



International workshop:

## How to unravel the interactions between soil structure and soil functions?

20-22 July 2015

Grenoble, France

# PROCEEDINGS



## PROTINUS

*This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N°645717.*



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## Workshop programme

July 20, 2015

### EXPERIMENTAL WORKS

**9h15-9h30: Duwig C.** (LTHE/IRD, France): presentation PROTINUS

**9h30-10h30: Baveye P.** (Rensselaer Polytechnic Institute, Troy, New York/ AgroPariTech, Paris): Invited Keynote 1: Working our way backward from soil functions to their architecture: Can we do it without ever talking about aggregates. **Invited speaker**

**10h30-11h00: Müller K, McLeod M., Young I., Scott J., Clothier B.** (The New Zealand Institute for Plant & Food Research (PFR), Hamilton): Linking soil form to function: Solute filtering.

11h00 -11h15: Café

**11h15-11h45: Dal Ferro N., Morari F.** (Univ. Padova Italy): From real soils to 3D printed soils: reproduction of complex pore network at the real scale is possible?

**11h45-12h15: Johannes A., Boivin P.** (Institute Land-Nature-Environment, Switzerland): Handling Variability of Soil Structure

**12h15-14h00: Lunch**

**14h00-14h30: Martins J.** (LTHE, Grenoble, France): Application of X-ray microTomography to the visualization of bacterial biofilms in porous media.

**14h30-15h00: Fujiki, Y., Oxarango, L. and Mukunoki, T.** (LTHE Grenoble, X-earth center, Kumamoto University, Japan and LTHE, Grenoble): X ray micro-CT analysis of retention and relative permeability curves.

**15h00-15h30 : Prado B., Gastelum Strozzi A., Huerta E, Duwig C., Zamora O., Delmas P., Casasola D., Márquez J.,** (UNAM, Mexico): 2,4-D mobility in two clay soils: impact of macrofauna abundance observed by CT-scan.

**15h30-16h00: café / Poster**

**16h00-16h30: Boukcim H, Braudeau E, Hedri E, Taugourdeau O.** (Valorhiz, France): From Soil Characterization With Typosoil® To Bio-Technosoil Building: The Valorhiz Approach Of Soils Functions.

**16h30-17h00: Podwojewski P., Aroui-Boukbida H., Smaili, L., L.Hovhannissian, G** (IRD, UMR 242, IEES-Paris). Study of the lateral extension of gullies in South Africa . Differential behavior of materials subjected to shrinkage and swelling.

#### Poster:

**Hamamoto S., Moldrup P., Kawamoto K., Sakaki T., Nishimura T., and Komatsu T.** (Graduate School of Agricultural and Life Science, The University of Tokyo, Japan). Pore Network Structure Linked by micro focus X-ray CT to Particle Characteristics and Mass Transport Parameters

**Caurel C., Rozenbaum O., Dupraz S., Garrido F., Bruand A.** (ISTO, Orleans, France): Pore scale processes governing biofilms location and development in a dual porous media: effect on CCA mobility.

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## IMAGING AND IMAGE PROCESSING

**9h00-9h30: Café, yesterday summary**

**9h30-10h30: Gimel'farb G.** (UoAuckland, New Zealand): Keynote 2: Texture characterisation in 2D/3D images: application to Environmental Sciences.

**10h30-11h00: Sammartino S., Lissy A.-S., Bogner C., Beltrame Ph., Van Den Bogaert R., Capowiez Y., Ruy S. and Cornu S.** (EMMAH, Avignon): A further step in visualizing and understanding preferential flow in undisturbed soil cores: identifying the functional macropore network. **Invited speaker**

**11h-11h15: café**

**11H15-11H45: Smet S., Leonard A., Degree A.** (Univ. Liège, Belgium): How And Where Is The Link Between The Soil Behaviour And Its Internal Architecture?

**11h&45-12h15: Delmas P.** (UoAuckland, New Zealand): 2/3D Image Processing in the context of Environmental Sciences.

**12h15-14h00: lunch**

**14h00-14h30: Watteau F., Jangorzo N.S., Hajos D., Leguedois S. and Schwartz C.** (Laboratoire Sols et Environnement, Vandoeuvre les Nancy, France): Direct visualization and quantification of the biological activity impact on the dynamics of technosol structure

**14h30-15h00: Rabot E , Lacoste M, Hénault C, Cousin I.** (CEA, Gif sur Yvettes, France): Using X-ray computed tomography to describe the dynamics of nitrous oxide emissions in soil

**15h00-15h30: Café/poster**

**Poster**

**Duwig C., Delmas P., Gastelum Strozzi A., Lefrancq M., Marquez J., Prado B., Charrier P.** Modelling of water flow through soil pores observed by x-ray tomography

**Gastelum Strozzi A.** X ray Tomography equipment at CCADET, Mexico

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July 22, 2015

## MODELLING SOIL FUNCTIONS

**9h00 – 9h30: Café, yesterday summary**

**9h30-10h00: Fayard B., Guiraud O. (NOVITOM Grenoble, France):** Synchrotron X-ray imaging - a multimodal approach for the analysis of complex structures.

**10h00-10h30: Tinet A.J. and Golfier F. (UoLorraine, Nancy, France):** Perspectives for pore-scale flow modeling with Lattice-Boltzmann method: multiphase behaviour and couplings.

**10h30-11h00: Gastelum Strozzi A. (UNAM Mexico):** From CT-scan imaging to SPH modelling: application to Environmental Sciences.

**11h00-11h15: café**

**11H15-11h45: Michel E., Majdalani S., van den Bogaert R., Cornu S., Di Pietro L. (INRA, Avignon):** What Are The Impacts Of Transient Flows On Colloid Mobilization And Retention In Macroporous Soils ?

**11h45-12h15: Qin C.-Z., Hassanizadeh M. S. (Utrecht University, The Netherlands):** Pore-network modeling of microbially-induced calcium carbonate precipitation: insights into scale-dependent reaction rates and permeability-porosity relationship

**12h15-14h00: lunch**

**14h00-17h00: PROTINUS internal meeting**

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## **PROTINUS project presentation.**

**Duwig C, PROTINUS coordinator**

IRD/Université Grenoble1/CNRS/G-INP, LTHE UMR 5564, F-38000 Grenoble, France.

In the Framework of **PROTINUS**, our new international network recently supported by H2020 Marie Sklodowska-Curie Research and Innovation staff exchange, we are pleased to welcome you to our first international workshop. The aim of this workshop is to get together experts in the different fields of soil science, image analysis and soil processes modelling. We hope to meet you in Grenoble in July 2015 to exchange around soil structure and soil functions, and to come out with new standards for soil science research in 2015, declared the **International Year of Soils** by the 68th UN General Assembly!

The project assembles a multi-disciplinary team from the EU and three associated countries, namely France, Italy, Denmark, New Zealand, Mexico and Japan, coming from Research Institute and Universities as well as private companies.

The aim of PROTINUS is to combine advanced, applied and theoretical research to create a new standard in imaging, analysing, modelling and predicting the interactions between soil structure and soil functions. Soil structure impacts a whole range of services soil renders to ecosystems, including for example contaminant filtering, carbon storage, root growth, and microbiological diversity.

