Call for Abstracts for Oral and Student Poster Presentations

2014 Borchardt Conference

University of Michigan, Ann Arbor, MI

February 25 & 26, 2014

Presentation Title:	Can we predict intermediate-radicals and stable-byproducts in aqueous phase Advanced Oxidation Processes using computational chemistry?
Has this presentation been given previously? Yes / No; If yes, when and where?	No
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In the space below or on a separate sheet, provide a one page maximum abstract.
E-mail your abstract to David Schendel and Lut Raskin by **November 12, 2013**:

Advanced Oxidation Processes (AOPs) that produce highly reactive electrophiles, hydroxyl radicals, at ambient temperature and atmospheric pressure are attractive and promising water and wastewater treatment technologies. AOPs can control trace level organic contaminants in water treatment and water reclamation processes as well as high strength industrial and municipal wastewater if adequate design parameters are given. However, hydroxyl radical induced radical-involved complex reaction mechanisms make it challenging to predict reaction pathways and formation of intermediate-radicals and stable-byproducts quantitatively. Critical components for predicting the fate of intermediate-radicals and stable-byproducts are understandings of reaction pathways and associated reaction rate constants.

This talk will shed light on development of aqueous phase reaction rate constants prediction tools including a group contribution method (GCM) and linear free energies relationships (LFERs). The GCM is a first comprehensive tool to predict the aqueous phase hydroxyl radical reaction rate constants for more than 500 organic compounds including emerging contaminants. We updated the original GCM by including a number of new functional groups that were not examined experimentally before. The updated GCM has an accuracy of difference of factor of two from the experimentally observed values. The LFERs relate the experimentally obtained reaction rate constants with the theoretically calculated aqueous phase free energies of activation. We developed the LFERs for the reactions in the aqueous phase AOPs including H-atom abstraction from a C-H bond by hydroxyl radicals, hydroxyl radical addition to a C=C double bond of alkenes and aromatic compounds, molecular oxygen addition to a carbon-centered radical, uni-molecular decay of peroxyl radicals, and peroxyl radical disproportionation reactions for tetroxide radical formation and bi-molecular decay, respectively. An appliction of computational chemistry enables us to elucidate the indivdual reaction mechanisms and predict associated reaction rate constants.

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