



Dr. Young is a Professor of Environmental Engineering at the University of California, Davis, who specializes In measuring and modeling the fate and transport of trace organic compounds and heavy metals and in assessing their environmental impacts. Dr. Young has a B.S. in Chemical Engineering, a master's degree in Public Policy and a PhD in Environmental Engineering. He has authored more than 75 peer-reviewed publications and currently serves as a member of the Environmental Engineering Committee and the Hydraulic Fracturing Advisory Committee of the US EPA's Science Advisory Board.

## ENVIRONMENTAL ENGINEERING SEMINAR SERIES

FRIDAY, FEBRUARY 7TH FROM 1:30PM-2:20PM

McDonnell Douglas Auditorium (MDEA)

## Tracking Pharmaceutical Degradation and Byproduct Formation in an Innovative Reactor for UV/H<sub>2</sub>O<sub>2</sub> Advanced Oxidation Using High Resolution LC-MS

Presented By: Thomas Young, Ph.D.

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## Abstract:

Most trace organic constituents in wastewater remain unidentified and are therefore not readily subject to conventional "targeted" monitoring approaches. Targeted analysis methods typically miss compounds that are: (1) newly introduced to commerce, (2) not within categories that are currently the focus of research, or (3) are transformation products of commercially produced chemicals produced during physical, chemical and biological treatment of wastewater. Consequently, monitoring and treatment may not be optimized to protect human and ecosystem health. High resolution mass spectrometry serves as one component of a potential response to this situation. With sufficient mass accuracy, especially combined with high resolution MS/MS information, plausible molecular formulas and ultimately structures can be discerned, eliminating the necessity of selecting all target constituents in advance of designing monitoring and treatment programs. Here the information that can be gained from this approach is illustrated with data from a pilot scale advanced oxidation (UV/H2O2) reactor operated at the UC Davis wastewater treatment plant. "Influent" samples consisted of secondary effluent collected prior to pilot reactor operation, and these samples were spiked with a mixture of pharmaceutical compounds selected as probe molecules. "Effluent" samples were collected from the basin at the top of the pilot reactor. Both types of samples were concentrated using solid phase extraction. The reactor was operated at several peroxide doses and detention times to examine the effects of these variables on reactor efficacy. Samples were analyzed with an Agilent 1200 HPLC combined with a 6530 quadruple time-of-flight mass spectrometer (QTOF). "Molecular features," (i.e., groups of isotopes, charge states, adducts, and multimers postulated to arise from individual compounds) were filtered to remove features present in the blank samples and to eliminate ions that were observed in a limited number of samples. As expected, the number of significantly transformed constituents generally increased as detention time and peroxide dose increased. A reaction pathway model was used to predict transformation products of the probe molecules and some of these products were tentatively identified in the effluent samples.

## Next Week's Seminar (Friday, February 14th)

Megan Rippy, Ph.D. University of California, Irvine