By using modern imaging, image analysis and modelling techniques, we will develop an integrated approach to perform experiments in soil physics, bio-chemistry, to reconstruct soil structure in 3D and to model soil processes. The evaluated models will be used for predicting the different services soil renders to ecosystems in a dynamic way and for testing classical theory, where soil structure is not directly taken into account. To do so we will bring together the theoretical and practical expertise of the involved researchers, infrastructure of the partnering institutes, soil samples and databases.

The first stage will investigate today's best practise in experimental soil science and imaging, data analysis and modelling. Our findings will enable our second stage approach where synergies between the different disciplines will be explored. The third stage will provide the cornerstone of a new unified methodology meant to modify practise and outcomes of current experimental/imaging, analysis and modelling approaches. Our final stage will look at the changes brought to each of the specific research area's practises and how it impacts the understanding of soil structure and its functions.

It is expected that our proposal will foster bilateral collaborations within Europe and with our overseas partners through local and international funding, shared database and infrastructure management, and lead to the creation of a sustainable international network of researchers, infrastructure and institutes.

Our project aims to answer the following questions:

- Can trans-disciplinary understanding and sharing of standards developed separately in different research areas provide a way to foster synergies between disciplines?
- Can synergies be found between the four pillars to develop a new trans-disciplinary approach?
- Can a trans-disciplinary approach to the understanding of the interaction between soil structure and functions improve current theoretical understanding?
- Can each of the four pillars benefit from a new trans-disciplinary approach?

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### **Linking soil form to function: Solute filtering.**

**Müller K<sup>1\*</sup>, McLeod M<sup>2</sup>, Young I<sup>3</sup>, Scott J<sup>4</sup>, Clothier B<sup>5</sup>**

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<sup>3</sup>School of Environmental & Rural Sciences, University of New England, Armidale NSW 2351, Australia

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<sup>5</sup>Production Footprints, PFR, Palmerston North, 4474, NZ

Soils deliver the ecosystem service of filtering. But filtering capacities differ between soils. Quick solute transport into aquifers cannot be excluded. We hypothesized that a soil's filtering capacity depends on its macropore structure, which is linked to texture. Tension disc infiltrometry can be used to measure hydraulic properties near saturation. The differentiation between hydrologically active and non-active pores at a given tension indirectly characterizes macropore continuity. Water flow through macropores is a function of the size distribution, tortuosity and connectivity of macropores. These characteristics can directly be derived by 3D X-ray computer tomography (CT). Our objective was to analyze the macropore network and to characterize the resulting filtering performance of soils with contrasting structures. For this purpose, an Andosol and a Gleysol with known filtering behaviour for microbes were selected. Each soil was separated into three horizons assuming that each horizon had a specific macropore structure. In March 2011, infiltration near saturation was measured in the field; hydraulic conductivity and flow-weighted mean macropore diameter for each soil horizon were derived. We extracted intact soil cores from the centre of the infiltration areas, determined the macropore architecture by X-ray CT and conducted bromide leaching experiments. Dye tracer visualized flow patterns in situ. Our results confirmed the better filtering capacity of the Andosol. The soil's comparatively low macroporosity was coupled with a high connectivity of the smaller macropores which led to a more homogeneous matrix flux. Similarly, all measurements confirmed the poorer filtering capacity of the Gleysol, which had a bi-modal pore system with a few very large, but well connected macropores. This resulted in preferential flows. We identified the macroporosity, mean pore diameter and connectivity as the relevant 'form' parameters to describe the 'function' of filtering.



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## **From Real Soils to 3D Printed Soils: Reproduction of Complex Pore Network at the Real Scale is Possible?**

**Dal Ferro N\*, Morari F**

Department of Agronomy, Food, Natural resources, Animals and Environment, Agripolis, University of Padova, Viale Dell'Università 16, 35020 Legnaro (Padova), Italy

Estimating the soil structure characteristics is a key aspect for understanding the biogeochemical processes affecting the vadose zone. Repeated experiments are needed, although the large micro-heterogeneity of the soil pore network renders each sample unique and not fully replicable. Using manufactured geometrically models mimicking the soil architecture is essential, but so far the pore system reproducibility was assured only with homogeneous packed columns of aggregates. 3D printing technology is maturing today to overcome these limitations and reproduce the physical heterogeneity of the soils at high resolution. In fact, operating at small spatial scale is now possible even for complex porous structures, reconstructing the surface of the samples with 3D printing techniques.

Here, we evaluated the feasibility of using 3D multijet printing technology, coupled with X-ray microtomography (microCT), in order to create replicated structures of a loamy soil and compare the hydraulic properties of original soil samples with those obtained from the soil-like prototypes.

MicroCT digital soil models were used to create 3D solid prototypes with a commercial ProJet® 3510 HD 3D printer (3D Systems). The 3D printer deposits a curing resin mixture slices by slices at a resolution of 16 µm (Visijet Crystal®) and was supported by wax during the printing process. Once printed, the prototypes were opaque, white and rigid.

Results showed that soil-like prototypes were similar to the original samples in terms of total porosity and pore shape. By contrast the pore connectivity was reduced by the incomplete wax removal from pore cavities after the 3D printing procedure. Encouraging results were also obtained in terms of hydraulic conductivity since measurements were successfully conducted on five out of six samples, showing positive correlation with experimental data.

We conclude that reproducing the soil structure with 3D printing technologies is a promising technique for understanding the role of its micro-heterogeneity in the soil-water dynamics, although advancements in resolution and cleaning treatments are key aspects that still need to be improved.

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## Handling Variability of Soil Structure.

Johannes A.\*<sup>1,2</sup>, Boivin P<sup>1</sup>

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<sup>2</sup> Soil Protection, Institute of Terrestrial Ecosystems, ETHZ, 8092 Zürich, Switzerland

Understanding seasonal and spatial variability of soil structure is a key to link micro-scale observations to large-scale soil properties. This study aimed at quantifying soil structure properties and the determinants of their variability on a soil unit at national scale.

### *Hypotheses*

(i) Shrinkage analysis (ShC) allows characterizing the soil pore systems, which show linear determination of their properties by the soil colloidal constituents. (ii) These relations are unique when colloidal constituents show similar surface properties, i.e. within a soil order with same parent material, whatever the spatial scale.

### *Material and Methods*

Undisturbed Cambi-luvisol samples were collected from spring 2012 to fall 2014 at 178 locations and from three land uses (permanent pasture, conventional tillage, no-till). Only soils showing a preserved structure, according to the VESS method (Ball et al., 2007) were sampled and analysed for soil organic carbon content (SOC), texture, CEC and shrinkage analysis. The shrinkage analysis enables among others to quantify the plasma and structural porosities. Plasma is defined as made of the soil colloids (SOC, oxides and clay minerals). Plasma porosity is made of inter colloidal particle voids, while the structural porosity is made of biopores, lacunar voids and cracks.

### *Results*

The SOC ranges were overlapping amongst the 3 land uses while the textures were not significantly different. The ShC parameters were linearly correlated to SOC, with  $R^2$  ranging from 50% to 80%, independently of land use, spatial coverage and sampling season. Considering additional soil properties only marginally improved the prediction of physical properties by colloidal constituents.

