A review of soil pore models

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Abstract

Phenomena occurring in soil pores can best be studied if the geometry of the pore space is understood. A number of models for the pore space have been proposed. These have included a Boolean grain process, fractals, packed sphere and other grain models, bubble processes, cracking processes and a range of models based on simple geometrical objects. This paper considers the issues raised by these models and their advantages and disadvantages.

1 Introduction

The traditional approach to modelling phenomena occurring in soil pores (such as gas diffusion and water transport) has been to regard the soil as a continuous medium. Characteristics of the pore space are aggregated over lengths large compared with individual pores, and modelling is done at this scale only. For many applications this should be satisfactory. When considering some phenomenon, suitable macroscopic characteristics are defined, and behaviour of the phenomenon analysed in terms of them. The characteristics are assumed to exist for any material, and can be estimated by appropriate laboratory measurements.

What this approach lacks is insight into what is going on at the level of individual pores. We cannot predict what will happen when the pore geometry changes. Soil is susceptible to changes from many influences: wetting, drying, compaction, plant growth etc. In addition, the 'continuous soil' models often lead to approximate results only. Anomalous phenomena (e.g. non-Fickian diffusion, see Crank, 1975 and Havlin & Ben-Avraham, 1987) cannot be easily handled.

It has been recognised that pores in porous material are highly complex, (e.g Scheidegger, 1974. Ch.1). Their study has usually been avoided because of its difficulty. Any description would need to be statistical since we are concerned with large assemblages of pore space. An analytical treatment has not yet proved tractable. An investigation based on simulation and numerical methods is computationally demanding, and has only recently become possible. Even now, computational considerations impose limits on what can be done.

In this article, the various attempts that have been made to model and study soil pore geometry are reviewed and compared. We will restrict attention to soil, while recognising that many other disciplines also study porous materials, and may have ideas to offer. It would be too wide a task to cover all classes of porous materials, many of which are nothing like soil.

Soil is formed from many constituents, and to represent it as a two-phase material, solid and pore, is often an oversimplification. The behaviour of water, gas and organisms in a pore can be affected by the differing materials enlosing it. However, this review would grow too large and unwieldy if it tried to encompass models of all aspects of soil structure, and so it concentrates on the pore space, referring to aspects of the solid phase only occasionally.

In order to give some structure to the discussion of pore models, a classification into 5 groups has been adopted: (i) Non-spatial, (ii) Schematic, (iii) Random set, (iv) fractal (v) other stochastic. This classification is not completely clear cut (like many aspects of soil classification!) and some models will have elements of more than one class. We use it help us to arrange our account of different models. There is no significance in the ordering of types listed.

In addition to outlining the general idea and some examples of each model type, we will draw attention to their advantages and disadvantages. It should be remembered that soil modelling is done for many reasons, and these advantages and disadvantages will be applicable to some aspects of the modelling only. They should not be read as a guide on which approach to select for any given application. It should also be remembered that a disadvantage of all models is that they are at best only approximate. Reality will always be more subtle and complex. We will not repeat this point in considering each model type.

2 Non-spatial models

A non-spatial model is one in which the details of how the soil phase and pores are distributed in space are not considered. This does not mean that the soil material is considered as homogeneous. There is generally explicit recognition that soil pores vary. However, this will be described in terms of such things as pore radius distributions without considering the arrangement of the pores in relation to each other in space.

The main advantage of considering pores in this way is that it generally leads to analytical results.

The above description should not be taken as implying that non-spatial models are simplistic. The consideration of soil and pore properties can be detailed and even hierarchical. A good example of this approach is presented by Gwo *et al.* (1995), who describe a multi-region model with different pore types, and use it to study surface mass transport. This is also studied with a two-region model by Li *et al.* (1994). Hall (1993) assumes two pores types, larger and smaller, in modelling leaching. A two-domain approach was also used by Chen *et al.* (1993) in estimating hydraulic properties, and by Gerke & Van Genuchten (1993) and Lenhard *et al.* (1991) in evaluating water flow. Geostatistical ideas were used to express heterogeneity of pore transport and other properties by Tseng & Jury (1993).

