# Environmental flows

I.M. Young, A.G. Bengough, J. Chessell, J.W. Crawford, L. Deeks, X. Zhang

Background Flows of water, solutes and gases are fundamental to the major biogeochemical cycles that sustain terrestrial life. An important, yet poorly understood, component of these flows are those within the top 2 metres of soil covering the land surface. This edaphic zone is not only crucial for plant growth, but is highly relevant to the many man-made environmental concerns, such as application of agrochemicals and the disposal of waste chemicals and sewage sludge.

Central to our approach is the hypothesis that the spatial heterogeneity of soil architecture influences the flow and activity of solutes, and organisms, within a soil profile. We also recognise implicitly that the size-scale within which flow mechanisms operate, impact directly on flow characteristics. For example, at the molecular scale, the position of a reactive chemical, moving in a water-filled pore, depends on the tortuosity and connectivity of the pore-space, at a larger scale, and the accessibility of reactive sites to the molecule. Under unsaturated conditions, the ambient matric potential, which controls the spatial distribution of retained water and the thickness of water films within soil, presents an additional variable to consider, which may also impact on the reactivity and residence time of the molecule over a given time.

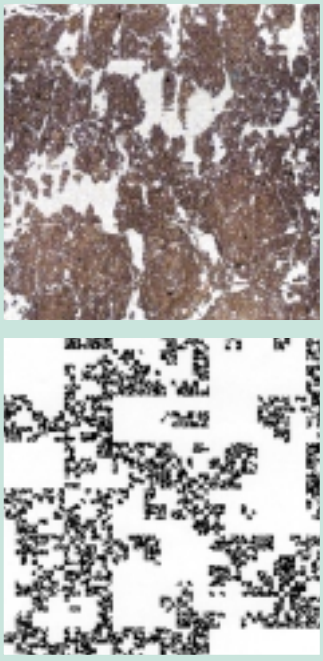


Figure 1 The link between complex soil architecture (top image) and fractal approximations (bottom image). Fractals capture the irregular and tortuous shapes that are ubiquitous in soil, and that impact on all soil processes.

Additionally, as we have shown in earlier work, the porosity of the soil can be scale-dependant; increasing as soil volume increases. The spatio-temporal heterogeneity of the architecture of soil thus impacts directly on the dispersal of pollutants and microbial contaminants to waterways and aquifers.

*Accounting for complex architectures*

The first step in our work was to describe mathematically the complex structures of all soils. The rough and tortuous shapes typically found are not usefully measured by classical geometry. From past work we have shown that fractal geometry can account for these complex structures, and has the added benefit of providing numerical approximations of the structural complexity that can be related directly to transport processes. Figure 1 shows how fractal geometry provides a useful description of real

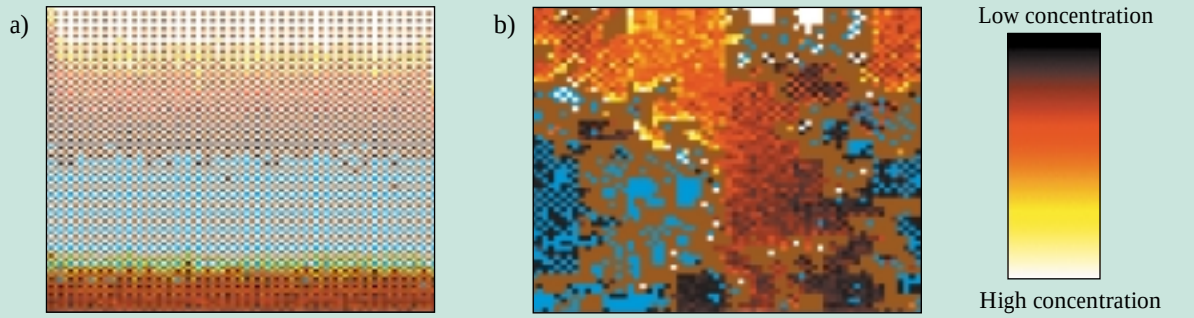


Figure 2 The effect of a heterogeneous physical structure on chemical adsorption. (a) Simulation of adsorption within a homogenous structure, and (b) adsorption within a heterogeneous fractal grid.

soils. By constructing model structures that account for complex pore shapes and connectivities, we can then use computers to simulate chemical, physical and biological processes. In this way we can test rigorously the hypothesis that the physical architecture of soil alone can have a significant impact on soil processes.