### *Discussion and Conclusions*

The working hypotheses were validated. The structure properties can be estimated robustly and accurately, by using SOC as covariate to explain the soil variability. This approach is fully compatible with the knowledge on soil structure at different scales: (i) the quantified pore systems are the same as those defined at micro-scale in micromorphology. (ii) the soil is characterized at clod scale as it is with visual assessment methods and (iii) accounting for the plasma constituents and their properties is at the basis of soil classification and mapping. The determined properties can be used at horizon and profile scale (e.g. for preferential flow mapping, Coppola et al., 2012) and spatialized at larger scale with plasma constituents content. The determined relations between soil structural properties and plasma constituents can be considered as pedotransfer functions, but they are neither empirical nor limited to the calibration area but to soil order only. We think this represents an opportunity to bridge soil science and soil physics, for a wide range of applications requiring spatial variability control.

Ball, B.C., T. Batey, and L.J. Munkholm. 2007. Field assessment of soil structural quality – a development of the Peerlkamp test. *Soil Use and Management* 23(4): 329–337.

Coppola, A., H.H. Gerke, A. Comegna, A. Basile, and V. Comegna. 2012. Dual-permeability model for flow in shrinking soil with dominant horizontal deformation. *Water Resources Research* 48.

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## **Application of X-ray microTomography to the visualization of bacterial biofilms in porous media.**

**Martins J.M.F.<sup>1\*</sup>, S. Rolland du Roscoat<sup>2</sup>, P. Séchet<sup>3</sup>, F. Pignon<sup>4</sup>, S. Mbaye<sup>3</sup>, C. Geindreau<sup>2</sup>, Z. Huang<sup>3</sup>, E. Vince<sup>1</sup> and A. Cartelier<sup>2</sup>**

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The study of biofilms in porous media spans a range of environmental applications going from subsurface ecosystems to industrial bioreactors. The development of bacterial biofilms in porous media is driven by complex processes that involve fluid flow, nutrient transport, microbial ecology and/or biotransformation. In practice, in order to describe the biological behaviour of a bioreactor that usually ends up with porous media clogging, it is almost impossible to account for all these biophysical processes at the pore scale, and continuum macroscopic modelling approaches are usually preferred although not satisfactorily from a pure mechanistic point of view.

The development of reliable models to accurately predict biofilm growth in porous media relies on a good knowledge of the temporal evolution of biofilms structure within the porous network. Since little is known on the true 3D structure of biofilms in porous media, this work aimed at developing a new experimental protocol to visualize the 3D microstructure of bacterial biofilms in order to improve the description of the main biophysical mechanisms occurring at the pore scale. For this purpose, small glass columns reactors have been developed, in which biofilms of *Pseudomonas putida* were grown under varying controlled conditions and observed by 3D X-ray microtomography. The main originality of the proposed procedure lies on the combination of the more recent advances in synchrotron microtomography (Paganin mode) and of a new contrast agent (1-chloronaphtalene) that has never been applied to biofilm visualization. It is shown that the proposed methodology takes advantage of the contrasting properties of 1-chloronaphtalene to prevent some limitations observed with more classical contrast agents such as barium sulfate. A quantitative analysis of the microstructural properties (volume fractions and specific surface area) of bacterial biofilms developed in columns of clay beads is also proposed on the basis of the obtained highly resolved 3D images.

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## **X-ray CT Characterisation Of The Retention And Relative Permeability Curves Of A Sandy Soil.**

**Fujiki<sup>1</sup> Y., Oxarango<sup>2\*</sup> L., Mukunoki<sup>1</sup> T.**

<sup>1</sup>X-earth center, Kumamoto University, Japan

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### **Abstract**

The objective of this study was to characterize the behavior of the unsaturated flow in sandy soil (*i.e.* Toyoura sand). The hanging column water retention curve test was performed using a specific centimetric cell. At each suction step, the sample is analysed using an micro focused X-ray Computed Tomography ( $\mu$ X-ray CT) scanner. The CT image is segmented in order to separate the 3 phases: solid, liquid and gas (figure 1). A methodology based on stochastic sub-sampling is used to select the minimum Representative Elementary Volume (REV) of a CT image sample to ensure the representativity of numerical analysis. From the experimental results and their CT image analysis, the distribution of water is analysed with respect to the pore diameter and its distribution in 3 dimensions. In a second part, the water flow is simulated using the Lattice Boltzmann Method (LBM) in order to estimate the relative permeability for each water content. A strong assumption is used considering that the water flow only occurs in pores filled by water, The obtained results present a satisfactory agreement with the classical Mualem model of relative permeability curve.

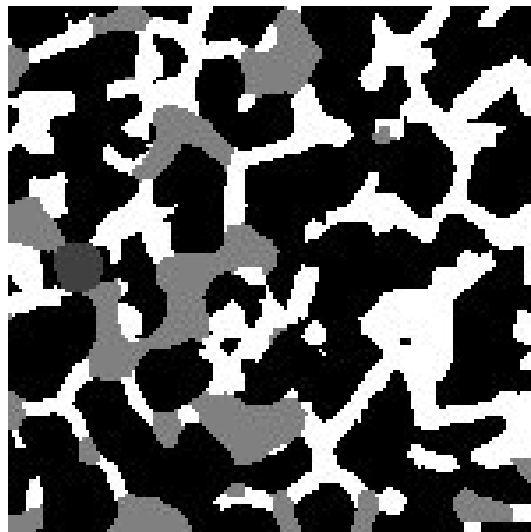


Figure 1 : Example of 3 phase segmentation

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## **2,4-D Mobility in Two Clay Soils: Impact of Macrofauna Abundance Observed by CT-scan.**

**Prado B<sup>1</sup>, Gastelum A<sup>2</sup>, Huerta E<sup>3</sup>, Duwig C<sup>4</sup>, Delmas P<sup>5</sup>, Márquez J<sup>2</sup>**

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### **Abstract**

The pesticide 2,4-D is one of the most widely used herbicides in the world, it belongs to the group of synthetic herbicides that control broadleaf weeds. In this paper the risk of groundwater contamination by 2,4-D and its major metabolite, 2,4-DCP, is studied in a context of high density of soil worms. We compared the adsorption, desorption, degradation and displacement of 2,4-D in soils from Tabasco Region having different properties: clay, organic matter, iron and aluminium oxides contents. In addition to the classical soil physicochemical characterizations, a 3D analysis of the soil structure and porosity was performed by analyzing images acquired by Computed Tomography. The objective was to evaluate the effect of soil properties and macroporosity produced by the macrofauna activity on solute movement.

All the soils studied sorbed the herbicide, the distribution coefficients were linear and varied between 1 and 4. The contents of iron and aluminum have an important role in the adsorption of the herbicide. In aerobic conditions, the herbicides half-life was about two days. Water movement occurred in physical equilibrium in three of the four soils. After 20 to 60 days depending on the soil, no 2,4-D leaching was observed through the soil columns, except for one soil where there was preferential flow. Earthworm burrows were exhibited and quantified in the soils samples through the analysis of Computer Tomography (CT) images, they appeared as small, snail-shaped, rounded volume of 3 to 7 mm radius with a higher density with respect to the surrounding soil. They were extracted from the original data using a combination of image processing and mathematical morphology operators. Based on the results obtained, it can be concluded that preferential flow caused by both high clay content and the presence of macrofauna pores significantly reduces the buffering capacity of the soil, increasing the risk of contamination by herbicides of the underlying aquifer.

