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Column experiments to simulate the transport of the basic beta-blocker atenolol in sandy aquifers under competitive conditions

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The ubiquitous occurrence of pharmaceuticals in the aquatic environment requires an advanced research and study of their interactions in all affected environmental compartments. Particularly sorption and degradation at the interfacial area between water and solid phase in aquifers play an important role as natural sink for such anthropogenic trace compounds. Previous column studies have shown that particularly cationic pharmaceuticals such as various beta-blockers were retarded strongly as protonated species on sediments with low organic content despite their strongly hydrophilic character. This may be explained by cation exchange despite the normally encountered extremely low concentration of pharmaceuticals in aquifers (ng L^{-1}) relative to the counteracting inorganic ions in groundwater (mg L^{-1}).

The objective of this study was to investigate the influence of selected competing inorganic cations on the transport behaviour of the basic beta-blocker atenolol (pK_a = 9,5) employing column experiments. The experiments were carried out at different concentrations and concentration ratios of the model compound atenolol and inorganic cations.

In the first experimental period two columns were filled with different natural sandy sediments with respect to cation exchange capacity (CEC) and content of total organic carbon (TOC). Model water containing atenolol (500 μg L^{-1}) and different Ca^{2+} concentrations (40 and 400 mg L^{-1}) was pumped in upflow mode consecutively through the same columns and the breakthrough curves of the respective ions were recorded. During the second experimental period, two columns were filled with the same sediment and the breakthroughs were observed at constantly high concentrations of inorganic cations and strongly varied concentrations of atenolol (1 and 500 μg L^{-1}).

As a result atenolol was clearly retarded in all cases but an increase in the Ca^{2+} concentration by a factor of 10 nearly yields to a halving of the retardation factor for atenolol, showing that the transport behaviour of atenolol is strongly influenced by other competing inorganic cations. On the contrary, a further decrease in the atenolol concentration showed no significant influence on its retardation.

In conclusion, the laboratory column experiments indicate that the relative concentration ratio between organic and inorganic cations is not the determinant control parameter for the cation transport. On the other hand, the experiments show that the mobility of the cationic model compound atenolol is more affected by concentration changes in the mg L^{-1} range than in the μg L^{-1} range. Therefore, it seems that absolute differences in concentration influence the cation exchange equilibrium stronger than relative differences. As a consequence the concentrations of organic cations in the trace level are not playing an important role for their transport behaviour. Instead, a variation of the main cation composition/water chemistry (such as during saltwater intrusions in coastal aquifers) causes much larger effects. Further experiments are planned to verify the results and to investigate the effect of other boundary conditions.