Linking chemistry and physics The ability of soil to supply nutrients to plants and retain potential chemical and microbial pollutants is crucial for food production and industries concerned with safe disposal of society's waste. The accepted protocols for measuring a soil's ability to adsorb and desorb chemicals (e.g. its cation exchange capacity) rely on destroying any natural physical architecture, through sieving and drying, and pouring chemicals onto the soil under saturated conditions. Therefore, the spatial relations between the chemical molecule, water, and the soil's natural architecture are completely lost. This leads to data based solely on artificial, structurally homogeneous, soil, bearing little relation to what really happens in the context of real soils.

When a solute is applied to such homogeneous structures, all reactive sites are accessible and adsorb solute until saturated (Fig. 2a). Essentially these methods give an adsorption capacity for the total reactive surface area of the soil. Clearly not all the reactive sites will be accessible to solute entering the soil. Site accessibility depends on both the soil structure and soil particle surface structure. We use a random recursive fractal lattice that accounts for the heterogeneity of the soil structure, and the random nature of soil particle surfaces (Fig. 1). When a solute is applied to this fractal lattice, a measure of the adsorption capacity of the accessible reactive surface of the soil is then determined. Figure 2b illustrates that the effect of structure on the chemical reactions is immediately apparent. It is interesting to note the occurrence of chemical 'hot spots' within the complex soil architecture, where solute has been trapped in, which are not seen in the simple architectures. This means that a proportion of solute is retained within the soil matrix rather than diffusing rapidly through the soil solution.

We use the Langmuir Adsorption Isotherm to express the proportion of occupied reactive sites at each solute

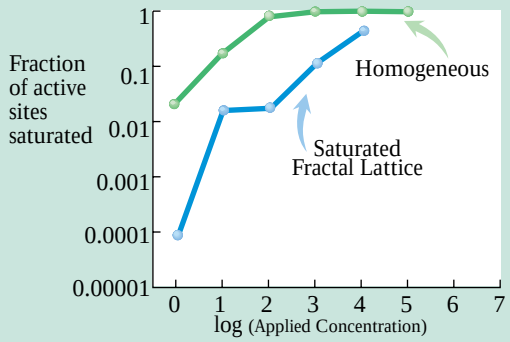


**Figure 3** Langmuir adsorption isotherms for a homogeneous and structured 2D soil.

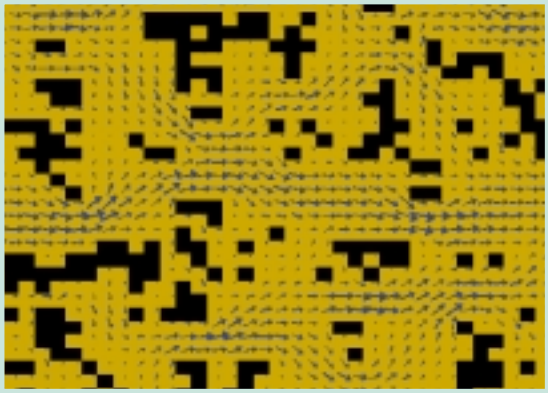

Figure 4 Lattice Boltzman simulation of solute flow through a random fractal lattice. The intensity and direction of flow are given by the blue arrows. Simulated soil is shown in black.

concentration, giving a measure of the adsorption capacity of the soil. Figure 3 compares the Langmuir adsorption isotherms for the unstructured, classical method and the structured, random recursive fractal lattice simulations. From these results it is clear that small-scale soil structure has a large effect on the adsorption of reactive solutes into soil.

Solute flow and structural complexity At the pore-scale, again using a fractal lattice as the basis of a complex architecture, we have modelled liquid and solute flow using the lattice Boltzmann equation discretized over a square lattice for 2D, and cubic lattice for 3D. Using the lattice Boltzmann algorithm, liquid flow is modelled by spreading a number of particles over the pore space within the lattice, which then move and collide according to the rules of conserving mass and momentum. We have shown that these simulations produce flow patterns entirely consistent with the solution of the classical Navier-Stokes equations that describe liquid flow at macroscopic scale. Two examples of simulated liquid flow for 2D and 3D soil structures using lattice Boltzmann algorithm are shown in Figure 4. From these simulations the major flow paths are clear. Additionally, areas where solute is present but little flow occurs are shown. These points show that only a relatively small portion of the pore space is involved in the main flow, and there are significant volumes where little or no flow occurs.

The two main areas of future research relate to the connection of the models for chemical reactivity and flow, which operate over two different scales, and to the development of the chemical model in 3D. In parallel we are conducting a joint experimental programme where we are developing methods which account for and measure the impact of complex soil structures on flow and chemical activity, with the ultimate aim of investigating the role of small-scale processes on flow and chemical activity at the catchment scale.

Whilst the examples illustrated in this article concentrate on physio-chemical processes, the concept of the rôle of the physical architecture of soil in controlling chemical processes, such as reactivity, is transferred easily to biological processes such as biocontrol, and pesticide efficacy.