International Conference on Applications of Radiation Science and Technology

Contribution ID: **388**

Type: **Oral**

Basic Radical Reactions in Water Treatment by Ionizing Radiation

Tuesday, 25 April 2017 11:15 (20 minutes)

Background of the study

In the so-called advanced oxidation processes (AOP) and in water treatment by ionizing radiation, which belongs to the class of AOP's, too, the main goal is to destroy, or at least to deactivate harmful water contaminants: pharmaceuticals, pesticides, surfactants, health-care products, etc. The chemical transformations are suggested to be initiated by hydroxyl radicals. However, some other inorganic radicals may also contribute to initiating the degradation.

Methodology

The changes due to irradiation were followed by taking the UV-Vis spectra and by measuring the chemical oxygen demand (COD) before and after irradiation. The degradation products were identified after LC separation with MS-MS detection. To obtain information about the degradation, kinetics pulse radiolysis with kinetic spectroscopic detection was used. The spectra of the intermediates were calculated from the kinetic curves (radical concentration versus time, on the μs time scale) taken at different wavelengths. These spectra give information about the structure of the intermediates.

Results

The kinetics and reaction mechanisms of a large variety of inorganic radicals with organic molecules were studied. It was shown that other inorganic radicals as $^\bullet$OH also contribute highly to the initiation of degradation in most AOP's. Cl^- and HCO_3^- in the treated water reacting with $^\bullet$OH transform to the $Cl_2^{\bullet-}$ and $CO_3^{\bullet-}$ oxidizing. Reactions of e_{aq}^- and $H^\bullet$ water radiolysis intermediates may also contribute to the degradation. In the primary reactions of all these radicals with organic molecules, carbon-centred radicals are produced. The reactions of the carbon-centred radicals with dissolved oxygen (DO) basically determine the oxidation rate. The peroxy radicals formed in the reactions of aliphatic carbon-centred radicals with DO may transform to peroxides and hydroperoxides, with the intervention of these intermediates gradual degradation takes place. Aromatic carbon-centred radicals (cyclohexadienyl radicals) in reversible processes react with DO, where the ring degradation is suggested to take place from the aromatic peroxi radicals. The primary carbon-centred radicals in uni- or bi-molecular processes may transform to other, e.g., oxygen or nitrogen centred radicals. These intermediates (e.g., phenoxy or anilino radicals) do not react with DO. Therefore, the initial degradation rate is low when, during the degradation reactions, there is a possibility for the formation of these radicals.

Conclusion

The carbon-centred radical formed in the reaction of a one-electron oxidizing radical with an organic molecule undergoes a second oxidation step when it reacts with DO. This reaction may be followed by further oxidations starting from the peroxy radical thus formed, or from the peroxide/hydroperoxide stabilization products. These reactions increase the degradation efficiency with a result that the one-electron oxidants induce 2–4 electron oxidations. When the radical does not react with DO, the degradation rate is low.

Country/Organization invited to participate

Hungary

Primary author: Mr WOJNAROVITS, Laszlo (Centre for Energy Research, MTA, Hungary)

Presenter: Mr WOJNAROVITS, Laszlo (Centre for Energy Research, MTA, Hungary)

Session Classification: A05

Track Classification: FUNDAMENTAL AND APPLIED RADIATION CHEMISTRY RESEARCH