Evaluation of QSPR Techniques for Wastewater Treatment Processes

This research assessed existing techniques known as quantitative structure property relationship (QSPR), used by water quality managers and scientists in predicting key wastewater processes such as sludge sorption, activated sludge biotransformation, and chlorine oxidation. Accurate QSPR predictions are essential inputs into mass balance models to effectively predict the fate and potential removal of trace organic compounds (TOrCs) during wastewater treatment processes. However, this fate treatment information was experimentally lacking for emerging trace organic compounds including pharmaceuticals, personal care products, and household chemicals.

The results of this research will help to accurately and effectively predict the fate and potential removal of TOrCs during wastewater treatment processes and their release into the environment.

The results of this research will assist water quality scientists and engineers to accurately and effectively predict the fate and potential removal of TOrCs during wastewater treatment processes and their release into the environment.

A comprehensive literature review of existing biodegradation, sorption, and chlorine oxidation QSPRs was performed. This review assessed the applicability of existing QSPRs for wastewater treatment systems and identifies which QSPRs require further evaluation. Selected predictive QSPRs were statistically evaluated by comparing estimated and experimentally determined fate parameters.

The sludge partitioning coefficients and biotransformation and chlorination rate constants are essential fate parameters necessary to predict the behavior of TOrCs during primary, secondary, and disinfection processes within a wastewater treatment plant that incorporates chlorine disinfection. However, accurate TOrC fate parameters that serve as the input to mass balance models are lacking. A few QSPRs exist that are potentially applicable to wastewater treatment processes, but they have not been comprehensively evaluated for today's relevant low level TOrCs, such as pharmaceuticals, endocrine disruptors, household chemicals, and personal care products.

Fate of TOrCs during Wastewater Treatment by Evaluating QSPR Techniques

The researchers investigated several mechanisms of removal for trace organic compounds such as 1) sorption to wastewater sludge, 2) biotransformation during activated sludge treatment, and 3) chlorine oxidation during disinfection. TOrCs representing compounds from suspected EDC and PhAC, and PCP classes of compounds were used as the

How Does QSPR Work?

QSPRs work by using measured or estimated physical/chemical structural properties to determine a fate treatment parameter (i.e. sludge portioning coefficient) to predict the removal of organic compounds during wastewater treatment.

BENEFITS

- Provides experimental sorption, biotransformation, and chlorine oxidation fate data for a structurally diverse set of suspected endocrine disrupting, pharmaceutically active, and personal care product compounds.
- Includes a thorough literature review and evaluation of existing quantitative structural relationships (QSPRs) as they relate to the fate of trace organic compounds (TOrCs) during wastewater treatment.

RELATED PRODUCTS

Removal of Endocrine Disrupting Compounds in Water Reclamation Processes (01HHE20T)

Contributions of Household Chemicals to Sewage and Their Relevance to Municipal Wastewater Systems and the Environment (03CTS21UR)

Fate of Pharmaceuticals and Personal Care Products through Wastewater Treatment Processes (03CTS22UR)

Trace Organic Compounds and Implications for Wastewater Treatment (CEC3R07)

RELATED ONGOING RESEARCH

Categorizing Wastewater Treatment Processes by Their Efficacy in Reduction of a Suite of Indicator TOrC (CEC4R08)

Diagnostic Tools to Evaluate Impacts of Trace Organic Compounds on Aquatic Populations and Communities (CEC5R08)

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validation datasets as these compounds frequently occur and are currently relevant. These types of compounds have not been commonly used in training and validation data sets applied towards QSPR development and/or evaluation. QSPRs were employed to estimate fate parameters by calculating or estimating appropriate compound descriptors as QSPR input parameters. Experimental biotransformation, sorption, and chlorine oxidation fate parameters for TOrCs were either obtained from the literature or measured in the laboratory via batch studies.

Table 1 shows some recent studies that have examined the sorption behavior of current day emerging TOrCs including, steroidal hormones, PhACs, and PCPs, to activated-sludge solids. These studies determined experimental partitioning coefficients and these data are compiled in Appendix A of the report. This literature data was used by the researchers as part of the validation set used to evaluate QSPRs for this project.

Table 1. Literature Sources on the Partitioning of TOrCs to Activated-Sludge Solids.

Experimental Values Reported in Appendix A of the Report.

# OF COMPOUNDS	TORC CLASS	REFERENCE
4	PhAC	Stuer-Lauridsen et al. (2000)
4	PhAC	Golet et al. (2001)
11	PhAC/PCP/Steroids	Ternes et al. (2004)
3	Steroids/Bisphenol A	Clara et al. (2004)
5	PhAC	Gobel et al. (2005)
3	Steroids	Andersen et al. (2005)
15	PhAC/PCP/Steroids	Urase and Kikuta (2005)
1	Steroids	Yi and Harper Jr. (2007)
1	PhAC	Maurer et al. (2007)
20	PhAC	Wick et al. (2009)
14	PhAC	Radjenovic et al. (2009)

Results of the Wastewater Treatment Fate Processes

Research gaps were noted for the application of QSPRs for the prediction of the fate of TOrCs during wastewater treatment in the report. The outcomes of this study include the generation of high-quality sorption, biotransformation, and chlorine oxidation fate data for a large and structurally diverse set of suspected endocrine disrupting, pharmaceutically active, and personal care product compounds. This experimental fate data can be directly applied to understand the fate and removal during wastewater treatment for the relevant TOrC examined in this study. In addition, QSPRs were statistically evaluated, where key QSPRs for wastewater treatment processes and research gaps for the application of QSPRs were identified.

The results of this project complement an ongoing WERF project, *Trace Organic Compounds Removal during Wastewater Treatment* (CEC4R08) led by Carollo Engineers, which will provide reliable mass balance modelling tools that describe and predict removal efficiencies for a wide range of Trace Organic Compounds.

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The research on which this report is based was funded in part by the U.S. Environmental Protection Agency (U.S. EPA) through Cooperative Agreement No. CR-83155901-1 with the Water Environment Research Foundation (WERF). Unless an U.S. EPA logo appears on the cover, this report is a publication of WERF, not U.S. EPA. Funds awarded under the agreement cited above were not used for editorial services, reproduction, printing, or distribution.

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