy level is designated by $i$, which increases as size decreases.
decomposed, the structure must be identical to that of the original PSF, and 2) self-similarity is maintained in aggregates at all scales. Using these rules, it is possible to derive equations that determine the partitioning of phases in the modified PSF system based on an original PSF geometry; we derive these equations later. As an example application, Fig. 4-3 shows that the ratio of pores to minerals to organics is 2:4.5:2.5, as required by the original PSF geometry in Fig. 4-2.

One assumption of the modified PSF model is that organic matter behaves as a solid mass fractal, and this assumption is supported by experimental observations at small scales (Rice et al., 1999). Other observations, such as the separation of “light” and “heavy” SOM in relatively large and small fractions, respectively, are indirect validations (Elliott et al., 1991; Six et al., 1998). This is because a solid mass fractal increases in density at smaller scales (Bird and Perrier, 2003). Another assumption of the modified PSF model is that mineral matter is redistributed to help form secondary aggregates; at some scales, this could correspond to the dispersion of clay flocculates (Fig. 4-1). Dispersal of clay and clay-SOM interactions are reversible processes, and these should not be confused with classical “mineral weathering.” It is also important to note that in the modified PSF model, the mineral blocks contain no pores and, therefore, cannot be mass fractals. This implies that the mineral blocks have scale-invariant density, which is a reasonable assumption for most minerals. However, a portion of mineral blocks are grouped with the organic matter blocks because they are necessary in forming secondary aggregates and ultimately creating a structure that resembles that of the original PSF (Fig. 4-2).
The inclusion of time in the modified PSF model provides a realistic context in which to view soil structure formation, with the original PSF model serving as a guide. A point of emphasis is that an original PSF structure comprises two true phases (solids and pores) and one virtual phase (secondary aggregates), as infinite resolution proves that the virtual phase is made up entirely of solids and pores. On the other hand, a modified PSF structure comprises three true phases (minerals, pores, and organics) and one virtual phase (secondary aggregates), in an attempt to incorporate principles from Fig. 4-1. Until most organic matter has been decomposed, the two models of structure are quite different. Nevertheless, we can utilize original PSF parameters to help understand the modified PSF structure.

We now quantify the relationships between the two PSF systems. In the modified PSF system, let \( F', S', \) and \( P' \) represent organic matter, mineral matter, and pore phase blocks, respectively. They combine to form the initial hierarchy (largest size class) of soil aggregates as follows:

\[
F'_0 + S'_0 + P'_0 = b^d .
\]  

Equations (4-6)-(4-7) show that the initial fractal aggregate comprises \( b^d \) subunits partitioned amongst three phases.

In the modified system, organic and pore subunits derive from larger organic matter blocks, while solid subunits derive from larger solid blocks. The subdivision of the initial hierarchy can be expressed as

\[
F'_i = k_f \cdot b^d F'_0 \\
S'_i = k_s \cdot b^d S'_0
\]
\[ P_i' = (1 - k_f) \cdot b^d F_0', \quad (4-10) \]

where \( k_f \) is the proportion of organic material yielding smaller organic matter blocks (i.e., the complement of the smaller pore blocks), and \( k_s \) is the proportion of solid blocks that subdivide. Because the number of subdividing blocks is equivalent in the two systems, we can also express the first subdivision as

\[ F'_i = F \cdot F'_0 \quad (4-11) \]
\[ S'_i = F \cdot S'_0 \quad (4-12) \]
\[ P'_i = F \cdot P'_0. \quad (4-13) \]

Combining Eqs. (4-8) and (4-11),

\[ F = k_f \cdot b^d, \quad (4-14) \]

and combining Eqs. (4-9) and (4-12),

\[ F = k_s \cdot b^d. \quad (4-15) \]

Equations (4-14)-(4-15) prove that

\[ k_f = k_s. \quad (4-16) \]

Furthermore, combining Eqs. (4-2), (4-14) or (4-15), and (4-16) yields

\[ f = k_f = k_s. \quad (4-17) \]

Equation (4-17) shows that the proportion of secondary organic material in organic matter blocks is identical to the proportion of secondary aggregates in the initial original PSF structure. The equality also reflects the proportion of solid blocks that subdivide. This reduces the number of unknowns and simplifies the task of relating phases in the two PSF systems.
In either system, the pore blocks fail to contribute to subdivision. Thus, in order for the modified structure to approximate that of the original, the following equality holds:

\[ P = P_0'. \] (4-18)

Likewise, the solid blocks that do not subdivide can be equated to the number of original PSF solid blocks:

\[ S = (1 - f) \cdot S_0'. \] (4-19)

It is then straightforward to express \( F \) as a function of modified PSF subunits.

Combining Eqs. (4-6)-(4-7) with Eqs. (4-18)-(4-19) yields

\[ F = F_0' + f \cdot S_0'. \] (4-20)

Explicit functions for modified PSF phases can now be achieved algebraically:

\[ P_0' = P \] (4-21)

\[ S_0' = \frac{S}{1 - f} \] (4-22)

\[ F_0' = F - \frac{f \cdot S}{1 - f}. \] (4-23)

Alternatively, by utilizing Eqs. (4-2)-(4-4), Eqs. (4-21)-(4-23) can be written as follows:

\[ P_0' = b^d (1 - f) \cdot \phi \] (4-24)

\[ S_0' = b^d (1 - \phi) \] (4-25)

\[ F_0' = b^d f \cdot \phi, \] (4-26)

where

\[ \phi = \frac{p}{p + s}. \] (4-27)
Equations (4-24)-(4-26) describe the proportion of pore, mineral, and organic blocks that must be considered in order to yield ultimately the proportion of pore \( P \), solid \( S \), and aggregate \( F \) blocks in the corresponding original PSF structure. Perrier et al. (1999) derived Eq. (4-27) in order to explain how the porosity of a PSF soil behaves; as resolution approaches infinity, it can be shown that the total porosity approaches \( \phi \), referred to here as the ultimate porosity. This value is a function only of pore and solid blocks of a given size. The incorporation of \( \phi \) into Eqs. (4-24)-(4-26) links the modified PSF model to a more physical soil trait determined by original PSF parameters.

**Comparison of fractal dimensions**

Because the organic matter phase in the modified PSF model is a classical mass fractal, we can derive its fractal dimension. Combining Eqs. (4-1)-(4-2) with Eq. (4-11) yields

\[
F'_{i'} = F'_0 \cdot b^{D_i}.
\]  

(4-28)

Since the subdivision process is iterative, Eq. (4-28) can be generalized as

\[
F'_{i'} = F'_0 \cdot b^{D_i},
\]  

(4-29)

where \( D \) is the fractal dimension of the organic matter phase. This can be shown via the scaling of organic mass of unit volumes—\( b^{-d} \) for a subunit in the 0\(^{th}\) hierarchy, and \( b^{-d(i+1)} \) for a subunit in the \( i^{th}\) hierarchy. Since there is complete conservation of mass after each subdivision, it is known that

\[
F'_{i'} \cdot m_f (i) = F'_0 \cdot m_f (0),
\]  

(4-30)

where \( m_f \) represents organic mass of unit volume. Equations (4-29)-(4-30) show that

\[
m_f (i) = m_f (0) \cdot b^{-iD},
\]  

(4-31)
which demonstrates that the mass fractal dimension of the organic matter phase is $D$, identical to the fractal dimension of the original PSF structure.

**Organic matter density and SOM scaling**

We can use the previous equations to solve for organic matter density as a function of scale. Equation (4-31) is divided by $b^{d(i+1)}$, the volume of a subunit in the $i$th hierarchy, to give

$$\rho_f(i) = \frac{m_f(0)}{b^{-d(i+1)}} \cdot b^{-id}.$$  \hspace{1cm} (4-32)

where $\rho_f$ is the organic matter density. Equation (4-32) can be rewritten as

$$\rho_f(i) = \frac{m_f(0)}{b^{-d}} \cdot b^{-i(D-d)},$$

which simplifies to

$$\rho_f(i) = \rho_f(0) \cdot b^{-i(D-d)}. \hspace{1cm} (4-33)$$

This demonstrates the density scaling of the organic matter phase, which is critical in determining SOM and soil organic carbon (SOC) as a function of size.

From this point on let $F', S',$ and $P'$ represent $F_0', S_0',$ and $P_0'$, respectively, since we need only consider numbers of blocks per phase in a representative hierarchy. Also, for simplicity, let $x=\rho_f(0)$; then Eq. (4-33) can be rewritten as

$$\rho_f(i) = x \cdot b^{-i(D-d)}. \hspace{1cm} (4-34)$$

The density of a representative aggregate, $\rho_t$, will be an average of the contributing phase densities:

$$\rho_t(i) = \frac{F' \rho_f(i) + S' \rho_s}{b^d}. \hspace{1cm} (4-35)$$
Equation (4-35) assumes that pore blocks have zero mass. Note that the density of solid blocks, $\rho_s$, is scale-invariant, and that each density is weighted according to its spatial presence in the aggregate.

