Predictive Models to Aid in the Design of Membrane Systems for Organic Micropollutant Removal

Funding Agency:
- **WateReuse Foundation (WRF-06-009)**

Principal Investigators:
- **Dr. Jörg Drewes**
- **Dr. Chris Bellona**
- **Dr. Shankar Chellam**
- **Dr. Mark Eberhart**

Students Participating:
- **Matt Sonnenberg**
- **Travis Jones**

Start date: August 2008

End Date: May 2011

Project Objectives

➢ Evaluate current molecular modeling methods and employ molecular modeling techniques to determine reliable and accurate solute descriptors that can be employed for quantitatve structure property relationship (QSPR) model development

➢ Develop and optimize modeling strategies that can be used for the prediction of organic micropollutant removal by NF and RO membranes

➢ Evaluate the efficiency of full-scale organic micropollutants removal and successfully predict the removal rates with developed model(s)

Methodology

➢ Three bench-scale flat sheet membrane units are in place to perform removal studies of a large set of organic contaminants

➢ Molecular Modeling Software is employed to generate descriptor values for the organic contaminants

➢ Statistical analysis of removal data by principle component analysis (PCA) and self-organized maps (SOM) will indicate molecular descriptors that may contribute to differences in removal trends among organic contaminants

➢ Descriptors identified during PCA and SOM will be incorporated in modeling strategies used during the study