Contribution ID: **620** Type: **Oral Presentation**

Assessing the fate of PFAS in subsurface from experimental studies and numerical simulations at soil-column scale

Monday, 22 May 2023 13:45 (15 minutes)

Per- and poly-fluoroalkyl substances (PFAS) are emerging contaminants of great importance, because of their spreading in subsurface, gradual bioaccumulation and toxicity. Assessing exposure risk, developing management strategies, and implementing remediation scenarios require an accurate understanding of the fate of PFAS in subsurface. In the present work, PFAS transport in saturated and unsaturated soil columns has been studied under varying initial concentration for two type of PFAS: perfluorooctanoic acid (PFOA) and perfluorodecanoic acid (PFDA). The PFAS surface tension and PFAS / n-dodecane (n-C12) interfacial tension were measured as functions of PFAS concentration and salinity with static (DuNouy ring) method, and fitted to Langmuir-Szyszkowski equation (Fig.1a,b). The capacity of PFAS solutions to emulsify non-aqueous phase liquids (NAPLs), commonly trapped in the saturated zone, was investigated by mixing PFAS solutions with n-C12 at various volume ratios with the aid of an ultrasound probe, inspecting their stability optically, and measuring transient changes of the shear viscosity. Moreover, the effects of PFAS on wetting properties were analysed by measuring the contact angles of PFAS drops surrounded by either air or n-C12 on glass surfaces (Fig.1c,d). A dried sandpack was evacuated and saturated with NaCl solution with free imbibition. Unsaturated and NAPL-polluted conditions were created by injecting air or NAPL at constant flow rate, reinjecting NaCl solution and monitoring the axial distribution of water saturation with a multiple-electrode resistivity meter [1]. PFAS flow tests were then conducted, and the concentration of PFAS was measured in aqueous samples collected at the outlet port with the methylene blue active substances (MBAS) method and UV-Vis spectrophotometry [2]. The spreading of PFAS in the soil column was simulated with a 3D field scale Computational Fluid Dynamic model which simulates the PFAS transport by solving the Navier Stokes equation inside infinite domain (field scale), where convection, dispersion and adsorption (on solid interfaces and air/water interfaces) terms were included. The simulations were developed on Comsol Multiphysics platform [3] and the numerically predicted PFAS concentration breakthrough curves under saturated and unsaturated conditions were compared with corresponding datasets of PFAS flow tests in soil column.

Acknowledgements
This work was performed under Grant Agreement 101037509 —SCENARIOS —H2020-LC-GD-2020 / H2020-LC-GD-2020-3 (project title: "Strategies for health protection, pollution Control and Elimination of Next generAtion RefractIve Organic chemicals from the Soil, vadose zone and water"- acronym "SCENARIOS") supported by the European Commission.

Participation

In-Person

References

REFERENCES
1. Aggelopoulos, C.A., and C.D. Tsakiroglou, "The effect of micro-heterogeneity and capillary number on capillary pressure and relative permeability curves of soils", Geoderma, 148, 25-34 (2008).
2. Sharma, R., Pyter, R., and P. Mukerjee, "Spectrophotometric Determination of PerfluoroCarboxylic Acids

(Heptanoic to Decanoic) and Sodium Perfluorooctanoate and Decyl Sulfate In Mixtures by Dye Extraction", Anal. Lett. 22(4), 999-1007 (1989).
3. COMSOL Multiphysics v.6.1 www.comsol.com COMSOL AB, Stockholm, Sweden (2022).

MDPI Energies Student Poster Award

Yes, I would like to submit this presentation into the student poster award.

Country

Greece

Acceptance of the Terms & Conditions

Click here to agree

Energy Transition Focused Abstracts

Primary authors: Mr MELITSIOTIS, Anastasios (Foundation for Research and Technology Hellas - Institute of Chemical Engineering Sciences (FORTH/ICE-HT)); Dr BALI, Nadia (Foundation for Research and Technology Hellas - Institute of Chemical Engineering Sciences (FORTH/ICE-HT)); Dr THEODOROPOULOU, Maria (Foundation for Research and Technology Hellas - Institute of Chemical Engineering Sciences (FORTH/ICE-HT)); Dr TSAKIROGLOU, Christos (Foundation for Research and Technology Hellas - Institute of Chemical Engineering Sciences (FORTH/ICE-HT))

Presenter: Mr MELITSIOTIS, Anastasios (Foundation for Research and Technology Hellas - Institute of Chemical Engineering Sciences (FORTH/ICE-HT))

Session Classification: MS18

Track Classification: (MS18) Innovative Methods for Characterization, Monitoring, and In-Situ Remediation of Contaminated Soils and Aquifers