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## From Soil Characterization With Typosoil® To Bio-Technosoil Building: The Valorhiz Approach Of Soils Functions.

Boukcim H<sup>1</sup>, Braudeau E<sup>2</sup>, Hedri E<sup>1</sup>, Taugourdeau O<sup>1\*</sup>

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\*: presenter

Soils are the origin of our alimentation. Better understanding the interactions between soil structure and functions is a key for sustainable agriculture and living soils management. Improving our understanding of soils is critical to build or restore soils with optimized functions (food production, water infiltration, contamination control, carbon sequestration etc.).

In this context, Valorhiz, in collaboration with IRD, has developed an innovative device for soil water functioning measurements: TypoSoil® (<http://www.typosoil.com>).

All along the drying process, TypoSoil® measures soil sample sizes (height and diameter), weight and suction. These measurements are taken, under controlled conditions, with high precision tools (spot lasers, tensiometers and precision scales) on eight soil samples per run; thanks to a rotating board, each sample is measured every 11 min.

Typosoil® allows measuring simultaneously the soil shrinkage curve and the water retention curve of soil samples (Fig. 1). These curves describe the interactions between substrate, water and air and can be used as inputs for modeling soil functioning. For instance, Typosoil® data can be used to calibrate a water retention model, a key input of the Richard's equation used to model water transport within multilayered rigid soils (e.g. Hydrus: Šimůnek *et al.* 2012).

Moreover, the water retention curve and the soil shrinkage curve provided by Typosoil® are used for the calibration of soil hydrostructural models with a thermodynamic perspective such as Kamel® (Braudeau *et al.* 2014a; Assi *et al.* 2014). Interestingly, this approach allows extrapolating soil water retention curve given by Typosoil® beyond tensiometers limits (Braudeau *et al.* 2014b): the model used the complete data (soil shrinkage curve) to infer the incomplete one (water retention curve).

Using the curves provided by Typosoil® allows taking into account, in a systemic way, soil functioning in agro-environmental engineering in different ways, especially in the current context of global changes:

- optimizing bio-technosoils (i.e. neoformed soil performed with technical raw materials inoculated with specific micro-organisms) for agricultural uses, land reclamation, water infiltration in urban context;
- improving the irrigation in cultivated soils in a perspective of sustainable agriculture;
- managing pollutant pathway trough soil layers.

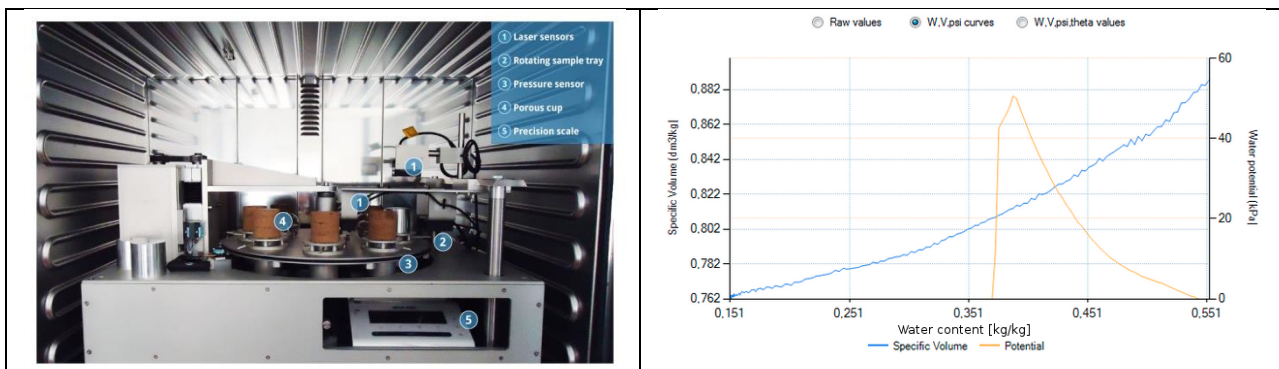


Figure 1. Typosoil® device setup (left) and measured data (right): soil shrinkage curve in blue and water retention curve in yellow (<http://www.typosoil.com> for details).

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**Mechanisms of lateral extension of gully banks with heterogeneous behaviour of horizons submitted to shrinkage and swelling in a subhumid grassland of South Africa.**

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The formation of deep gullies in KwaZulu-Natal province in South Africa rangeland is a natural phenomenon. In order to understand the strong lateral expansion of the gullies due to the collapse of their side-walls, this study is based on the continuous measurement of the shrinkage curve of the different horizons.

Reconstituted cylindrical samples of approximately 100cm<sup>3</sup> of different horizons were prepared and moistened to follow their shrinkage by a laser retractometer during their drying in an oven at 30°C. The retractometer measures with great precision simultaneously the height, the diameter and the weight of the samples each 10 minutes during a few days, in order to obtain the curve of volumic shrinkage related with the water loss. A model, based on physical parameters characterizing the hydro-structural behavior of soil, was applied to fit the experimental shrinkage curves, with the aim to extract the characteristic parameters, such as the shrinkage slope, the air inlet point and the content of different types of water

The soils in which the dongas have developed are duplex soils such as Luvisols formed on mudstone or unconsolidated colluvium. The A horizon was a sandy loam with only illite in the clay fraction and a high structural stability, which decreased rapidly towards its base. The shrinkage of this horizon was very regular and limited. It overlaid with a sharp contact a Bt loamy clay horizon with illite as the sole clay mineral, a high structural stability and a strong shrinkage potential of the macrostructure only. At the base of the profile, the colluvial C horizon also contained interstratified illite-smectite swelling clay with very low structural stability, and presented a saturation curve at low water-contents and a residual shrinkage.

It was concluded that the different soil horizons present clear and sharp differences in physical properties and heterogeneous shrink-swell properties, which are the major cause of sidewall instability. Therefore it can be assumed that the retreat of the donga sidewalls is generated by the collapse of different horizons by anisotropic shrink-swell processes and is not associated with heavy rainfall events.



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## **Pore Network Structure Linked by Micro Focus X-ray CT to Particle Characteristics and Mass Transport Parameters.**

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### **Abstract:**

Mass transport in soils occurs through the soil-pore network, which is highly affected by the physical properties of soil particles (i.e., particle size and shape). However, there have been few studies on the relation among the particle size and shape, soil pore network, and mass transport parameters such as a hydraulic conductivity. In this study, using sands with different size fractions and particle shapes, the pore structure (i.e., pore size distribution, pore tortuosity) was analyzed by micro focus X-ray CT images. Mass transport parameters including gas diffusion coefficient and air permeability at variably saturated conditions were measured on the same repacked columns using standard methods, and literature data on saturated hydraulic conductivity for the same materials were analyzed. Comparison between X-ray CT derived pore network structure and physical parameters showed that the round sands and glass beads exhibited larger pores, higher pore coordination number, and lower volumetric surface area as compared to the angular sands at the same particle size. The X-ray CT derived mean pore diameter and pore coordination number for each material correlated well with key gas transport properties such as percolation thresholds and pore network connectivity. A predictive gas diffusivity model from wet to dry conditions based fully on X-ray CT derived parameters was developed and showed a good agreement with measured data for both round and angular sands.