The geometric shape of the pores is sometimes considered. For example, Arah & Vinten (1995) look at a random distribution of cylindrical pores, whereas Freijer (1994) assumes they are jointed tubes. Mualem (1976) modelled hysteresis phenomena based on pores in the shape of tubes with a central bulge. Golden (1980) uses the parameters of cylinders (radius, length) in a pore model, while maintaining that this is not equivalent to assuming that they are cylinders. Arya & Paris (1981) assume that soil material consists of spherical particles and that the pore space consists of cylinders. Although unrealistic, this model was helpful in understanding experimental results.

There is some overlap with the fractal category in that some models assume fractal structure for soil material or the pore space or surface. They do not explicitly specify a fractal model for the pore arrangement, but instead summarize it by properties such as a fractal dimension, and analyse the soil properties analytically in terms of it. Examples of this approach are described by Perfect & Kay (1995a), Pachepsky *et al.* (1995), Crawford (1994), Rawls *et al.* (1993) and Booltink *et al.* (1993).

In addition to the advantage of leading to analytical results, the non-spatial approach to modelling enjoys the advantage that aspects of the pore space relating to connectivity need not be a concern, and may be treated at the macroscopic level. This gives the approach some flexibility, at the cost of obscuring any insight into how pore connectivity details affect macroscopic properties. Becsuse of this, we cannot hope to predict how external influences on soil will affect these connectivity properties, or the result of these effects.

3 Schematic models

We classify as schematic any models which prescribe a spatial structure for the soil pores, but which do so in terms of simple arrangements of basic geometric structures such as sphere, cubes and cylinders.

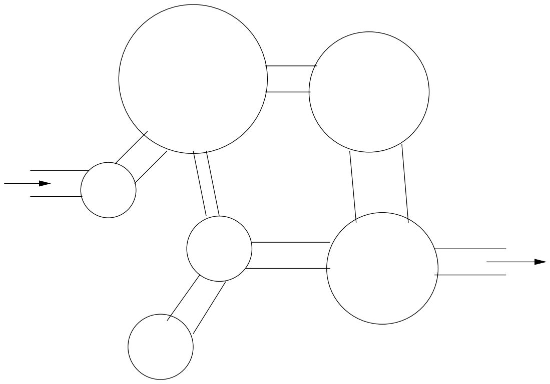

Figure 1: *A schematic model of soil pores. Here the pores are modelled as spheres of variable radius connected by cylinders of variable length and radius*

Figure 1 shows an example of the sort of model we term schematic. The pores space consists mainly of spheres with a random distribution of radii linked by cylinders of random length and radius. This model is spatial, in that the pore space is linked, although it is reduced to a network whose 3 dimensional nature has not needed to be specified.

Figure 1 is not intended to mimic any published model. However, it is similar to some, such as that described by Lowry & Miller (1995), who studied the formation and removal of nonwetting-phase residual. This form of network is a convenient choice for a model, since it allows separate specification of the 'storage' and 'transport' roles of pores. Another example is given by Steele & Nieber (1994), and a complex network model is developed by Mann *et al.* (1986). Wise (1992) regards the pore space as cylinders arranged in a cubic mesh.

Spherical geometry is a natural way to model soil particles, the pores being the space that remains. Gvirtzman & Roberts (1991) examine the adhesion of water to spheres packed in regular arrays, while Wan *et al.* (1995) calculate rates of bacterial transport in a medium of spherical particles. Arah & Ball (1994) model the pore space as a sequence of individual arterial and marginal pores.

Fractures are important in soil structure, and these have also been modelled by structural schemes. A good example is Cacas *et al.* (1990). Many fracture models have also been fractal, and are considered below.

