

## Abstract

# Numerical Simulation of Coupled Processes of Membrane Filtration and Advanced Oxidation (AOPs) in Photolysis Reactors for Water Decontamination <sup>†</sup>

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**Abstract:** (1) Introduction: Chemical pollutants disposed of various branches of industry pose a significant threat to both the aquatic environment and human health. A specific class of pollutants is given by hardly biodegradable organic compounds coming mainly from pharmaceuticals, personal care products and industrial dyes. These pollutants are identified in water bodies (surface or underground) used as a source of water in drinking water treatment plants, the classic technologies for their elimination being inefficient. Exploring new processes and transposing them on an industrial scale in order to develop innovative, operationally and energy-efficient technologies is a complex approach, supported by both theoretical and experimental investigations, numerical modeling and virtual experiment, being basic steps in shortening the time required and increasing accuracy for developing new methods. (2) Materials and methods: Based on laboratory-level and functional model studies, the combined advanced oxidation processes (by photolysis and photocatalysis) and separation at the interface of photocatalytic ultrafiltrating membranes impregnated with elements based on carbon nanotubes (MWCNTs) decorated with ZnO particles, in the presence of active oxygen species (dissolved ozone), were investigated. The paper presents a methodology and a numerical model for modeling hybrid processes of advanced oxidation and membrane separation in photolysis reactors, as a preliminary step in the development of a water decontamination technology on an industrial scale. The model deals with a coaxial reactor configuration, being based on concepts from fluid mechanics (CFD—Computational Fluid Dynamics) assembled in a multi-physical model that incorporates elements of fluid flow, radiation distribution in the reactor and the dynamics of dissolved ozone photolysis processes, both in the reactor volume and at the filter membrane interface. (3) Results: The results obtained from virtual experiments, at different operating parameters of the reactor allowed the determination of the flow regime in the reactor by highlighting active areas, evaluating the efficiency of disinfection processes and photochemical processes (photolysis, photocatalysis) and by analyzing the reaction dynamics of dissolved ozone in the presence of UV radiation, useful in establishing the technical specifications necessary to make the model on a real scale.

**Keywords:** water decontamination; membrane filtration; photolysis; photocatalysis

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