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# Influence of non-hydrophobic factors on the sorption of ionizable xenobiotics to solids

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## 1. Short abstract

It is well known that xenobiotics sorp to solid phases like soil and sediment, depending on their inherent properties and environmental conditions. Traditionally it was accepted, that the hydrophobicity of the chemical, i.e. the  $\log K_{ow}$ , as well as the solid's content of organic carbon (OC) were the parameters describing the extent of sorption. Realizing that ionizable chemicals like weak acids and bases not always sorb according to their hydrophobicity, a correcting factor has been suggested. Correcting the hydrophobic sorption according to the Henderson-Hasselbalch equation has recently shown to improve the predicted sorption of weak acids significantly, however, weak bases do still show discrepancies compared with experimental data. In this investigation it was studied how a range of electrostatic parameters have influence on the sorption of weak bases to solid phases. Besides  $\log K_{ow}$ , pH and OC content of the solids, this investigation also included parameters like clay, silt and sand content, cation exchange capacity, zeta potential and other properties of the solids, and the impact on the sorption of weak bases to solids. Weak bases with  $pK_a$ -values differing about half a unit in the range 4-9, resulting in ionization within an environmental relevant pH range, are selected for the study. Literature is searched for data on distribution coefficients ( $\log K_D$ ) where also information about the experimental conditions regarding electrostatic parameters was reported. Taking the above mentioned parameters into consideration, predictions and regressions of the distribution to solids shall be improved.