77e Detailed Chemical Kinetic Modeling of Ammonia Oxidation in Supercritical Water

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We constructed a detailed chemical kinetic model (DCKM) to describe the homogeneous supercritical water oxidation (SCWO) of ammonia, a model nitrogen-containing compound. The model is a subset of our previous model for methylamine oxidation and pyrolysis in supercritical water, and represents the first known application of detailed chemical kinetic modeling to ammonia SCWO. The ammonia model is based on a free-radical reaction mechanism containing 29 species and 171 elementary reactions. Ammonia SCWO is modeled from 723-973 K and 14-30 MPa, which encompasses the range of experimental ammonia SCWO investigations in the literature. Computer simulations reveal that the base mechanism under-predicts the overall reactivity of ammonia during SCWO. However, the model does capture the global reaction orders for ammonia and oxygen, as revealed by recent experiments. The predicted activation energy agrees with the experimentally determined value, within uncertainty limits. Reaction pathway and sensitivity analyses are used to identify the main routes of chemical transformations and most important elementary reactions during homogeneous SCWO of ammonia.