A SYSTEMS APPROACH TOWARDS THE STUDY OF PHOTOCATALYTIC ADVANCED OXIDATION PROCESSES

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ABSTRACT

As the number of emerging chemical contaminants continue to grow and the reality that traditional treatment techniques prove to be ineffective in removing this waste the access to clean water is becoming an increasing concern for our nation. The desire to develop novel water treatment techniques is quickly becoming a major focus in the engineering community. One such treatment technique that has become very popular over the last decade is the use of Advanced Oxidation Processes (AOP) to chemically oxidize organic compounds. In this work I describe the use of one such process known as photocatalysis (the use of photon energy to mineralize organic compounds). I present a novel photocatalytic reacting system and with the use of optimization based techniques I develop a framework that gives insight into the operation and design of the system and the photocatalytic particles.

First I provide a discussion of state-space representation approaches and how they have been applied to chemical networks allowing for these systems to be decomposed into unit operations. I then extend this approach to represent and model the Circulating Fluid Bed (CFB) system that I have adapted for application in AOP referred to as a Pressure-regulated Recycle Reactor (PRR). I describe the formulation of a nonlinear program (NLP) and a general annual cost objective function that can be used for analysis and synthesis of both the PRR system, and the bulk properties of the composite particles.

Using empirically and theoretically determined correlations and equations to describe the unit operations that comprise the PRR system (transportation, adsorption, and photocatalytic reaction) and using parameters that have been referenced in literature to describe the properties of the contaminant species and composite particles I perform a variety of case studies that discuss the operation and design of the PRR system, the optimal bulk properties of the particles, and the overall performance for a multicomponent system (respectively).

The first case study employs a TiO_2-activated carbon composite immobilized on 2mm silica beads to degrade reactive red dye at an initial concentration of 10 ppm.

This framework identified successive globally optimal particle circulation rates and draft-tube fluid flowrates at minimum utility cost based on transport costs (pumping requirements), photocatalytic costs (UV power requirements), and catalyst utilization.

The second case study investigates the optimal weight loading, substrate selection, overall particle diameter, and catalyst shell thickness of a TiO_2-activated carbon composite particle for the degradation of methyl orange dye at an initial concentration of 20 ppm. This investigation identified the limitations and tradeoffs between the adsorptive, photocatalytic, and transport abilities when designing composite particles to be utilized in this PRR system.

The final case study investigates the performance of the PRR system and a TiO_2-activated carbon composite particle for an inlet stream containing a binary mixture of pollutant species. The model contaminants for this study are vinyl chloride, benzene, toluene, chlorophenol, and dichlorobenzene. This investigation identified that any compound with low relative adsorptive properties with respect to the other pollutant constituents is considered to be a performance limiting species in this system.

Broadening the approach of water treatment, I extend the use of this state-space modeling approach to investigate the directed design of filtration networks. I describe the formulation of a mixed integer non-linear program and a general flow distribution objective function that can be used to construct filter configurations having the ability to effectively remove a given particle contamination load, increasing overall filter lifetime.