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Quantitative modelling of soil-water partition coefficients for tetracycline antibiotics in a typical karst wetland

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Antibiotics are discharged into the environment as metabolites when taken as drugs by human, ultimately leading to worldwide detection of antibiotics in environmental media such as soil, surface water, groundwater and sediments to varying degrees. Although the concentration of antibiotics in the environment is low, their prolonged presence can affect the population structure and nutrient transfer patterns of bacteria, aquatic organisms, soil organisms in environmental ecosystems, disrupting their balance and generating large numbers of drug-resistant bacteria, posing a threat to human health. The development of models to predict the distribution coefficients of antibiotics between the aqueous and sediment has been studied. However, most models have been developed considering only soil physicochemical factors and not water chemistry characteristics.

In our study, the distribution characteristics of sixteen groups of tetracycline antibiotics (TC, DOX, CTC, DMC) samples collected from aqueous and soil of the largest karst wetland in China were analysed. The results showed that the concentrations of antibiotic in the environment is influenced by a combination of factors. The soil-water partition coefficients (LogKd) of each antibiotic were calculated using redundancy analysis (RDA) method to screen out Fe^{3+}, NO_3^- and PO_4^{3-} as the main contributing factors in the aqueous, while the soil clay, organic matter, bulk weight and pH were the main contributing factors in soil. A prediction model for the Log K_d of various TCs and the seven major contributing factors in the aqueous and soil was developed using partial least squares (PLS) analysis. Four models were developed to provide quantitative methods for predicting the distribution coefficients of antibiotics and emerging contaminants with structures similar to tetracycline antibiotics in natural water-sediment systems. Compared with previous studies, the inclusion of water chemistry indicators in this study does complement the model construction and improves the indicator system for model construction. The results provide insights into the influence of soil and water physicochemical properties on the distribution of antibiotics, predict the transport and fate of antibiotics, and assess the exposure and risk of antibiotics to aquatic ecosystems.

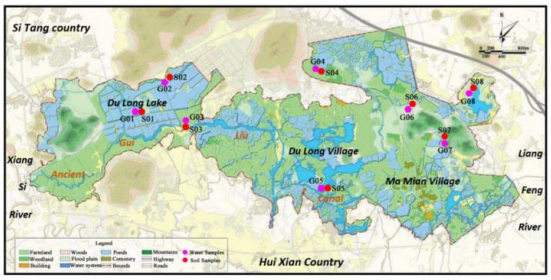

Fig. 1 Distribution of sampling points in Huixian karst wetland

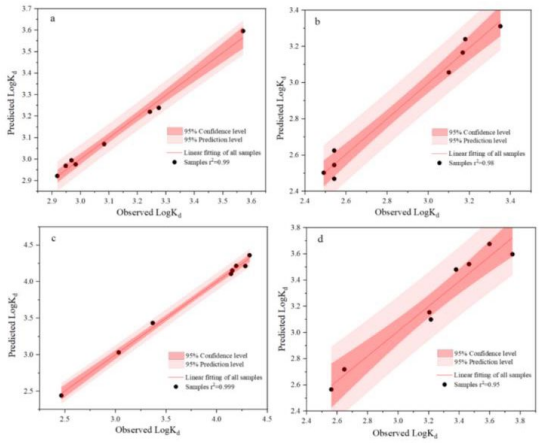

Figure 2 Fitted curve of measured and predicted of tetracycline antibiotics (a:TC, b:DMC，c:CTC，d:DOX)