We now require an equation for the mass quantity of SOM, $Q_{SOM}$. This is the ratio of the mass of organic matter blocks, $F' m_f(i)$, to the mass of the housing aggregate, $m_t(i)$:

\[ Q_{SOM}(i) = \frac{F' m_f(i)}{m_t(i)}. \] (4-36)

Equation (4-36) can be expressed, then, in terms of corresponding densities as

\[ Q_{SOM}(i) = \frac{F' b^{-(i+1)} \rho_f(i)}{b^{-d} \rho_s(i)}. \] (4-37)

The numerator of Eq. (4-37) derives from Eqs. (4-31)-(4-32), while the denominator utilizes similar logic. The only difference is that the volume of an organic matter subunit is $b^{-d(i+1)}$, but for an aggregate it is $b^{-d}$. Combining Eqs. (4-34)-(4-35) and (4-37) yields

\[ Q_{SOM}(i) = \frac{F' b^{-D-d} b^{-i}}{F' b^{-D-d} + S' \rho_s}, \] (4-38)

which relates SOM to modified PSF parameters. Therefore, SOM relates indirectly to original PSF parameters, Eqs. (4-21)-(4-23).

**Internal aggregate development**

We have demonstrated that original PSF parameters are useful in describing the proportion of SOM in undeveloped aggregates. Essentially, an aggregate without internal aggregates can be modeled by Eq. (4-38). However, as organic matter decomposes, it forms secondary organic matter particles that bind minerals into secondary aggregates.
Fig. 4-1); Fig. 4-4 summarizes this process in a fractal context. Theoretically, organic matter is conserved over short time frames, which assumes that the rate of organic matter loss from the aggregate is small relative to the rate of decomposition of individual organic matter particles. In this sense, $Q_{SOM}$ does not change, and Eq. (4-38) is still valid. Eventually, organic matter losses must be accounted for, and this can be achieved with the implementation of a minimum size for organic matter particles. This is equivalent to imposing a scale range limit on the fractal model, which allows us to relax the constraint on organic matter conservation for the decomposition of the smallest organic matter particles. In other words, once an organic matter particle has undergone a certain number of decompositions, some (but not all) of its resultant fragments are oxidized completely.

We can modify Eq. (4-38) to include organic matter losses via internal aggregate development. Let $A$ be the maximum number of aggregates that can form within a larger aggregate:

$$A_i = F^i. \quad (4-39)$$

Note that when $i=0, A=1$, which reflects the initial housing aggregate. After each $i^{th}$ subdivision, the maximum number of aggregates that can form via recombination is equal to the number of subdividing organic matter particles and minerals. If $n$ is the maximum number of levels of internal structure that can form, then Eq. (4-39) can be rewritten as

$$A_n = (vF)^n, \quad (4-40)$$

where $v$ is the proportion of organic matter particles and minerals that actually subdivide. The coefficient $v$ ranges from 0, with no aggregate development, to 1, with complete
Figure 4-4. Internal development of a modified PSF aggregate. In this example, there is a 1:1 recombination ratio of solid and organic blocks, and the structure is developed completely when all organic blocks (gray blocks) have decomposed; the end product is an original PSF aggregate.
aggregate development. $A_n$ represents the number of the smallest aggregates contained within the initial aggregate.

To obtain the number of organic matter blocks that oxidize completely, we require the number of smallest aggregates given by Eq. (4-40). The number of smallest organic matter blocks is exactly $A_n F'$, but only some of these will actually be completely degraded. Continuing with the scale-invariant subdivision process, let $\nu$ also be the proportion of smallest organic matter blocks that are completely degraded. Then,

$$O = (vF)' \cdot vF', \quad (4-41)$$

where $O$ is the number of oxidized organic matter blocks. From Eqs. (4-2) and (4-26) we know that $F'' = \phi F$, so Eq. (4-41) can be expressed as

$$O = (vF)' \cdot v\phi F', \quad \text{or, more simply,}$$

$$O = \phi \cdot (vF)^{n+1}. \quad (4-42)$$

Equation (4-42) reveals the number of small organic matter blocks that are oxidized, for different degrees of internal development, $\nu$. To modify Eq. (4-38), we use the unit volume of a small organic matter block, $b^{-d(n+1)}$, and Eqs. (4-34) and (4-42) to calculate the total oxidized organic matter mass, $M$:

$$M = \phi \cdot (vF)^{n+1} xb^{-(nD+d)},$$

or, utilizing Eq. (4-2),

$$M = \phi \cdot (vf)^{n+1} xb^{-n(D-d)}. \quad (4-43)$$

Similarly, the total oxidized organic matter volume, $V$, is

$$V = \phi \cdot (vF)^{n+1} b^{-d(n+1)},$$
or, from Eq. (4-2),

\[ V = \phi \cdot (\nu f)^{n+1}. \]  \hspace{1cm} (4-44)

Finally, \( M \) is subtracted from the numerator and denominator of Eq. (4-38):

\[ Q_{\text{SOM}}(i) = \frac{F'xb^{-i(D-d)} - M}{F'xb^{-i(D-d)} + S' \rho_i - M}. \]  \hspace{1cm} (4-45)

Equation (4-45) describes how SOM changes in an aggregate, from any size class, as its internal structure develops. Equation (4-44) is useful when considering corresponding changes to the aggregate density. Specifically, as the aggregate loses organic matter, it loses mass, given by \( M \), as well as some volume; without evidence to the contrary, we will assume that the lost volume corresponds to that of the oxidized organic matter, given by \( V \). To update aggregate density, we must express Eq. (4-35) as a ratio of mass to volume. Using the unit aggregate volume, \( b^{-d_i} \), and Eq. (4-35), the aggregate mass is

\[ m_i(i) = b^{-d(i+1)}(F' \rho_j(i) + S' \rho_s). \]

Thus, the updated mass is

\[ m_i(i) = b^{-d(i+1)}(F' \rho_j(i) + S' \rho_s) - M. \]  \hspace{1cm} (4-46)

Likewise, the updated aggregate volume is \( b^{-d_i} - V \), which, utilizing Eq. (4-34), yields the following expression for \( \rho_i \):

\[ \rho_i(i) = \frac{b^{-d(i+1)}(F'xb^{-i(D-d)} + S' \rho_s) - M}{b^{-d_i} - V}. \]  \hspace{1cm} (4-47)

Equations (4-45) and (4-47) can be applied to actual data representing aggregate SOM and aggregate density, respectively. Thus, we have utilized the PSF framework to derive expressions for two quantities in direct correspondence, which can help test the
modified PSF model. Furthermore, as time is an implicit component of the model, implications for soil carbon dynamics might emerge.

Materials and Methods

To test their soil fractal models, Rieu and Sposito (1991b) and Bird and Perrier (2003) used the data set of Wittmuss and Mazurak (1958), which appears to be the only study available in the literature that reports soil aggregate density and SOM for corresponding size classes (Table 4-1). Wittmuss and Mazurak (1958) used the Chepil method to measure density, and the Walkley-Black method to measure SOM, of aggregates from Sharpsburg silty clay loam—a smectitic, mesic, Typic Argiudoll. Corresponding measurements were recorded for aggregates ranging in size from 18.5 µm to 4.76 mm. Here, we re-examine those measurements in order to test Eqs. (4-45) and (4-47).

Aggregate density and SOM data were plotted using geometric mean sizes, rather than arithmetic means as used by Rieu and Sposito (1991b) and Bird and Perrier (2003). This was done in order to represent more accurately the assumed exponential number-size distribution of aggregates. MATLAB 6 (The MathWorks Inc., Natick, MA) was used to perform simultaneous nonlinear curve fitting of the two quantities. Five parameters were used as unknowns: the ultimate porosity ($\phi$), the inverse of the similarity ratio ($b$), the proportion of blocks that subdivide ($f$), the large-scale organic density ($x$), and the degree of internal aggregate development ($v$). The first three parameters dictate
Table 4-1. Aggregate properties of Sharpsburg silty clay loam (Wittmuss and Mazurak, 1958).

