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Numerical simulation of dissolved PFAS transport in unsaturated soil columns

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A 2-dimensional and dynamic numerical model of PFAS fate in unsaturated porous media is developed by accounting for the most important PFAS flow and mass-transfer mechanisms: convective flow, hydrodynamic dispersion, adsorption on solid grains and adsorption on air/water interfaces. Experimental measurements of the transient evolution of the shape of pendant and sessile drops are combined with image analysis software to develop equations describing the dynamics of the surface tension [1] and contact angle, associated with the surfactant (PFAS) sorption on the air/water interfaces, and formulate relevant models. Likewise, equilibrium and kinetic studies of PFAS sorption on soil grains are used to estimate all relevant (Langmuir, Freundlich, 1^{st}-order, 2^{nd}-order) sorption parameters [2]. Earlier work conducted on the immiscible two-phase flow in glass-etched pore networks [3] and soil columns [4] is used to model the dependence of capillary pressure and gas/water relative permeability curves on gas and water capillary numbers, regarded as dynamic parameters expressing the transient variation of the ratio of viscous to capillary forces. All aforementioned information is incorporated into the numerical code (JavaScript) so that a true-to-the physics model is obtained. The algorithm is developed in the platform of Comsol Multiphysics®.

First, forced imbibition in a soil column is simulated by considering the injection of uncontaminated water at a constant flow rate, until reaching the residual non-wetting phase (air) saturation. Then the water is replaced by PFAS-contaminated water, the flow rate is kept identical, and changes caused on the temporal and spatial distribution of water saturation and PFAS concentration across the soil column are mapped. Parametric analyses are done with respect to the type and concentration of PFAS, water injection flow rate, soil properties, and water composition. The numerical results could be used as a database for assessing the spreading of PFAS in vadose zone under varying conditions. The numerical model could be calibrated with regard to corresponding results from soil column tests, when such data become available.

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Literature

[1] Berry, J.D., Neeson, M.J., Dagastine, R.R., Chan, D.Y.C., Tabor, R.F., “Measurement of surface and interfacial tension using pendant drop tensiometry”,*J. Coll. Interface Sci.* **454** (2015) 226-237.

[2] Stavrinou, A., Aggelopoulos, C.A., Tsakiroglou, C.D.,“Exploring the adsorption mechanisms of cationic and anionic dyes onto agricultural waste peels of banana, cucumber and potato: Adsorption kinetics and equilibrium isotherms as a tool”,*J.Env. Chem. Eng.* **6** (2018) 6958–6970.

[3] Tsakiroglou, C.D., Avraam, D.G., Payatakes, A.C., “Transient and steady-state relative permeabilities from two-phase flow experiments in planar pore networks”, *Adv. Water Res.* **30** (2007) 1981-1992.

[4] Tsakiroglou, C.D., “The Correlation of the Steady-State Gas / Water Relative Permeabilities of Porous Media with Gas and Water Capillary Numbers”, *Oil & Gas Science and Technology - Revue d' IFP Energies nouvelles* **74** (2019) 45, 11p.