NUMERICAL MODEL TO EXPLAIN TRANSPORTATION OF ORGANIC CATIONS BASED ON ION EXCHANGE PROCESSES IN GROUNDWATER: TESTED WITH OBSERVATIONS OBTAINED BY LABORATORY AND FIELD EXPERIMENTS

Pubudu Kalinga[a,*], Tobias Licha[a], Ekkehard Holzbecher[a]

[a] Department of Applied Geology, Geoscience Center, University of Goettingen, Germany

ABSTRACT

Understanding the transportation of organic pollutants which are present as cationic form in groundwater is essential since it exerts a great risk for living beings by adding pollutants to the groundwater. It is a hugely challenging task to model organic cation transport since sorption mechanisms based concepts of hydrophobic partitioning which are used for non-ionic organic compounds are not valid for organic cations.

A numerical model has been developed to incorporate ion exchange equilibrium which describes reversible sorption reaction. The Gapon convention in the model describes the cation exchange process. Series of partial differential equations were used to explain transportation of cation due to ion exchange processes for both organic and inorganic species in both aqueous and sorbed phases. The model was evaluated with atenolol sorption experiments for various Ca^{2+} concentrations in column experiments.

The model explains sorption of organic cations in laboratory conditions successfully and retardation of cation exchange with inorganic cation concentration. But, it fails to yield retardation at field conditions. Organic cation concentration in field conditions is negligible compared that of inorganic ion concentration. At such a situation, the sorption of organic cations does not depend on their concentrations, but on the concentrations of inorganic cation concentration and it can be explained using the model. Further, according to the model, the ion exchange process wouldn't be happening when the retardation is equal to one. It could be because of ion exchange process is not determined by the sorption processes of organic cation and there may be other sorption mechanisms and water chemistry which affect on organic cation sorption.

Key words *– Organic cations, ion exchange equilibrium, selectivity coefficient, CEC, retardation, sorption.*