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Quantitative-Structure-Activity-Relationship (QSAR) Models for the Reaction Rate and Temperature of Nitrogenous Organic Compounds in Supercritical Water Oxidation (SCWO)

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Abstract

Supercritical water oxidation (SCWO), in which hazardous wastes are removed from water at high temperature and pressure, is an effective method for wastewater treatment. To gain a better understanding of the removal rules for nitrogenous organics in SCWO, a Quantitative-Structure-Activity-Relationship (QSAR) approach was applied to establish the relationship between quantum chemical parameters and removal behaviors. In this study, 41 nitrogenous organics were used to study the removal behaviors, including the reaction rate constants of total nitrogen (k_{TN}) and the temperature at which the total nitrogen removal efficiency is 50% ($T_{TN_{50}}$). QSAR models were subsequently developed and evaluated. The two optimal models for k_{TN} and $T_{TN_{50}}$ were stable, robust and accurate, with the associated statistical indices of R^2= 0.725 and 0.951, q^2= 0.568 and 0.931, Q^2_{ext}= 0.847 and 0.987, respectively. The two optimal models both contained $f(-)_n$, E_{gap}, $q(N)$ and BO_x, but varied in the correlation between these four parameters and dependent variables. A three factors theory was thus proposed based on the two optimal models: the selectivity of active site, the transfer of electrons, and the breaking of chemical bond. These two models not only offer theoretical methods for predicting k_{TN} and $T_{TN_{50}}$, but also have predictive power for the removal behaviors of other nitrogenous organics in SCWO, reducing the need for further experiments.

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