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Trace Organics

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Trace Organic Compound Indicator Removal During Conventional Wastewater Treatment

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TRACE ORGANIC COMPOUND INDICATOR REMOVAL DURING CONVENTIONAL WASTEWATER TREATMENT

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ABSTRACT AND BENEFITS

Abstract:

Because of concerns related to public and aquatic health, there is increasing interest in evaluating occurrence and removal of trace organic compounds (TOrC) during conventional wastewater treatment. TOrC comprise various groups of compounds including pharmaceuticals, personal care products, food additives, and other high production chemicals. Due to the large number and variety of compounds present in municipal wastewater influents and effluents, guidance is needed for assessing the removal efficiencies for a wide range of TOrC in conventional wastewater treatment. The objective of this study was to identify a small number of suitable performance indicators that allow for a rapid characterization of performance efficiency of conventional wastewater treatment facilities. The study focused primarily on investigating the performance of activated sludge treatment processes.

The study identified a suite of 22 compounds that represent a range of sorption characteristics and biotransformation kinetics in mixed liquor. Based on these characteristics, these indicator compounds were grouped into nine bin categories that represent a larger group of TOrC with similar sorption and biotransformation. Each bin category was described in terms of anticipated range of removal efficiency and the accuracy and reliability of predicting fate during activated sludge treatment using current fate models. Solid retention time (SRT) was found to drive the biotransformation of indicator compounds that are moderately biotransformed. Threshold SRTs were defined for each indicator that exhibited more than 80% removal.

Benefits:

- Provides guidance to the wastewater treatment industry on which compounds to monitor to assess the efficiency of conventional wastewater treatment for broader groups of TOrC.
- Quantifies the impact of solid retention time, hydraulic retention time, wastewater temperature, and TOrC influent concentrations on the removal efficiency of TOrC.
- Assesses the reliability and accuracy of current fate modeling for predicting TOrC removal during activated sludge treatment.
- Places conventional secondary treatment for TOrC removal into perspective with the costs and benefits of alternative attenuation processes such as activated carbon adsorption, ozone, and membrane treatment.

Keywords: Secondary treatment, indicator, biotransformation, sorption, modeling.

TRACE ORGANIC COMPOUND INDICATOR REMOVAL DURING CONVENTIONAL WASTEWATER TREATMENT

What was the focus of this project?

Answer: Every domestic wastewater contains thousands of organic compounds at trace concentrations that originate from consumer products, pharmaceutical use, or food products. While we are today able to detect and quantify many of these compounds in wastewater influents and effluents, our understanding on their ecological and toxicological relevance for aquatic ecosystems and human health is still growing.

We currently have limited knowledge on the removal efficiency of trace organic compounds (TOrC) in conventional wastewater treatment. Furthermore, it is not feasible to monitor all of the TOrC that would be entering a wastewater treatment plant. Thus, this project helped fill important data gaps by comparing the efficiency of different conventional wastewater treatment processes for the removal of select TOrC. We focused on identifying a small group of indicator organic compounds that are helpful in assessing the removal efficiency of a broad range of TOrC in secondary treatment for removing a broad number of trace organic compounds present in domestic wastewater influents. The evaluation of indicator compounds allows us to draw conclusions on the removal of a much broader number of TOrC that share similar sorption and biotransformation characteristics.

Why should I read this report?

Answer: The findings of this report are of interest to wastewater utilities that seek a better understanding of TOrC removal in their existing conventional treatment process. The study allows the reader to compare TOrC removal efficiency for different conventional wastewater processes and operational conditions.
Findings of this work will help utilities, planners, design engineers and researchers to better predict which types of trace organic compounds are, or are not, efficiently removed during conventional treatment depending on the treatment configuration and operational conditions. The study will also help in assessing whether specific trace organic compounds are attenuated by biotransformation during treatment or removed from the liquid process stream through sorption onto biosolids.

How is this report useful for my utility?

Answer: Conventional wastewater treatment was not designed for the purpose of removing trace organic compounds. Nevertheless, many TOrC are removed during conventional treatment to varying degrees, while other compounds are persistent. Knowing the level of removal that existing primary and secondary treatment processes provide for different types of TOrC groups is a critical first step for risk awareness and for communication with external stakeholders. This knowledge also helps with treatment process optimization and upgrade decisions.

QUESTIONS AND ANSWERS ABOUT WERF'S CEC4R08 RESEARCH

My state has no limits or monitoring requirements for these substances so why should I care?

Answer: Even though regulatory requirements that define discharge limits for TOrC do not exist today in the United States, it is anticipated that regulations will be developed in the coming years. Some regions of the U.S. require monitoring for certain TOrC and such requirements could be adopted by your state in the future.

While there may be no pressing need for you to take action on TOrC removal from a compliance point of view, it is prudent to consider future regulatory trends in today's planning process. Many utilities are currently required to invest in process upgrades in order to comply with more stringent nutrient limits for nitrogen and phosphorus. This study helps to define synergies between specific process upgrades that may improve both nutrient and TOrC removal. Integrating treatment processes capable of attenuating TOrC in current master planning efforts could reduce compliance costs in the long-term.

What is the benefit to my facility of this work if I was not included in the study?

Answer: The utilities included in this study for full-scale field testing were selected to represent a variety of secondary treatment processes and operational conditions. Data collected from these sites were used to develop general relationships between process operation and TOrC removal efficiency. These relationships were found to be generally useful for predicting TOrC removal performance at secondary treatment facilities.

I'm a state water quality manager, how is your research relevant to me?

Answer: The suite of compounds in this study was selected for the function of addressing treatment efficacy of different processes for compounds sharing similar chemical structures and biotransformation properties rather than for reduction of risk. A suite of target TOrC from a risk perspective can, however, be mapped amongst the suite of performance indicators based on shared physical and bio-kinetic properties. Linking compound databases on basis of physical, bio-kinetic, and risk data allows identifying, engineering, and evaluating treatment process configurations to achieve a target whole effluent toxicity.

What kind of TOrC removal performance can I expect at my utility?

Answer: The degree to which TOrC are removed during conventional wastewater treatment is very compound specific and depends on process, operational, and seasonal conditions. This study describes different groups of TOrC that are present in wastewater influents and their anticipated removal efficacy depending on these factors. For example, the removal of moderately fast biotransformed compounds like DEET (insect repellent) and gemfibrozil (lipid regulator) can range between 30-100% depending on the secondary treatment process operation. Rapidly biotransformed compounds like ibuprofen and caffeine have been found to be effectively removed (80-100%) at all secondary treatment facilities. Compounds like carbamazepine (an antiepileptic drug) that are slowly biotransformed and poorly sorbable onto solids show typically very low removal (0-25%) independent of process operation.

QUESTIONS AND ANSWERS ABOUT WERF'S CEC4R08 RESEARCH

Can you highlight one of the key research findings that have advanced our knowledge of TOrC in wastewater treatment processes?

Answer: One of the key findings pertains to the relevance of solid and liquid stream interactions during wastewater treatment for TOrC attenuation. Our research indicates that highly and moderately sorbable TOrC are found in significant amounts on the wasted solids from secondary treatment systems (10% to more than 100% of secondary influent loads). The slow-to-degrade and highly sorbable TOrC triclocarban accumulated on the solids in systems operating under long SRTs. Additional investigations we conducted at a full-scale anaerobic digestion process revealed that several recalcitrant TOrC were not reduced during anaerobic digestion, but were found in increased concentration in the digested sludge in relationship to the solid destruction achieved (i.e., carbamazepine, TCEP, TCPP). This finding highlights the potential for accumulation of hydrophobic, non-degradable TOrC sludges in liquid stream processes and on biosolids. Methods need to be investigated that can effectively reduce such compounds in solid process streams. Conventional liquid and solid stream treatment proved to be ineffective.

How does this project link to WERF's project (Stock No. CEC5R08) on *Diagnostic Tools to Evaluate Impacts of Trace Organics in the Aquatic Environment*?

Answer: CEC5R08 developed a screening framework to determine the risk of TOrC exposure in the aquatic environment. CEC5R08 proposed general characteristics of discharge locations to assess the risk for aquatic life. This project links into CEC5R08 by providing predictive capabilities for effluent TOrC concentrations, which can then be used to predict exposure concentrations in aquatic environments. In particular, insights gained from this project allows us to estimate the removal of other trace organic compounds of concern when basic compound properties, such as charge, water-octanol partitioning coefficient and biotransformation rate constant are known.

How is this project part of WERF's larger Trace Organics Program?

Answer: WERF's Trace Organics program has funded research in three focus areas related to TOrC in the natural environment. The focus areas are: 1) Risk Communication, 2) Aquatic Impacts, and 3) Treatment Efficiency. This project (CEC4R08) primarily supports the Treatment Efficiency focus area, though results from this project also support the Risk Communication and Aquatic Impacts focus areas.

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ABI	Aeration Basin Influent
AD	Anaerobic digester
ADAF	Average daily annual flow
ADMMF	Average daily maximum month flow
A2O	Anaerobic-anoxic-aerobic process
Alk	Alkalinity
AOP	Advanced oxidation process
APEC	Alkylphenoxy carboxylate
APEC	Alkylethoxycarboxylates
ASE	Accelerated solvent extraction
BNR	Biological nutrient removal
BOD	Biochemical oxygen demand
CAS	Conventional activated-sludge
CBOD	Carbonaceous biochemical oxygen demand
CDPH	California Department of Public Health
CEPC	Chemically enhanced primary clarification
cm	Centi meter
COD	Chemical oxygen demand
CSM	Colorado School of Mines
CT	Disinfectant concentration × contact time
D	Day
DAFT	Dissolved air floatation thickener
DEET	N,N-Diethyl-meta-toluamide
DF	Detection frequency
DI	Deionized
DNA	Deoxyribonucleic acid
DO	Dissolved Oxygen
DOC	Dissolved organic carbon
D_{ow}	Octanol-water partitioning coefficient at pH 7
DR	Detection ratio
EE2	17α-ethinylestradiol
ESI	Electrospray ionization
F/M	Food to microorganism
GAC	Granular activated carbon
g	gallons
gph	Gallons per hour
gpd	Gallons per day
GS/MS	Gas chromatography-mass spectrometry
GT	Gravity thickener

h	Hour
HPO	High purity oxygen
HPV	High production volume
HRT	Hydraulic retention time
IFAS	Integrated fixed-film activated sludge
K_b	First-order biodegradation rate constant [d^{-1}] or normalized by TSS concentration [L/g_{ss}-d^{-1}]
K_{ow}	Octanol-water partitioning coefficient [-]
K_d	Sorption distribution coefficient [m^3/kg]
L	Liter
LC/MS-MS	Liquid chromatography-tandem mass spectrometry
LFB	Laboratory fortified blank
LFSM	Laboratory fortified sample matrices
MBR	Membrane bioreactor
MDL	Method detection limit
mgd	Million gallons per day
Min	Minute
mJ	Milli Joule
mL	Milli liter
ML	Mixed liquor
MLE	Modified Ludzack-Ettinger Process
MLR	Mixed liquor recycle
MLSS	Mixed liquor suspended solid
mM	Milli mole
MMSD	Milwaukee Metropolitan Sewerage District
MQL	Method quantification limit
MQO	Measurement quality objective
MRL	Method reporting limits
MWCO	Molecular weight cutoff
NaN_3	Sodium azide
ng	Nano gram
NH_3	Ammonia
NO_3^-	Nitrate
NPEO	Nonylphenol ethoxylate
O_3	Ozone
OECD	Organization for Economic Co-operation and Development
OP	Orthophosphate
P	Phosphorus
PAC	Powdered activated carbon
PDF	Peak day flow
PFOA	Perfluorooctanoic acid
PFOS	Perfluorooctane sulfonate
POTWs	Publicly owned treatment works

PPCPs	Pharmaceutical and personal care products
ppt	Parts-per-trillion
QA/QC	Quality assurance/quality control
RAS	Return activated sludge
RO	Reverse osmosis
rpm	Revolutions per minute
RSD	Relative standard deviation
SBR	Sequencing bioreactor
SCCWRP	Southern California Coastal Water Research Project
sCOD	Soluble COD
sf	Square foot
SNWA	Southern Nevada Water Authority
SOR	Surface overflow rate
SPE	Solid phase extraction
SRT	Solid retention time
TCEP	Tris (2-carboxyethyl) phosphine
TCPP	Tris (chloroisopropyl) phosphate
TKN	Total Kjeldahl nitrogen
TOrC	Trace organic compound(s)
TP	Total phosphorus
TPS	Thickened Primary Sludge
TS	Total solids
TSS	Total suspended solids
TWAS	Thickened waste activated sludge
UF	Ultrafiltration
µg	Micro gram
UNSW	University of New South Wales
U.S. EPA	United States Environmental Protection Agency
UV	Ultraviolet
VS	Volatile solids
VSS	Volatile suspended solids
WAS	Waste activated sludge
WRRF	WateReuse Research Foundation
WWTP	Wastewater treatment plant

EXECUTIVE SUMMARY

ES.1 Background

There is increasing interest in evaluating the occurrence and removal of trace organic compounds (TOrC) during wastewater treatment and water reclamation, due to concerns related to potential adverse public and aquatic health effects. TOrC present in municipal wastewater influents and effluents contain thousands of chemicals, which are comprised of pharmaceuticals, personal care products, food additives, and other high production volume (HPV) chemicals with a wide range of physical and chemical properties. As we can only monitor a very small fraction of all TOrC that are present in wastewater, strategies are needed to describe and predict removal efficiencies for a representative number of TOrC. The strategy in this study is based on TOrC performance indicators that were selected by considering key removal mechanisms and compound properties that are critical for TOrC attenuation during conventional wastewater treatment.

