**Sorption interactions of ionizable organic compounds in soil environment**

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Soil sorption of ionizable organic compounds (IOCs) is typically described by distributions of molecular and ionic species between a sorbent and a liquid phase. The analysis of sorption interactions involves modeling experimentally determined distribution coefficients of species and/or relating them to (i) the properties associated with the IOC molecular/ion structure (e.g., molecular size, types of present functional groups, capability of specific interactions), (ii) the sorbent characteristics (e.g., mineral composition, surface area, ion exchange capacities, ionization of functional groups, sorbent polarity and presence of „non-polar" surfaces), and (iii) the properties of a solvent phase (pH, ionic strength, the presence of competing ions and dissolved organic matter – DOM etc). All these three groups of factors, i.e., representing the sorbate structure, sorbent properties and the medium, are generally well recognized in the literature, however, their accounting may become very complexed regarding multiple IOCs found in various soil environments. The presentation identifies and discusses several issues associated with sorption of IOCs in soil environments that are worth of more attention.

(i) IOCs found in soil environment are often characterized by complex chemical molecular structure. For example, in addition to different synthetic organic pesticides used in agriculture and various anthropogenic pollutants (e.g., pharmaceuticals and personal care products) originating from treated wastewater used for irrigation or sewage sludge-based biosolids, IOCs may include natural allelochemicals and plant growth regulators. Identification of ionizable functional groups in IOCs may not be straightforward, the data on pKa are not always available, and the presence of several ionizable groups in a molecule has to be taken into account. The complexity of IOCs becomes even more distinctive when DOM is explicitly considered as a part of IOCs. DOM having a poorly defined chemical composition, characterized by various ionizable functional groups demonstrating functional group - pKa distributions is well known to play a profound role in soil functioning and may act as a pollutant (or result in a further formation of contaminants, as, for example, in the case of formation of chlorination byproducts during water treatment).

(ii) Chemical soil inhomogeneity, due to the presence of clay minerals, different types of chemically and physically heterogeneous organic matter, and metal oxides contributes to the complexity of interactions of organic compounds with soil sorbents. The non-additive contributions of soil components to the total sorption of IOCs, blocking of mineral surfaces by organic matter and the role of natural inorganic nano-phases need to be addressed.

(iii) The often analysis of soil sorption of IOCs is based on the assumption that the species distribution coefficients are concentration-independent, despite the presence of non-linear sorption isotherms is often well-documented. This assumption makes more difficult accounting for the effect of sorption site heterogeneity on soil sorption of IOCs (as well as it does not allow estimating the limiting soil sorption capacities). How does non-accounted concentration-dependence of distribution coefficients correlate with additional efforts to improve the quality of their prediction? Soil sorption of IOCs characterized without specific attention to the possibility for sorption-desorption hysteresis should limit usefulness of the soil sorption data.

(iv) In a mechanistic analysis of IOC interactions in a sorbed state, their interactions in a solution may need to be explicitly accounted for. This can be easily made for sorption of non-ionized species but not for organic ions thus masking real nature of magnitude of IOC interactions in a sorbed state. The analysis of IOC distribution coefficients needs to be adapted to the real soil solution environment characterized by the presence of DOM potentially complexing IOCs, variable salinity, the presence of multivalent bridging inorganic cations and competing anions (e.g., due to the land use of gypsum and inorganic fertilizers) or surfactants used in agrochemical formulations.