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A trend prediction model of natural attenuation in groundwater based on machine learning and microbial community

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Natural attenuation is a commonly observed phenomenon in most contaminated sites.(Kao et al. 2010; Kawabe and Komai 2019) Natural attenuation describes naturally occurring processes in soil and groundwater that lead to a reduction in the mass, toxicity, mobility, volume, or concentration of contaminants without human intervention.(Jin et al. 2020) Natural attenuation combined with long-term monitoring (known as monitoring natural attenuation, MNA) has been proven to be a resultful remediation technology in petroleum-contaminated sites in which the biodegradation was the mainspring study conduct at contaminant removal.(Chiu et al. 2013; Naidu et al. 2010) Trends analysis and prediction are important segments for MNA application, in which complex biotic and abiotic factors need to be considered.

Microbiome data has been shown to work in combination with machine learning in parsing or predicting the degradation process of organic pollutants.(Bellino et al. 2019; Wijaya et al. 2023) Microbial communities acclimatized themselves to the local physicochemical conditions as well as to the pollutants in a historically contaminated site.(Guo et al. 2019; Yu et al. 2023; Sperlea et al. 2022) Due to their susceptivity to discrepancies of their surroundings, microorganisms could be regarded as "first responders"to environmental changes.(Sperlea et al. 2022) The microbial information carries additional information about environmental conditions and should be of great advantage in simplifying natural attenuation predictions, but there are few reports on this area.

In this work, the long-term monitoring of BTEX/CAHs and microbial community in the groundwater of a pesticide plant was conducted. A machine learning approach for natural attenuation prediction was developed with RFC model followed by either RFR or ANN model, utilizing both microbial information and contaminant attenuation rates for model training and cross-validation. The performance of the models in the prediction of the feasibility and/or rates of natural attenuation of BTEX and CAHs was subsequently evaluated and compared.

Results showed that the RFC model could achieve high accuracy (above 99%) for the feasibility prediction of natural attenuation for both BTEX and CAHs, and could successfully identify the key functional microbial genera. The RFR model was sufficient for BTEX natural attenuation rate prediction, and the MAPE was 8.1% ~ 19.6%. However, the predicted natural attenuation rates of CAHs by RFR were unreliable, with the MAPE as high as 22.0% ~ 153.9%. The ANN model showed better performance in the prediction of attenuation rates for both BTEX (with MAPEs from 2.1% to 4.6%) and CAHs (with MAPEs from 6.9% ~ 19.7%). Based on the assessments, a composite modeling method of RFC and ANN models was proposed, which could reduce the MAPE to as low as 2.1% ~ 4.6% for BTEX and 6.9% ~ 19.7% for CAHs. This study reveals that the combined machine learning approach under synergistic use of site microbial data has promising potential for predicting natural attenuation.

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