Although not designed for this purpose, conventional treatment removes a variety of TOrC to various degrees. The degree to which TOrC should be removed during wastewater treatment is not yet defined for the majority of compounds. Strategies are needed for integrating trace organic removal with technical solutions addressing other treatment challenges, such as removal of nutrients or pathogens. Effluent limits for TOrC may in the future be defined for individual TOrC, groups of compounds, whole effluent toxicity, and/or ecotoxicological endpoints to manage the risk imposed by these compounds on the environment and public health. This study investigates the mechanisms driving the removal of individual TOrC during wastewater treatment. Results gained by these investigations provide a general basis for assessing the anticipated treatment efficiency for TOrC that are or become of interest based on their eco- or human toxicological relevance.

The core process of conventional wastewater treatment is secondary treatment focusing on reducing the organic and nutrient load in wastewater. The activated sludge process is the predominant type of secondary treatment in the U.S. and other parts of the world. Activated sludge treatment has been designed in many different process configurations depending on the level of treatment required. There are a number of factors which have been identified in previous work to affect the attenuation of TOrC in activated sludge systems, among them hydraulic residence time (HRT), solid retention time (SRT), pH, and temperature. *Quantitative* relationships between these factors and TOrC removal have not yet been systematically established; therefore, our ability to predict TOrC removal during conventional wastewater treatment is limited.

ES.2 Project Approach

This study was initiated with a comprehensive literature review on the existing knowledge on the fate of TOrC during conventional treatment and relevant characteristics of TOrC to assess their suitability to serve as potential performance indicators. The removal of TOrC during secondary treatment was studied on full-, pilot-, and bench-scale levels to assess the influence of operational parameters on TOrC removal efficiency. Biotransformation and sorption characteristics of selected TOrC were quantified in controlled laboratory-scale experiments to support modeling efforts for predicting TOrC reduction during full-scale treatment.

ES.3 Indicator Compounds

Twenty-two TOrC performance indicators were selected from a database of over 240 compounds on the basis of occurrence levels and detection frequency in wastewater influents and effluents, physicochemical properties (i.e., sorption, biotransformation), and analytical amenability. TOrC indicators were quantified in this study using liquid chromatography-tandem mass spectrometry (LC MS/MS). This method was selected based on its ability to cover a comprehensive list of indicator compounds in one method and its high accuracy. Toxicological relevance of the indicator compounds was a secondary selection criterion. The compounds were classified into different bin groups based on their biotransformation kinetics and sorption characteristics during activated sludge treatment (Table ES-1).

Table ES-1. Summary Matrix of TOrC Indicators Based on Biotransformation and Sorption Fate Parameters.

Sorption (log K_d)		Biotransformation (k_b, L/g-d)		
		Slow <0.1	Moderate 0.1-10	Rapid >10
Low	<2.5	Carbamazepine Meprobamate Primidone TCEP Sucralose	DEET Sulfamethoxazole Gemfibrozil Iopromide Trimethoprim	Acetaminophen Caffeine Naproxen Ibuprofen Atenolol
Moderate	2.5-3	TCPP	Cimetidine	Benzophenone Diphenhydramine Bisphenol A
High	>3	Triclocarban		Triclosan Fluoxetine

The indicators selected exhibited a high detection ratio (>10) and detection frequency in wastewater influents. Only two of the targeted indicator compounds, DEET and caffeine, quantified in wastewater influent concentrations at different facilities throughout the U.S. exhibited a strong seasonal and regional dependency. All compounds can be analyzed with LC/MS-MS with isotope dilution, to date the most accurate and reliable method for quantifying TOrC in challenging matrices, such as raw wastewater. As the bin matrix in Figure ES-1

illustrates, the indicators cover a broad range of biotransformation and sorption characteristics relevant for removal during secondary treatment.

ES.4 Indicator Removal During Secondary Wastewater Treatment

The efficiency and mechanisms of TOrC removal were evaluated during full-scale activated sludge treatment under steady-state process conditions. Full-scale sampling was conducted at seven wastewater facilities in the U.S. during 13 independent sampling campaigns. This resulted in detailed TOrC mass balances primarily around the secondary treatment processes quantifying removal by sorption and biotransformation for each TOrC indicator. The selected facilities used Conventional Activated Sludge (CAS), High Purity Oxygen (HPO), Modified Ludzack-Ettinger (MLE), Biological Nutrient Removal (BNR), and Membrane Bioreactor (MBR) processes. Plant influent flows ranged from less than 1 mgd to over 90 mgd and operating SRTs from less than two to over 50 days.

The observed TOrC removal during secondary treatment could be linked to the bin categories established for the indicators on the basis of sorption and biotransformation properties measured in the mixed liquor of various wastewater treatment facilities (Table ES-1). The measured sorption and biotransformation characteristics were predictive of the removal efficiencies for the majority of TOrC indicators during full-scale secondary treatment. Table ES-2 summarizes the anticipated removal efficiencies of TOrC indicators during activated sludge treatment based on the nine bins. It is anticipated that similar efficiencies will be achieved for other TOrC that fall into the respective bin grouping based on their biotransformation and sorption characteristics.

Table ES-2. Anticipated Overall Removal of TOrC Based on Biotransformation and Sorption Characteristics.

Sorption (log K_d)	Biotransformation (k_b, L/g-d) Slow <0.1	Moderate 0.1-10	Rapid >10
Low <2.5	0-30% (Typical: 5%)	0-100% (Typical: 70-90%)	70-100% (Typical: 95%)
Moderate 2.5-3	0-60% (Typical 20%)	0-100%** (Typical 30-50%)	60-100% (Typical: 70%)
High >3	0-95% (Typical 50%)*	n.a.	0-100%*

Note:

* Data basis weak to estimate removal for this group.

** The anticipated removal can be narrowed for a specific compound and process operation by using the threshold $SRT_{80\%}$ identified in this study.

n.a.: not available

The selected 22 TOrC indicators distributed fairly evenly into the nine bins that characterize TOrC based on expected sorption and biotransformation. Generally, more TOrC indicators fell into the bins for TOrC with low sorption potential compared to the bins for TOrC with high sorption potential. None of the selected indicators represents TOrC with high sorption potential and moderate biotransformation.

Triclocarban represented TOrC with high sorption potential and slow biotransformation. This compound was not more than 50% removed during full-scale treatment independent of process and operational conditions. TOrC indicators that are rapidly biotransformed were almost completely removed in less than 3 hours hydraulic retention time during activated sludge treatment. Facilities operating at SRTs above 7-10 days are anticipated to see similar high removal efficiencies (> 80%) for all TOrC indicators in the bin category rapid transformation and low sorption (i.e., acetaminophen, caffeine, naproxen, and ibuprofen). Only facilities operating at much shorter SRTs are anticipated to experience distinct differences in the removal efficiencies of compounds that fall into this bin.

TOrC indicators that were moderately biotransformed ranged in removal anywhere from 0 to 100% removal depending on activated sludge operation. Threshold SRT values could be identified for all bioamenable TOrC indicators ranging from 2 to 30 days. Operation above the threshold SRT is anticipated to result in at least 80% removal of the respective TOrC during secondary treatment (Table ES-3).

Several indicators were not effectively removed during secondary treatment independent of process operation (less than 30% reduction). They included TOrC that were low in sorption and biotransformation potential (i.e., carbamazepine, primidone, TCEP, and sucralose). Advanced wastewater treatment is required to effectively attenuate these types of compounds. Implementation of advanced treatment processes is anticipated to also enhance the removal of TOrC in other bin categories.

Seasonal sampling revealed consistently higher TOrC removal efficiencies under summer compared to winter conditions during activated sludge treatment. The relationship between the biotransformation rates of TOrC removal and the removal efficiency was not linear during full-scale treatment. The removal of moderately biotransformed TOrC drastically increased in mixed liquor when biotransformation rates exceeded 0.2 to 1 L/g-d. The biotransformation rates for DEET and caffeine were generally multiple times greater in mixed liquor systems that received higher concentrations of these TOrC in the aeration basin influents.

Centrate return streams from anaerobic digestion contributed a significant fraction of certain TOrC to the overall secondary influent load. For the compounds carbamazepine, TCPP, ibuprofen, bisphenol A, and gemfibrozil the mass contribution to the secondary influent amounted to 5-65%.

Table ES-3. Threshold SRT Values to Achieve at Least 80% TOrC Removal.

	SRT, days
Acetaminophen	2
Caffeine	2
Ibuprofen	5
Naproxen	5
Bisphenol A	10
Triclosan	10
DEET	15
Gemfibrozil	15
Atenolol	15
BHA	15
Iopromide	15
Cimetidine	15
Diphenhydramine	20
Benzophenone	20
Trimethoprim	30

ES.5 Modeling the Fate of TOrC During Secondary Treatment

Several TOrC fate models were evaluated for their ability to predict the removal of different TOrC indicators during full-scale treatment. Of these fate models, ASTreat was selected for further evaluation because of its simplicity of input requirements and ability to model the fate of TOrC during solid and liquid stream treatment. Given our current level of understanding on the mechanisms driving TOrC removal during conventional treatment and the current sophistication of TOrC fate models, the goal of the model evaluation was to assess the usefulness of such tools as screening approaches for estimating the fate of TOrC during conventional treatment.

One of the biggest limitations with existing mass balance models is the lack of appropriate fate parameter values (i.e., biotransformation rate constants, sorption coefficients) that are needed as model inputs. While sorption properties for most compounds are often already published or can be easily quantified, biotransformation rates are not easily measured and are system specific.

The ability of ASTreat to predict TOrC indicator removal was validated for several full-scale facilities. The model input included the sorption coefficients and biotransformation rates determined for the TOrC indicators for different operational regimes as well as general process characteristics and process conditions. The reliability and accuracy for the different bin categories are summarized in Table ES-4. Twelve compounds exhibited less than 10% deviation from model predictions (i.e., acetaminophen, caffeine, carbamazepine, DEET, ibuprofen, meprobamate, naproxen, primidone, sucralose, TCEP, triclocarban, and triclosan). Seven compounds exhibited agreement with model predictions in 40-60% of all modeled cases

(atenolol, cimetidine, diphenhydramine, gemfibrozil, iopromide, sulfamethoxazole, and trimethoprim). Thus, the accuracy of ASTreat to predict the TOrC removal efficiency during wastewater treatment was compound and bin specific.

Table ES-4. Anticipated Modeling Accuracy for TOrC Using ASTreat.

Sorption (log K_d)	Biotransformation (k_b, L/g-d) Slow <0.1	Moderate 0.1-10	Rapid >10
Low <2.5	High accuracy, reliable	Medium accuracy, partially reliable	High accuracy, reliable
Moderate 2.5-3	n.a.	Medium accuracy, partially reliable	Low accuracy
High >3	High accuracy, reliable	n.a.	Variable* (Low for certain compounds, High and reliable for others)

Notes:
High accuracy: Anticipated model prediction generally within 10% of actual removal (light gray shading)
Medium accuracy: Anticipated model prediction within 20% of actual removal for approximately half of attempted field sites (medium gray shading).
Low accuracy: Anticipated model prediction poor and generally not within 30% of actual removal.
* The accuracy and reliability of TOrC in the group of rapidly degradable and highly sorptive compounds was very compound specific.
n.a. Modeling of representative TOrC Indicators in this group was not conducted in this study.

Compounds with moderate biotransformation kinetics were difficult to predict. The most challenging compounds were those with both high biotransformation rates and sorption coefficients. Improving model predictions for these challenging compound groups hinges on the ability to better predict biotransformation in the field, and the possible dynamics of TOrC accumulation on solids and desorption in the activated sludge system (i.e., for highly sorbable and rapidly degradable compounds such as fluoxetine).

Despite the accuracy of model predictions for certain bin groups (i.e., rapid biotransformation and low sorption as well as slow biotransformation), specific inaccuracies with model predictions identified in this study limited the reliability of TOrC removal predictions for other bins (i.e., rapid biotransformation and moderate or high sorption). The following model limitations were identified:

- Biotransformation rate measurements in the laboratory were inconsistent for a few of the investigated compounds. Thus, the reliability for model outputs was low because this input parameter significantly affects model predictions for bioamenable compounds.
- Desorption kinetics, which are currently not being modeled in ASTreat, could play an important role in the overall removal of moderately sorptive and biodegradable compounds.
- Other process parameters, such as anoxic zones, may affect sorption, desorption, or biotransformation in the field, and are currently not sufficiently understood to quantify their effects (i.e., the effect of redox conditions) in a mass balance model.

ES.6 TOrC Removal During Anaerobic Digestion

Selected TOrC indicators were monitored at Facility A to assess the fate and removal efficiency of TOrC during full-scale anaerobic digestion. Two compounds with very different properties (caffeine and triclocarban) were detected in significant concentrations (lower µg/g TSS) in thickened primary sludge (TPS) at Facility A, indicating that two groups of TOrC compounds are likely to show significant mass fluxes in primary sludges: a) hydrophilic TOrC like caffeine (low sorption) present in high concentrations (µg/L range) in wastewater influents, and b) hydrophobic TOrC like triclocarban (high sorption) with low biotransformation potential even if present at low concentrations (lower ng/L range) in wastewater influents.

Thickened waste activated sludge (TWAS) generally carried lower solid concentrations than TPS for TOrC indicators that are low in sorption and either slowly or rapidly biodegraded (i.e., carbamazepine, TCEP, caffeine, atenolol). Compounds with moderate or high sorption were generally detected at higher solid concentrations in TWAS compared to TPS (TCPP, triclocarban, fluoxetine).