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### **Pore scale processes governing biofilms location and development in a dual porous media: effect on CCA mobility.**

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Research has sustained a tremendous interest on soil about coupling the spatial heterogeneity of soil structure and microbiological functions, especially when it comes to the understanding of *in situ* processes. Due to technical limitations, spatialization of processes in soil porosity remains complicated. Until recent works, experimentations approach soil microbial activity through indirect lab testing, by controlling soil parameters at mesocosm scale (cm<sup>3</sup> to m<sup>3</sup>). It still remains difficult to use direct and non-destructive methods to switch from macro down to micro-scale, *i.e.* from a monitoring of the community activity to individual scale processes in soil.

Indeed this knowledge and technical gaps about soil microbial habitat localization depend on the heterogeneity and characteristic of soil material (numerous phases, composition and complex interfaces). Some non-invasive technics such as X-ray microtomography (X-ray  $\mu$ CT) are more and more used for soil characterization even if the observation of biofilms requires more complex image processing such as phase contrast observations.

Here, the aim is to understand if there are preferential microbial habitats inside soil porosity. The influence of both water and nutrient availability on the development and function of bacterial biofilms is studied. The next experimental devices to set up here are based on two different scales:

- Using mini columns filled of quartz particles with a bimodal distribution thus enabling the set-up to simulate a simplified dual porous media. Unsaturated conditions would allow activation of a specific range of pore according to their size, and subsequently specific processes. The column would be analyzed by X-ray  $\mu$ CT for location of biofilm;
- Using microfluidic devices with a microscopic kinetic monitoring of biofilm activity in a dual porous media.

Bacteria of interest will be chosen regarding direct redox activities for Chromated Copper Arsenate (CCA) which induce soil pollution after wood treatment. Result of microfluidic devices would allow to identify and target bacteria on the column experiment.

Key word: porosity, biofilm, microfluidic device, X-ray  $\mu$ CT, CCA.

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## **Soil and Image Texture - What's Common? Challenges of Image Modelling and Analysis.**

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Image texture, or visual appearance of soil samples in 3D CT scans has almost nothing in common with soil texture. Specified by relative contents of sand, silt, and clay, the soil texture only implicitly and rather weakly affects spatial distributions of X-ray attenuations of all soil components. Due to limited spatial resolution of CT scanners, the images depict individual sand grains on a continuous silt-clay background, together with visible pores and possible non-organic (e.g., mineral) and organic (e.g., roots) matters of different density. Soil image analysis has to relate functional soil characteristics to measurable visual appearance in terms of 3D morphology, e.g., sizes, shapes, and spatial distributions of distinct soil components.

Building useful probabilistic models of visual appearance and shape of these components is hindered by the absence of reliable databases of CT images of soil samples. The databases are expected to collect samples from different places over the world and have, at least, in part, comprehensive "ground-truth" maps of the components and other descriptions, provided by soil experts. The maps and descriptions facilitate accurate image modelling towards establishing quantitative relations between soil visual appearance and quality (functioning).

Even simple thresholding of voxel-wise signals, which is widely used at present to separate soil components in an image, is too inaccurate without reliable training data. The thresholds are derived from an empirical marginal probability distribution of densities, which is often unimodal. Thus, it cannot be partition accurately without prior learning its components, because the handpicked models produce different segmentation maps that can be evaluated only by soil experts. The databases also facilitate analysing soil samples with more advanced texture modelling, classification, and segmentation techniques involving, e.g., Markov random field and marked point process models of images.

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## **A Further Step in Visualizing and Understanding Preferential Flow in Undisturbed Soil Cores: Identifying the Functional Macropore Network.**

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Water flow in soils does not occur uniformly but is localized in some preferential paths. This phenomenon, which is known to be more a rule than an exception in most soils, controls mass transfer processes in the vadose zone such as water flow and solute transport. Thus, identifying the preferential flow paths and the functional part of the soil structure which is associated is still of major importance to take into account this phenomenon in models. Indeed, understanding of water flow processes in macropores and estimating the real surface accessible for mass exchanges with the soil matrix are still opened questions nowadays. Therefore, we recently proposed a new method to identify the functional part of a soil structure. This approach was based on the acquisition of time-resolved image sequence with a X-ray CT to visualize water flow in undisturbed structures of soil cores. The fast tomographic acquisitions were realized during simulated rainfall events in a medical scanner. The Brilliant Blue dye was added to the infiltrating water to simultaneously stain the preferential paths. The water voxels acquired during the experiment were converted in a data which reflected their frequency of detection in the structure during the rain, named the local detection frequency. We showed that 1) the part of the structure where water voxels were mostly detected during the simulated rainfall was almost identical to the active structure stained by the dye and 2) water flows through the largely opened, interconnected and continuous macropores that were easily detected despite the rough spatial resolution of the scanner. Consequently, the geometrical properties of the entire and functional structures strongly differ and the latter would be more relevant to be used in mass transfer models.

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## **How And Where Is The Link Between The Soil Behaviour And Its Internal Architecture?**

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Due to its central role in many agricultural and environmental processes, a good understanding of the soil behaviour is required (water, air and heat transfers). However, it is still vague how to consider the pore space structure as a variable in the prediction of the soil's physical functionalities, in other words, how to weigh up the microscopic scale, where the pore is the main constituent, to the macroscopic soil behaviour, namely at the core scale. Nowadays, there is an attempt to analyse the soil hydraulic conductivity and soil air permeability from the soil pore architecture. This is being done by statistical comparisons of measurements or by pore scale modelling with a main focus on preferential flows. To our knowledge few studies have compared the micro-and macroscopic soil's characteristics and even less have compared these features for the same soil core sample. Therefore, the objective of our study is to explore the relationship between macroscopic physical properties and microscopic pore network structure. Saturated hydraulic conductivity, air permeability, retention curve and others classical physical parameters are measured in laboratory. The pore network is quantified with the non-invasive x-ray microtomographic technique (micro-CT system Skyscan-1172). Several parameters at different levels (pore, pore network and sample) are calculated. For instance, the pore volume and orientation, the network connectivity, tortuosity and anisotropy are measured. Within the scope of this study, disturbed and undisturbed samples will be tested at different water content. We expect to find good correlation between parameters that express the large porosity and the hydraulic conductivity at saturation. We also count on explaining variations in retention curve between similar soil sample by their variations in pore orientation, size, tortuosity and connectivity. Eventually, we expect to find an exponential or log-log linear relationship between air permeability and hydraulic conductivity measurements, relationship which will be correlated to pore parameters that express size and connectivity.

Sarah Smet, as a research fellow, acknowledges the support of the National Fund for Scientific Research (Brussels, Belgium).

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## **2/3D Image Processing in the context of Environmental Sciences.**

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After a brief introduction of the Intelligent Vision Systems Lab (IVSLab) current research, I will give an outline of the research outputs in Image Processing and Imaging for Environment Sciences applications in the context of the research collaboration between the LTHE, Plant and Food Research Ltd, The Collegio de Postgrados and la UNAM since 2003. I will encompass results in fluorescent, optical, microscope and CT-scan imaging. I will conclude with a glimpse on the current IVSLab research progress in 2/3D image Processing for Environmental Sciences applications at large.

