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Modelling micropollutant degradation in UV/H_2O_2 systems: Lagrangian versus Eulerian method

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HIGHLIGHTS

- Modelling of organic micropollutant removal in UV/H_2O_2 systems.
- Methodology of combining fluid dynamics and photochemistry models at different degrees of complexity is provided.
- Models were validated with measured data for different UV systems (collimated beam and pilot-scale reactors).
- Lagrangian and Eulerian techniques are both applicable to predict micropollutant degradation in UV/H_2O_2 systems.

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ABSTRACT

The UV/H_2O_2 system is an effective barrier against micropollutants. The degradation of micropollutants largely differs due to variations in target compounds, water matrix composition and UV system. Models can account for these varying hydraulic and photochemical conditions. Computational fluid dynamics (CFD) models are combined with UV radiation, transport and (photo)chemical models to compute the degradation of compounds in a UV system. In this paper several modeling approaches with different levels of complexity are discussed. Depending on the type of UV system, a full CFD model, that resolves the hydraulics, UV radiation and transport of compounds, or simplified approaches that assume analytical hydraulic profiles and/or take the average of the fluence rate distribution. For the transport of chemical compounds, two methods were evaluated: the Lagrangian method and the Eulerian method. The Eulerian method calculates compound's concentrations at a fixed computational mesh and is most often used for compound degradation prediction in UV/H_2O_2 systems. The Lagrangian method calculates compound's concentrations along the tracks of individual particles. For a collimated beam and a pilot-scale flow-through reactor, both methods resulted in similar degradation predictions. This research shows that both methods can be used for oxidation predictions in UV/H_2O_2 systems.

1. Introduction

Treatment of water by advanced oxidation processes (AOPs) is an effective technique for micropollutant removal [1,2]. In the AOPs highly reactive hydroxyl radicals are generated that effectively degrade a wide range of organic compounds. Photochemical AOPs use UV radiation in combination with a chemical species (such as hydrogen peroxide, ozone, persulfate) to generate the hydroxyl radicals. The UV/H_2O_2 system is most often used to degrade organic compounds by the combined mechanisms of direct UV photolysis and hydroxyl radical reactions.

The degradation of organic compounds may largely differ due to variations in target compounds, water matrix composition, H_2O_2 concentration and UV system. Each compound has its specific sensitivity towards UV and hydroxyl radicals. The target compounds have to compete for UV photons and hydroxyl radicals with other water matrix constituents. In addition, the operating conditions and geometry of the UV system determine the UV radiation distribution. This distribution, in combination with the hydraulics, determines the exposure of compounds towards UV and hydroxyl radicals.

Models are being developed that account for all these varying hydraulic and photochemical conditions: Computational fluid dynamics (CFD) models are combined with UV radiation, transport and (photo)chemical models to compute the degradation of compounds in a UV system. Computational fluid dynamics is widely used in UV disinfection processes as a design tool for UV reactors and to assess UV reactor performance [3–5]. Modelling also offers the

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