Compounds with moderate to high sorption potential in activated sludge were found to increase in solid concentration during anaerobic digestion, even if these compounds showed rapid biotransformation during aerobic activated sludge treatment (i.e., bisphenol A, fluoxetine). The increase in solid bound TOrC concentration during anaerobic digestion may be positively related to the VSS destruction efficiency. Biotransformation kinetics for all compounds were significantly slower during anaerobic digestion compared to aerated activated sludge treatment (the kinetic rates were several orders of magnitude lower on basis of a normalized TSS concentration). During a total HRT of 35 days in the two-stage anaerobic digestion, only rapidly and some moderately biotransformed TOrC were reduced in solid concentration (i.e., atenolol, caffeine, and trimethoprim). Other moderately biotransformed compounds (i.e., meprobamate and TCEP) were not reduced during digestion.

The mass flux of highly sorbable TOrC indicators in the dewatered biosolids cake can constitute a significant portion of the TOrC mass flux in the plant influent. These groups of compounds deserve specific attention in risk assessments of biosolid land applications.

Full-scale testing confirmed that TOrC with a biotransformation rate constant in excess of approximately 0.07 d^{-1} measured under laboratory conditions demonstrated more than 90% overall removal during full-scale anaerobic digestion (i.e., atenolol, caffeine, and trimethoprim).

ES.7 Key Study Conclusions

Indicator Selection

- The suite of TOrC performance indicators included in this study provided a useful screening tool for assessing the performance of secondary treatment processes for the attenuation of TOrC representing different biotransformation and sorption amenabilities. The suite of 22 compounds was categorized in this study into nine bins depending on their demonstrated removal efficiency by sorption and biotransformation. The indicators were not selected because they are regarded as compounds of highest concern. Instead they are proposed to provide a useful representation of the large number of TOrC in wastewater influents for the purpose of assessing treatment performance.

- The list of TOrC indicators investigated in this study and the proposed bin categorization provides a logic TOrC monitoring approach for wastewater treatment plants who are trying to assess their site-specific treatment efficiency for a large variety of TOrC. The list in its current form provides a reasonable distribution of the 22 indicators into the nine bin categories. However, there remains a need to amend the current proposed list specifically with additional TOrC indicators of medium to high sorption and low to medium biotransformation characteristics to better cover the full range of TOrC potentially present in wastewater influents and effluents.
- The 22 TOrC indicators provided a useful suite of compounds to characterize the TOrC removal performance of a variety of treatment plants. Depending on process and operational conditions at a specific treatment plant the list of key performance indicators may be further narrowed. For example, facilities operating at long SRT may find that compounds in the bin "rapid biotransformation and low sorption" provide redundant information (i.e., very efficient removal for all compounds). It should be noted that reducing the number of TOrC does not necessarily reduce the analytical costs of a sampling program as commercially offered analysis may target a large number of TOrC as part of a single analytical method.
- The suite of compounds in this study was selected for the function of addressing treatment efficacy of different processes for compounds sharing similar chemical structures and biotransformation properties rather than for reduction of risk. A suite of target TOrC from a risk perspective can, however, be mapped amongst the suite of performance indicators based on shared physical and bio-kinetic properties. Linking compound databases on basis of physical, bio-kinetic, and risk data may allow identifying, engineering, and evaluating treatment process configurations to achieve a specific target whole effluent toxicity.

Liquid Stream Treatment Efficiency

- Solid retention time, hydraulic retention time, wastewater temperature, solids recycles, redox conditions, overall process stability, and TOrC influent concentrations were important factors affecting the removal efficiency of TOrC through sorption and biotransformation. These relationships could be quantified in this study and are helpful to predict TOrC removal during conventional treatment on basis of process configuration and operational boundary conditions.
- Facilities that operated at long SRTs demonstrated generally higher removal efficiencies for TOrC that are amenable to biotransformation than facilities operating at short SRTs. This finding indicates treatment synergies between TOrC removal and nitrification for facilities that are operating at a high level of secondary treatment to meet low ammonia limits.
- Conventional secondary treatment does not provide a significant barrier against TOrC that fall into the bin slow biotransformation and low sorption. Removal of these compounds requires advanced treatment processes beyond conventional wastewater treatment.
- Primary treatment removed TOrC indicators that were moderately to highly sorbable between 5-35% with slightly higher removal performances (additional 10-30%) when chemically enhanced primary clarification was practiced.
- Findings of this study did not indicate that the addition of anoxic conditions during secondary treatment at facilities operating in denitrification mode improved the removal of TOrC indicators. Several moderately biotransformed compounds showed an increase in liquid phase concentration after anoxic treatment before being removed in the aerobic portion of the aeration basins. Thus, anoxic conditions did not compromise the overall

treatment efficiency for TOrC during secondary treatment. The increase in liquid phase concentration after anoxic treatment could have been caused by desorption of solid bound TOrC under oxygen deficient conditions. Similar desorption processes may also occur when solids are temporarily stored in secondary clarifiers and may lead to temporary increased TOrC concentrations in secondary effluents.

- The TOrC load associated with solids in the secondary effluents was significant for highly sorbable TOrC such as triclocarban, triclosan, and fluoxetine (5-70% of the secondary effluent TOrC load in the liquid phase). This suggests that tertiary processes targeting additional particle removal (such as filtration) will also significantly reduce the concentration of hydrophobic TOrC in the final effluent. For the majority of TOrC indicators that were low or moderately sorbable TOrC loads associated with secondary effluent TSS were less than 5% of the total secondary effluent loads.

Occurrence of TOrC in Solid Streams

- Some highly and moderately sorbable TOrC were found in significant amounts on the waste activated sludge solids from secondary treatment systems (10 to more than 100% of secondary influent loads). The recalcitrant and highly sorbable TOrC triclocarban accumulated on the solids in systems operating under long SRTs. Several recalcitrant TOrC were not reduced during anaerobic digestion but were found in increased concentration in the digested sludge (i.e., carbamazepine, TCEP, TCPP). This finding highlights the importance of investigating means to reduce TOrC associated with solids during the wastewater treatment process to minimize internal recycling and TOrC loads in biosolids.
- The relevant loads of certain TOrC detected in recycle streams from solid treatment suggest that increasing the attenuation of TOrC during wastewater treatment through side stream treatment of filtrate and centrate deserves further consideration.

Predicting TOrC Removal during Conventional Wastewater Treatment

- TOrC modeling was conducted in this study using ASTreat, due to its free access, simplicity, and suitability from a utility perspective regarding easily available input parameters. The fundamental effort of this study to develop indicator-specific fate parameters for sorption and biotransformation provides the necessary basis for the application and evaluation of other TOrC fate models that could not be considered within the scope of this study.
- The accuracy and reliability of TOrC fate modeling was improved by determining accurate compound-specific biotransformation rate parameters and sorption coefficients as model inputs. The library of fate parameters developed in this study can give guidance for selecting appropriate biotransformation rate constants and sorption coefficients for the TOrC indicators for future use based on general activated sludge process conditions.
- ASTreat proved to be a useful screening tool for predicting the removal of most TOrC indicators under full-scale treatment. The accuracy of predicting the removal for TOrC that are moderately fast biotransformed was improved by recognizing that TOrC biotransformation rates are a function of the operating SRT. The fate prediction of TOrC that are sorbable and rapidly biotransformed remains a major challenge, as these compounds appear to accumulate on the solids during treatment, making a steady-state performance analysis, as attempted in this study, challenging.

Cost Evaluation

- This study helps define the costs and benefits of process alternatives targeting TOrC removal for both conventional and advanced treatment.
- While there is for many utilities no pressing need to take action on TOrC from a compliance point of view, it is prudent to consider future regulatory trends in today's planning processes. Many utilities are currently required to invest in process upgrades in order to comply with more stringent nutrient limits for nitrogen and phosphorus. This study helps to define and quantify synergies between specific process upgrades that may find consideration for improving nutrient removal and benefit TOrC removal. Integrating considerations in today's master planning efforts on how the implementation of treatment processes or modifications for near-term permit compliance effect the attenuation of TOrC could result in more comprehensive, cost-effective compliance strategies in the long term.

CHAPTER 1.0

INTRODUCTION

1.1 Introduction

Trace organic compounds (TOrC) are discharged from multiple sources into municipal wastewater. Because of concerns related to public and aquatic health, there is increasing interest in evaluating occurrence and removal of TOrC during wastewater treatment and water reclamation. No systematic and comprehensive work has fully described the dimensions of TOrC issues in wastewater treatment, including origins, fate, and transport. Various approaches have been proposed to estimating TOrC concentrations in raw sewage and treated effluents. Some of these studies have focused on closed systems such as hospitals (Kümmerer et al., 1997), utilization of prescription rate data in combination with per-capita sewage volume (Stuer-Lauridsen et al., 2000; Huang et al., 2001; Sedlak and Pinkston, 2001), production data of high-production volume chemicals (Drewes et al., 2008), and physicochemical information and mass balances approaches (Ternes et al., 2004; Khan and Ongerth, 2004) to predict the concentration of TOrC in secondary treated wastewater. Up to now, concentration predictions derived from these studies for raw sewage and secondary treated effluent qualities can only be considered as illustrative due to our limited understanding of process performance for the removal of large numbers of TOrC during wastewater treatment.

There are a number of factors which have been identified in previous work to influence the removal of TOrC in activated sludge systems, among them hydraulic residence time (HRT), solid retention time (SRT), food-microorganism ratio (F/M ratio), mixed liquor suspended solids (MLSS), pH, and temperature. *Quantitative* relationships between these factors and TOrC removal have not yet been systematically established.

Facilities attempting to assess treatment performance for TOrC removal often monitor TOrC based upon commonly available laboratory capabilities. This approach does not consider the wide range of physical and chemical properties of TOrC and thus does not evaluate removal over a range of characteristics. Naturally, we can only monitor a very small fraction of all TOrC that are present in wastewater influents and effluents as TOrC analysis is still in development and expensive. Deciding on the compounds that should be analyzed depends on the goals of the monitoring campaign. Is a study driven by the concern of a potential endocrine disrupting effect in the receiving water? Does a utility seek to gain a general understanding of treatment performance for TOrC removal during specific operational conditions? The recommended compounds to analyze for and even the analytical methods to be used will be different depending on the question asked. This study attempted to provide guidance to utilities on the question related to *treatment performance* for TOrC with a range of physical and chemical properties. A limited toxicological review was, however, included for the indicators focused on in this study.

The identification of TOrC performance indicators must be based on a logical selection considering removal mechanisms and compound properties that are critical during treatment. Those indicators are only useful in practice if analytical methods are robust and commercially available. Although regulatory requirements that define discharge limits for TOrC in the United

States do not exist today, a growing number of facilities are proactively addressing the concerns related to TOrC in the aquatic environment through master planning efforts, while a selected few are adding treatment in advance of regulations. Since discharge of treated wastewater effluent must protect beneficial uses of receiving streams, including fishing, swimming, recreation, and municipal drinking water supply, minimizing the discharge of harmful TOrC is desirable. Even though conventional wastewater treatment has not been designed with the goal to remove TOrC specifically, it is known that TOrC are partially removed during primary and secondary treatment and to some extent during final disinfection. Continuous progress is being made in understanding the toxicological effects of specific TOrC on the environment, with the goal of determining environmentally acceptable concentrations for TOrC in domestic effluents. From the perspective of a facility operator, it is valuable to understand the performance of *existing* wastewater treatment processes for TOrC removal, which may be used to assess the viability of advanced treatment needs.

The suite of TOrC performance indicators must be comprehensive and cover compounds representing a wide spectrum of removal observed for TOrC during conventional treatment: Compounds that are generally very easily removed those that are persistent, and compounds for which removal efficiencies vary dependent on site-specific wastewater treatment and operational conditions. TOrC released to wastewater by consumers are numerous and they are diverse in structure, size, persistence, and occurrence patterns. Claiming that any suite of indicators fully represents the diversity of chemicals and their behavior during wastewater treatment would be inaccurate. At the same time, it is obvious that without categorization and indicator identification the task to understand and predict the fate of TOrC during wastewater treatment is not manageable. Linking mechanisms of TOrC indicator removal to specific operational factors provides a means by which wastewater treatment plant operations can be generally categorized and optimized for TOrC removal. Studying a limited number of these indicator compounds in detail may allow quantifying minimum process criteria to achieve a certain removal for a broader TOrC group, e.g., “moderately fast degradable compounds” or “highly sorptive compounds”. Even though this approach to predict TOrC removal is still empirical from a process standpoint, it is similar to traditional design approaches commonly used for conventional wastewater constituents, such as BOD, nitrogen, or phosphorus. In this study, biotransformation and sorption properties are evaluated as the basis for linking a wide range of TOrC to specific indicators.

1.2 TOrC Removal During Conventional Wastewater Treatment

Findings from previous studies have demonstrated that sorption onto suspended solids, aerobic and anaerobic biotransformation, chemical (abiotic) attenuation (via processes such as hydrolysis), and volatilization are the primary removal mechanisms for TOrC during conventional wastewater treatment (Clara et al., 2005; Stevens-Garmon et al., 2011). Aqueous solubility and hydrophobicity determine whether and to which extent compounds are physically removed. For the majority of more polar TOrC, removal during primary treatment by sorption onto primary sludges is negligible (Dickenson et al., 2010). As chemical attenuation is very compound specific it was not a focus of this study. Equally, volatilization is only relevant for specific compounds with high vapor pressures, not for the majority of TOrC found in wastewater and wastewater effluents.

Physicochemical properties will influence whether a TOrC will remain in the aqueous phase (like many of the acidic, neutral, and basic hydrophilic pharmaceuticals) or interact with solid particles (such as estrogens or certain antibiotics, which have a higher potential to be

sorbed to sewage sludges). Sorption and volatilization are physical processes and their relevance for specific contaminants can be predicted using physicochemical property information (Rogers, 1996). Hydrophobic contaminants may partition onto primary or secondary sludge solids and the tendency to accumulate in sludge solids can be assessed using the octanol-water partition coefficient (K_{ow}).