## Direct visualization and quantification of the biological activity impact on the dynamics of technosol structure.

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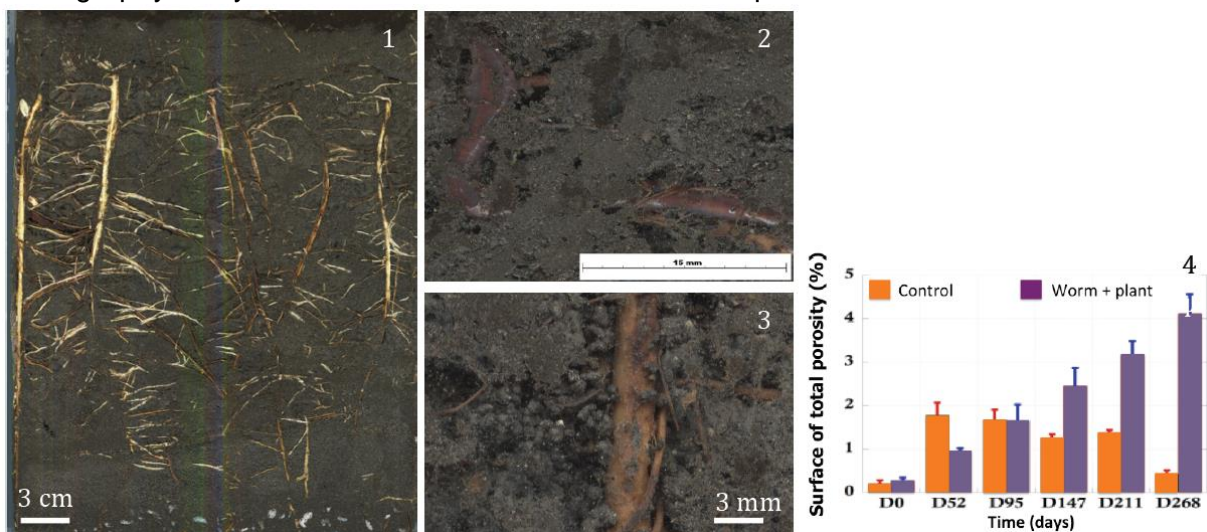
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Evaluate the dynamics of soil structure, particularly under the influence of biological factors is a major challenge in an objective of their pedogenesis modeling. By using an innovative device of automatic acquisition of high-resolution images, SOILINSIGHT<sup>®</sup>, we specified in rhizotrons during 14 months the porosity and aggregation dynamics of a constructed Technosol within the rhizosphere of a leguminous plant (*Lupinus albus*) in presence of earthworms (*Lumbricus castaneus*). The constructed Technosol is, by definition, considered as a good candidate for the pedogenesis modeling, insofar as its initial characteristics and implementation conditions are controlled (Séré *et al.*, 2010).

A video can show the dynamics of biological agents: root system architecture from germination to senescence of plants, formation of symbiotic nodules, movements of earthworms within rhizotron. Specific image processings were used to quantify total porosity (50µm-2mm), total area of aggregates (100µm-2mm) and various descriptive parameters of pores or aggregates: number, size, diameter, form index (Janquorzo *et al.*, 2013). "Actions" of worms - digging or filling burrows, crossing - were recorded over time. After 14 months, the pore surface is 10 times higher in rhizotrons with plant and macrofauna in comparison with the controls. If the biological activity promoted the genesis of aggregates, their dynamics was irregular in that the proportion of aggregates increased or decreased depending on the actions of worms.

The used device of non-destructive observation of soil profiles is an innovative way of monitoring and quantifying the impact of pedogenetic factors on the functioning and evolution of soils. Currently we attempt to link these results with data obtained through tomography analysis of the cosmes at the end of the experimentation.



(1) View of the rhizosphere at the rhizotron surface. (2) Detail of worm/soil interface (3) Detail of the root/soil interface (4) Quantification of total porosity

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## **Using X-ray computed tomography to describe the dynamics of nitrous oxide emissions in soil.**

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Soils are a major source of nitrous oxide (N<sub>2</sub>O), a gas involved in stratospheric ozone depletion and global warming. Soil water saturation, partly controlled by soil structure, is a key factor for controlling N<sub>2</sub>O emissions. We thus hypothesized that soil structure partly controls N<sub>2</sub>O dynamics in soils.

We proposed a method to image the soil water and structure with X-ray computed tomography, while controlling the hydric state (with a multistep outflow system) and monitoring N<sub>2</sub>O fluxes. An undisturbed soil sample (13 cm inner diameter, 7 cm height) was saturated for three days, and then submitted to a -100 hPa pressure at its bottom. This wetting-drying cycle was applied two times (C1 and C2 cycles). N<sub>2</sub>O fluxes were measured using the closed-chamber technique. The soil core was scanned with X-ray computed tomography (resolution 300 μm), once during wetting and several times during drying (7 for C1, 9 for C2).

Image processing was done with the ImageJ software and the C library QuantIm. Air and water phases were separated from the soil matrix and gravels using the watershed segmentation method. Quantitative and qualitative indicators of the pore network were calculated: volume of air and water-filled macropores, relative gas diffusion coefficients and Euler number (characterizing the pore space connectivity).

Fluxes increased quickly after the beginning of the drying phase to reach a peak after 5 h (55 and 19 mg N m<sup>-2</sup> d<sup>-1</sup> for C1 and C2). Maximum N<sub>2</sub>O fluxes were reached at approximately -45 cm water column, when pores with radius >66 μm were drained. Differences in the N<sub>2</sub>O emissions intensity between the two cycles were attributed to differences in the water saturation, air-phase connectivity, and relative gas diffusion coefficient, which led to more or less N<sub>2</sub>O production, consumption, and entrapment in soil. The speed of the N<sub>2</sub>O emissions at the beginning of the drying phase depended on the rate of increase of the air-filled pore volume and connectivity, and was especially well described by the relative gas diffusion coefficient. This study highlighted the need to find and measure dynamic indicators of soil structure to enhance our understanding of the N<sub>2</sub>O emissions dynamics in soils.

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**Perspectives for pore-scale flow modelling with Lattice-Boltzmann method:  
multiphase behaviour and couplings.**

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Soil functions such as entrapment capacity of the soil, flow behaviour, reactive transport require a better understanding of pore-scale multiphase and/or multiphysic behaviour. Developments of pore-scale experiments from micromodels to CT observations allow a better understanding of such processes. Meanwhile, pore-scale numerical models such as Lattice Boltzmann models are being developed and take advantage of the improvement of computing capacities. Comparisons between numerical simulations and experiments for pore scale properties as well as dynamic effects are of importance to enhance the description of multiphase flow processes. Moreover, Lattice-Boltzmann methods coupled with other pore-scale methods are more and more used for modelling complex behaviour such as reactive transport.

A discussion on the validation of the pseudopotential Lattice-Boltzmann model for multiphase multicomposant flow using drainage experiment on a quasi-2D pore network micromodel. The results show good agreements for the characterisation of preferential pathways due to porosity variation and entrapment even though the scaling from lattice units to physical units remains questionable.

Moreover, an insight of modelling reactive transport at the pore scale using Lattice Boltzmann with immersed boundaries is given with promising results for the representation of biodegradation of LNAPL pollution.

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## **From CT-scan imaging to SPH modelling: application to Environmental Sciences.**

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### **Abstract**

In this work the pore form study and numerical flow simulation software SMAS is presented. SMAS was implemented in the CUDA architecture in order to improve the computational time per study.

