ABSTRACT

Student, Beibei Z. Sun Ph.D., Purdue University, December 2009. Numerical Simulation of Inorganic Fouling of Quartz Surfaces in Ultraviolet Photoreactor.
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Inorganic mineral accumulation along the quartz sleeves that protect the ultraviolet (UV) lamps from water immersion has been observed as a major problem in UV photoreactor performance in water treatment process. Previous research has indicated that inorganic fouling is largely attributable to thermally-enhanced precipitation of metal-ligand pairs. Accumulation of these precipitates on the quartz surfaces that cause lamps reduces the transmission of UV radiation to the fluid that is being treated, thereby degrading reactor performance.

The central hypothesis of this research was that thermally-enhanced precipitation of metal:ligand pairs was responsible for fouling of quartz surfaces in UV photoreactors. Based on this hypothesis, a series of numerical models were developed to simulate the dynamics of fouling and its effect on process performance.

Analysis of the chemical composition and optical characteristics of foulants allowed identification of contributors to UV absorbance. A chemical equilibrium model was used to demonstrate that $Fe(OH)_3$ and MnO_2 among foulants are representative chemical forms for the two major foulants. Due to the availability of thermal properties from past research results, Fe was selected as a surrogate for Fe-based foulants. Calcium carbonate was also selected as a surrogate for Ca-based foulants because of the common observation of Ca mineral accumulation in fouling studies, even though Ca-based foulants do not appear to contribute significantly to UV absorbance. FLUENT coupled with GAMBIT were used as a computational fluid dynamics

(CFD) tool to simulate the kinetics of the fouling reactions for calcium and iron based on a combined mass, heat, and momentum balance (i.e. multiphysics) approach.

The results of these two models were then incorporated into a third model to allow simulation of the effects of fouling on UV photoreactor performance. This model involved a modified intensity field submodel to account for the effects of foulants on the irradiance-field. This information was linked with simulated particle trajectories to develop a simulation of the UV dose distribution delivered by a reactor under a fouled condition. In turn, these results were applied to a segregated-flow model to simulate the effects of fouling on microbial inactivation.

The modeling tools developed in this research are intended to serve as aids in the design and application of UV-based photoreactors in water treatment. The information developed from these models will allow for a quantitative assessment of the potential for fouling to take place and its effect on process performance.