Structural properties of TOrC will also determine the likelihood for biotransformation of the parent compound. The susceptibility of TOrC for microbial biotransformation and sorption differs widely during activated sludge treatment. Biotransformation of TOrC might occur during secondary treatment, which involves the biological treatment of wastewater constituents in fixed film or suspended growth systems, and during sludge digestion. Secondary treatment can occur under aerobic, anoxic, and/or anaerobic conditions in many different process configurations targeting different levels of nutrient removal. Although the mechanism of degradation of the bulk organic matter of wastewater during aerobic and anaerobic processes is well understood (Tchobanoglous, 2003), the effects of such processes on TOrC occurring at the parts-per-trillion (ppt) level have received relatively little focused study. For degradable compounds, several operational factors such as SRT (Oppenheimer et al., 2006) seem to be correlated with removal, resulting in lower effluent TOrC concentrations for longer SRTs. However, the factors affecting TOrC attenuation during secondary wastewater treatment have not been systematical identified yet or been described in a way that would allow predicting removal efficiencies. This will help identifying those compounds that are partially or completely persistent through biological treatment processes because of properties that impede degradation and/or attenuation and that may therefore require additional treatment.

There is also a need for developing and assessing the accuracy of fate models to improve our ability to accurately and broadly predict the removal of TOrC during secondary treatment processes. Modeling the TOrC removal mechanisms allows a comparison between model predictions and field observations. In the case that the model predictions are in close agreement with actual removal observed in the field this supports that the major TOrC removal mechanisms are adequately identified and accurately described in the form of quantitative functional relationships. If, however, model predictions vary significantly from field observations, this reveals that the mechanisms for TOrC removal may be more complex than we are currently able to express in mathematical equations.

1.3 Objectives

This study was designed to address the general knowledge gaps summarized in the previous section. Specifically, this study was tailored to address six primary objectives related to occurrence and fate of TOrC during conventional wastewater treatment. These six objectives are listed below with a brief description of the research approach selected by the project team. The objectives were:

1. **To identify suitable candidate indicator TOrC that allow for a rapid characterization of performance efficiency of conventional wastewater unit operations.**

This objective was addressed by conducting a comprehensive review on occurrence and fate of TOrC in raw sewage and treated wastewater effluents. This review generated a short list of proposed indicator TOrC that allow a rapid preliminary characterization of secondary

treatment process efficiencies for TOrC removal. The selected indicators were further used for fate model calibration and validation.

2. To generate performance data at full-scale that allowed an assessment of mechanisms responsible for TOrC attenuation in secondary treatment unit operations.

Detailed mass balances for TOrC were generated at seven full-scale facilities employing different secondary wastewater treatment processes. Treatment processes that were evaluated included non- or partly-nitrifying activated sludge systems, fully nitrifying activated sludge systems, denitrifying activated sludge systems, and biological phosphorus removal processes. Evaluations in this study focused on suspended growth activated sludge processes, as those systems comprise the majority of secondary treatment operations in the U.S. and elsewhere.

3. To elucidate the effect of wastewater treatment operational parameters on the fate of TOrC indicators during laboratory- and pilot-scale studies.

Full-scale efforts were augmented by controlled experiments at the laboratory- and pilot-scale to enable the further development and thorough evaluation of observed relationships between operational parameters and TOrC removal. Functional relationships between critical process variables (e.g., SRT) or biological nutrient removal (BNR) process combinations and TOrC removal efficiencies were developed for various secondary treatment unit operations. In addition, biotransformation rate constants and sorption coefficients for various operational conditions were derived that were utilized in TOrC fate modeling.

4. To develop guidance on how to describe and predict removal efficiencies for a wide range of TOrC.

This effort comprised a critical evaluation of existing TOrC fate models for conventional wastewater treatment operation, the calibration of a viable fate model based on the performance of full-scale facilities, and validation tests of this fate model at full-scale using various process configurations and operational conditions.

5. To assess the removal of TOrC indicators during anaerobic digestion.

Controlled laboratory-scale studies were conducted to investigate the fate of TOrC during anaerobic digestion. The fate model was expanded to a simulation of TOrC removal during anaerobic digestion and was calibrated based on laboratory-scale data and field monitoring efforts at a full-scale digestion facility.

6. To assess the costs of various treatment system modifications to achieve TOrC removal.

This study assessed the performance and costs of modifying and operating a secondary process for a given target TOrC reduction and compared these costs to those of alternative treatment processes effective at achieving TOrC reduction, such as membrane filtration, ozonation, or carbon based ballasted sedimentation.

1.4 Background and Significance

The following illustrates still existing data gaps related to the focus of this study. Sampling strategies employed in many previous studies were not adequate in drawing detailed conclusions on the efficacy of treatment processes for TOrC removal (e.g., grab vs. flow-based composite sampling during dry or wet weather, duration of composite sample collection, etc.). Previous research has focused in detail on investigating processes at batch- or laboratory-scale conditions that limit performance extrapolation to full-scale settings. Limited work has been done to date to systematically explore the impact of different operational factors on TOrC removal. Other times, analytical methods have been utilitized that did not properly account for matrix effects resulting in an underestimation of TOrC concentrations. Studies have often been limited to a short list of target chemicals or were not able to distinguish between sorption and biotransformation for TOrC attenuation during liquid and solid stream treatment.

1.4.1 Removal During Primary and Secondary Treatment

Among others, Moehle and Metzger (2001) conducted controlled batch experiments with pharmaceutical residues simulating activated sludge treatment and observed an initial loss in concentrations of fortified wastewater after 15 minutes of exposure to activated sludge. This removal of acidic and neutral drug residues (e.g., diclofenac, propyphenazone, carbamazepine, primidone) was attributed to initial sorption to the sludge although these compounds span a wide range of hydrophobicities (log K_{ow}), which would not suggest a high tendency to sorb onto biosolids. Likely, the sorption observed in these experiments was not in equilibrium and Ternes et al. (2004) reported no appreciable sorption of carbamazepine onto biosolids in their controlled experiments. Kreuzinger et al. (2004) investigated highly loaded activated sludge plants with a SRT of 1 day or less and observed no removal of select pharmaceutical residues (i.e., ibuprofen, diclofenac, bezafibrate). During activated sludge treatment, ibuprofen and naproxen were removed by 60-70% and 40-55%, respectively (Carballa et al., 2004). Clara et al. (2005) reported no removal of ibuprofen in a non-nitrifying full-scale facility with short SRT (2 days), but a removal of 98% in a denitrifying facility with a SRT of 48 days. Findings of this study allowed deriving a critical SRT of 10 days for complete removal of ibuprofen in activated sludge systems. Additional findings derived from controlled laboratory studies revealed a residence time of wastewater in excess of 6 hours for complete removal of ibuprofen (Buser et al., 1999).

In the studies conducted by Clara et al. (2005) and Strenn et al. (2004), contradictory results were obtained for diclofenac where a significant removal was observed in some facilities, whereas in other wastewater treatment plants at comparable SRTs no or only slight removal was obtained. Similar contradictory results are documented in the literature for diclofenac. Buser et al. (1999) and Heberer (2002) reported no significant removal of diclofenac during wastewater treatment. Two studies (Ternes, 1998; Ternes et al., 1999) reported an elimination of diclofenac in excess of 70%, and one study (Clara et al., 2005) listed a removal between 40 and 60%, respectively. On the other hand, the results of Ternes (1998) and Stumpf et al. (1999) documented a removal of 15% during trickling filter treatment, 34% during activated sludge treatment, and 51% in an activated sludge system using ferric chloride. The reasons for these performance differences are unknown.

Steroid hormones, including 17α-ethinylestradiol (EE2), are deconjugated quickly through enzymatic hydrolysis in the wastewater collection system or primary treatment process introducing the biologically active form of EE2 into wastewater (Huang and Sedlack, 2001; Andersen et al., 2003; D'Ascenzo et al., 2003). Facilities employing nitrogen removal (nitrifying or nitrifying/denitrifying) can achieve effluent concentrations of EE2 consistently below 1 ng L^{-1}. During a pilot-scale study simulating an activated sludge process, Onda et al. (2003) were unable to establish strong correlations between estrogen removal and BOD loading or other operational conditions. By measuring mass fluxes of EE2 at a full-scale nitrifying/denitrifying facility, Andersen et al. (2003) were able to quantify that about 90% of the EE2 was eliminated through aerobic degradation. The sorbed load of EE2 onto the excess and digested sludge at this facility was lower than 6% of the inlet load suggesting little removal of EE2 through sorption onto suspended solids, which is supported by rather small sorption coefficients for EE2 onto colloidal organic carbon derived from activated sludge as determined by others (Ternes et al, 2004; Holbrook et al., 2004; Yamamoto and Liljestrand, 2003). The plant targeted in this study had just been updated to achieve nutrient removal at SRTs of 11-13 days. Prior to the update, the facility operated at SRTs of less than 4 days and a previous study at the same facility had revealed only minor reductions of estrogens (Ternes et al, 1999). In a study reported by Drewes et al. (2005), a non-nitrifying facility with a SRT of less than 1.7 days achieved only a 70% removal of EE2 with an effluent concentration of 4.1 ng L^{-1}, whereas all nitrifying plants employing longer SRTs exhibited effluent concentrations of less than 0.7 ng L^{-1}. Consistently higher concentrations of EE2 in non-nitrified effluents representing short SRTs were also reported in other studies (Desbrow et al., 1998; Huang and Sedlack, 2001) stressing the fact that longer SRTs seem to promote the growth of microorganisms capable of degrading EE2. Longer SRTs can also result in modified sorbent characteristics as suggested by Holbrook et al. (2000), which might be beneficial for estrogen mineralization as well. Controlled experiments conducted by Shi et al. (2004) with nitrifying activated sludge collected from a facility employing longer SRTs demonstrated very similar degradation rate constants for natural hormones and the synthetic hormone EE2. The study also confirmed that a consortium of bacteria rather than an individual species (such as *Nitrosomonas europaea*) is likely responsible for the biotransformation of estrogens including EE2. Since nitrifying bacteria have a lower growth rate at lower temperatures, prevalent during winter operation, ammonia removal is usually lower during winter months. Monitoring studies available today; however, do not suggest that a declining nitrification activity will also result in a less efficient removal of EE2 (Baronti et al., 2000; Desbrow et al., 1998; Belfroid et al., 1999).

The removal efficiencies of TOrC during primary and secondary treatment have been highlighted in previous review articles authored by members of the research team (Drewes and Shore, 2001; Drewes, 2007; Snyder et al., 2008). Lessons learned from these reviews are that many studies published in the peer-reviewed literature regarding TOrC removal during conventional wastewater treatment have either utilized simplistic batch reactors receiving synthetic feed water that poorly represents municipal wastewater qualities, employed spiked target compounds orders of magnitude above ambient levels, conducted experiments that did not allow full adaptation of biocommunities, failed to report the operational boundary conditions of laboratory-, pilot- or full-scale reactors employed in these studies, or used analytical methods that did not properly account for matrix effects resulting in underestimation of TOrC concentrations. Findings of these studies do allow some qualitative estimation of key removal pathways of TOrC during conventional wastewater treatment and the relationship between

operational parameters and physicochemical characteristics of the compounds, but the knowledge base is insufficient to develop accurate and predictive fate models.

1.4.2 Modeling the Fate of TOrC During Secondary Treatment

During the last two decades, several steady-state models have been developed to predict the fate of chemicals during wastewater treatment plants (Sruijs et al., 1996; Cowan et al., 1993; Clark et al., 2002; McAvoy et al., 1999; Khan and Ongerth, 2004). It is noteworthy that these models are not intended to simulate conditions in an actual plant in detail, but instead provide a screening level model of chemical fate. In general, these mass balance models account for partitioning (between biomass, aqueous, and gaseous phases), transport, and transformation processes that affect TOrC through primary and secondary wastewater treatment. One of the biggest limitations with existing mass balance models is the lack of appropriate fate parameters (i.e., degradation rate constants, partitioning coefficients) that are needed as model inputs.

1.4.3 The Fate of TOrC During Anaerobic Digestion

Wastewater treatment plants have been identified as a major source of TOrC to receiving environments (aquatic and terrestrial). While implications of their release to the environment are still being evaluated, most research to date has focused on liquid phase removal during wastewater treatment (i.e., primary and secondary treatment) and effluent concentrations entering aquatic environments. Since a significant amount of biosolids in the U.S. are land applied for beneficial use, recent concerns about TOrC exposure in terrestrial environments have illustrated the importance of understanding the fate of TOrC during sludge digestion as well as the need to predict TOrC concentrations in biosolids.

The goal of the anaerobic digestion evaluation was to fill knowledge gaps between the removal of TOrC in primary and secondary treatment, and TOrC attenuation during anaerobic sludge digestion. This goal was accomplished by investigating the fate of select indicator TOrC in laboratory-scale bioreactors, determining sorption coefficients and biotransformation rate constants using existing standard laboratory test methods, and analyzing sludge and biosolids samples at a full scale wastewater treatment plant to characterize the mass balance of select indicator TOrC in anaerobic sludge digestion and dewatering.

1.5 Study Overview

The following chapters of this report contain relevant information on the procedure, findings, and conclusion of this study. More detailed information on methods and data is available in the appendices of this report. The study included a literature review that resulted in a database summarizing existing knowledge on the fate of TOrC during conventional treatment and relevant characteristics of TOrC to assess their value as potential performance indicators. The removal of TOrC during secondary treatment was studied on full-, pilot-, and bench-scale level to assess the influence of operational parameters on TOrC removal efficiency. Biotransformation and sorption characteristics of selected TOrC were quantified in controlled laboratory experiments to support modeling efforts to predict TOrC reduction during treatment. The study of TOrC removal during anaerobic treatment included full-, and pilot-scale investigations, as well as the quantification of biotransformation and sorption characteristics of selected TOrC specific for an anaerobic digestion environment.