The main advantage of schematic modelling of soil structure is flexibility. We can choose how to vary different geometric properties of the pore space, and this variation can be arranged independently for different properties. The main disadvantage follows from this: it leads us too readily to characterise the pore space in a particular way and we may wrongly believe that the features we select are all, and the only, ones relevant to the soil phenomenon being investigated. For example, a separation of pore space into storage and transport areas is surely artificial.

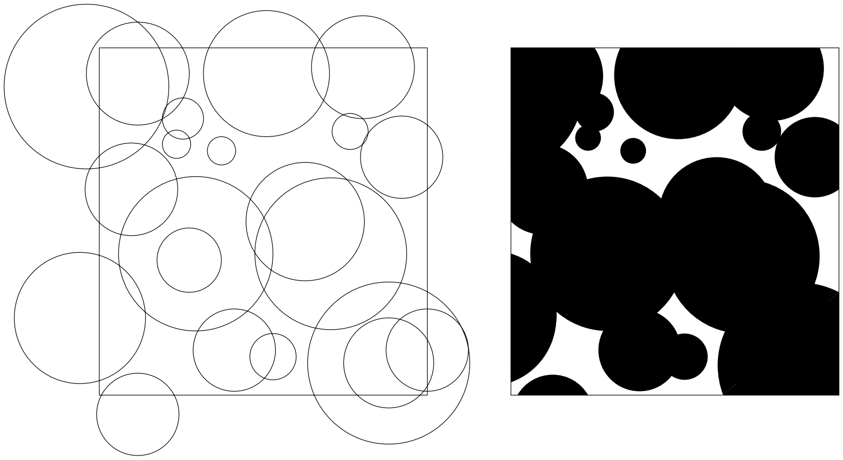

Figure 2: *Illustration of the Boolean random set model for soil pores. Randomly placed spheres define the soil material. The remaining space (white) is the pore space.*

4 Random set models

Random set models generate a random subset of the plane or of space by placing sets at random positions. In this context, a set means a set of points, such as a disc or line. The set placed at each position will in general be chosen from some random distribution of sets. The random set model divides the plane or space into two disjoint components: points which are members of a random set and those which are not. One component will be assumed to be soil material, the other the pore space. Many random set models have been proposed and studied, for their mathematical interest and in a variety of applications. A good introduction can be found in Stoyan, Kendall and Mecke (1995). A bibliography is maintained by Molchanov (1996 + updates).

The simplest and most commonly studied random set model is the Boolean model. Sets chosen randomly and independently from some distribution are placed at points generated by a Poisson point process. This is illustrated in Figure 2. Such a model has been used to simulate soil pores by Glasbey *et al.* (1991) and Horgan and Ball (1994). It has also been used to model soil surface roughness (Bertuzzi *et al.*, 1995; Goulard *et al.*, 1994). The sets can also be used to model the pore space — Sills *et al.* (1991) consider spherical bubbles in gassy offshore soil.

Another category of random sets is packed sphere models. It is assumed that we have an ensemble of rigid hard particles, and we try to pack them as closely as possible. This model has been widely studied for many applications in materials science. A review of applications in the earth sciences is presented by Rogers *et al.* (1994). An example of their use in soil science is given by Bures *et al.* (1993), who examined the effect of different particle size distributions on soil shrinkage. For a flavour of some of the many other approaches to packed sphere modelling, see Stillinger & Lubachevsky (1993), Alonso *et al.* (1995) or Martys *et al.* (1994). Related to packing is sedimentation, in

