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学　位　論　文　内　容　の　要　旨

博士の専攻分野の名称　　博士（工学）　　氏名　SHI Gang

学　位　論　文　題　名

Development of a versatile computational fluid dynamics-based model for optimization and implementation of vacuum ultraviolet photoreactor for drinking water treatment

(真空紫外線の浄水処理への導入と最適化に向けた汎用的流体力学モデルの開発)

To overcome the problem of organic micropollutants (OMPs) occurring in the drinking-water supply, additional purification processes especially advance oxidation processes (AOPs) have been applied to improve the conventional drinking-water-treatment processes. Vacuum ultraviolet (VUV) processes, a chemical-free AOP, have recently been found to be a promising technique for OMPs in lab-scale research. However, the lack of a proper simulation model is among the key factors hindering the implementation. Some computational models predicting the behavior of OMPs during VUV processes have been proposed. However, these models: (1) only assessed bicarbonate and natural organic matter as water matrices, the other inorganic ions found ubiquitously in natural drinking water sources have not been included; (2) only applied in specific reactors with limited conditions, the effects of design parameters and operation conditions have not been systematically analyzed. This doctoral work attempted to fill in the blanks. To evaluate the performance of the VUV photoreactor, the polar cyclic diether 1,4-dioxane, a representative OMP, was chosen as a target because of its ubiquitous presence, carcinogenicity, and refractoriness in the drinking-water-treatment process. According to the experimental results and CFD model simulations, some findings were concluded.

Firstly, a kinetic model, which was set up by a series of partial differential equations of chemical and photochemical reactions, was developed to investigate the relationship between VUV dose and 1,4-dioxane degradation. In batch mode experiments, coexisting inorganic ions (i.e. carbonate/bicarbonate, chloride, and nitrate/nitrite) were discovered to have a great impact on the degradation: the increase in concentrations suppressed the degradation. The effects of these inorganic ions on the degradation were then incorporated into the model. The model successfully predicted the 1,4-dioxane degradation in the batch mode experiments even under different water matrices. After introducing a term for hydraulic correction into the model to predict the degradation with a flow-through-type reactor, the model successfully predicted the 1,4-dioxane degradation in actual contaminated groundwater. This result clearly demonstrated that the model was accurate enough to predict the 1,4-dioxane decomposition during VUV treatment of contaminated waters, even though the prediction was limited to a given VUV reactor under a given operation condition. The model simulation finally showed that 1,4-dioxane degradation during the VUV treatment could be reasonably assumed to follow a pseudo-first-order reaction depending on the water matrices.

Secondly, based on the kinetic model above, a novel CFD model taking into account the effects of operation conditions (i.e. flow rate and radiation exitance) was developed for predicting degradation with flow-through type reactors. To reduce the cost of computational resources, the kinetic model was simplified as a pseudo-first-order reaction, whose reaction constant is the only parameter to be determined in advance and can be easily obtained by a simple batch experiment. After experimentally verified and validated the CFD model in a flow-through-type pilot-scale reactor, a virtual photoreactor was set up to precisely and systematically investigate the effects of the operation conditions on the degradation efficiency. Simulation results revealed that both increasing flow rate and decreasing radiant exitance increased the reactor performance, which agreed with the experimental results. Through EEO analysis, the following operations were finally recommended to be employed in actual drinking water treatment plants: VUV treatment using low-power lamps and a high flow rate was the most economical set-up under laminar flow, whereas VUV treatment using high-power lamps at a high flow rate under turbulent flow.

Thirdly, to discuss the effects of photoreactor configurations on the degradation efficiency, more experiment data were collected from three types of flow-through-type reactor. After the CFD model was validated by the experimental data, virtual photoreactors with different design configurations were set up. Simulations with the virtual photoreactors showed that (1) both increasing reactor gap (the depth of the water path) and increasing radiant reactor length increased EEO (i.e., decreased the efficiency), and (2) performance was improved by introducing some baffles into the reactor under laminar flows, but was not so obvious under turbulent flows. Based on the simulation results, the following configurations were recommended. For laminar flows, VUV configurations consisting of several short reactors, with a thin reactor gap, in series were recommended. Incorporating baffles was necessary in case of using long reactors. In contrast, for turbulent flows, VUV configurations with a thin reactor gap was recommended, and other parameters were not so important because the reactor gap was the only parameter significantly affecting the cost-effectiveness.

Overall of the research, a methodology for designing and optimizing the VUV reactor was proposed. From engineering points of view, for small and remote treatment plants that small and rural communities often possess, reactors with a thin reactor gap and short-multi-reactors configuration operating under laminar flow are recommended to be employed with low power lamps. In contrast, for large treatment plants with centralized water-treatment processing, long reactors employed with high power lamps and operation under turbulent flow are recommended.