CHAPTER 2.0

MATERIALS AND METHODS

2.1 Project Approach

A comprehensive literature review was conducted that targeted the occurrence and fate of TOrC in full-scale wastewater treatment plants (WWTPs) in North America with emphasis on the influence of secondary treatment process type and operational parameters on TOrC removal.

2.1.1 Indicator Compounds

The available scientific publications concerning TOrC in full-, pilot-, and lab-scale activated sludge, biological, and membrane bioreactor WWTPs were screened. The database is based on the review of 56 papers and reports detailing full-scale sampling campaigns carried out in 18 countries. The database comprises information for 242 TOrC representing polar pollutants, pharmaceuticals, personal care products, natural and synthetic hormones, flame retardants, fungicides, herbicides, illicit drugs, plasticizers, X-ray contrast media, and the metabolites and degradation products of several TOrC.

Papers were selected if the concentration of TOrC had been analyzed in the plant influent and effluent. In order to be included, concentrations in the influent had to be above the limit of detection or limit of quantification (MDL and MQL, respectively). At a minimum, the studies had to report the percent compound removal. Papers or studies were not added to the database if influent or effluent concentrations were averaged across different treatment plants and not further distinguished for individual processes. Studies were also not considered in this review if treatment processes were not adequately defined (e.g., in terms of type of treatment process or key operational conditions). In the case of compounds that were rarely reported (i.e., organophosphates), papers with very few WWTP details were included.

Recently, the United States Environmental Protection Agency (U.S. EPA) published results from a review of the recent literature on wastewater treatment technologies and their ability to remove a number of emerging TOrC (U.S. EPA, 2010). However, the study was not as comprehensive as the review performed herein for activated sludge systems and the U.S. EPA study provided limited operational parameters, such as SRT and HRT.

Table A-1 in Appendix A contains the database of the literature review in electronic format. As available from the peer-reviewed literature the database includes details on the:

Operational condition of the treatment plants studied (i.e., capacity, type of treatment, basic water quality parameters),

- TOrC influent and effluent concentrations.
- Operational parameters (HRT, SRT, temperature, MLSS, BOD, TSS, TKN),
- Sampling strategies (i.e., preservation technique).
- Analytical methods employed (i.e., method detection limits, recoveries, accounting for matrix effects, use of isotope standards for recovery correction, sensitivity using tandem mass spectrometry, laboratory and field blanks, proper quality assurance/quality control (QA/QC) to demonstrate proficiency).

- Type of data reported (i.e., mean, median, average, standard deviation, number of replicates).

In a second database, potential TOrC indicator candidates were summarized and compared (Table A-2 in Appendix A submitted in electronic format). This list contained over 200 TOrC that were assessed in terms of four criteria to select indicator compounds for this study:

1. Detection frequency and occurrence
2. Analytical amenability
3. Physicochemical compound properties
4. Toxicological relevance.

Occurrence was assessed using the concept of the "detection ratio (DR)", which is defined as the ratio of the median observed concentration and the method detection limit (MDL). Table A-1 in Appendix A lists the occurrence of TOrC and their corresponding concentrations in plant influent or after primary clarification. In this study, TOrC were considered as potential indicator candidates if the detection ratio was larger than 10 and the detection frequency (DF) was larger than 80%. In addition, reported TOrC concentrations in raw sewage or primary effluents needed to exceed 1,000 ng/L for a compound to be considered in the list of potential indicators for this study.

As an example, perfluoroacetic acid (PFOA) and perfluorooctane sulfonate (PFOS) along with nonyl- and alkylethoxycarboxylates (NPEO, APECs) were considered in the evaluation, but they present an "occurrence" challenge as they are either formed or transformed into breakdown products during wastewater treatment, thus making degradation difficult to track. Accordingly, these compounds were not recommended for further evaluation as indicators in this project.

The removal of TOrC during conventional wastewater treatment depends on their physicochemical properties, i.e., volatilization, sorption, and biotransformation characteristics. For this study, it is proposed that the fate of an indicator compound during conventional wastewater treatment will offer insight into the treatability for other TOrC that have similar physicochemical properties. The potential of a compound for sorption on primary and secondary sludges can be estimated by physicochemical compound properties, such as the octanol-water partitioning coefficient K_{ow}. Biotransformation depends on the presence and character of compound fragments or functional groups, which can enhance or retard biological attack and breakdown.

Physicochemical properties relevant for treatment performance indicators include:

- The molecular weight.
- The octanol-water partitioning coefficient at pH 7 (log D_{ow}).
- The state of ionization (whether a compound is neutral, or negatively or positively charged).
- The structure of the compound.

Significant compound structural fragments are shown in Table A-2 and are sorted according to fragments that have an enhancing effect on biological attack and fragments that have a retarding effect on biological attack. This analysis was based upon the examination of Organization for Economic Co-operation and Development (OECD) ready biodegradation tests for 884 discrete TOrC (Tunkel et al., 2000). In general, fragments that are important to

enhancing the effect of biodegradability include long unbranched alkyl chains with the number of carbon atoms ≥ 3, one or more hydroxyl groups attached to a chain structure, and one or more carbonyl, ester or acid groups attached to either a chain or ring structure. Fragments that commonly lessen biodegradability include the presence of one or more aromatic ring structures, one or more halogen substituents on either the chain or ring structure, a nitro group, four branched carbon atoms and anilines. In this study, the evaluation of TOrC indicators during wastewater treatment was limited to the parent compound. Metabolites of TOrC indicators were not identified nor quantified.

The ability to accurately analyze target compounds in raw sewage, treated wastewater, and solids samples at environmentally relevant concentrations is not a trivial task but critical in order to produce meaningful results. For example, due to frequent blank issues during analysis not only in our laboratories, phthalate compounds were not considered viable indicator TOrC for performance assessments.

In this study, selection preference was given to compounds that can currently be analyzed by the liquid chromatography-tandem mass spectrometry (LC/MS-MS) isotopic dilution method (Vanderford and Snyder, 2006). This method accounts for matrix effects and potential recovery losses, and provides the most accurate and reliable results to date for quantifying TOrC in challenging matrices, such as raw sewage, treated effluents, and on solids. The TOrC database presented in Table A-1 indicates whether a compound can currently be analyzed using the LC/MS-MS isotopic dilution method. Some TOrC groups that are of public interest cannot be analyzed using this method and were thus not included in the suite of indicator candidates, among them brominated flame retardants (gas chromatography-mass spectrometry (GC/MS) analysis needed). For cimetidine and diphenhydramine new isotopic dilution LC/MS-MS methods were established in this study.

The toxicological relevance of TOrC was of minor importance for the selection of indicator candidates in this study, as the purpose was to develop a suite of indicators for treatment *performance*. The selected indicators for this study and a brief summary of the toxicological assessment of the selected compounds is included in Chapter 3.0.

2.2 TOrC Mass Balances at Full-Scale Wastewater Facilities

Full-scale sampling was conducted at seven wastewater treatment utilities to establish mass balances on the TOrC indicator candidates. For anonymity, utility names were kept confidential. A general description of each field site is presented below. As available, information on treatment characteristics, discharge location, capacity, influent composition, industrial contributions, and relevant information on discharge limits were included.

A process flow schematic of each facility is provided in Appendix C with the identification of the TOrC sampling locations at each site. The sample locations were selected to enable the team to establish mass balances on TOrC removal in secondary treatment by taking all relevant recycle streams into account. At selected sites, additional sample locations were added to complete the picture on TOrC removal during primary treatment, tertiary treatment, or final disinfection. Data collected at these additional sampling locations is included in Appendix E for completeness, even though these results are not included in the results and discussion provided in Chapter 3.0.

A process overview of each facility is provided in Table 2-1. Specific operational and performance data is summarized in Appendix D for each sampling event conducted in this study. Sampling was conducted during a time that represented steady-state performance of the secondary treatment process. Parameters used to assess steady state conditions were influent flow and loads, process operation (SRT, MLSS concentration, etc.), and process performance.

2.2.1 Facility A

Facility A is a secondary treatment facility utilizing primary clarification followed by an Modified Ludzack-Ettinger (MLE) activated sludge process. The MLE process is fully nitrifying and partially denitrifying without biological P-removal. Primary clarification at the facility removes about 50% of the BOD and more than 60% of the TSS load coming into the plant. The facility discharges into a creek after disinfection, which recently received increased public attention on the potential effects of TOrC on aquatic life. The activated sludge process came on line in the fall of 2007 and is currently treating 14 mgd average daily annual flow (ADAF). The influent composition is mostly residential sewage with small contributions of industrial waste.

2.2.2 Facility B

Facility B uses flow equalization upstream of secondary treatment so that incoming flow peaks downstream of primary treatment are largely limited to wet weather events. Treatment consists of conventional primary and secondary treatment with single-stage nitrification in a complete-mix activated sludge configuration after an anoxic selector. Tertiary treatment consists of chemically enhanced flocculation for P-removal using slaked lime, two-stage recarbonation for hardness removal, multimedia filtration, and activated carbon adsorption for removal of COD. The secondary treatment consists of older and newer unit processes, and under current flow conditions, only the newer portion of the treatment plant is in operation. Secondary treatment is conducted at comparatively longer SRT (16.5 days) and high MLSS concentrations (above 4,000 mg/L in winter). The facility discharges into a creek after final disinfection that drains into a reservoir, which serves as a principal water supply reservoir.

Facility B currently treats close to 30 mgd in ADAF. The wastewater influent of Facility B is mainly of residential origin with about 10% of the flow originating from a microchip manufacturer and small contributions from other industry, commercial sources, and water plant sludge. Discharge limits require TKN in the effluent of less than 1 mg/L, COD of less than 10 mg/L, TP of less than 0.1 mg/L on a monthly average basis and partial denitrification.

2.2.3 Facility C

Treatment at Facility C consists of conventional primary clarification followed by high purity oxygen (HPO) secondary treatment. The secondary effluent is neither nitrified nor denitrified. The TKN/BOD ratio (about 6.7) and the F/M ratio (about 0.8) entering the aeration basin is higher than for other facilities included in this study. The HRT in the aeration basin is approximately 2 hours on average. The facility operates throughout the year consistently at an SRT of about 1.4 days.

Table 2-1. Comparison of Treatment Processes of Facility A to G.

Facility	Primary treatment	Secondary treatment	Nutrient removal	Tertiary treatment	Disinfection	Digestion
A	Primary Clarification	Modified Ludzack-Ettinger (MLE), secondary clarification	Nitrification and partial denitrification	NA	Chlorination/ Dechlorination	Anaerobic digestion
B	Primary Clarification	Modified Ludzack-Ettinger (MLE), secondary clarification	Nitrification and partial denitrification	Chemical P-removal, two-stage recarbonation, multi-media filtration, activated carbon adsorption.	Chlorination/ Dechlorination	Anaerobic digestion
C	Primary Clarification	High purity oxygen, secondary clarification	BOD/TSS removal	NA	Chlorination/ Dechlorination	Anaerobic digestion (but no recycle flows)
D	Primary Clarification	Modified Ludzack-Ettinger (MLE) with Centrate side stream aeration, secondary clarification	Nitrification and partial denitrification	NA	Chlorination/ Dechlorination	Anaerobic digestion
E	NA	Membrane Bio-Reactor (MBR)	Nitrification and partial denitrification	NA	UV Disinfection	NA
F	Chemically Enhanced Primary Clarification	Single-stage activated sludge, secondary clarification	Nitrification and partial denitrification	NA	NA	Anaerobic digestion (but no recycle flows)
G	Chemically Enhanced Primary Clarification	Anaerobic-anoxic-aerobic process (A2O), secondary clarification	Nitrification and partial denitrification, biological P removal	Chemical P removal	UV Disinfection	Not onsite

The effluent of Facility C is discharged to a river that serves downstream users as a drinking water resource. Facility C currently receives about 70 mgd ADAF, which is predominantly residential in origin. The secondary effluent after clarification cannot be sampled before final chlorination at Facility C. Therefore, the aeration basin effluent sample needed to be sampled before final clarification as a mixed liquor sample.

2.2.4 Facility D

Treatment at Facility D consists of conventional primary clarification followed by secondary treatment using the MLE process. A side-stream aeration process is also used for centrate nitrification. The facility operates at an SRT of 4-5 days. Facility D operates at complete nitrification with ammonia effluent concentrations below 2 mg/L and partial denitrification.

Facility D currently receives a flow of about 80 mgd ADAF mainly of residential origin. Facility D discharges into a river that is used by downstream users as a drinking water source.

2.2.5 Facility E

The process of Facility E consists of preliminary treatment followed by a membrane bioreactor for complete nitrification. The aeration basins are equipped with anoxic and aerobic

zones for denitrification, but maintaining anoxic conditions is challenging due to high oxygen concentrations in the RAS returned from the membrane tanks. The MLSS concentration in the membrane bioreactor is about 8,000 to 10,000 mg/L. Facility E started operation in spring 2008 and is currently treating an ADAF of 0.1 mgd. Wastewater influent is primarily residential in nature. Incoming flows are relatively constant over the course of a year. However, the plant is essentially not running during the night due to drastic diurnal flow variations.

2.2.6 Facility F

The secondary effluent of Facility F is treated in an activated sludge process and is mainly used for groundwater recharge. For this study, the aeration basin process stream was sampled. In November 2009, operation of the secondary process was modified to assess nitrification and denitrification performance in the aeration basins. The sampling campaign was conducted in late April 2010, when the plant was operating in nitrification / denitrification mode in a step feed configuration.

