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Exploring the Potential of Water Quality Sensors-Based Predictions of Hydrocarbon Levels in Groundwater: Virtual Experiments with Reactive Transport Modelling

MR. CHEN LESTER REÑON WU[1,2], R. MARTIJN WAGTERVELD[1] AND BORIS M VAN BREUKELEN[2]

[1]Wetsus, European Centre of Excellence for Sustainable Water Technology

[2]Delft University of Technology

Presenting Author: lester.wu@wetsus.nl

Petroleum products have caused groundwater contamination by harmful organic compounds, such as benzene, toluene, ethylbenzene, and xylenes (BTEX). Collecting and analysing contaminated groundwater samples is expensive, dangerous, and not frequently done. Relatively cheap water quality sensors (e.g. pH, electrical conductivity (EC), oxidation-reduction potential (ORP), and dissolved oxygen (DO)) may have the potential to predict hydrocarbon levels early, in real-time, and continuously through a virtual sensor, which would be advantageous in contaminated site management. As the first step towards this goal, we determined the correlation between water quality sensor data and BTEX concentrations. Since suitable datasets are limited, we used reactive transport modelling (RTM) to simulate hydrocarbon groundwater pollution plumes under realistic conditions to obtain a spatiotemporally dense virtual dataset for further analysis. We considered, over a two-dimensional cross-section, continuous dissolution from a stationary oil source zone at the top of a heterogeneous and shallow sandy aquifer. We simulated transient conditions (fluctuating water table) and assumed spatially uniform hydrogeochemical composition. BTEX concentrations have strong negative correlation with pH, DO, and ORP at all observation points except at the source zone ($r > |-0.70|$, mutual information score > 0.7), and moderate positive correlation with EC ($r > |0.60|$ mutual information score > 3). We further evaluated the effect of variations in hydrochemical and hydraulic aquifer conditions on the correlation coefficients. An increase in water table fluctuation, salinity, and nitrate concentration decreased the correlation of BTEX with pH and EC but increased the correlation with ORP. An increase in hydraulic conductivity also decreased the correlation of BTEX with DO and ORP. As the next step, these correlation coefficients are considered sufficiently high to develop a prediction model for detecting and estimating BTEX levels based on water quality sensor data at polluted sites.