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Estimation of groundwater CO_2 concentrations on a catchment scale using Random Forest

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Water-rock-interactions in the saturated and unsaturated zone govern the natural variability of CO_2 in groundwater. However, anthropogenic pollutions such as excessive input of organic and inorganic fertilizers or sewage leakage can cause shifts in the carbonate-pH system in an aquifer. Additional dissolution of minerals and associated mobilization of harmful heavy metals are possible consequences. Anthropogenic groundwater pollution is especially an issue where a protective confining layer is absent. On the other hand, addressing an environmental hazard such as fertilizer input to a single parameter remain intricate due to the high number of possible competing reactions such as microbial-controlled redox reactions. To overcome these obstacles, machine learning based statistical methods become increasingly important.

This study attempt to predict the CO_2 concentration in groundwater from a multi-feature selection by using Random Forest. For this purpose, groundwater chemistry data (in situ measured bulk parameter, major ions, nutrients, trace elements and more) from more than 23000 wells and springs in Germany were collected and homogenized in a single database. Measured or calculated CO_2 concentrationsare used to train the Random Forest algorithm and later to validate model results. Beside chemistry data, features about hydrogeology, soil characteristics, land use land cover and climate factors serve as predictors to build the “forest”. The intention of this study is to establish comprehensive CO_2 predictions based on surface and climate features and to identify trends in local CO_2 production. Gained knowledge can be used as input for groundwater quality management processes and adaptation policies.