Core Ideas

- Noninvasive, high-resolution imaging is important for visualizing water flow and transport processes.
- Most important are X-ray CT, MRI, and neutron CT.
- Image processing techniques are mandatory for maximum benefit from the images.

Noninvasive Imaging of Processes in Natural Porous Media: From Pore to Field Scale

Andreas Pohlmeier,* Sarah Garré, and Tiina Roose

Noninvasive, high-resolution imaging techniques are important for visualizing water flow and transport processes in soils, which are natural porous media. They are a key to understanding effects such as crop production, water resource restoration, CO_2 sequestration, or the transport and fate of pollutants. During the last two decades, the development of three-dimensional imaging techniques such as nuclear magnetic resonance imaging (NMR and MRI), X-ray computed tomography (CT), and neutron CT has made significant progress possible in the study of soil processes. This special section presents examples of X-ray CT and NMR from the small-column scale to the application of portable NMR equipment in the field, along with some important advances in image processing that make it possible to extract optimal physical information from the original data.

Abbreviations: 3D, three-dimensional; CT, computed tomography; MRI, magnetic resonance imaging; NMR, nuclear magnetic resonance; XCT, X-ray computed tomography.

Characterization and prediction of water flow and transport processes in soils as natural porous media is a key in understanding and managing climate change, plant production, restoration of water resources, CO_2 sequestration, and waste disposal. Traditional techniques for measuring structure, water content, or solute transport are mainly invasive or restrictive in dimensionality or resolution. Nevertheless, noninvasive imaging from the pore to the soil core or mesocosm scale with appropriate high resolution is necessary for the fundamental understanding of the interaction between the soil and plant structure, fluid flow, and solute transport. In the past two decades, the development of three-dimensional (3D) imaging techniques such as magnetic resonance imaging (MRI), X-ray computed tomography (XCT), and neutron computed tomography has enabled rapid advancement in the investigation of soil states. Moreover, these methods are also necessary for imaging of processes such as the flow and redistribution of water, and solute and particle transport because they are strongly affected by the structure of the pore system.

Micro-X-Ray Computed Tomography

Micro-X-ray computed tomography (X-ray CT or XCT) is the most common technique due to its broad availability. X-rays, emitted from a source, are focused on an object and interact with the electron shell of atoms, and a projection image is recorded. A full set of projections at different rotation angles of the sample covers typically >1000 individual images, from which the 3D image is finally created by reconstruction techniques. The sensitivity of X-rays increases with the atomic number of the elements present in the sample. This makes it an excellent tool to study the microstructure of soil, i.e., the spatial distribution of minerals containing heavy atoms such as Si, Fe, or Mn. Furthermore, advanced methods have been developed in the past decade that allow imaging of organic matter and water in soils in combination with appropriate image analysis techniques (Gregory et al., 2003; Heeraman et al., 1997; Pierret et al., 1999; Roose et al., 2016; Tracy et al., 2015). The spatial resolution has been greatly improved to 10 µm for routine instruments and <1 µm using synchrotron X-ray source devices (Keyes et al., 2013). In this special section, Weller et al. (2018) demonstrated the improvement of water quantification by correction of beam hardening effects. They developed a calibration protocol and tested

A. Pohlmeier, Research Center Jülich–IBG-3, Jülich 52425, Germany; S. Garré, Faculte des Sciences, Gembloux Agro-Bio Tech, Univ. de Liege, TERRA, Passage des déportés 2, BE-5030 Gembloux, Liege 4000, Belgium; T. Roose, Faculty of Engineering and Environment, Univ. of Southampton, University Road, Southampton SO17 1BJ, UK. *Corresponding author (a.pohlmeier@fz-juelich.de).

it as an example on the infiltration of water into several soil cores, monitored by two-dimensional X-ray radiography. Their success was proved by comparison with gravimetric analysis. Katuwal et al. (2018) determined the macropore systems from 3D X-ray CT images of several soil cores from Denmark representing different texture classes from pure sand to silty loam. In a second step, they correlated the macroporosity and the CT matrix density with the organic clay mineral content obtained from visible–near-infrared spectroscopy analysis and showed its convenience for the prediction of soil hydraulic and preferential flow properties.

Neutron imaging (neutron tomography or neutron CT) is less common in soil science mainly because it requires access to relatively few facilities. Methodologically, it is comparable to XCT in the sense that it is a transmission technique, too, although the basic physics, the neutron scattering by certain nuclei, is very different. The most popular nucleus in soil science with a high scattering cross-section is the H atom, making the technique highly sensitive for water content imaging. Similar to XCT, neutron CT records many projections through a rotating object, from which the 3D image is finally reconstructed (Haber-Pohlmeier et al., 2017; Oswald et al., 2015; Tötzke et al., 2017; Vontobel et al., 2008). In comparison to XCT, the neutron-imaged samples are radioactive after scanning, requiring a special disposal protocol, and hence these scans are almost always terminal scans or near terminal with less scope for time-resolved studies.