<table>
<thead>
<tr>
<th>Size (geometric mean) (mm)</th>
<th>Aggregate Density (g cm$^{-3}$)</th>
<th>Soil Organic Matter (SOM) (g org. matter g$^{-1}$ aggregate)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.366</td>
<td>1.373</td>
<td>0.037</td>
</tr>
<tr>
<td>1.683</td>
<td>1.410</td>
<td>0.037</td>
</tr>
<tr>
<td>0.838</td>
<td>1.480</td>
<td>0.039</td>
</tr>
<tr>
<td>0.419</td>
<td>1.510</td>
<td>0.040</td>
</tr>
<tr>
<td>0.210</td>
<td>1.540</td>
<td>0.043</td>
</tr>
<tr>
<td>0.105</td>
<td>1.650</td>
<td>0.044</td>
</tr>
<tr>
<td>0.052</td>
<td>2.100</td>
<td>0.026</td>
</tr>
<tr>
<td>0.026</td>
<td>2.360</td>
<td>0.025</td>
</tr>
</tbody>
</table>
the geometry of the model soil (Eqs. (4-24)-(4-26)), including the fractal dimension, while the last two parameters help predict the prevalence of SOM. Over all scales considered, $\rho_s$ was assumed to be 2.65 g cm$^{-3}$, a common value for particle density in soils. The range in aggregate sizes considered was 0.026 mm to 3.366 mm (Table 4-1), and organic matter particles smaller than 0.026 mm were subject to oxidation according to $\nu$.

**Results and Discussion**

Figure 4-5a shows the aggregate density fitted curve, and Fig. 4-5b shows the SOM fitted curve, for the data of Wittmuss and Mazurak (1958). Because Gauss-Newton iterative fitting was extremely sensitive to changes in the five input parameters, confidence intervals for the returned values were always large. As a result, we opted for a manual trial-and-error procedure to produce the fits in Fig. 4-5. Clearly, any information regarding the statistical significance of the returned values was lost, but the presence of five unknowns precludes significance automatically. In this case, the fitting results are best viewed as a way to test acceptable values for the five unknowns in capturing a satisfactory proportion of the data variability.

Several combinations of the five parameters produced relatively high $r^2$ values, but most of the combinations required a low value for $b$. Presumably, this was necessary to capture the sharp curvature of aggregate density scaling (Fig. 4-5a). Low $b$ values tend to correspond to clay-rich soils (Tyler and Wheatcraft, 1992; Perfect et al., 2002), which
Figure 4-5 (following page). Nonlinear estimation of (a) aggregate density, $\rho_t$, and (b) aggregate organic matter, $Q_{SOM}$, scaling in Sharpsburg soil. The curves were produced by trial and error with $\phi, b, f, x$, and $v$. See text for details.
\begin{align*}
\phi &= 0.525 \\
b &= 2.150 \\
f &= 0.785 \\
x &= 1.000 \\
v &= 0.985 \\
r^2 &= 0.890
\end{align*}

\begin{align*}
\text{SOM (g organic matter g}^{-1}\text{aggregate}) \\
r^2 &= 0.711
\end{align*}
is the case for Sharpsburg soil. Large-scale organic matter density was set arbitrarily to 1 g cm\(^{-3}\), mainly to account for light POM, and \(\phi\) was set close to 0.5 since this is a realistic value for soil porosity. Because there was no precedent for \(f\) and \(v\), these parameters were varied most. However, almost all fits with small \(v\) values were poor, particularly for SOM (Fig. 4-6). Likewise, fits were improved generally by increasing \(f\). While an aggregate density fit yielding \(r^2=0.966\) is possible with the modified PSF approach, optimizing for both density and SOM produced \(r^2\) values of 0.890 and 0.711, respectively.

One of the most interesting patterns observed was the necessity for large values of \(v\). As Fig. 4-6 illustrates, the model curves were highly sensitive to small changes in \(v\), particularly over the range \(v=0.75\) to \(v=1\) (all other parameter values are identical to those in Fig. 4-5). Clearly, as the conceptual aggregates develop towards the original PSF structure (\(v=1\)), their ability to represent the real aggregates improves. This is due to the fact that, in the modified PSF model, organic matter density increases as size decreases, according to a power law with \(D\) (Eq. (4-34)). Thus, an equivalent volumetric proportion of organic matter in small and large aggregates will produce greater SOM among small aggregates. Since \(D\) controls the rate of increase in aggregate density and SOM at smaller scales, a balance had to be achieved between the effects of \(v\) and \(D\) when fitting the two corresponding curves. From Eq. (4-1) and the values in Fig. 4-5a, \(D\) was estimated at 2.684, a relatively low value compared to other published values for soils of various texture (Tyler and Wheatcraft, 1992), but necessary in fitting aggregate density scaling. As a result, SOM was exaggerated at smaller scales for all but the highest values of \(v\) (Fig. 4-6b).
Figure 4-6 (following page). Model results for (a) aggregate density, $\rho$, and (b) aggregate organic matter, $Q_{SOM}$, scaling in Sharpsburg soil. The curves were produced by using the parameter values derived from Fig. 4-5, and by allowing $v$ to range from 0 to 1.
a) 

aggregate density (g cm$^{-3}$)

aggregate size (mm)

$v=0$
$v=0.25$
$v=0.50$
$v=0.75$
$v=0.985$
$v=1$

$\phi=0.525$
$b=2.150$
$f=0.785$
$x=1.000$

b) 

SOM (g organic matter g$^{-1}$ aggregate)

aggregate size (mm)

$v=0$
$v=0.25$
$v=0.50$
$v=0.75$
$v=0.985$
$v=1$
As described, one of the reasons \( \nu \) must be large is to balance parameters that allow for a pronounced aggregate density scaling. However, another interpretation, based on the physical nature of the soil, is also justified. Specifically, large \( \nu \) values in the modified PSF model depict a soil that has experienced significant loss of organic matter over time. This is quite realistic for the soil under consideration, which belonged to an experimental farm at the time of analysis (Wittmuss and Mazurak, 1958). Note that \( \nu \) only has a relative association with time, but that the uncultivated soil \((t=0)\) would exhibit \( \nu<0.985 \) and higher levels of SOM for all aggregate size classes (Fig. 4-6). However, even if initial \( \nu \) is known, it would be impossible to calculate total SOM loss without knowledge of the past and present aggregate size distributions. Despite the fact that there is a downward trend in SOM at extremely small scales (Fig. 4-5b), it is likely that most SOM loss was due to large aggregates. This is because a single large aggregate can release orders of magnitude more organic matter than a single small aggregate, and because soil degradation is experienced initially in larger aggregates (Six et al., 2000a). Specifically, research has shown that soil cultivation can lead to a loss of carbon-rich macroaggregates and an increase of carbon-poor microaggregates (Six et al., 2000b). This may also explain why SOC scaling is so inconsistent (Ashman et al., 2003): among other things, it depends on soil age and management history.

In an attempt to understand the effects of some of the other fractal parameters, model curves were produced for an artificial soil with the following values: \( \phi=0.500 \), \( b=\{5.000, 15.000\} \), \( f=0.750 \), \( x=1.000 \), and \( \nu=\{0, 0.25, 0.50, 0.75, 0.985, 1\} \). The focus was on larger \( b \) values, especially since values of \( b \) are difficult to ascertain and estimates have been greater than 20 (Tyler and Wheatcraft, 1992). Figure 4-7 summarizes the
Figure 4-7. Model results for (a)-(b) aggregate density, $\rho_t$, and (c)-(d) aggregate organic matter, $Q_{SOM}$, scaling in artificial soils. The panels on the left represent a soil with $b=5$, while the panels on the right represent an otherwise identical soil, except that $b=15$. As in Fig. 4-6, $v$ was allowed to range from 0 to 1.
results. One of the most striking features is that aggregate density decreases over time for $b=5$, but increases over time for $b=15$. Again this probably reflects the fact that smaller $b$ values lead to smaller $D$, which amplifies scaling effects for density and SOM. Since both scenarios in Fig. 4-7 use an organic matter density of 1 g cm$^{-3}$ for 3.366 mm diameter aggregates, $b=5$ must yield greater SOM than $b=15$ for sizes smaller than 3.366 mm at $v=0$ (Eq. 4-38). As a result, removal of organic matter will remove more mass per aggregate in the $b=5$ scenario, which leads to decreasing density over time (Fig. 4-7a). This is not the case with $b=15$, where organic matter is light enough to increase aggregate density over time (Fig. 4-7b).

Figure 4-7 illustrates another important point. Because SOM is more recalcitrant within aggregates of small size (Puget et al., 2000; Six et al., 2000a; Plante et al., 2002), it is apparent that a small $b$ value will distribute naturally more organic matter into the recalcitrant fractions (Fig. 4-7c and Fig. 4-7d). This is a direct result of our initial assumption that SOM behaves as a solid mass fractal. If this assumption is accurate, then it would imply that soils with smaller $b$ values might have a greater capacity for carbon storage.