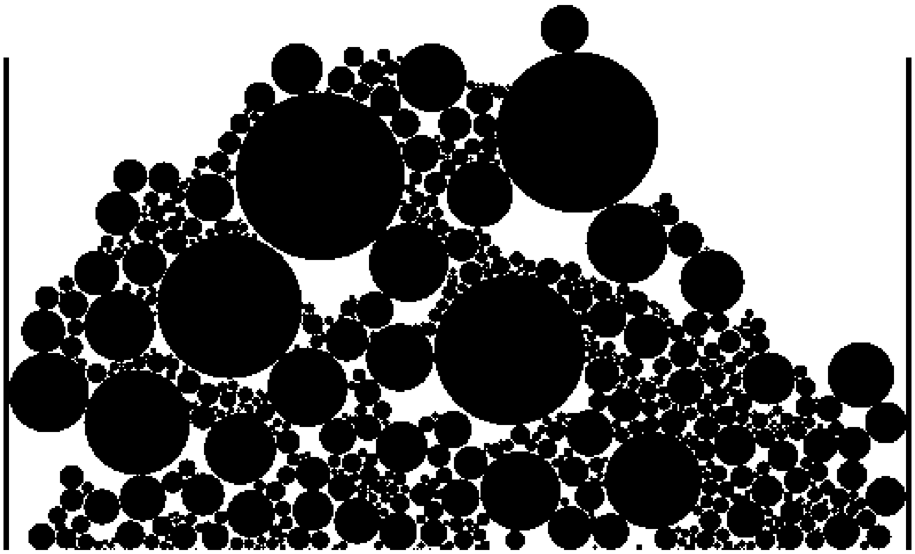

Figure 3: *Simulation of a two-dimensional sedimentation process of discs with a log-normal distribution of radius.*

which particles fall under gravity and pile on top of each other. Figure 3 shows an example. Aspects of such a model are considered by Ghilardi *et al.* (1993). Åberg (1992 & 1996) considers random sets of non-overlapping, but not packed, particles, and derives some analytical results.

An advantage of random set models is that they can generate very tortuous pore networks which seem realistic. Unlike some simpler models, there need be no constraint that pores have a simple shape or connectivity structure. Some models, particularly packed spheres, appeal in that they may resemble the way soil is formed. The major disadvantage of random sets is that they are mathematically intractable, and computationally demanding to simulate and handle.

5 Fractal models

In terms of numbers of models and resulting publications, this is the largest category. Fractals have enjoyed much popularity in recent years, since it has been discovered that they are a better description of much of the natural world than classical geometry. The basic idea is that many natural processes have no natural size scale and so generate similar structures over a wide range of scales (hence the term 'self-similar'). In practice, the self-similarity will extend only over a bounded range of scales. If this covers some orders of magnitude, a fractal model may be useful. Figure 4 shows an example of a simulated random fractal. It was generated by thresholding a non-stationary two dimensional autoregressive process. Several authors have convincingly demonstrated the fractal nature of soil (e.g. Bartoli *et al.*, 1991; Young & Crawford, 1991). Either

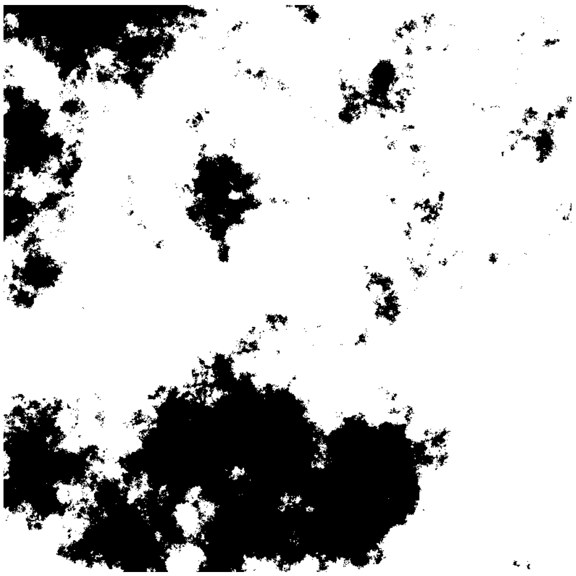

Figure 4: *Fractal set generated by thresholding a non-stationary two-dimensional autoregressive process*

the pore space or its surface may be fractal (Wang, 1987).

There are several approaches to fractal modelling of soil. We have already mentioned the analytical approach based on fractal dimensions. Where this approach does not suffice, we need to look at the geometry of the fractal. This is done in a number of ways: through size distributions, fracture processes, regular structures and random structures.