Nuclear Magnetic Resonance

Nuclear magnetic resonance is a well-known technique in chemical analysis, medical diagnostics, and material sciences (Blümich, 2000; Blümich et al., 2014; Callaghan, 1991). Its physical operating principle, based on the nuclear magnetic resonance (NMR) effect, is fundamentally different from that of XCT and neutron CT. While the XCT and neutron CT techniques are based on source (X-ray or neutron) ray attenuation by the object imaged, in NMR atomic nuclei are excited and their excitation response is monitored in terms of the emitted radiation in the time domain. Many atomic nuclei, such as ^{1}H, ^{23}Na, ^{19}F, or ^{13}C, possess a finite microscopic magnetic moment related to their spin. Of these, the H atom in water is the most commonly used nucleus in soil science. If placed in an external magnetic field, the spin system of water can be excited by interaction with radio-frequency radiation and subsequently relaxes to its equilibrium. The response signal in the time domain is controlled by the water content and relaxation times and contains information about the chemical environment, the pore system, and the local motion of the spins. Consequently, NMR is directly sensitive for water (^{1}H$_2$O) in the voids of the porous medium. In nuclear magnetic resonance imaging (MRI), additional magnetic field gradients encode the spatial resolution of the NMR signal in the time domain and the image is reconstructed in the real space domain by inverse Fourier transformation. The wealth of information obtained by NMR and MRI is due to the use of additional encoding and decoding filters that make the image sensitive to chemical shift, diffusion, flow characteristics, or T_1 and T_2 relaxation times, reflecting the pore environment. After spectroscopy for chemical analysis of soil components, NMR relaxometry, either integral or spatially resolved, is the most widespread technique for the exploration of the interaction of water with the pore system.

A general rule of thumb is that the relaxation times scale inversely with the mobility. Mobile water in large pores relaxes more slowly than immobile water narrowly confined (Coates et al., 1999) or, as an extreme case, frozen water. Consequently, by analysis of relaxation time distributions, Tian et al. (2018) used NMR relaxometry for the differentiation of mobile, capillary bound water, and adsorptive water in freeze–thaw cycles in some soil cores. Correlation with water potential measurements supported their findings.

Water is found in natural soils mostly in small pores, and its relaxation times are relatively short and become even shorter with decreasing saturation. Therefore, quantitative imaging of water in soils requires special NMR pulse sequences with very short detection times after the excitation. Merz et al. (2018) used the SPRITE method for investigation of evaporation processes from the topsoil and could confirm the development of a dry surface layer due to the interruption of capillary continuity. This strongly hinders further evaporation (Merz et al., 2016). In their contribution to this special section, they continued this work by analysis of the observed water content patterns by numerical modeling. It turned out that the use of a fully coupled liquid, vapor, and heat flow model is necessary for a correct description of evaporative drying (Merz et al., 2018).

Classical NMR requires a device where the magnetic field is highly homogeneous inside a cylindrical magnet. In contrast, NMR is also applicable in field studies by using a magnet whose field is directed outward and the radio-frequency coil generates exciting pulses in a defined region outside the magnet. Such dedicated equipment has been historically developed by the petroleum industry for well-logging purposes (Coates et al., 1999), and during the past few years it has been adopted for hydrological purposes (Kirkland et al., 2015; Sucre et al., 2011). Using a small-scale instrument, Kirkland and Codd (2018) demonstrated the usefulness of a mobile NMR borehole device to quantify the soil moisture distribution as well as biofilm and precipitate formation at the field scale. By analysis of one-dimensional resolved NMR relaxation data, they were able to derive hydraulic conductivity profiles from the surface to a depth of 10 m.

Image Processing

After multidimensional images have been correctly reconstructed from the raw data by appropriate computing techniques, further image processing algorithms are necessary for the extraction of relevant soil physical information, a rapidly growing field of methodologies in soil science. Especially for the analysis of high-resolution XCT images, semi- and fully automated programs are under development. An important step is the segmentation of the pore space and the differentiation of liquid phases and organic matter

therein. This is the basis of further quantification of these soil components and their correlation with other image information.

In this special section, Koestel (2018) integrated several tools for automated processing into a new plugin for the open platform ImageJ or Fiji (Schindelin et al., 2012). The plugin "SoilJ" bundles several tools for column outline recognition, correction of intensity bias, segmentation, extraction of particulate organic matter and roots, soil surface topography detection, as well as morphology and percolation analyses and was tested on some soil columns with a high organic matter content.

Also, Smet et al. (2018) tested three segmentation algorithms for their performance of segmentation and noise reduction. Using examples of simulated and real images from the literature, they showed that pre-segmentation noise reduction significantly improves image quality in contrast to post-segmentation procedures.

The top surface of soils is a very sensitive zone because it is the interface between the atmosphere and deeper layer compartments. All flux processes such as precipitation, evaporation, and gas exchange must pass this interface. Therefore, the extraction of information about this zone from images requires special attention. This was addressed by Garbout et al. (2018), who demonstrated the performance of the ImageJ plugin "TopCap" for an automated capture of the 3D morphology of the soil surface texture and roughness and a segmentation of the local pore structure.

Concluding Remarks and Outlook

This special section addressed the application of noninvasive techniques for noninvasive imaging of soil structure, water redistribution, and transport properties. Special focus was on the processing of X-ray CT images to extract relevant soil physical information. Nuclear magnetic resonance imaging was mostly applied in terms of integral and spatially resolved relaxometry. The focus was on the analysis of relaxation time spectra reflecting the degree of confinement in the porous system. In the future, the combination of noninvasive techniques and the addition of further invasive methods promise a more detailed understanding of soil physical processes. Especially, the implication of advanced image processing techniques and statistical analysis will allow a reliable extraction of information from the original multidimensional images.

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