**Conclusions**

The modified PSF model is a model for soil aggregate structure, designed to mimic the original PSF model as time approaches infinity. The modified PSF model incorporates organic matter as a distinct soil phase, which also serves as the medium for
secondary aggregate development. These attributes help link abstract fractal concepts to the current understanding of aggregate and SOM dynamics illustrated in Fig. 4-1. One benefit of the model is that it predicts aggregate density and SOM scaling simultaneously, which can be tested against actual data. Another benefit of the model is that the effects of time, or internal aggregate development, are represented by a separate parameter. This is important, as our understanding of soil measurements depends greatly on the effective age of the soil.

Results showed that fractal parameters, such as $b$, and therefore $D$, can have a profound effect on the expected aggregate density and SOM scaling. By default, since different sized aggregates have different soil residence times (Plante et al., 2002), fractal parameters should influence the soil organic carbon capacity. Specifically, smaller values for $b$ or $D$ may distribute naturally more organic matter into microaggregates, which have longer residence times. This, in turn, would increase the capacity for carbon storage in the soil. One confounding factor is the aggregate size distribution, which could lessen or enhance the effect of fractal parameters. However, in a highly degraded state, soils would have disproportionately more microaggregates than macroaggregates; in this case, the soil with the lowest $b$ value should retain its carbon the longest, thus allowing it to be more resilient. The utility of the modified PSF model in describing time-dependent dynamics of soil aggregates and SOM is promising, but it requires further research.
References Cited


## Table A-1

Chemical, biological, and physical data of the Continuous Corn (CC) and Rotation (RO) soils from the Hunter Rotation Experiment (HRE), averaged over a five year period (1996-2000).

<table>
<thead>
<tr>
<th>Soil</th>
<th>pH</th>
<th>Carbon* (%)</th>
<th>Nitrogen (%)</th>
<th>Microbial Biomass C* (µg C g⁻¹ soil)</th>
<th>Aggregate Stability* (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CC</td>
<td>5.8</td>
<td>1.5</td>
<td>0.14</td>
<td>163</td>
<td>11</td>
</tr>
<tr>
<td>RO</td>
<td>6.6</td>
<td>1.7</td>
<td>0.15</td>
<td>557</td>
<td>60</td>
</tr>
</tbody>
</table>

# Data are from Tables 2.5 and 5.2 of Bucher (2002): (Bucher, A. 2002. Soil quality characterization and remediation in relation to soil management. Doctoral dissertation. The Pennsylvania State University, University Park, PA, 143 pp.)

* Significantly different ($p<0.05$), according to Duncan’s Multiple Range Test. Measurements for pH were not subjected to statistical analysis.
Table A-2. Meteorological data for two sampling times, summarized from the Penn State University Automated Weather Observation System at Rock Springs, PA.

<table>
<thead>
<tr>
<th></th>
<th>June, 2002</th>
<th>July, 2002</th>
<th>May, 2003</th>
<th>June, 2003*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total precipitation</td>
<td>4.94</td>
<td>1.32</td>
<td>4.71</td>
<td>4.65</td>
</tr>
<tr>
<td>(inches)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Normal precipitation</td>
<td>4.28</td>
<td>3.59</td>
<td>3.70</td>
<td>4.28</td>
</tr>
<tr>
<td>(inches)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Percent of normal#</td>
<td>115%</td>
<td>36.8%</td>
<td>127%</td>
<td>109%</td>
</tr>
<tr>
<td>Days 0.01+ in.</td>
<td>15</td>
<td>14</td>
<td>24</td>
<td>18</td>
</tr>
<tr>
<td>Days 0.10+ in.</td>
<td>8</td>
<td>4</td>
<td>12</td>
<td>12</td>
</tr>
<tr>
<td>Days 0.50+ in.</td>
<td>4</td>
<td>1</td>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td>Days 1.00+ in.</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Monthly temperature</td>
<td>+3.0</td>
<td>+3.3</td>
<td>-1.4</td>
<td>-1.2</td>
</tr>
<tr>
<td>departure (ºF)#</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

# Estimated using monthly normal precipitation and temperature, as reported for State College, PA by AccuWeather (www.AccuWeather.com, 2004).
* Months in which soil samples were collected at Rock Springs, PA.
Appendix B

MATLAB PROGRAMS

function [PoreData,output]=fractal2(n1,n2,n3,n4,filename)

% Fractal2.m
% Written by Jody Gibson, 2000-2005
%
% This function uses a "linked list" philosophy to distinguish
% individual pore (or solid) grains within 2-D aggregate images.
% The method involves processing an image to remove external noise,
% followed by defining pixels belonging to pores. Next, pore
% pixels are grouped based on orthogonal adjacency--if two pixels
% do not meet this criterion then they belong to different pores.
% The fractal density scaling is obtained by using boxes of
% different size to sample the "solid" portion of the aggregate.
% Pore sizes are used in the following way: if they are larger
% than the box size then they are excluded from the calculation
% of density at that scale.
%
% n1,n2,n3,n4 describe coordinates for boxes that must be placed
% over the image to eliminate faulty CT units used by the scanner
% to quantify extremely dense areas; filename is just the
% directory of the image files; PoreData is a matrix describing
% different pores and their sizes; output includes the density
% values, b values, and total number of pixels in the aggregate.
%
% This function is called as a subroutine by various main programs.
% These include:
% Mainoldb.m, Mainoldg.m, Mainbad.m, Maingood.m

A=imread(filename,'tif');

A64=double(A)+1;
clear('A')
A=A64;
clear('A64')

M=1024;
N=M;
%A=A(434:945,414:925);
%M=512;
%N=M;

%%%USE THIS FOR LARGE AGGS%%% 

%M=1024;
%N=M;
%
%fid2=fopen(filename,'r');
%A,Anum]=fscanf(fid2,'%g
',[M,M]);
%fclose(fid2);

m1=max(max(A));
m0=min(min(A));

B=A;
clear('A')

%lowcut=10000; % old aggs
lowcut=6000; % small aggs
%lowcut=3000; % medium aggs
%lowcut=700; % large aggs

for i=1:M % go left to right
    for j=1:M
        if (B(i,j)>=lowcut)
            break
        else
            B(i,j)=0;
        end
    end
end

%done w/ part 1'

for i=1:M % go right to left
    for j=M:-1:1
        if (B(i,j)>=lowcut)
            break
        else
            B(i,j)=0;
        end
    end
end

%done w/ part 2'

for j=1:M % go down to up
    for i=1:M
        if (B(i,j)>=lowcut)
            break
        else
            B(i,j)=0;
        end
    end
end
for j=1:M  % go up to down
  for i=M:-1:1
    if (B(i,j)>=lowcut)
      break
    end
    B(i,j)=0;
  end
end

if (n1==0)  % done w/ part 4'
else
  for i=n1:n2
    for j=n3:n4
      if (B(i,j)<100)
        B(i,j)=m1;
      end
    end
  end
end

A=B;
clear('B')
AA=A;

figure(2)
pcolor(A)
colormap gray
shading flat
axis square 'paused'
pause

Amain=zeros(M+2,M+2);
Amain(2:M+1,2:M+1)=A;
A=Amain;
M=M+2;
N=M;

A=((Amain>0)+(Amain>=lowcut));
[ro,co]=find(A==2);
Nblacks=length(ro)
SolidListX=ro;
L=length(SolidListX);
SolidListY=co;
[ro,co]=find(A==1);
Nwhites=length(ro)
IndexList=[ro co];  % this is the master list of pore coords for referencing row nos.
aggsize=Nblacks+Nwhites
'paused'
pause