If we have a collection of objects of variable size, this collection may exhibit fractal properties for certain distributions of size. The simplest way to see this is to consider a size distribution with density

$$f_S(s) = \frac{1}{s^2}.$$

We might imagine S to be the radius of a sphere, for example. This distribution is improper, in that

$$\int_0^\infty \frac{1}{s^2} \mathrm{d}s = \infty,$$

and so in practice there must be a lower limit to the size. One intuitive way to see that this can give rise to fractal behaviour is to note that $f_S(s)$ is the apparent distribution, at the origin, of radii of spheres of constant radius randomly scattered in three dimensional space. If we made on image of what would be observed, looking at it more closely would be equivalent to magnifying the image to see what is farther away — it would look the same. Thus we have the fractal property of self similarity. More generally, size densities of the form

$$f_S(s) = \frac{1}{s^D}$$

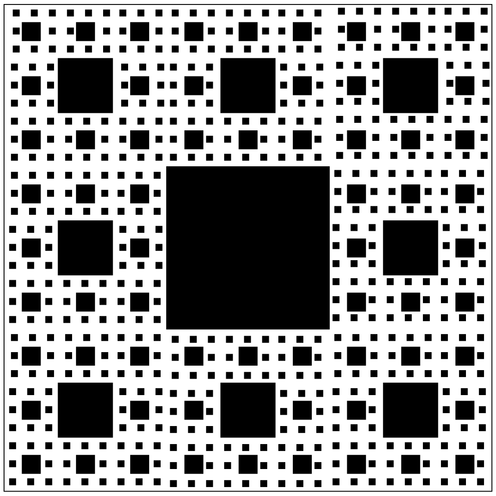

Figure 5: *Regular Sierpinski carpet*

will give rise to fractals with different fractal dimensions — see Mandelbrot (1983). The distribution of soil particle sizes has been considered in this light by Tyler & Wheatcraft (1992) and Perfect *et al.* (1993). Logsdon (1995) uses particle size distributions in studying hydraulic conductivity.

Consideration of size distributions is often associated with models of fracturing — the way in which particles repeatedly fragment into smaller particles. It may be shown that many fracturing processes give rise to fractal size distributions. Fracturing is seen as an important element of soil formation. The fractal nature of these processes is examined by Perfect & Kay (1991, 1995b) and its implications for hydraulic conductivity by Rieu & Sposito (1991) and Perrier *et al.* (1995).

The most detailed use of fractals in modelling introduces the full structure of the fractal. This may use either a regular fractal, such as the well-known Sierpinski carpet (Figure 5) or Menger sponge, or a random fractal, which may be a randomised version of a regular construct, or one generated by an intrinsically random process, such as that shown in Figure 5. Regular fractals are used to model hydraulic conductivity by Toledo *et al.* (1990), Rawls *et al.* (1993) and Shepard (1993), to study macroporosity by Brakensiek *et al.* (1992), to investigate pore microstructure by Ghilardi *et al.* (1993). Random fractals are considered for predicting water properties by Rieu and Sposito (1991), in modelling soil fabric by Moore & Krepfl (1991) and in investigating water retention by Perfect *et al.* (1996). Crawford *et al.* (1993) use a pore space based on real soil images to predict diffusion properties. Both regular and random fractals are used by Ewing & Jaynes (1995) and a number of different fractal models are compared by Rieu & Sposito (1991) and by Li *et al.* (1996).

