Machine Learning Modeling in Environmental Science and Engineering for Sustainable Development

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Abstract

To effectively remove numerous contaminants from contaminated water to achieve sustainable environments, we need accurate predictive models that can readily provide reasonable estimates of the contaminant reactivity during important water and wastewater treatment processes, including advanced oxidation processes (AOPs) and adsorption. However, conventional models rely heavily on quantitative structure-activity relationships (QSARs) between molecular descriptors and chemical activity which have multiple limitations, such as small numbers and narrow-scopes of contaminants involved, tedious calculations of molecular descriptors, and ignorance of adsorbent properties. In this talk, we'll discuss our recent progresses in using machine learning algorithms to develop more powerful, robust, and trustworthy predictive models. Specifically, we have 1) mined the literature and available databases to obtain large datasets of contaminant reactivity in AOPs and adsorption; 2) experimentally quantified the activity of selected contaminants in AOPs or adsorption; 3) developed predictive machine learning models for the activity of contaminants based on the data from the above two objectives; and 4) interpreted the obtained machine learning models to make them trustable and defined their applicability domains. These models will also help us design next-generation sustainable adsorbents and catalytic materials for more cost-effective water treatment.