A=(A==1);

stash=Nwhites;
List=IndexList;
PoreData=[ ];
number=0;
while (stash>0)

number=number+1
xi=ceil(rand(1,1)*stash);
Xpt=List(xi,1);
Ypt=List(xi,2);
A(Xpt,Ypt)=-1;
DataSet=[Xpt Ypt 0 0 1 1 1 1];
rows=1;
position=rows;
IndexLinked=DataSet(position,3);
BranchOrder=DataSet(position,4);
OptionsLeft=DataSet(position,5:8);
cnt=0;
finished=0;
while (~finished)
cnt=cnt+1;
x1=Xpt-1;
x2=Xpt+1;
y1=Ypt-1;
y2=Ypt+1;
options=[Xpt y1; Xpt y2; x1 Ypt; x2 Ypt];
done=0;
while (~done) % try each direction (option) in turn
   opts=DataSet(position,5:8);
   ind=find(opts);
   if (isempty(ind)) % equivalent to saying if (sum(opts)==0)
      if (position==1)
         done=1;
         finished=1;
         break
      end
      position=IndexLinked;
      Xpt=DataSet(position,1);
      Ypt=DataSet(position,2);
      IndexLinked=DataSet(position,3);
      BranchOrder=DataSet(position,4);
      OptionsLeft=DataSet(position,5:8);
      done=1;
      break
   else
      ind=ind(1);
   end
   if (isempty(ind)) % equivalent to saying if (sum(opts)==0)
      if (position==1)
         done=1;
         finished=1;
         break
      end
      position=IndexLinked;
      Xpt=DataSet(position,1);
      Ypt=DataSet(position,2);
      IndexLinked=DataSet(position,3);
      BranchOrder=DataSet(position,4);
      OptionsLeft=DataSet(position,5:8);
      done=1;
      break
   else
      ind=ind(1);
   end
   ...
end

x=options(ind,1);
y=options(ind,2);
Avalue=A(x,y);
DataSet(position,4+ind)=DataSet(position,4+ind)-1;  % erase one of the options
if (Avalue<1)
    IndexLinked=position;
    BranchOrder=DataSet(position,4)+1;
    rows=rows+1;
    position=rows;
    Xpt=x;
    Ypt=y;
    OptionsLeft=[1 1 1 1];
    dataset=[Xpt Ypt IndexLinked BranchOrder OptionsLeft];
    DataSet=[DataSet; dataset];
    A(Xpt,Ypt)=-1;
    %plot(y,x,**)
    %'paused'
    %pause
done=1;                                              % stack is added to, come back later
end
end                                              % end while ('done')
end                                                              % end while ('finished')

List2=DataSet(:,1:2);
List=setdiff(List,List2,'rows');
[ro,co]=size(List);                                              % List is list of remaining pore pixels
stash=ro;
[ro,co]=size(List2);
GrainSize(number)=ro;                                           % number of pixels in this particular pore

fixer=ones(ro,1);
PoreData=[PoreData;List2(:,1) List2(:,2) fixer*number fixer*GrainSize(number)];
end                                                              % end while ('stash')

A=AA;
M=1024;
%M=512;
N=M;
clear('AA')

if (isempty(PoreData))
    bvalue=-1.5;
else
    maxporesize=max(PoreData(:,4))
    bvalue=sqrt(aggsize)/sqrt(maxporesize)
    PoreData(:,1:2)=PoreData(:,1:2)-1;
    [rosize,cosize]=size(PoreData);
    for i=1:rosize
        A(PoreData(i,1),PoreData(i,2))=-PoreData(i,4);
    end
end
boxsizes=[241 193 155 123 99 79 63 51 41 33 27 21 17 13 11 9 7 5 3];
boxsizes=[123 99 79 63 51 41 33 27 21 17 13 11 9 7 5 3];
boxsizes=[63 51 41 33 27 21 17 13 11 9 7 5 3];
Rho=[];
for J=1:5
cnt=0;
for i=boxsizes
    cnt=cnt+1;
tendril=(i-1)/2;
    Density=[];
    for j=1:1000
        done=0;
        while (~done)
            ind=ceil(L*rand(1,1));
            ro=SolidListX(ind);
            co=SolidListY(ind);
            rows=[ro-tendril:ro+tendril];
            cols=[co-tendril:co+tendril];
            if (min(rows)<1)
                elseif (min(cols)<1)
                elseif (max(rows)>M)
                elseif (max(cols)>M)
                else
                    B=A(rows,cols);
                    C=(B>=lowcut);
                    solidpix=sum(sum(C));
                    C=B.*C;
                    totalmass=sum(sum(C));
                    C=(B>0);
                    porepix=sum(sum(C));
                    kk=(cnt-1)*100+j;
                    pps=porepix+solidpix;
                    if (pps>0.5*i^2)
                        density(kk)=totalmass/(porepix+solidpix);
                        ruler(kk)=sqrt(porepix+solidpix);
                        Density(j)=density(kk);
                        done=1;
                    end
                end
            end
        end
    end
end
rho(cnt)=mean(Density);
end
X=log(boxsizes)';
Y=log(rho)';
X(:,2)=1;
[b,bint,r,rint,stats]=regress(Y,X);
D=2+b(1)
rsquared=stats(1)
pvalue=stats(3)
xval=X(:,1);
Rho=[Rho;rho];
end % end for J

output=[Rho [bvalue;bvalue;bvalue;bvalue;bvalue] [aggsiz;aggsiz;aggsiz;aggsiz;aggsiz]];
% Mainoldb.m
% Written by Jody Gibson, 2000-2005
%
% This program calls the Fractal2.m subroutine for analyzing
% single-slice scans from 10 'CC' soil aggregates.
%
% The output is written to two text files:
% 'fractaldataoldb_1.txt' and 'fractaldataoldb_2.txt'
% The first contains pore information and the second
% contains basic fractal parameters data. These files are
% opened and analyzed further by Readin2.m.

clear;

nn1=0;
nn2=0;
nn3=0;
nn4=0;
filename='C:/Documents and Settings/Jody/My Documents/CTdata/Spring_2003/Single-
Slice/Low_Organic/SB_0';
x=filename(1:91);
lastbit=48;
for i=1:9
    y=lastbit+i;
x(92)=char(y);
[PoreData,output]=fractal2(nn1,nn2,nn3,nn4,x);
fid=fopen('fractaldataoldb_1.txt','a');
fprintf(fid,'%g
',PoreData)
fclose(fid);
 fid=fopen('fractaldataoldb_2.txt','a');
 fprintf(fid,'%g
',[-1 ])
 fclose(fid);
end

filename='C:/Documents and Settings/Jody/My Documents/CTdata/Spring_2003/Single-
Slice/Low_Organic/SB_10';
[PoreData,output]=fractal2(nn1,nn2,nn3,nn4,filename);
fid=fopen('fractaldataoldb_1.txt','a');
fprintf(fid,'%g
',PoreData)
fclose(fid);
fid=fopen('fractaldataoldb_2.txt','a');
fprintf(fid,'%g
',[-1 ])
fclose(fid);
% Mainoldg.m
% Written by Jody Gibson, 2000-2005
%
% This program calls the Fractal2.m subroutine for analyzing
% single-slice scans from 10 'RO' soil aggregates.
%
% The output is written to two text files:
% 'fractaldataoldg_1.txt' and 'fractaldataoldg_2.txt'
% The first contains pore information and the second
% contains basic fractal parameters data. These files are
% opened and analyzed further by Readin2.m.

clear;

nn1=0;
nn2=0;
nn3=0;
nn4=0;
filename='C:/Documents and Settings/Jody/My Documents/CTdata/Spring_2003/Single-
Slice/High_Organic/SG_1_1';
[PoreData,output]=fractal2(nn1,nn2,nn3,nn4,filename);
fid=fopen('fractaldataoldg_1.txt','a');
fprintf(fid,'%g
',PoreData)
fclose(fid);

fid=fopen('fractaldataoldg_2.txt','a');
fprintf(fid,'%g
',[-1])
fclose(fid);

filename='C:/Documents and Settings/Jody/My Documents/CTdata/Spring_2003/Single-
Slice/High_Organic/SG_0';
x=filename(1:92);
lastbit=48;
for i=2:9
    y=lastbit+i;
x(93)=char(y);
    [PoreData,output]=fractal2(nn1,nn2,nn3,nn4,x);
    fid=fopen('fractaldataoldg_1.txt','a');
    fprintf(fid,'%g
',PoreData)
    fclose(fid);
    fid=fopen('fractaldataoldg_2.txt','a');
    fprintf(fid,'%g
',[-1])
    fclose(fid);
end
filename='C:/Documents and Settings/Jody/My Documents/CTdata/Spring_2003/Single-Slice/High_Organic/SG_10';
[PoreData,output]=fractal2(nn1,nn2,nn3,nn4,filename);
fid=fopen('fractaldataoldg_1.txt','a');
fprintf(fid,'%g
',PoreData)
fprintf(fid,'%g
',[-1])
fclose(fid);
fid=fopen('fractaldataoldg_2.txt','a');
fprintf(fid,'%g
',output)
fprintf(fid,'%g
',[-1])
fclose(fid);
% Mainbad.m
% Written by Jody Gibson, 2000-2005
%
% This program calls the Fractal2.m subroutine for analyzing
% 410 single-slice scans from Aggregate 2a ('CC' soil).
%
% The output is written to two text files:
% 'fractaldatabad_1.txt' and 'fractaldatabad_2.txt'
% The first contains pore information and the second
% contains basic fractal parameters data. These files are
% opened and analyzed further by Readin2.m.