The study of the pores forming a soil core using computational models can be done using soil volumes obtained from X-ray microtomography. The volume slices are process with a multidimensional filter in order to reduce the noise and the voxels belonging to pores are segmented using a k-means classification approach.

The segmented pore voxels are label using a 26 connectivity approach, each connected pore is label and the soil core porosity obtained.

The morphological properties for each pore are obtained. The software consist on fifty different two-dimensional and three-dimensional measurements. The pores are classified using the linear dimensional reduction method principal component analysis and a fuzzy c means clustering implementation.

The numerical flow simulation is obtained using a parallel implementation of the smoothed particle hydrodynamics method, the lineal correlation of the morphological properties and the numerical solution is obtained in order to evaluate which form properties have a higher relation to the simulated flow in the pore.

The obtained results are used to classified soil core samples and the morphological properties that are more correlated to the flow.

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## **What Are The Impacts Of Transient Flows On Colloid Mobilization And Retention In Macroporous Soils ?**

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Colloidal particle naturally occurring in the soil can act as vectors of adsorbed pollutants from the soil surface to the groundwater. Although much effort has been devoted to understand and model the mobilization and retention mechanisms of colloids in soils, most of the studies have focused on single rains or irrigation events, while in field conditions soils undergo successions of rain and drying cycles.

We performed long series of successive irrigations on undisturbed macroporous soil columns, and monitored the concentration, in the column effluents of (i) natural soil colloids (SC) mobilized inside the soil and (ii) labeled colloids (LC) brought with the irrigation water. All irrigation events were in every respect identical (duration, intensity, water chemistry) but were separated by irrigation Interruption Durations (ID) of increasing length.

We found that the amount of leached SC and LC was much affected by the irrigation interruption duration. As the ID before the irrigations increased, the amount of leached SC increased, reached a maximum value and decreased. Maximum SC leaching occurred for IDs of about 250 hours and was up to an order of magnitude higher than leaching recorded at the shortest and longest IDs. Interestingly, the fraction of LC recovered at the column outlet also increased with ID, but leveled out for IDs greater than about 250 hours.

We showed that SC and LC leaching variations are (indirectly) linked to water content variations in the active macropores and proposed a mechanistic model to account for the SC leaching variations. It is based on the hypothesis that non-uniform water loss from the macropore walls during an irrigation interruption induces differential capillary stresses that weaken the structure of the walls and promotes colloid mobilization during the passage of a new infiltration front. The model reproduces well the experimental results and has been validated with data obtained in different experimental conditions. Finally, we discuss how the model can also reproduce the observed variations of LC retention.

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**Pore-network modeling of microbially-induced calcium carbonate precipitation: insights into scale-dependent reaction rates and permeability-porosity relationship.**

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**Abstract**

Over the past few years, ureolysis-driven biofilm-induced calcium carbonate precipitation, as a novel geotechnique, has received much attention. It is promising to be used in a number of engineering applications, such as carbon dioxide sequestration, groundwater remediation, and soil stabilization. A primary research focus has been controlling the temporal and spatial precipitation by manipulating parameters that influence the saturation state to achieve specific engineering goals [1]. Besides laboratory- and field-scale experiments [2, 3], the numerical modeling also plays an important role in improving our understanding and prediction of the precipitation process. With the ultimate goal of developing a predictive field-scale model, a few scale-dependent parameters and material coefficients need to be obtained with the help of the upscaling technique, which has a long history in porous media research. These parameters and material coefficients, for instance, include ureolysis rate, calcium carbonate precipitation rate, permeability porosity relationship, and biofilm growth rate. To this aim, the pore-scale modeling is needed. Basically, there exist two levels of pore-scale models, namely, direct simulations and pore-network models (PNMs). In direct simulations, the pore space is discretized by many computational grids, on which physics-based governing equations for biofilm growth, solute transport, and calcium carbonate precipitation are solved. Its merit is that most model parameters are directly measurable. This helps us understand fundamental bio-geo-chemophysical processes. However, up to now, its computational effort is still very expensive and even prohibitive to a REV (representative elementary volume)-scale study. Alternatively, the pore-network modeling can serve as the bridge between the direct simulation of a few pore spaces and the field-scale modeling. The basic idea of a pore-network model is as follows [4]. First, the porous medium of interest is characterized by a proper pore network. Pore bodies of proper shapes are used to represent large pore spaces, while pore throats are used to represent narrow regions which connect neighbouring pore bodies. Then, pore-element-based thermodynamic properties like pressure and species concentrations, in common, are defined. Their flow and transport are solved by rule-based governing equations (note that at this stage, some local rules should be obtained by pore-element-scale direct simulations [5]). Finally, REV-scale parameters and material coefficients are computed in the postprocessing which will be provided to a field-scale model.

In this talk, we will present a developed framework for pore-network modeling of microbially-induced calcium carbonate precipitation. First, we build a stochastic model for the

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unstructured pore network generation. A generated network can be calibrated against a soil sample in terms of pore size distribution and coordinate number, etc. (see Fig. 1). Then, pore-scale governing equations for biofilm growth, calcium carbonate precipitation and dissolution, and reactive species transport are rigorously formulated. Meanwhile, the temporal evolution of pore structure is taken into account because of the biofilm growth and calcite precipitation. The speciation of geochemical components is computed by an open geochemistry module PHREEQC, which is coupled with the flow and transport in the pore network. Finally, the methodology of upscaling scale-dependent reaction rates and permeability-porosity relationship is developed.

As a demonstration of the developed pore-network model, we will present two case studies (high and low flow rates) of the inject strategy employed in the calcium carbonate precipitation. Here, the inject strategy includes three stages. The first stage is to stimulate the biofilm growth for 15 hours. In the second stage, two pore-volume calcium-rich medium is injected to create high saturate state in the domain. In the third stage of precipitation, the injection system is closed for 4 hours. Fig. 2 shows the biofilm distribution along the network in stage 1. Fig. 3 shows the biofilm and calcite distributions along the network at the end of stage 3. With these case studies, we will discuss about the influence of various operating and physical parameters on controlling the calcite precipitation distribution. Also, we will provide insights into scale-dependent reaction rates and permeability-porosity relationship.

