Announcing the Final Examination of Carlyn Higgins for the degree of Doctor of Philosophy

Time & Location: June 26, 2020 at 1:00 PM in Virtual Defense https://ucf.zoom.us/j/96874640160
Title: Removal of Chemicals of Emerging Concern and Mass Transfer Modeling in a Nanofiltration Membrane Process

An investigation that studied the mass transfer of 1,4-dioxane and enantiomeric ibuprofen in a nanofiltration (NF) membrane process has been completed. Pilot-scale experiments using a 267 gallon per minute split-feed, center-port NF process treating pH 6.5 groundwater containing between 180 nanogram per liter (ng/L) to 38,400 ng/L of 1,4-dioxane consistently removed approximately 12 percent of the chemical despite the variable feed content when the water flux and temperature were held constant. Bench-scale, flat-sheet membrane experiments also revealed that nanofiltration operating at pH 4.0 conditions removed ibuprofen between 34.5 and 49.5 percent from a feedwater containing between 1 and 1,500 microgram per liter (µg/L) of the racemic chemical. Although 1, 4-dioxane was not found to exhibit adsorptive tendencies, as much as 25 percent of ibuprofen adsorbed onto the metal surfaces of the testing equipment. Mass balances determined that ibuprofen's S-enantiomer was primarily responsible for the adsorption. Density functional theory (DFT) computations exposed a 6.4 Å³ smaller molecular volume and 1.10 x 10^-29 Coulomb-meters (Debye) longer dipole moment of S-ibuprofen than R-ibuprofen, which could explain the S-enantiomers stronger affinity to stainless-steel equipment components. The rejection of S-ibuprofen was consistently greater than R-ibuprofen, explained by the dissimilar polarity of the two molecules outlined by DFT calculations. Feedwater ibuprofen concentration, pH and operating pressure affected ibuprofen adsorption onto the equipment and membrane components. Contact angle measurements revealed a direct relationship between membrane hydrophobicity and adsorbed ibuprofen concentration. Langmuir and Freundlich isotherms also accurately modeled S-ibuprofen adsorption. Additionally, application of the Homogeneous Solution Diffusion Model was found to provide accurate predictions of 1,4-dioxane and R-ibuprofen permeate content based on statistical analysis; however, the model was less predictive for the S-enantiomer due to adsorptive tendencies of the molecule. At least 24 hours of equilibration is required prior to conducting hydrophobic solute membrane rejection studies.

Major: Environmental Engineering

Educational Career:
Bachelor's of Environmental Engineering, BS, 2016, University of Central Florida
Master's of Environmental Engineering, MS, 2017, University of Central Florida

Committee in Charge:
Steven J. Duranceau, Chair, Civil, Environmental, and Construction Engineering
Woo Hyoung Lee, Civil, Environmental, and Construction Engineering
A H M Anwar Sadmani, Civil, Environmental, and Construction Engineering
Melanie J. Beazley, Chemistry

Approved for distribution by Steven J. Duranceau, Committee Chair, on June 8, 2020.

The public is welcome to attend.