clear;

nn1=0;
nn2=0;
nn3=0;
nn4=0;
filename='C:/Documents and Settings/Jody/My Documents/CTdata/Spring_2003/3D_Scans/agg_b2/number2_b_vol_0000';
x=filename(1:94);
lastbit=[48 48 48];
for i=1:410
    i
    n1=floor(i/100);
n2=floor((i-ii)/10);
n3=floor(i-ii-iii);
y=lastbit+[n1 n2 n3];
x(95:97)=char(y);
    [PoreData,output]=fractal2(nn1,nn2,nn3,nn4,x);
    fid=fopen('fractaldatabad_1.txt','a');
    fprintf(fid,'%g
',PoreData)
    fprintf(fid,'%g
',[-1])
    fclose(fid);
    fid=fopen('fractaldatabad_2.txt','a');
    fprintf(fid,'%g
',output)
    fprintf(fid,'%g
',[-1])
    fclose(fid);
end
% Maingood.m
% Written by Jody Gibson, 2000-2005
% This program calls the Fractal2.m subroutine for analyzing
% 369 single-slice scans from Aggregate 7b ('RO' soil).
% The output is written to two text files:
% 'fractaldatagood_1.txt' and 'fractaldatagood_2.txt'
% The first contains pore information and the second
% contains basic fractal parameters data. These files are
% opened and analyzed further by Readin2.m.

clear;
nn1=0;
nn2=0;
nn3=0;
nn4=0;
filename='C:/Documents and Settings/Jody/My
Documents/CTdata/Spring_2003/3D_Scans/agg_g7/number7_g_vol_0000';
x=filename(1:94);
lastbit=[48 48 48];
for i=1:369
    n1=floor(i/100);
    n2=floor((i-n1*100)/10);
    n3=floor(i-n1*100-n2*10);
    y=lastbit+[n1 n2 n3];
    x(95:97)=char(y);
    [PoreData,output]=fractal2(nn1,nn2,nn3,nn4,x);
    fid=fopen('fractaldatagood_1.txt','a');
    fprintf(fid,‘%g
’,PoreData)
    fprintf(fid,‘%g
’,[-1])
    fclose(fid);
    fid=fopen('fractaldatagood_2.txt','a');
    fprintf(fid,‘%g
’,output)
    fprintf(fid,‘%g
’,[-1])
    fclose(fid);
end
% Readin2.m
% Written by Jody Gibson, 2000-2005
%
% This program performs a variety of tasks, for both
% 2-D and 3-D fractal analysis. The files produced by
% Mainoldb.m, Mainoldg.m, Mainbad.m, and Maingood.m
% are used here.
%
% First, this program opens the pore data files for
% the hundreds of single-slices corresponding to
% Aggregate 2a ('CC' soil) and Aggregate 7b ('RO' soil).
% Using a connectivity algorithm, sequential slices
% within an aggregate are analyzed to define real
% individual pores in 3-D space, which are plotted
% as different colored "blobs" using the plot3 function.
% The pore information is written to the files
% 'poredatabad.txt' and 'poredatagood.txt'. These files
% are required for the 3-D fractal subroutine called
% Real3d.m. Next, all 2-D density scaling data are
% analyzed and plotted on the same set of axes
% (yielding many of the data in Chapter 2).
%
% In order to fit curves for the density scaling data,
% this program calls two functions:
% Simplefun.m and PSFfun.m

clear

fid=fopen('fractaldatabad_1.txt','r');
%fif=fopen('fractaldatagood_1.txt','r');
[A,cnt]=fscanf(fid,'%g
');
fclose('all');
indices=find(A==-1);
k=1;
N=length(indices);
pores=0;
lastvalue=0;
PoreInfo=[];
a1=0;
a2=0;
b1=0;
b2=0;
for i=1:N
    if (indices(i)>k)                          % if there's any pore data to be had
        B=A(k:indices(i)-1);
        k=indices(i)+1;                      % update position in data vector
        LB=length(B);
        nopix=LB/4;
    end
    if (indices(i)>k)                          % if there's any pore data to be had
        B=A(k:indices(i)-1);
        k=indices(i)+1;                      % update position in data vector
        LB=length(B);
        nopix=LB/4;
    end
end
poreinfo=reshape(B,nopix,4);
poreinfo(:,4)=i; % column 4 now indicates z coordinate (not grain size)
poreinfo(:,3)=poreinfo(:,3)+lastvalue; % column 3 is the pore label/identifier
X=poreinfo(:,1);
Y=poreinfo(:,2);
if (pores>0) % do this only if you had pores on the previous level
  for jj=1:pores % loop over each pore in the previous level
    j=oldIDs(jj); % actual pore identifier
    ind=find(pinfo==j); % ind is never empty
    prevpts=pts(ind,:);
    newpts=[X Y];
    [compts,i1,i2]=intersect(newpts,prevpts,'rows'); % do this only if you had pores on the previous level
    newinfo=poreinfo(i1,3); % the pore labels (new level) of the common pixels
    % ...j is the pore label from the previous level
    labels=unique(newinfo);
    LL=length(labels)+1; % number of distinct labels, including j
    replabel=min(labels); % this is the value you will use to replace all connections with
    rep1ind=[];
    rep2ind=[];
    for jjj=1:LL % loop over all possible labels involved
      rep1=find(poreinfo(:,3)==labels(jjj));
      rep1ind=[rep1ind;rep1];
      rep2=find(PoreInfo(a1+1:a2,3)==labels(jjj));
      rep2ind=[rep2ind;rep2];
    end
    if (~isempty(rep1ind))
      poreinfo(rep1ind,3)=replabel;
      end
    end
    PoreInfo(a1+rep2ind,3)=replabel;
  end % end for j
endif % end if pores
IDs=unique(poreinfo(:,3)); % IMPORTANT
nopores=length(IDs);
pores=nopores;
oldIDs=IDs;
pts=poreinfo(:,1:2);
pinfo=poreinfo(:,3);

lastvalue=max(pinfo);
[a1,b1]=size(PoreInfo);
PoreInfo=[PoreInfo;poreinfo];
[a2,b2]=size(PoreInfo);
else % IMPORTANT STUFF...(when no pore data to be had)
  k=k+1; % update position in data vector
  pores=0;
  oldIDs=];
  pts=;]
  pinfo=;]
end % end if indices
end % end for i

[Y,I]=sort(PoreInfo(:,3));
unY = unique(Y);
NY = hist(Y, unY);                          % number of pixels in each pore!
[Dummy, NYI] = sort(NY);
NYI = NYI([length(NYI): -1: 1]);
NY = NY(NYI);
unY = unY(NYI);

for cnt = 1:1
    cnt
    i = unY(cnt);
    ind = find(PoreInfo(:, 3) == i);
    xs = PoreInfo(ind, 1);
    ys = PoreInfo(ind, 2);
    zs = PoreInfo(ind, 4);
    measure1(cnt) = length(ind)^(1/3);    % size of pore defined by the cube root of its volume
    volume1(cnt) = length(ind);
end

for cnt = 2:length(unY)
    cnt
    i = unY(cnt);
    ind = find(PoreInfo(:, 3) == i);
    xs = PoreInfo(ind, 1);
    ys = PoreInfo(ind, 2);
    zs = PoreInfo(ind, 4);
    measure1(cnt) = length(ind)^(1/3);    % size of pore defined by the cube root of its volume
    volume1(cnt) = length(ind) + volume1(cnt - 1); % total volume subtracted at scale 'measure1'
end

aggsize = 20786746;                                   % Agg 2a
%aggsize = 14874503;                                  % Agg 7b
V = aggsize - volume1;
plot(measure1, 0.031 ./ V, 'r+')

cmatrix = colormap(jet);
figure(1)
hold on
for i = 1:max(PoreInfo(:, 3))
    ind = find(PoreInfo(:, 3) == i);
    if (~isempty(ind))
        plot3(PoreInfo(ind, 1), PoreInfo(ind, 2), PoreInfo(ind, 4), 'o', 'Color', cmatrix(mod(i, 64) + 1, :))
    end
end

fid = fopen('poredatabad.txt', 'w');
%f fid = fopen('poredatagood.txt', 'w');
fprintf(fid, '%g
', PoreInfo);
fclose(fid);

