Soil structure, water and solute transport: from 3D soil images to particle tracking

J-F. Delerue, S. Fournier

UR Geodes, Centre de recherche IRD Ile de France, 32 avenue Henri Varagnat, 93143 Bondy
delerue@bondy.ird.fr

Solute transport is closely linked to hydraulic behaviour. Our research deals first with the determination of soil unsaturated hydraulic properties by collecting information from 3D soil images and by modelling the geometric structure of the pore space, then we investigate computer tools to simulate solute transport in such a context.

Much work has been done in Soil Science to relate hydraulic properties to structural data. From a deterministic and physical point of view, fluid dynamics are fully constrained by the boundary of the void space, but solving the Navier-Stockes within such complex geometry as that of soils is difficult. It needs a lot of power computation and memory. Such attempts have been made in monoscale porous media to predict the saturated hydraulic conductivity by direct solving of Navier-Stockes equations or, using lattice gases simulations in saturated soils (Heijs et all., 1996)Many models.have been developed which represent porous media in a simplified approach as a connected set of individualised voids, cylindrical pores or parallepipedal fractures, where simple, integrated forms of the Navier-Stockes equations are available (namely, the Poiseuille Law in cylindrical tubes). In unsaturated conditions, i.e. a soil partially filled with water, the active network is reduced to the smaller, water-filled pores according to the Laplace law and the displacement of air-water boundary with varying capillary pressures. This so-called pore network modelling approach is mainly used in theoretical studies, where a given type of pore network is calibrated by available data, mainly to match a measured pore size distribution (e.g. a given fractal pore size distribution in Perrier et al, 1995). The connectivity of the network has been shown to be crucial, but it is difficult to measure it and different types of modeling assumptions are tested.

We propose a complete framework to actually extract a pore network from nowadays rather easily available 3D soil data. For example computer tomography (CT) provides a new, valuable type of soil structure investigation (Timmerman et al., 1999). A 3D Soil image is first acquired and converted to binary image where the white voxels represent the pore space (a more of less continuous void space) and the black ones represent the solid space. Then a set of computer vision tools (Delerue, 2001) allows to analyse the structure of the pore space. We begin to extract the 3D skeleton of the pore space using a Voronoï based algorithm. This skeleton, gives all local information about local aperture and connectivity. An aperture map is created from this skeleton by mapping balls on the skeleton. This aperture map is a first step in the description of the pore space. Using this map, it is possible to know the local aperture at any point within the pore space.

The next step consists in dividing the pore space in pores. We define a pore as a part of the pore space where all the points belong to the same local aperture class, and which is located between the boundaries of the pore space. A growing area segmentation algorithm is used to actually define these pore objects. Using the skeleton extracted previously, seeds are placed in the pore space. Those seeds consist in maximum balls touching opposite boundaries of the pore space. During the second part of the growing area algorithm, we make those seeds grow in a synchronous way in the pore space until each area reaches boundaries or other pore areas. The result is a partition of the pore space in pores.

For each pore, it is possible to know its aperture, volume, localisation and neighbours. All this information is used to calibrate a pore network model. This model provides hydraulic properties for the whole sample. I.e. it gives the equivalent hydraulic conductivity for the whole soil sample. This pore model also gives local hydraulic properties for each pore, such as local hydraulic conductivity, fluid pressure, flow intensities etc…
All that information, i.e. local hydraulic properties and pore map can then be used to develop a multiagent-oriented approach for solute particle tracking. In this model, two classes of agents are defined: spatial pore agents and moving particle agents. For each pore in the pore map an agent is defined who knows its local hydraulic properties such as local pressure and flow speed as a function of the imposed global pressure gradient. Then particle agents are defined which_know their localisation at any time and physical properties like the amount or type of solute they carry At each time step, each particle moves according to the intensity and direction of the water flow given by the pore where they are located. Up to now this model enables_particle tracking in the pore space using a simple convection model as the pore scale and computing statistics about repartition in the pore space and time needed to go across the whole medium.
However, the agent oriented design is open to lots of extensions : The local direction of particle agent be influenced by local diffusion within the pore or by other simulated physical phenomena. In particular, modelling continuous displacements within the pore space allows to modify particle agent directions when they collide with the interface between solid and void space. Interaction between particle agents could allow particles to split or to merge when two particles collide. Interaction between particle and pore could allow considering probabilities for the particle to be infiltrated in the solid part when particle collide with the void / solid interface. Finally, interaction between pores could allow the model to reorganise itself automatically in case of dynamic modification of the geometry of the pore space. The main originality of the agent-based approach through giving "life" to individualised agents, consists in the straightforward possibility to register individual trajectories and to simulate tracing experiments

References

Heijs, A.W.J., JF. Th Schoute & J. Bouma, 1996. On 3D-flow in macropore systems, from computed tomography imaging to lattice Boltzmann simulations. In P.A.C. Raats, H. Rogaar and A.H. van del Heuvel (Eds.), Soil structure and transport processes: implications for water, gases, nutrients, pesticides and contaminants in soils. *Wageningen, Neth. Integr. Soil Research program. Rep.6 pp 45-53*

Perrier, E, C. Mullon, M. Rieu and G.D. Marsily, 1995. Computer construction of fractal soil structures. Simulation of their hydraulic and shrinkage properties. *Water Ressources Research, 31 (12) pp 2927-2944*

Timmerman A., K. Vandersteen, T. Fuchs, J. Vancleynenbreugel & J. Feyen, 1999. A flexible and effective pre-correction algorithm for non medical applications with clinical CT scanners. *In: Proceedings of the international workshop on modeling of transport processes in soils at various scales in time and spaces. Leuven, Belgium*

Delerue J.F., 2001. Segmentation 3D, application à l'extraction de réseaux de pores et à la caractérisation hydrodynamique des sols. *Ph.D. Thesis, Université Paris XI.*

Delerue J.F., E.Perrier, Z. Yu, B.Velde, 1999. New methods in 3D image analysis and their application to the measurement of pore size distributions in soils, *Physics and Chemistry of the Earth, Vol. 24, No. 7, Part A.*

Delerue J.F., E.Perrier, A.Timmerman, M.Rieu, 1999. New computer tools to quantify 3D porous structures in relation with hydraulic properties. *Actes du colloque Modelling of transport processes in soils, 24-26 Novembre 1999, Leuven, J.Feyen & K.Wiyo.Eds, Wageningen Pers, The Netherlands, pp.153-163.*

Delerue J.F., 2001, Segmentation 3D appliquée à la modélisation des milieux poreux. *Récents progrés en génie des procédés, pp. 175-179 No.78, Volume 15.*