The influent of Facility F is comprised of approximately 80% residential/commercial and 20% industrial flows. The industrial customers are businesses such as food processors, metal finishers, and hospitals.

2.2.7 Facility G

Facility G operates a secondary treatment plant that operates in a full nitrification, partial denitrification, and biological P-removal mode. After chemically enhanced primary clarification, secondary treatment consists of a Biological Nutrient Removal (BNR) treatment with a three-stage anoxic, anaerobic, aerobic configuration. Tertiary treatment at the plant consists of tertiary filtration for chemical P-removal followed by final disinfection. The SRT is approximately four and eight days during winter and summer months, respectively. Aeration basins and associated secondary clarifiers can be isolated as independent parallel trains. This process control allowed for testing the effect of various SRTs on TOrC removal in the same sampling campaign. Solids are not treated on site, but are stored for a few hours in a holding tank before being pressed and hauled off-site.

Facility G is currently treating close to 100 mgd ADAF. Disinfection consists of ultra-violet (UV) disinfection, only a minor portion of the flow is treated by chlorination. The plant discharges into an ecologically sensitive surface water that also serves as a drinking water source.

2.3 TOrC Fate Parameters

Both sorption and biotransformation rates were measured.

2.3.1 Sorption

Sorption partitioning coefficients were measured for TOrC onto activated sludge solids using the following method. Sorption experiments were performed in 15 mL glass centrifuge tubes as the reactor vessels, with triplicates for each isotherm point. Freshly collected mixed liquor (ML) was kept shaken to maintain solids in suspension prior to being added to centrifuge tubes. Enough ML volume was added to reactor vessels in order to target a TSS concentration of 5000 mg/L during the experiments. Separate sorption tests were performed for triclosan and triclocarban where a lower solids-to-liquid ratio was used for these tests. The reactor vessels were centrifuged at 2000 rpm for 5 minutes and the supernatant was decanted and discarded.

Each reactor of sludge solids was then resuspended in 10 mL synthetic wastewater (pH 7), vortexed and centrifuged again. The synthetic wastewater recipe was modified from Kerr et al. (2000) and included: ammonium chloride (2.0 mg/L), magnesium sulfate (22.5 mg/L), calcium chloride (47.7 mg/L), ferric chloride (0.3 mg/L), and phosphate salts for buffering. This washing step was performed a total of three times, with the supernatant being discarded each time. The goal of the washing procedure was to reduce background levels of TOrC from the original sample.

After the third washing step, 10 mL of synthetic wastewater containing biocide (0.5% NaN_3, 5mM $BaCl_2$, 5mM $NiCl_2$) was pipetted into each vessel. Six spiking concentrations were used for six isotherm points (500, 1000, 2000, 2500, 5000, 10000 ng/L), as well as a non-spiked point. After spiking, the vessels were capped and vortexed to mix completely. In addition to sorption reactors, a no-solids control was performed in triplicate. For the no-solids control, three concentrations of mixed TOrC were spiked into reactor vessels containing 10 mL of synthetic wastewater with biocide. The three spike concentrations used for the controls were 0, 1000, and 10000 ng/L.

All reactor vessels were placed on their sides and equilibrated on a shaker table at room temperature (~23°C) in the dark covered with foil for 72 hours. Thereafter, all glass reactor vessels were centrifuged and the aqueous phase was measured by a direct-injection-LC-MS/MS method, where isotope surrogate standards were used for each compound. The technique for measuring the solid phase TOrC concentrations is still a work in progress, where an accelerated solvent extraction method is being examined.

The fraction of organic carbon f_{oc} for solids was measured between 45-50%. Sorption data for individual TOrC to solids were fitted by the Freundlich isotherm model:

$$q_{eq} = K_F (C_{eq})^{1/n}$$

where q_{eq} is the solid phase concentration, C_{eq} is the aqueous phase concentration, and K_F and $1/n$ are Freundlich isotherm constants. K_F is a measure of adsorption capacity and $1/n$ indicates adsorption strength for a given activated carbon and aqueous matrix. The experimental data was fitted with the transformed Freundlich adsorption equation, in order to solve for the variables $\log K_F$ and $1/n$:

$$\log q_{eq} = \log K_F + (1/n) \log C_{eq}$$

2.3.2 Biotransformation

Biotransformation rates for indicator TOrC were measured in batch biotransformation experiments. The tests examined the disappearance of the parent compound (primary biodegradation). Rates were determined for activated-sludge mixed-liquor samples from full-scale systems operated under varying operational conditions. The rate of primary biodegradation was measured according to OECD 3xxB proposed guidelines (OECD, 2007). The OECD guidelines are based on a procedure originally published by Federle and Itrich (1997). The principle of the method is to incubate a test chemical with an activated-sludge sample under realistic environmental conditions.

A fresh ML sample was initially buffered at pH 7 with a 10 mM carbonate buffer. Then a 4 L amber-glass open-batch reactor was filled with 2 L of ML sample (Figure 7-1). Biotransformation experiments were performed in triplicate, thus three 4 L reactors were utilized

in parallel. At time zero, target TOrC were spiked at ~3000 ng/L. The TOrC stock standard was initially dissolved in methanol, where methanol was used to assure all the compounds would dissolve in a subsequent water matrix. The stock standard in methanol was nitrogen-dried to minimize the introduction of methanol into reactors (0.4 mg-C/L introduced to reactors coming from methanol), as methanol could be a desirable carbon source and thus potentially alter the composition of the microbial community.

The reactors were continuously stirred via a shaker table and aerated. Air was passed through a water trap before introduction into reactors. The reactors were closed with a foam stopper to minimize evaporative loss of water. During the experiment, the reactors were topped off with ultra pure water to take into account observed evaporation of water due to aeration. The reactors were maintained at ambient laboratory temperature, 23^{o}C, and between 2 and 5 mg/L of dissolved oxygen prior to and during the experiment. After the initiation of the experiment, TOrC samples were collected for the following time points: 1 min, 10 min, 25 min, 45 min, 1.25 h, 2 h, 4 h, 8 h, 14 h, 1 d, 2 d, and 5 d.

Environmental blank (laboratory ultra-pure water) and ML background blank (before spiking) samples were collected. An abiotic control was performed in parallel to biotransformation experiments. The abiotic control contained a mixture of sodium azide (5%) and nickel/barium chloride (5 mM). The chemical biocide was allowed to mix with the ML for six minutes prior to spiking of TOrC. In addition, an ultra-pure water control was performed to assess other removal mechanisms besides sorption to solids. The abiotic and ultra-pure water controls were sampled in triplicate. TSS was measured initially and after 2 and 24 h. Ammonia, nitrate, temperature, soluble chemical oxygen demand (sCOD), dissolved organic carbon (DOC), alkalinity, suites of inorganic anions (i.e., chloride, sulfate, phosphate, nitrite, bromide, fluoride), metals (e.g., calcium, potassium, sodium, magnesium), and pH were monitored for time points 0, 1, 4, 8, 14, and 24 h, and 5 days. The reduction of the parent compound was measured in the aqueous phase. Aqueous phase samples were obtained by centrifugation and then measured by a direct-injection LC-MS/MS method, where isotope surrogate standards were used for each compound.

The kinetic disappearance of a TOrC due to biotransformation was described by a pseudo first-order model as described in Appendix G.

2.4 Effect of Treatment Conditions on TOrC Removal

Both laboratotory-scale and pilot-scale investigations were conducted. See below for more detailed information.

2.4.1 Laboratory-Scale Investigations

Three laboratory-scale activated-sludge systems were operated in parallel from the summer of 2010 to 2011. The goal of the laboratory tests was to evaluate the effects of SRT, temperature, and different secondary treatment configurations on TOrC removal (Table 2-2).

The systems consisted of an aerobic basin followed by a solids separation basin housing a customized Puron hollow-fiber ultrafiltration membrane where sludge was recycled from the membrane chamber back to the aerobic basin. The total volume for both chambers was 75 L. The aerobic and membrane chambers contain level switches to prevent the overflow of tanks and keep the membrane module submersed below the water level. The membrane permeate pump was programmed to reverse flow (69.4 mL/min) and to back flush and clean the membranes

every 4 minutes and 36 seconds for a 20 second duration. In addition, the membranes were back flushed at 20 mL/min with 6% chlorine solution once a week for one hour, followed by a deionized water rinse at 20 and 140 mL/min for 15 and 1 min, respectively. The systems were originally seeded with nitrified activated sludge from a 10 gpm pilot-scale sequencing MBR system operated on site. The feed for the lab-scale systems consisted of underground holding tank sewage from a local student residential community (400-unit student apartment complex). Influent wastewater entered the 9.5 m^3 (2500 gallon) tank, and a submerged grinder pump transferred mixed sewage to the laboratory-scale systems. The wastewater was intermittently fed every hour into a 55-gallon equalization tank. The feed line into the equalization tank contained a fine mesh screen to filter large solids. The feed to the system was continuously amended with a carbonate buffer (Na_2CO_3) and TOrC compounds (spiked at ~1000 ng/L). The system's pH (i.e., 7-8), temperature, and dissolved oxygen (i.e., ~5 mg/L) were continually monitored. Also, the reactor tank walls were scrubbed weekly to minimize attached biomass growth on the walls. For each reactor system the feed flow rate, sludge recycle rate to feed rate ratio, and hydraulic retention time was approximately 70 L/d, 4 and 20 hours, respectively.

Three experiments were performed in chronological order and their operational durations are provided in Table 2-2.

The analytical program included weekly monitoring for nutrients (i.e., ammonia, nitrate, and total nitrogen), alkalinity, influent and effluent COD, MLSS, and TSS in final effluent and waste activated sludge (WAS).

COD was significantly removed in all three reactors during experiment set #1 (see Appendix G for data from July 2010 to November 2010). At an SRT of 10 and 20 days, the majority of the influent ammonia was nitrified with ammonia effluent concentrations below 2 and below 1 mg-N/L, respectively, and nitrate above 30 mg-N/L. For the most part, the total nitrogen concentration in the effluent corresponded with the total nitrogen concentration in the influent, indicating that nitrification but no denitrification occurred. At a temperature of 20°C and at the lowest SRT of 5 days the ammonia concentrations in the effluent fluctuated ranging from 0.3 to 15 mg-N/L. Nitrate concentrations in the effluent varied from 7 to 50 mg-N/L. Nitrification was at times incomplete resulting in nitrite formation. Treatment performance for experimental Sets 2 and 3 are also presented in Appendix G.

Table 2-2. Laboratory-Scale Experiments.

Operational Condition	SRT (days)	Temperature (°C)
Set 1: SRT; July – November 2010		
Conventional Activated Sludge (CAS)	~20 days	~20
Conventional Activated Sludge (CAS)	~10 days	~20
Conventional Activated Sludge (CAS)	~5 days	~20
Set 2: Temperature; December 2010 – February 2011		
Conventional Activated Sludge (CAS)	~10 days	29.6±0.3
Conventional Activated Sludge (CAS)	~10 days	20.1±0.4
Conventional Activated Sludge (CAS)	~10 days	13.0±2.7
Set 3: Treatment Configuration; April 2011 – June 2011		
Modified Ludzack-Ettinger Process (MLE)	~10 days	20.4±1.5
Integrated Fixed-Filmed Activated Sludge Process (IFAS)	~10 days	19.6±2.1

2.4.2 Pilot-Scale Investigations

In parallel to the laboratory-scale experimental Set 1, a pilot-scale sequencing bioreactor (SBR)-membrane bioreactor (MBR) was used to compare results for TOrC removal at a completely nitrifying system at an SRT of approximately 35 days.

The pilot SBR-MBR and laboratory-scale systems were fed by the same wastewater. Influent and effluent samples from the pilot system were sampled in November 2010 at which time the pilot-scale reactor had been in continuous operation for over a year. Raw, screened wastewater was transferred to the pilot SBR-MBR system. The SBR-MBR system consisted of two parallel bioreactor tanks equipped with submerged membrane tanks (PURON® hollow fiber ultrafiltration membrane cassettes, Koch Membrane Systems, KMS, Wilmington, MA). The membrane cassettes were intermittently aerated during operation and operated with frequent backwashing to control the transmembrane pressure. Influent wastewater was subjected to SBR cycles consisting of a non-aerated fill stage (Mix Fill), an intermittently-aerated fill stage (React Fill), and an intermittently aerated discharge phase (React Draw). When one bioreactor was in Mix Fill or React Fill mode, activated sludge was pumped from the second bioreactor (React Draw) to the shared membrane tanks for permeate production and sludge recycle.

2.5 Anaerobic Digester Investigations

Both full-scale and laboratory-scale anaerobic digestion processes were studied.

2.5.1 Indicator Compounds

The indicator compounds selected for the anaerobic digestion study were based on the availability of analytical methods (from indicator candidate list from this study), their occurrence in sludges and biosolids (based on information gathered in this study and previous publications), and their physical and biochemical properties. For a TOrC to be present in sludges and biosolids it must be moderately to highly sorptive, and moderately to poorly biodegradable. Based on these criteria, the following compounds were selected for the anaerobic digester evaluation: atenolol, benzophenone, caffeine, carbamazepine, cimetidine, diphenhydramine, fluoxetine, gemfibrozil, ibuprofen, naproxen, sulfamethoxazole, triclocarban, triclosan, TCPP, TCEP, and trimethoprim.

2.5.2 Full-Scale Anaerobic Digester TOrC Mass Balance

Facility A was used to evaluate the fate of selected indicator compounds during the sludge thickening, anaerobic digestion, and dewatering processes (see Table 2-1; Section 2.2.1). The process flow schematic for Facility A includes the solid treatment process train (Appendix I).

