ABSTRACT

The objective of this thesis is contributing to the development of a systematic modelling approach for a more efficient and sustainable water management.

The main aim is introducing Chemical and Process System Engineering methods and tools to provide a contribution to the AOPs (Advanced Oxidation Processes) investigation field by proposing process models that can be exploited to progress towards efficient management strategies for practical AOPs operation and inclusion in wastewater treatment networks.

First, different advanced oxidation processes, namely Fenton, photo-Fenton and VUV photo-oxidation, were investigated and compared for the treatment of paracetamol (PCT) aqueous solution, by evaluating a series of performance indicators. Among the selected AOPs, VUV photo-oxidation and photo-Fenton showed the most promising results. Both processes allowed attaining total removal of the target compound and high mineralization levels.

The second and main part of the thesis was focused on transforming "data into knowledge" by proposing different modelling approaches. The modelling effort focused on Fenton/photo-Fenton processes that showed the need of improving operating conditions.

Accordingly, two practical kinetic models for Fenton and photo-Fenton degradation of organic compounds have been proposed and validated:

- A conventional First Principles Model, based on a line source radiation model with spherical and isotropic emission, developed for the prediction of Fenton and photo-Fenton degradation of PCT and the oxidant (H_2O_2) consumption;
- A general non-conventional First Principles Model, based on a wide-ranging contaminant degradation mechanism considering a variable number of carbon atoms for the characterization of the intermediates.

Both models were experimentally validated and showed that were able to satisfactorily reproduce the system behavior. Particularly, the non-conventional First Principles Model showed to be a successful modelling approach for the Fenton/photo-Fenton degradation of different wastewater systems composed by single or multiple organic contaminants by means of lumped parameters (e.g. Total Organic Carbon-TOC). Thus, the approach proved to offer practical characterization of complex mixtures of chemicals.

Once process models are proposed and validated, they can be systematically exploited to determine efficient operation modes or design alternatives. Accordingly, the thesis addressed two cases of practical interest: the optimization of a control recipe and the design of a treatment network.

Particularly, a dynamic optimization framework for taking advantage of available kinetic models and determining the best hydrogen peroxide dosage profile, was proposed. Economic and environmental objectives and constraints were included to develop a dynamic optimization problem that was implemented in JModelica and solved using a direct simultaneous optimization method (IPOPT).

Finally, the combination of cheaper conventional biological processes with more expensive AOPs was explored. A Mixed-Integer Non Linear Programming (MINLP) model for the optimization of a general wastewater network was proposed based on a superstructure of alternative designs, which was implemented and solved in GAMS. The novel formulation includes the BOD_5/COD

ratio method, describing the removal efficiency of BOD_5 and COD of a treatment for modelling the variation of the biodegradability of the influents. This novel formulation allows determining the extent of the AOP treatments when combined with biological treatments, and paves the way for more complex models aimed at solving the trade-off between cost and treatment efficiency.