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Development of mechanistic models for photooxidative degradation of priority pollutants

Matija Cvetnić[1], Mirjana Novak Stankov[1], Daria Juretić Perišić[1], Ana Lončarić Božić[1], Šime Ukić[1], Marko Rogošić[1], Bakhtiyor Rasulev[2], Hrvoje Kušić[1] and **Tomislav Bolanča[1]**

[1]University of Zagreb, Croatia
[2]North Dakota State University, USA

Water can be loaded with various toxic pollutants whose degradations result with additional compounds which can be less or even more toxic than the starting pollutants. Therefore, conversion of the initial pollutant cannot be the only guideline in searching for a successful degradation method; it is highly desirable to understand the degradation mechanism as well as the degradation products. Mechanistic mathematical models (MM models) can provide better understanding of the degradation mechanism. This research was focused on UV-C/H_2O_2 and UV-C/S2O82- degradation of priority pollutants and development of related semi-empirical MM models. Toxicity and biodegradability were environmental aspects of the interest. The degradation was performed in batch reactor. In order to perform modeling, an analytical monitoring of the system was required. Further data were determined: conversion of pollutant's degradation, total organic carbon (in order to calculate mineralization), oxidant consumption and pH value of the media. The system temperature was considered constant. The systems of appointed differential equations were solving in mathematica 10 (Wolfram Research) software using GEAR numerical method.

mcvetnic@fkit.hr