Fractal models appeal in that they capture an aspect of soil not easily handled in other models — that soil is heterogeneous at many scales. However, saying that soil is fractal

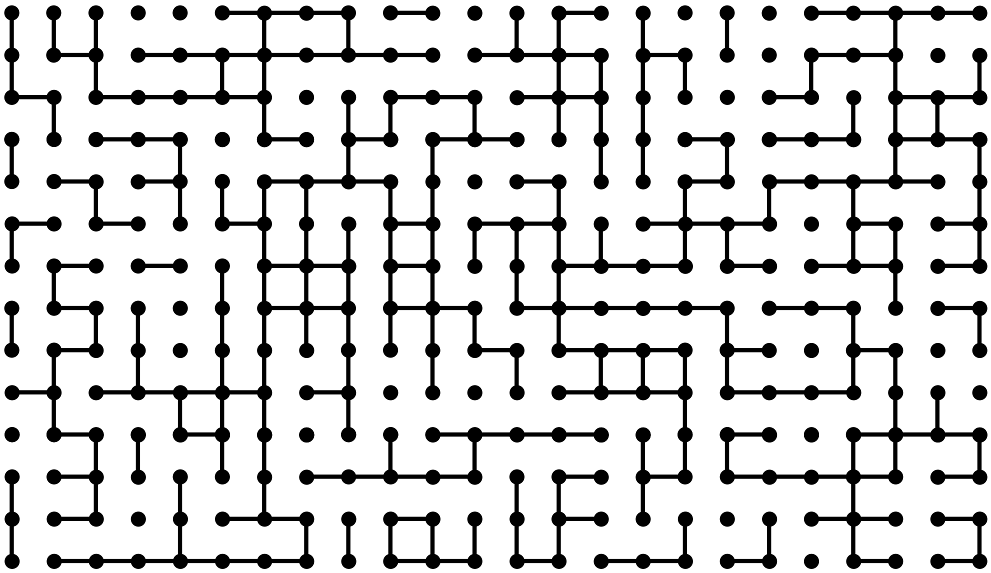

Figure 6: *A bond percolation network. Each lattice point is connected to its 4 nearest neighbours with probability* $p = 0.5$.

does not specify its nature in detail. It is clearly not a regular Menger sponge, although a consideration of the sponge may of course shed light on some soil properties. More realistic fractals are possible, although their random nature may then mean they are difficult and computationally intractable to handle.

6 Other models

It is inevitable that any classification of models will have an 'other' section to gather together those that do not readily fit into other categories.

Eggleston and Pierce (1995) use very simple models of independent or simply blocked groups of pixels to generate images to illustrate dynamic programming tools for analysing pore space. Percolation networks are of considerable mathematical interest and have been used in a wide variety of physical applications, particularly in view of their leading to critical point phenomena. Good introductions may be found in Stauffer (1985) and Grimmett (1989). An example of a bond percolation network is shown in Figure 6. Ideas of percolation theory are used in a discussion of wetting by Blunt & Scher (1995).

Two dimensional lattices offer a wide range of possibilities for creating transport models. Di Pietro *et al.* (1994) base a model on interacting lattice gas cellular automata, originally developed by Appert & Zaleski (1990). Ewing & Gupta (1993a,b) look at permeability and percolation using regular networks with various toplogies. Shcherbakov*et* *al.* (1995) base their model on the Wiener random process, and discover fractal properties.

Ringrose-Voase & Bullock (1984) consider soil pores as being of three types, namely vughs, channels and planes which are intrinsically of zero, one and two dimensions, and use image analysis to identify the different types in soil section images. These ideas are further developed by Ringrose-Voase (1991). Pietruszczak & Pande (1996) analyse the behaviour of gas which is present in the soil in the form of bubbles, and consider how their size will affect their properties.

With an 'other' group of models, we cannot discuss in general their advantages and disadvantages, except to cite the obvious benefit of flexibility. We can choose an approach which best achieves our desired balance between model realism, convenience of handling, computational efficiency, insight generated and compatibility between predicted and experimental results.

7 Conclusions

It is apparent that there have many attempts, from a broad range of approaches, to model and understand soil pore structure. No approach has dominated. It is likely that this is because any model captures only some aspects of real soil behaviour, with different models being useful for different topics of interest.

Research will undoubtedly continue. The principal trend we may expect to observe is increasing use of computer simulation as computing speed becomes faster and more readily available. Analytical descriptions of the soil medium will not cease, however, as the wish to describe soil behaviour in terms a modest number of parameters will remain.

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