The solids handling at Facility A includes primary sludge thickening in a gravity thickener and secondary activated sludge thickening using dissolved air flotation. Overflow from gravity thickener (GT) is returned to the grit removal tank, whereas underflow from the dissolved air floatation thickener (DAFT) is returned to the influent of the activated sludge process (i.e., blended with the primary clarifier effluent). Primary and secondary thickened sludges enter the first-stage anaerobic digester (HRT = 15-20 days) and then flow into a second-stage anaerobic digester (HRT = 15 days). Following anaerobic digestion, the biosolids are temporarily stored prior to dewatering in a batch centrifuge process. The centrifuges are typically run twice per week for 8 hours.

2.5.3 Laboratory-Scale Anaerobic Digestion

A laboratory-scale anaerobic bioreactor experiment was conducted to assess the removal of selected indicator TOrC during anaerobic digestion under controlled operating conditions (e.g., SRT, temperature). The anaerobic bioreactor was designed as a completely mixed reactor, with a diameter of 15 cm and an effective liquid volume of 13.3 L. A flow-through water-based heat exchanger was installed in the bioreactor to ensure a constant operating temperature of 35°C. Mixing was ensured with four propellers connected to a variable speed motor. The biogas was directed to the outdoors where it was flared. Design criteria for the anaerobic bioreactor are provided in Table 2-3. A schematic of the bioreactor is provided in Appendix I.

The bioreactor was fed daily with 665 mL of primary settled solids, which was generated in a laboratory-scale primary clarifier (effective volume of 96 L and an HRT of 2 hours). The raw wastewater feed to the primary clarifier was obtained from a student housing complex located at the Colorado School of Mines. The loading of the primary settled solids to the bioreactor corresponds to an HRT of 22 days.

The performance of the anaerobic bioreactor was monitored weekly (influent and effluent) for total solids (TS), volatile solids (VS), total suspended solids (TSS), volatile suspended solids (VSS), chemical oxygen demand (COD), alkalinity, pH, total nitrogen (TN), nitrate (NO_3^-), ammonia (NH_3), total phosphate (TP), and orthophosphate (OP). The performance samples were collected in 250 mL amber bottles and stored at 4°C until processed for analysis.

After the system had reached steady-state conditions (after approximately 3 HRTs or 60 days), samples were collected for TOrC analysis during the next HRT cycle (20 days). For the TOrC analysis, influent primary sludge was sampled on a daily basis (to account for day to day concentration variation in the feed) and then composited to form a 7-day composite sample. The bioreactor effluent samples were collected on a weekly basis since the completely mixed bioreactor represents a composite sample. This sampling scheme resulted in three 7-day composite samples of influent and effluent. The samples were preserved with 1 g/L sodium azide and kept at 4°C until processed for analysis.

Table 2-3. Design Information for Laboratory-Scale Anaerobic Digester.

Parameter	Design criteria
Anaerobic Digester	
Diameter, cm	15
Side Water Depth, cm	75
Volume, L	13.3
Hydraulic Residence Time, days	22
Volatile Solid Loading Rate, mg/L/d	15,000
VSS destruction, %	50
Temperature, °C	35

2.5.4 TOrC Fate Parameters for Anaerobic Digestion

The biotransformation rate constants and sorption distribution coefficients were determined using anaerobic digester sludge collected from Facility A. The procedures used are provided below.

2.5.4.1 Biotransformation

The indicator compounds selected for the digester evaluation were incubated at environmentally relevant concentrations in anaerobic digester sludge collected from Facility A. At test initiation, the test compounds were added directly to the anaerobic digester sludge with constant mixing in an anaerobic chamber. The spiked anaerobic digester sludge was then transferred into individual 50 mL glass serum bottles and capped. The serum bottles were then purged with N_2 to ensure the samples remained anaerobic. Abiotic, biotic, and dosing controls were included in the experiment. All samples were incubated at 35°C ± 3°C. To simulate the relatively static conditions within an anaerobic digester, the serum bottles were gently agitated for a few minutes 2 to 3 times per week. Biogas production was monitored via a pressure gauge.

For the biotransformation rate analysis, triplicate serum bottles were collected at various times (2 and 8 hours, and 2 days, and 3 and 7 weeks). The duration of the test was sufficiently long to assess the extent and rate of biotransformation for the test chemicals. The collected serum bottles were flash frozen at -80°C and then lyophilized prior to Accelerated Solvent Extraction (ASE) of the dried residue. Instrumental analysis was performed using LC-MS/MS and quantification was performed by isotope dilution. Data was collected in two acquisition periods for both the ESI negative and positive modes. Results were fit to a first-order kinetic model according to

$$dC_T/dt = -K_bC_T$$

Where C_T is the total compounds concentration (ng/L), t is the time (days), and K_b is the first-order rate constant (1/day).

2.5.4.2 Sorption

Sorption distribution coefficients were determined at ambient laboratory temperature (23°C) using anaerobic digester sludge collected from Facility A. At test initiation, the test compounds were added directly to the anaerobic digester sludge in 15 mL glass centrifuge tubes. Seven concentrations were used in the isotherm experiments (typically ranging from 0 to 10,000 ng/L). The solid-to-water ratio was set to ensure an acceptable measurable range for each TOrC in the aqueous fraction (within 20-80% of the spike concentration). Blank controls (without solids) were also included in the experiments. The centrifuge tubes were capped and then equilibrated on a shaker table at room temperature for 6 hours. After equilibration, the samples were centrifuged and the supernatant was transferred to microcentrifuge tubes for later TOrC analysis. The remaining sludge solids were then extracted using ASE. Instrumental analysis for both the aqueous and solid phase samples was performed using LC-MS/MS and quantification was performed by isotope dilution. Data was collected in two acquisition periods for both the ESI negative and positive modes. Results were fit with a Freundlich sorption model, which was used to determine sorption distribution coefficients (K_d) for each TOrC under field conditions.

2.6 TOrC Analytical Protocols

Brief descriptions of the analytical protocols are given below. Complete details and QA/QC results may be found in Appendix B.

2.6.1 Preservation and Sampling Protocols

The following sections provide more specific details of the preservation study and sampling protocols.

2.6.1.1 Preservation Study

A preservation study was performed on three different wastewater matrices from Facility G to determine the suitability of the preservative sodium azide (NaN_3) for reducing biotransformation during sampling, storage, and shipping. Complete details of the preservation study can be found in Appendix B. With the exception of caffeine, which is highly amenable to biotransformation, the data suggested that the proposed preservation protocol (i.e., 1 g/L of NaN_3 during sampling and storage at 4ºC) was sufficient for the full-scale sampling phase.

2.6.1.2 Sampling Protocols

A sampling protocol was set up and customized for each facility to guide the full-scale field sampling campaigns to assure QA/QC compliance by staff during sample collection and handling (see Appendix B, Section B.2).

2.6.2 TOrC Analysis

The following sections provide more specific details of the extraction protocols and instrumental analysis.

2.6.2.1 Extractions

In brief, aqueous samples were extracted using solid phase extraction (SPE) protocols based on work by Vanderford and Snyder (2006). Solid-containing samples (i.e., primary influent, return activated sludge (RAS), etc.) were filtered using a 1 μm glass fiber filter and a vacuum filter apparatus. The filtrate was extracted using the SPE procedure employed for aqueous samples. Extraction of the solids remaining on the filter was performed using a method based on work by Radjenovic et al. (2009). The resulting extract was subjected to the SPE method as described above, with the exception of using a 500 mg SPE cartridge (Waters Corporation (Millford, MA).

2.6.2.2 Instrumental Analysis

Instrumental analysis was performed using LC-MS/MS (API 4000 triple-quadrupole mass spectrometer, Applied Biosystems, Foster City, CA) and quantification was performed using isotope dilution. Data was collected in two separate acquisition periods for ESI negative mode and two acquisition periods for ESI positive mode to allow for a minimum acquisition time of 25 msec for each transition monitored. The process of optimization of the mass spectrometer has been previously published (Vanderford, 2003).

2.6.3 Quality Control

A number of quality control measures were used. They are described in this section.

2.6.3.1 Method Detection and Reporting Limits

Aqueous method reporting limits (MRL) were based on MDL calculated from 12 replicate measurements of deionized water samples fortified with analytes at their expected detection limits and extracted as previously described. MRLs for each analyte were set at greater than three times the MDL.

The MDL for solid samples was determined from the analysis of a least eight samples processed through the procedure described above. The MRL of each analyte in the solids method was calculated by multiplying the MDL value by a minimum factor of five. The MRLs were then adjusted for each sample by dividing the MRL by the mass of the solids calculated to be present on the filter paper from TSS measurements performed on samples taken during the same sampling event. It should be noted that background contamination prevented a meaningful MRL from being established for N,N-Diethyl-meta-toluamide (DEET) and pushed the MRL for trimethoprim to values significantly higher than that established in the liquid method.

2.6.3.2 Blanks

Twelve field blanks were analyzed during the study to quantify the degree of contamination present during sampling and twelve rinse blanks were conducted to determine the degree of contamination introduced by the sampling equipment. Five field blanks had detections of five of the target analytes and some of the rinse blanks displayed contamination of several of the target compounds.

Laboratory deionized (DI) water blanks were also extracted alongside project samples to quantify the degree of blank contamination during extraction and analysis. Thirty-three DI blanks were analyzed during the project and the majority of analytes were not detected in any of the blanks.

In addition, ASE blanks were analyzed to determine the degree of contamination introduced during the solids extraction. Most compounds were not detected in the ASE blanks; however, five compounds (carbamazepine, naproxen, TCEP, triclocarban, and triclosan) showed varying degrees of blank contamination.

2.6.3.3 Laboratory Fortified Blanks

A total of 27 laboratory fortified SPE blanks (LFBs-SPE) and 12 LFBs-ASE were extracted and analyzed to determine and monitor the accuracy of the analytical method without matrix interference. All mean SPE recoveries were between 98-118% and %RSDs were all $\leq$ 12% with one exception (bisphenol A = 22%). ASE recoveries ranged from 88-112% and %RSDs were $\leq$ 15% with three exceptions (benzophenone = 27%, BHA = 36%, diphenhydramine = 18%).

2.6.3.4 Laboratory Fortified Sample Matrices (LFSMs)

Twelve LFSMs were conducted over the course of the project to determine the accuracy of the method in the sample matrices and its susceptibility to matrix interferences. The following matrices were represented in the 12 LFSM samples: primary influent, aeration basin influent, centrate, mixed liquor, secondary effluent, and centrate side stream reaeration. Mean recoveries for all analytes ranged from 93-125%.

2.6.3.5 Replicates

Overall, 30 sets of aqueous replicate samples, and 14 sets of solid samples (either duplicates or triplicates) were analyzed to assess and monitor analytical precision during extraction and analysis of aqueous matrices. Percent relative standard deviations (%RSDs) were calculated for each analyte on each set of duplicates/triplicates and the averages of those %RSDs are shown in Appendix B. For a given analyte, sample sets in which two or more samples were non-detect were not used in the calculation.

Musk ketone (16%), detected in only one sample set, was the only compound with an average %RSD > 15%; the remaining compounds had average %RSDs ≤ 10%. Solid replicates were also relatively precise with all analytes having %RSDs ≤ 17%, with one exception (caffeine = 49%).

2.6.4 Data Reporting

Sample extracts with compound concentrations greater than the calibration range were diluted and reanalyzed. All reported aqueous values accounted for sample-specific dilution or concentration. The calculation of analyte concentration for the solid samples required that two factors be applied to the value obtained by the LC-MS/MS method. The first factor was applied to relate the obtained value to the mass of solids that were present on the filter paper at the beginning of the extraction. The second factor applied was a concentration factor needed to relate the final extract (0.5 mL methanol) to the calibration curve, which was in units of ng/mL. Therefore, the following calculation was used to convert the obtained values into final values in ng/g:

$$Final\ concentration\ \left(\frac{ng}{g}\right) = \frac{Measured\ value}{2 * solids\ mass\ (g)}$$

Due to contamination problems, meaningful MRLs were unable to be calculated for DEET and therefore it was not reported for solid samples.

CHAPTER 3.0

RESULTS AND DISCUSSION

3.1 Indicator Selection

Using the criteria occurrence levels, detection frequency, physicochemical properties, and analytical amenability, a list of indicator compounds was selected from the overall TOrC database (Table 3-1). Toxicological relevance of the indicator compounds, reviewed below, was not a key criterion for inclusion. Past studies indicate that the selected candidates frequently occur at quantifiable concentration levels in the primary effluents of municipal wastewater treatment facilities. The selected candidates had detection ratios (ratio between median occurrence concentration and method detection limit) larger than 10. Selecting indicator compounds with detection ratios of less than 10 (e.g., 17α-ethinylestradiol, 17β-estradiol) limits an accurate assessment of removal efficiency (above 1-log removal) during treatment. Analytical methods using LC-MS/MS with isotope dilution were established and previously Round Robin tested for the selected candidates.

Table 3-1 summarizes toxicological information for the selected indicator compounds as far as this information is currently available. It should be noted that the list of performance indicator TOrC identified in this research is not identical to the list produced by the WERF TOrC project CEC5R082 (Diagnostic Tools to Evaluate Impacts of Trace Organic Compounds). This is expected because the criteria used to prioritize TOrC for evaluation in that project were different from the criteria used in this research. Two of the selected compounds in this study overlap with the toxicologically-driven list of indicators proposed in WERF project CEC5R082, namely bisphenol A and triclosan.