R = NY.^(1/3);

fid = fopen('fractaldatabad_2.txt', 'r');
indices = find(A == -1);
k = 1;
N = length(indices);
boxsizes = [123 99 79 63 51 41 33 27 21 17 13 11 9 7 5 3];
realsizes = boxsizes .* 9.46 .* 10.^-3; % size, in mm
x = realsizes(4:16);
figure(2)
hold on
for i = 1:N
    B = A(k:indices(i)-1);
    LB = length(B);
    if (LB < 90)
        % if (LB < 75) % toggle when necessary
        b(i) = B(1);
        aggsize(i) = B(6);
    else
        density = reshape(B, 5, 18);
        b(i) = density(1, 17);
        aggsize(i) = density(1, 18);
    end
    dstd = std(density(:, 1:16));
    dmean = mean(density(:, 1:16));
    y = dmean(4:16);
    plot(x, y, 'y')
    % density = reshape(B, 5, 15);
    % b(i) = density(1, 14);
    % aggsize(i) = density(1, 15);
    % dstd = std(density(:, 1:13));
    % dmean = mean(density(:, 1:13));
    % y = dmean
    % plot(x, y, 'y')
end
rhomax = 1.25;
rhomax = rhomax * 5430 + 3750;
D = 1.80;
b0 = [rhomax D];
[BETA, R, J] = nlinfit(x, y, @simplefun, b0);
p0(i) = BETA(1);
D1(i) = BETA(2);
SSE = sum(R.^2);
SSTO = sum((y - mean(y)).^2);
rs1(i) = 1 - SSE / SSTO;
CI = nlpardci(BETA, R, J);
% plot(x, y - R, '--', 'LineWidth', 1)
% 'paused'
% pause
% rhomax=1.25;
% rhomax=rhomax*5430+3750;
% rhoPSF=1.50;
% rhoPSF=rhoPSF*5430+3750;
% D=1.80;
% b0=[rhomax rhoPSF D];
% [BETA,R,J]=nlinfit(x,y,@PSFfun,b0);
% p0(i)=BETA(1)*1.84*10^-4-0.69;
% pPSF(i)=BETA(2)*1.84*10^-4-0.69;
% D2(i)=BETA(3);
% SSE=sum(R.^2);
% SSTO=sum((y-mean(y)).^2);
% rs1(i)=1-SSE/SSTO;
% CI=nlparci(BETA,R,J);
end
k=indices(i)+1;
end

D1ind=find(D1);
figure(3)
D1x=D1(D1ind);
boxplot(D1x)
mean(D1x)
median(D1x)
% D2ind=find(D2);
% figure(3)
% D2x=D2(D2ind);
% boxplot(D2x)
% mean(D2x)
% median(D2x)
bind=find(b);
figure(4)
bx=b(bind);
boxplot(bx)
mean(bx)
median(bx)
% sagg=sum(aggsize)
% db=sagg^(1/3)/(max(NY))^(1/3)
% mean(b)
% figure(3)
% hist(b)
function yhat=simplefun(beta,x)

% Simplefun.m
% Written by Jody Gibson, 2000-2005
%
% This function is used with the MATLAB function
% nlinfit.m to perform nonlinear curve fitting of
% aggregate density scaling data. This is the solid
% mass fractal (not PSF) model.
%
% beta is the vector of parameters that are fitted
% upon convergence; the vector includes the large-
% scale density (rhoL) and the fractal dimension (D);
% x is the vector of sizes for which density
% measurements exist.
%
% This function is called by a variety of programs,
% including Readin2.m and Analy3d.m.

L=0.82577;
rhoL=beta(1);
D=beta(2);
rhoR=rhoL.*(x./L).^(D-3); % IMPORTANT: toggle from D-3 (for 3-D data) to D-2 (for 2-D data)
yhat=rhoR;
function yhat=PSFfun(beta,x)

% PSFfun.m
% Written by Jody Gibson, 2000-2005
% 
% This function is used with the MATLAB function
% nlinfit.m to perform nonlinear curve fitting of
% aggregate density scaling data. This is the PSF
% (not solid mass fractal) model.
% 
% beta is the vector of parameters that are fitted
% upon convergence; the vector includes the large-
% scale density (rhoL), the mineral+pore density
% (rhoPSF), and the fractal dimension (D);
% x is the vector of sizes for which density
% measurements exist.
% 
% This function is called by a variety of programs,
% including Readin2.m and Analy3d.m.

L=0.82577;
rhoL=beta(1);
rhoPSF=beta(2);
D=beta(3);
rhoR=rhoPSF-(x./L).^(D-3).*(rhoPSF-rhoL);       % IMPORTANT: toggle from D-3 (for 3-D data) to D-2
% (for 2-D data)
yhat=rhoR;
% Real3d.m
% Written by Jody Gibson, 2000-2005
%
% This program performs 3-D fractal analysis for Aggregate 2a
% ('CC' soil) and Aggregate 7b ('RO' soil). The technique is
% comparable to that of Fractal2.m, but for 3-D structures.
% Because of the memory requirements of 3-D computations, this
% program allows for the aggregate to be analyzed 1/8th at a
% time.
%
% This program utilizes output from Readin2.m for incorporating
% pore information (full sizes and locations). Density output
% is written to 'real3d_bad2.txt' and 'real3d_good2.txt' for
% further analysis/plotting.

clear

M=256;
N=M;
MM=205;
% stpt=1;                             % small z
stpt=MM+1;                             % big z

%M=256;
%N=M;
%MM=185;
% stpt=1;                                 % small z
% MM=184;                                 % these two lines are for big z, good only
% stpt=MM+2;

filename='C:/Documents and Settings/Jody/My
Documents/CTdata/Spring_2003/3D_Scans/agg_b2/number2_b_vol_0000';
%filename='C:/Documents and Settings/Jody/My
Documents/CTdata/Spring_2003/3D_Scans/agg_g7/number7_g_vol_0000';
x=filename(1:94);
lastbit=[48 48 48];
for i=stpt:MM+stpt-1
    i

    n1=floor(i/100);
    ii=n1*100;
    n2=floor((i-ii)/10);
    iii=n2*10;
    n3=floor(ii-iii);

    y=lastbit+[n1 n2 n3];
    x(95:97)=char(y);

    B=imread(x,'tif');
B64=double(B)+1;
clear('B')
B=B64;
clear('B64')

B=B(434:945,414:925);
BB=zeros(512,512);
BB(1:512,1:491)=B(1:512,22:512);
B=BB;
%B=B(434:945,414:925);
%BB=zeros(512,512);
%BB(32:512,10:490)=B(1:481,1:481);
%B=BB;

%A(:,:,i-stpt+1)=B(1:M,1:M); % small x, small y
%A(:,:,i-stpt+1)=B(1:M,M+1:2*M); % small x, big y
%A(:,:,i-stpt+1)=B(M+1:2*M,1:M); % big x, small y
A(:,:,i-stpt+1)=B(M+1:2*M,M+1:2*M); % big x, big y
end
% we now have our 3-D matrix

lowcut=10000;
B=(A>=lowcut);
A=B.*A;
clear('B')
ro=[];
co=[];
ho=[];
for i=1:M
    Aslice=reshape(A(i,:,:),M,MM);
    [coslice,hoslice]=find(Aslice);
    co=[co;coslice];
    ho=[ho;hoslice];
    Lho=length(hoslice);
    roslice=ones(Lho,1).*i;
    ro=[ro;roslice];
end
SolidListX=ro;
SolidListY=co;
SolidListZ=ho;
L=length(SolidListX);
clear(ro')
clear(co')
clear(ho')

fid=fopen('poredatabad.txt','r');
%fid=fopen('poredatagood.txt','r');
PoreData=fscanf(fid,'%g
');
fclose(fid);
whos
LPD=length(PoreData)
%PoreData=reshape(PoreData,LPD/5,5);
PoreData=reshape(PoreData,LPD/4,4);

[Y,I]=sort(PoreData(:,3));
unY = unique(Y);
N = hist(Y, unY);
placement = 0;
for i = 1:length(unY)
    PoreData(I(placement+1:placement+N(i)),5) = N(i);
    placement = placement + N(i);
end
'first part done''

%inds = find(PoreData(:,4) < MM+1); % for small z
inds = find(PoreData(:,4) > MM); % for big z
PoreData(:,4) = PoreData(:,4) - MM; % for big z
%inds = find(PoreData(:,4) > MM+1); % for big z, good only
PoreData(:,4) = PoreData(:,4) - MM - 1; % for big z, good only
PoreData = PoreData(inds,:);
clear('inds')

%inds = find(PoreData(:,1) < M+1); % for small x
inds = find(PoreData(:,1) > M); % for big x
PoreData(:,1) = PoreData(:,1) - M; % for big x
PoreData = PoreData(inds,:);
clear('inds')

%inds = find(PoreData(:,2) < M+1); % for small y
inds = find(PoreData(:,2) > M); % for big y
PoreData(:,2) = PoreData(:,2) - M; % for big y
PoreData = PoreData(inds,:);
clear('inds')