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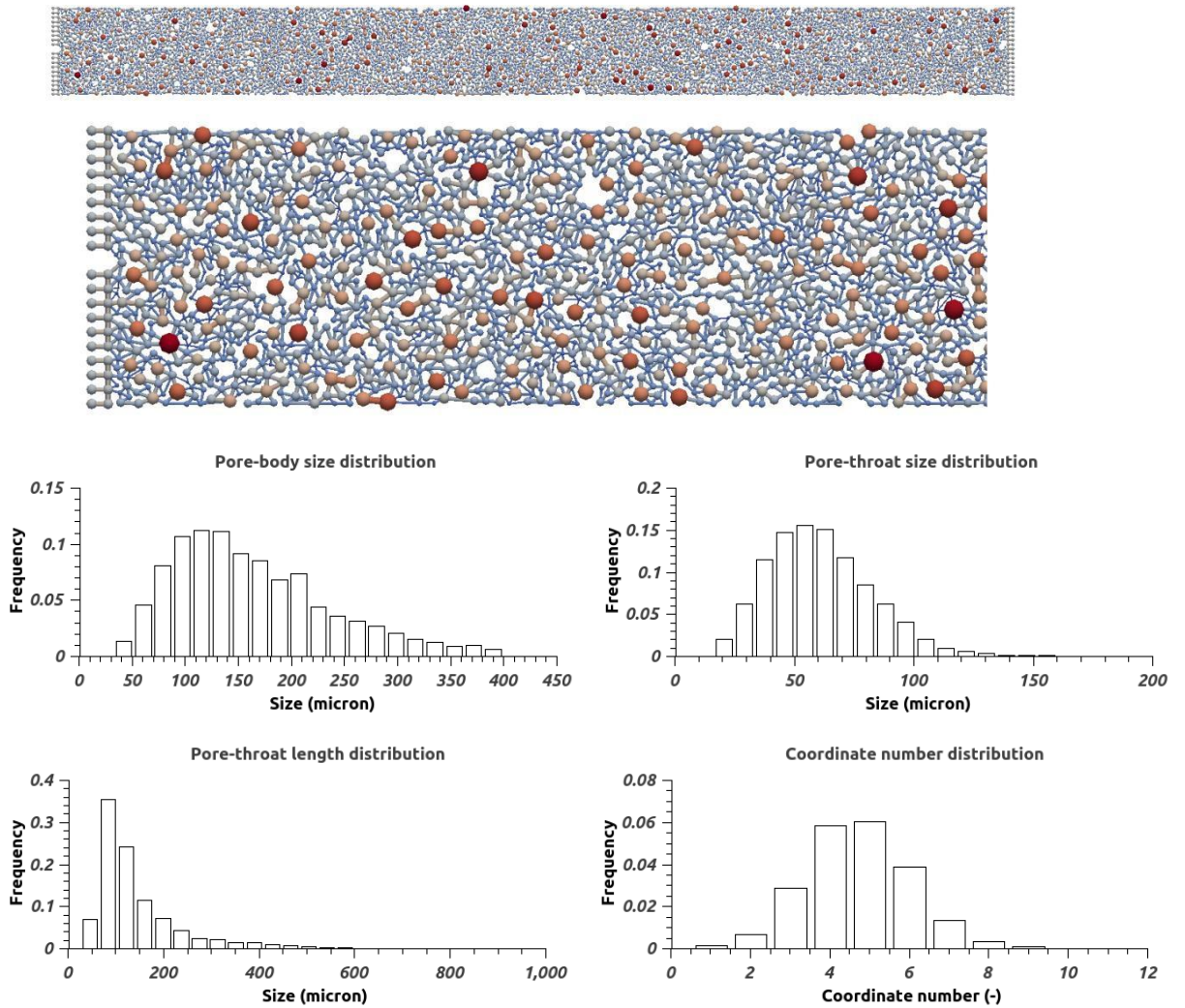


Figure 1: the generated pore network of a general soil sample, and its pore structure information.

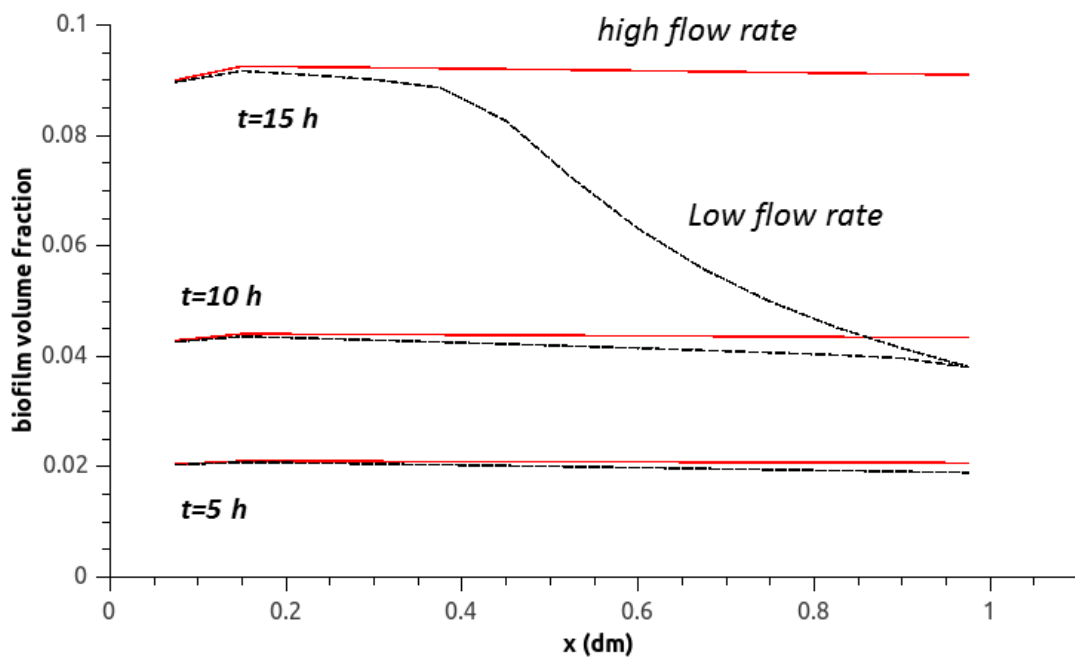


Figure 2: biofilm growth in the stage 1.

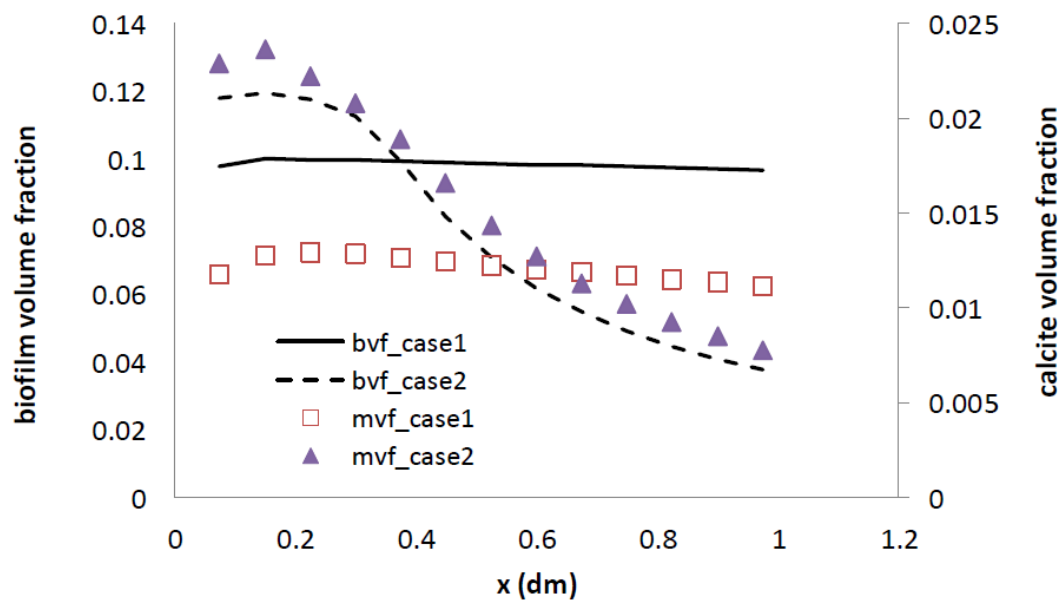


Figure 3: biofilm growth and calcite precipitation in the stage 3.