# DRUG TRANSPORT IN URBAN SOIL THROUGH THE SEASONS IN A COMBINATION OF X-RAY COMPUTED TOMOGRAPHY AND CHEMICAL ANALYSES: PRELIMINARY RESULTS

Victory A. J. JAQUES<sup>a,\*,\*\*</sup>, Petra ZÁVODSKÁ<sup>b,\*\*</sup>, Martina KLUČÁKOVÁ<sup>b</sup>, Miloslav PEKAŘ <sup>b</sup>, Tomáš ZIKMUND<sup>a</sup>, Jozef KAISER<sup>a</sup>

- <sup>a</sup> CEITEC Central European Institute of Technology, Brno University of Technology, Purkyňova 123, 61200 Brno, Czech Republic
- <sup>b</sup> Institute of Physical and Applied Chemistry, Faculty of Chemistry, Brno University of Technology, Purkynova 118, 612 00 Brno, Czech Republic
- \* Contact email: <u>victory.jaques@ceitec.vutbr.cz</u>
- \*\* Student

## **KEYWORDS**

Drug Transport; Seasonal changes; microCT; Chemistry; Urban soil; Diffusion

### ABSTRACT

We combined X-ray computed tomography with common chemical analyses to observe seasonal changes (Spring, Summer, Autumn) in natural urban grassland soil and the impact on drug transport.

Soil is an essential material for life on earth due to its numerous functions. Its modification has important long term economic, environmental, and ecological impacts [1]. Drug diffusion and permeability of soil impact its functions through its contamination rate and spread, which changes its usability.

Soil is heavily structured by its organic content (fauna, flora) [2], which creates voids and networks. Also, soil disaggregation and solubility impact the movement of drug molecules [3,4].

Most studies focus on croplands or natural soil [5], on transport studies realized under artificial laboratory conditions or on computer solute transport modelling [6,7]. We think that a study on natural soil is important to assess the reality in a more comprehensive way.

For this work, the top layer (10 cm) from an urban soil was sampled, which is directly impacted by the climate and its direct environment. It is also the entrance point of the drugs (Fig. 1).

The soil just sampled was scanned with a microCT system directly in its sampling device and then its humidity and chemistry (thermogravimetry, FTIR, elemental analysis) were analysed as well as its diffusion coefficient with chosen drug molecules (sulfapyridine, sulfamethoxazole).

The scanned soil was segmented into organic matter, pores (open/closed) and the matrix with VG Studio (Fig. 1A). The segmentation between organic matter and pores was challenging as they have low contrast.

We ran molecular diffusion and permeability simulation (Fig. 1B) based on the chemical parameters and results measured on the same soil sample and then compared the CT analyses to the chemical ones.



**Figure 1** Spring soil core **(A)** 3D volume segmented in an organic matrix (light green), pores (dark green) and matrix (brown-yellow). **(C)** 3D representation of the permeability paths with the liquid pressure from the soil surface (purple grid) to the core bottom (yellow grid; 10 cm depth)

### REFERENCES

[1] R. Lal, "Soil carbon sequestration impacts on global climate change and food security.," Science, vol. 304, no. 5677, pp. 1623–1627, Jun. 2004, doi: 10.1126/science.1097396.

[2] S. De Gryze, L. Jassogne, J. Six, H. Bossuyt, M. Wevers, and R. Merckx, "Pore structure changes during decomposition of fresh residue: X-ray tomography analyses," Geoderma, vol. 134, no. 1–2, pp. 82–96, Sep. 2006, doi: 10.1016/j.geoderma.2005.09.002.

[3] L. Luo, H. Lin, and S. Li, "Quantification of 3-D soil macropore networks in different soil types and land uses using computed tomography," J Hydrol (Amst), vol. 393, no. 1–2, pp. 53–64, Oct. 2010, doi: 10.1016/j.jhydrol.2010.03.031.

[4] L. Luo, H. Lin, and J. Schmidt, "Quantitative Relationships between Soil Macropore Characteristics and Preferential Flow and Transport," Soil Sci. Soc. Am. J., vol. 74, no. 6, pp. 1929–1937, Nov. 2010, doi: 10.2136/sssaj2010.0062.

[5] C. E. Carducci, Y. L. Zinn, D. F. Rossoni, R. J. Heck, and G. C. Oliveira, "Visual analysis and X-ray computed tomography for assessing the spatial variability of soil structure in a cultivated Oxisol," Soil and Tillage Research, vol. 173, pp. 15–23, Nov. 2017, doi: 10.1016/j.still.2016.03.006.

[6] Y. Mehmani and H. A. Tchelepi, "Minimum requirements for predictive pore-network modeling of solute transport in micromodels," Adv. Water Resour., vol. 108, pp. 83–98, Oct. 2017, doi: 10.1016/j.advwatres.2017.07.014.

[7] C.-Z. Qin, S. M. Hassanizadeh, and A. Ebigbo, "Pore-scale network modeling of microbially induced calcium carbonate precipitation: Insight into scale dependence of biogeochemical reaction rates," Water Resour. Res., vol. 52, no. 11, pp. 8794–8810, Nov. 2016, doi: 10.1002/2016WR019128.

- Abstracts should be submitted as a Word Document NOT a PDF
- Abstracts should be a maximum of 300 words
- Please include a full title, all authors and affiliations
- Include keywords
- Images/diagrams are acceptable
- Indicate if you are a student
- Presenting authors are required to register, pay and attend the symposium
- Please indicate from the list below which session you feel is most appropriate

#### SUGGESTED SESSION

- Correlative Tomography and Complimentary Techniques
- Materials Science
- Culture Heritage
- Life Sciences
- Manufacturing and Industry
- Outreach and Public Engagement
- New X-ray Technologies and Future Advances
- Data
- Quantification