'second part done'

[Y, I] = sort(PoreData(:,3));
unY = unique(Y);
LunY = length(unY);
N = hist(Y, unY);
placement = 0;
for i = 1:LunY
    Xs = PoreData(I(placement+1:placement+N(i)),1);
    Ys = PoreData(I(placement+1:placement+N(i)),2);
    Zs = PoreData(I(placement+1:placement+N(i)),4);
    for j = 1:N(i)
        A(Xs(j), Ys(j), Zs(j)) = -PoreData(I(placement+1),5);
    end
    placement = placement + N(i);
end
clear('PoreData')
'third part done...'
tendril=(i-1)/2;
Density=[];
for j=1:1000
    done=0;
    while (~done)
        ind=ceil(L*rand(1,1));
        ro=SolidListX(ind);
        co=SolidListY(ind);
        ho=SolidListZ(ind);
        rows=[ro-tendril:ro+tendril];
        cols=[co-tendril:co+tendril];
        hoes=[ho-tendril:ho+tendril];
        if (min(rows)<1)
            elseif (min(cols)<1)
            elseif (min(hoes)<1)
            elseif (max(rows)>M)
            elseif (max(cols)>M)
            elseif (max(hoes)>MM)
            else
                B=A(rows,cols,hoes);
                C=(B>=lowcut);
                totalmass=sum(sum(sum(C)));
                C=(B>i^3);
                B=B.*C;
                % zeros assigned to pore pixels belonging to oversized pores
                C=(B<0);
                porepix=sum(sum(sum(C)));
                % true pore pixels
                kk=(cnt-1)*100+j;
                pps=porepix+solidpix;
                if (pps>0.5*i^3)
                    density(kk)=totalmass/(porepix+solidpix);
                    Density(j)=density(kk);
                    done=1;
                end
            end % end if min(rows)
        end % end while (~done)
    end % end for j
    rho(cnt)=mean(Density);
end % end for i
X=log(boxsizes)';
Y=log(rho)';
X(:,2)=1;
[b,bint,r,rint,stats]=regress(Y,X);
D=3+b(1)
rsquared=stats(1)
pvalue=stats(3)
xval=X(:,1);
Rho=[Rho;rho];
end % end for J

output=Rho;
fid=fopen('real3d_bad2.txt','a');
fprintf(fid,'%g\n',output)
fclose(fid)
% Analy3d.m
% Written by Jody Gibson, 2000-2005
%
% This program analyzes and plots the density scaling
% output from Real3d.m.
%
% This program calls Simplefun.m and PSFfun.m to
% perform nonlinear curve-fitting of the 3-D density
% scaling for Aggregate 2b ('CC' soil) and Aggregate
% 7b ('RO' soil).

clear

%fid=fopen('real3d_bad2.txt','r');
%fid=fopen('real3d_good2.txt','r');
[A,cnt]=fscanf(fid,'%g
');
fclose(fid);

boxsizes=[63 51 41 33 27 21 17 13 11 9 7 5 3];
realsizes=boxsizes.*9.46.*10.^-3;                   % size, in mm
LA=length(A);
amnt=LA/8;
k=0;
output=[];
for i=1:8
    data=A(k+1:k+amnt);
    density=reshape(data,5,13);
    output=[output;density];
    k=k+amnt;
end

ostd=std(output);
omean=mean(output);
errorbar(realsizes,omean,ostd,'k')
hold on

x=realsizes;
y=omean;
rhomax=1.25;
rhomax=rhomax*5430+3750;
D=2.80;
b0=[rhomax D];
[BETA,R,J]=nlinfit(x,y,@simplefun,b0);
D=BETA(2)
SSE=sum(R.^2)
SSTO=sum((y-mean(y)).^2);
rs=1-SSE/SSTO
CI=nlparci(BETA,R,J)
plot(x,y-R,'k','LineWidth',2)
'paused'
pause

rhomax=1.25;
rhomax=rhomax*5430+3750;
rhoPSF=1.50;
rhoPSF=rhoPSF*5430+3750;
D=2.80;
b0=[rhomax rhoPSF D];
[BETA,R,J]=nlinfit(x,y,@PSFfun,b0);
rhomax=BETA(1)*1.84*10^-4-0.69
rhoPSF=BETA(2)*1.84*10^-4-0.69
D=BETA(3)
SSE=sum(R.^2)
SSTO=sum((y-mean(y)).^2);
rs=1-SSE/SSTO
CI=nlparci(BETA,R,J)
function [yhat1,yhat2]=finfun(beta,x)

% Finfun.m
% Written by Jody Gibson, 2000-2005
% % This function uses modified PSF theory to calculate
% % aggregate density and soil organic matter (SOM)
% % scaling for real or artificial soil.
% % yhat1 is aggregate density; yhat2 is SOM; beta is an
% % input vector of phi (ultimate porosity), b (inverse of
% % similarity ratio), f (fractal proportion), pf0 (large
% % organic density), and v (internal development factor);
% % x is the vector of sizes for which output is desired.
% % This function is called by the programs Finale2.m.

d=3;
ps0=2.65;

phi=beta(1);
b=beta(2);
f=beta(3);
pf0=beta(4);
v=beta(5);

D=d+log(f)/log(b)                       % fractal dimension of organic matter and ultimate PSF structure
bb=b^d;
F=f*bb;
p=phi*(1-f);
P=p*bb;
S=bb-F-P;
s=S/bb;

F1=F-f*S/(1-f);
P1=P;
S1=S/(1-f);
f1=F1/bb                           % proportion of fractal material
p1=P1/bb;
s1=S1/bb;

L=x;
LL=length(L);
L0=max(L);                           % largest size, in mm
pt0=(F1*pf0 + S1*ps0)/bb;            % largest agg density

i=log(L0./L)./log(b);
n=max(i);                           % n is the maximum iteration level, corresponding to the smallest L
n=n-i;                               % now n is a vector, 0 for the smallest agg size allowed
pf=pf0./b.^(i.*(D-d));                  % organic density for all sizes

NO=phi.*((v.*F).^(n+1));                % number of smallest orgs vanished (in aggs of diff size classes)
Ovol=(L(LL)/(10*b))^d;                  % unit volume of smallest organics, in cm^3
Odens=pf(LL);                           % density of smallest organics, in g/cm^3 (by default)
Omass=Ovol*Odens;                       % unit mass of smallest organics, in g
Ovol=Ovol.*NO;                          % total vanishing volume (can increase density with degradation)
Omass=Omass.*NO;                        % total vanishing mass (in aggs of diff size classes)

% now, since mass is conserved, all we must do is calculate the mass of the undeveloped aggs...
Vol=(L/10).^d;                          % agg volumes, in cm^3
subvol=Vol./(b.^d);                     % pore, solid, or organic constituent volume
Mass=pf.*subvol.*F1 + ps0.*subvol.*S1;  % agg masses, in g
Vol=Vol-Ovol;                           % agg volumes, accounting for lost organics
Mass=Mass-Omass;                        % agg masses, accounting for lost organics

pt=Mass./Vol;                           % **actual aggregate densities**
OMmass=pf.*subvol.*F1-Omass;            % organic mass in each agg size class
SOM=OMmass./Mass;                       % **soil organic matter (kg per kg soil)**

figure(1)
hold on
plot(L,pt,'k','LineWidth',1)
figure(2)
hold on
plot(L,SOM,'k','Linewidth',1)

NumAggs=(0.25*F).^i;                    % agg number-size distribution
MassAggs=NumAggs.*Mass;                 % agg mass-size distribution
MassOrgs=NumAggs.*OMmass;               % organic mass-size distribution
Tester=sum((Mass+Omass).*NumAggs)
smo=sum(MassOrgs)
TotalSOM=smo/sum(MassAggs)              % **soil organic matter (kg per kg soil) of bulk soil**

yhat1=pt;
yhat2=SOM;
% Finale2.m
% Written by Jody Gibson, 2000-2005
%
% This is the main program for calling the subroutine
% Finfun.m. Arbitrary input values (phi, b, f, pf0, V)
% are declared, along with the desired size range (x).
% Output is aggregate density and SOM scaling (yhat).
%
% Plotting is done by Finfun.m, but additional information
% can be plotted on the same axes by using this program.
% For example, any data for which you are attempting to
% simulate can be included in this program and plotted.

clear

phi=0.525;
b=2.150;
f=0.785;
 pf0=1.000;
 V=0.985;
k=[log10(3.366):-0.001:log10(0.026)];
x=10.^k;
for j=1:1
    v=V(j);
    beta=[phi b f pf0 v];
    yhat=finfun(beta,x);
end
VITA

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Publications


Academic Awards
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