

Determination and Qsar Modelling of Partitioning Coefficients for Some Xenobiotics in Soils and Sediments

Authors : Alaa El-Din Rezk

Abstract : For organic xenobiotics, sorption to Aldrich humic acid is a key process controlling their mobility, bioavailability, toxicity and fate in the soil. Hydrophobic organic compounds possessing either acid or basic groups can be partially ionized (deprotonated or protonated) within the range of natural soil pH. For neutral and ionogenic xenobiotics including (neutral, acids and bases) sorption coefficients normalized to organic carbon content, K_{oc} , have measured at different pH values. To this end, the batch equilibrium technique has been used, employing SPME combined with GC-MSD as an analytical tool. For most ionogenic compounds, sorption has been affected by both pH and pK_a and can be explained through Henderson-Hasselbalch equation. The results demonstrate that when assessing the environmental fate of ionogenic compounds, their pK_a and speciation under natural conditions should be taken into account. A new model has developed to predict the relationship between $\log K_{oc}$ and pH with full statistical evaluation against other existing predictive models. Neutral solutes have displayed a good fit with the classical model using $\log K_{ow}$ as $\log K_{oc}$ predictor, whereas acidic and basic compounds have displayed a good fit with the LSER approach and the new proposed model. Measurement limitations of the Batch technique and SPME-GC-MSD have been found with ionic compounds.

Keywords : humic acid, $\log K_{oc}$, pH, pK_a , SPME-GCMSD

Conference Title : ICASTE 2016 : International Conference on Agricultural Science, Technology and Engineering

Conference Location : Prague, Czechia

Conference Dates : March 30-31, 2016