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Coupled effects of pH and competing cations on metoprolol mobility: column experiments and parameter estimation using reactive transport modeling

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The fate of charged organic contaminants in the environment remains poorly understood due to the complexity of natural systems and the contaminants themselves. To isolate transport influencing factors, laboratory experiments are well suited. The transport behavior of metoprolol (MTP), a readily soluble beta-blocker, was studied in laboratory column experiments filled with quartz-sand under water saturated conditions. MTP is a weak base with an acid dissociation constant (pK_a) of 9.7 and is therefore predominantly cationic at pH<9.7 and increasingly uncharged at higher pH. Experiments were performed over the range of pH 3 to pH 11 and NaCl concentrations between c(NaCl)=1 and c(NaCl)=100 mmol l^{-1}. A significant dependence of MTP retardation on pH and c(NaCl) was observed ranging from an over 10-fold retardation at pH 6 and 1 mmol l^{-1} NaCl to nearly no retardation at pH 11. The findings suggest that transport behavior is mainly related to sorption of the cationic species of MTP for the used sediment. Modelling of retardation was done using a sorption model that considers (1) the speciation of MTP, (2) the surface reactions of MTP^+, and Na^+ with negatively charged surface silanol groups SiO^- of quartz and (3) the protolysis reaction between SiO^- and SiOH. The model was applied to the complete data set of 43 retardation values. Surface silanol quantity, as well as the equilibrium constants for reactions stated in (2) were modeled simultaneously. The model fits the transport behavior of MTP over the whole range of pH and c(NaCl) using the proposed transport equation and fitted parameters. This approach allows for predicting the transport behavior of charged organic species under a broad range of physico-chemical conditions if a set of required experimental data is available.