The indicator compounds were also selected based on their physicochemical properties relevant to the attenuation by sorption and biotransformation. Their sorptive properties are summarized in Table 3-2. Compounds are organized by their state of ionization and octanol-water partitioning at pH 7 (D_{ow}). Positively charged compounds are expected to be removed by electrostatic attraction to the generally negatively charged surfaces of mixed liquor flocs. The indicator compounds comprise a range of various structural fragments. Table 3-3 lists structural properties of the indicator compounds that may serve as initial attack sites for compounds undergoing biotransformation. Some selected compounds are not likely to undergo biotransformation due to the lack of sites easily amenable to biological attack.

Table 3-1. Toxicological Information of Selected Indicator TorC.

Compound	CASRN	Category	Human toxicological relevance	Other concerns	References
Acetaminophen	103-90-2	Analgesic (PhAC)	175 μg/L DWG (Paracetamol) (based on ADI 50 μg/kg/day)		EPHC, 2008
Atenolol	29122-68-7; 60966-51-0	Beta-blocker (PhAC)	70 μg/L ADI-DWEL (based on ADI 0.0020 mg/kg/day)		Snyder et al., 2008
Benzophenone	119-61-9	UV Blocker (PCP)		Known or possible endocrine disrupter	
Bisphenol A	80-05-7	Plasticizer (HHC)	200 μg/L DWG (based on TI 0.05 mg/kg/day)	Effects reported in fish and invertebrates; Known or possible endocrine disrupter; Identified as High Priority TOrC indicator in WERF5R082.	EPHC, 2008
			1,800 μg/L ADI-DWEL (based on ADI 50 μg/kg/day)		Snyder et al., 2008
Caffeine	58-08-2	Psychoactive stimulant (HHC)	0.35 μg/L DWG (based on TTC 1.5 μg/kg/day)		EPHC, 2008
Carbamazepine	298-46-4	Anticonvulsant (PhAC)	12 μg/L ADI-DWEL (based on ADI 0.00034 mg/kg/day)		Snyder et al., 2008
			100 μg/L DWG (based on S-ADI 2.8 μg/kg/day and LDTD 200 mg/day)		EPHC, 2008
Cimetidine	51481-61-9 [1]	Anti-acid reflux (PhAC)	200 μg/L DWG (based on S-ADI 5.7 μg/kg/day and LDTD 400 mg/day)		EPHC, 2008
DEET	134-62-3	Insecticide (HHC)	2,500 μg/L DWG (based on derived ADI 0.75 mg/kg/day)		EPHC, 2008
Diphenhydramine	58-73-1	Antihistamine (PhAC)			
Fluoxetine	54910-89-3	Antidepressant (PhAC)	10 μg/L DWG (based on S-ADI 0.28 μg/kg/day and LDTD 20 mg/day)	Affects spawning in certain invertebrate species; Known or possible endocrine disrupter	EPHC, 2008
			34 μg/L ADI-DWEL (based on ADI 0.00097 mg/kg/day)		Snyder et al., 2008

Compound	CASRN	Category	Human toxicological relevance	Other concerns	References
Gemfibrozil	25812-30-0	Antilipidemic (PhAC)	45 µg/L ADI-DWEL (based on ADI 0.0013 mg/kg/day)		Snyder et al., 2008
			600 µg/L DWG (based on S-ADI 17 µg/kg/day and LDTD 1,200 mg/day)		EPHC, 2008
Ibuprofen	15687-27-1	Analgesic (PhAC)	400 µg/L DWG (based on S-ADI 11.4 µg/kg/day and LDTD 800 mg/day)		EPHC, 2008
Iopromide	73334-07-3	X-ray contrast media (PhAC)	750 µg/L DWG (based on S-ADI 21.4 µg/kg/day and LDTD 1,500 mg/day)		EPHC, 2008
Meprobamate	57-53-4	Anxiolytic (PhAC)	260 µg/L ADI-DWEL (based on ADI 0.0075 mg/kg/day)		Snyder et al., 2008
Naproxen	22204-53-1	Analgesic (PhAC)	220 µg/L DWG (based on S-ADI 6.3 µg/kg/day and LDTD 440 mg/day)		EPHC, 2008
			20,000 µg/L ADI-DWEL (based on ADI 0.570 mg/kg/day)		Snyder et al., 2008
Primidone	125-33-7	Anticonvulsant (PhAC)			
Sucralose	56038-13-2	artificial sweetener (HHC)			
Sulfamethoxazole	723-46-6	Antibiotic (PhAC)	35 µg/L DWG (based on ADI 10 µg/kg/day)		EPHC, 2008
			18,000 µg/L ADI-DWEL (based on ADI 0.51 mg/kg/day)		Snyder et al., 2008
TCEP	115-96-8	Flame retardant (HHC)	0.3 µg/L DWG (based on TTC 1 µg/kg/day)		EPHC, 2008
			0.6 mg/kg/day ATSDR MRL Oral Intermediate (15-364 days); Neurological; (Draft: 09/2009) [2]		ATSDR, 2010
			0.3 mg/kg/day ATSDR MRL Oral Chronic (1 yr or longer); Hepatic; (Draft: 09/2009) [2]		ATSDR, 2010

Compound	CASRN	Category	Human toxicological relevance	Other concerns	References
TCPP	13674-84-5	Flame retardant (HHC)			
Triclocarban	101-20-2	Antimicrobial (PCP)		Known or possible endocrine disrupter	
Triclosan	3380-34-5	Antimicrobial (PCP)	0.35 µg/L DWG (based on TTC 1.5 µg/kg/day)	Known or possible endocrine disrupter; Identified as High Priority TOrC indicator in WERF5R082.	EPHC, 2008
			2,600 µg/L ADI-DWEL (based on ADI 0.075 mg/kg/day)		Snyder et al., 2008
Trimethoprim	738-70-5	Antibiotic (PhAC)	70 µg/L DWG (based on ADI 20 µg/kg/day)		EPHC, 2008
			6,700 µg/L ADI-DWEL (based on ADI 0.19 mg/kg/day)		Snyder et al., 2008

Abbreviations:
PhAC – Pharmaceutical Active Compound,
HHC – Household Chemical,
HVP – High Volume Production Chemical
PCP – Personal Care Product
ADI – acceptable daily intake; ADI-DWEL – acceptable daily intake-drinking water equivalent level; ATSDR MRL – Agency for Toxic Substances and Disease Registry Minimal Risk Level; DEET – diethyltoluamide; DWG – drinking water guideline; LDTD – lowest daily therapeutic dose; S-ADI – surrogate acceptable daily intake; TCEP – tris (2-chloroethyl) phosphate; TCPP – tris (2-chloro-isopropyl) phosphate; TI – tolerable intake; TTC – threshold of toxicological concern

Notes:
1. Cimetidine hydrochloride, CASRN 70059-30-2
2. The MRL is an estimate of the daily human exposure to a hazardous substance that is likely to be without appreciable risk of adverse noncancer health effects over a specified duration of exposure. These substance specific estimates, which are intended to serve as screening levels, are used by ATSDR health assessors and other responders to identify contaminants and potential health effects that may be of concern at hazardous waste sites. (ATSDR 2010)

Table 3-2. Selected Indicator TOrC that Represent Various Potential Sorptive Properties.

Neutral or Ionic (-) log D_{ow} at pH 7				Ionic (+) log D_{ow} at pH 7	
<2	2-3	3-4	>4	<-2	0-2
Caffeine	TCEP	TCPP	Triclosan	Cimetidine	Diphenhydramine
Acetaminophen	Carbamazepine	Benzophenone	Triclocarban	Atenolol	Fluoxetine
Ibuprofen(-)	DEET		Bisphenol A		Trimethoprim
Naproxen (-)					
Sulfamethoxazole (-)					
Gemfibrozil (-)					
Sucralose					
Primidone					
Meprobamate					
Iopromide					

Table 3-3. Selected Indicator TOrC that Represent a Range of Structural Fragments Affecting Biological Attack.

Biotransformation likely	Type	Biotransformation likely	Type	Biotransformation *unlikely*	Type
Acid		Ether		Halogenated	
Ibuprofen	*aliphatic*	Fluoxetine	*aromatic*	TCEP	*phosphate ester*
Naproxen[a]	*aliphatic*			TCPP	*phosphate ester*
Gemfibrozil[a]	*aliphatic*	Nitrile		Triclocarban	*aromatic amide*
		Cimetidine[d]		Sucralose	*cycloalkane alcohol*
Carbonyl					
Benzophenone	*aliphatic*	Heterocyclic N Ring			
		Caffeine	*2 N; 5 ring*	Non Halogenated	
Alcohol		Trimethoprim[a]	*2 N; 6 ring*	Primidone	*amide ring*
Bisphenol A	*aromatic*			Meprobamate	*carbamate*
BHA[1]	*aromatic*	Sulfonamide		Carbamazepine	*anzepine amide*
Triclosan	*aromatic*	Sulfamethoxazole	*aromatic*		
Amide		Amine			
DEET	*aliphatic*	Diphenhydramine	*aliphatic*		
Acetaminophen[2]	*aromatic*				
Atenolol[3,4]	*aliphatic*				

Notes:
1. Other attack site: aromatic ether
2. Other attack site: aromatic alcohol
3. Other attack site: aliphatic alcohol
4. Other attack site: aliphatic amine

3.2 TOrC Mass Balances at Full-Scale Facilities

The selected indicator compounds were used in this study to assess and compare the removal efficiency of secondary treatment processes for TOrC during full-, pilot-, and bench-scale testing.

3.2.1 Operational Conditions at Facilities During Sampling Campaigns

Table 3-4 summarizes relevant operational conditions at the facilities sampled in this study. More detailed information on steady-state process operation at the time of sampling is presented in Appendix D for each sampling campaign.

Table 3-4. Comparison of Operational Conditions During Sampling Campaigns at Facilities A-G.

	Date of Sampling	Sec. Inf. Flow, mgd	Total / Aerobic SRT, days[1]	MLSS, mg/L	HRT in ABs, hours[2]	Redox Condition in Aerobic Basins	WW Temp., °C
A (winter)	3/28-31/2011	14.9	10/8.2	1,590	11/3.7	Anx./Aer.	13.8
A (summer)	7/11-14/2011	19.9	12.5/8.7	1,740	6.7/2.1	Anx./Aer.	20
B (winter)	2/7-10/2011	39.8	16-20/11-14	4,480	8.8/5.5	Anx./Aer.	14
B (summer)	8/16-19/2010	36.4	18.2/18.2	3,620	9.6/5.7	Aer.	25.8
C (winter)	3/15-18/2010	66.9	2/2	2,560	2.4/0.9	Aer.	15
C (summer)	9/20-23/2010	54.7	1.4/1.4	2,230	2.3/1.0	Aer.	22
D (summer)	9/20-23/2010	83.2	6.7/4.6	2,590	5.3/1.6	Anx./Aer.	22
E (winter)	4/12-15/2010	0.11	>50	7,860	4.1/0.5	Anx./Aer.	17
E (summer)	8/23-26/2010	0.1	>40	8,050	4.2/0.3	Anx./Aer.	24
F (summer)	4/26-29/2010	91	6.5/4.9	3,700	3.7/2.6	Anx./Aer.	25
G (high SRT)	1/14-17/2011	5	42/34	5,070	11.1/6	An./Anx./Aer.	22.6
G (medium SRT)	1/14-17/2011	6.5	20/16	5,650	8.5/5.7	An./Anx./Aer.	22.6
G (low SRT)	1/14-17/2011	9.7	6/4.8	2,260	5.8/4	An./Anx./Aer.	22.6

Abbreviations:
an. – anaerobic, anx. - anoxic, aer. – aerobic.
Notes:
Values reported are typically averages of daily composite samples collected for process monitoring during 72-hour sampling events.
1. Total System SRT includes aerobic, anoxic, and anaerobic zones of aeration basins. Aerobic SRT includes solid inventory in aerobic zones of aeration basins only.
2. First HRT value calculated is based on forward flows (without internal secondary recycle streams (mixed liquor recycle (MLR) and RAS)). Second value calculated includes RAS and MLR flows.

Secondary influent flows ranged from less than 1 mgd to over 90 mgd at the different facilities sampled. Typically, two sampling events were conducted at each facility to assess treatment performance during different seasonal flow and load conditions. Facility C operated a high purity oxygen (HPO) treatment for BOD removal only at the lowest SRT of 1.4 days. Facility E operated an MBR at the highest SRT of 40-80 days, although the exact SRT could not be determined for this facility as the secondary process is operated under MLSS control and not SRT control.

The total HRT in the secondary treatment reactors varied from approximately 2 hours to 11 hours for all field sites. When internal recycle flows (RAS and MLR) are considered in the HRT calculation, the HRT ranged from less than 1 hour to approximately 7 hours.

TSS was used as a conservative parameter to assess the mass balances around the secondary clarifiers (or MBR) at each facility (see Appendix F for equations). TSS recovery was generally between 80 and 120% (Table 3-5). The TSS recovery for Facility D (Winter) was only 68%. This event was not considered for TOrC mass balance analysis as TOrC results gained from this sampling event were for unknown reasons generally inconsistent and unreliable. TSS recoveries around the secondary clarification at Facility F (Winter) and A (Winter) were 71 and 49%, respectively, indicating inaccuracies with process flow and/or TSS measurements. For both events, the TOrC mass balance errors for slow/recalcitrant compounds (e.g., carbamazepine) were, however, acceptable (see Appendix E). Therefore, TOrC data from both sampling campaigns was further used in this study despite the TSS inconsistency.

Table 3-5. Recovery of Solids for Secondary Clarification Mass Balances.

Facility	TSS recovery, %
A (winter)	49
A (summer)	120
B (winter)	80
B (summer)	106
C (winter)	95
C (summer)	99
D (winter)*	68
D (summer)	83
E (winter)	98
E (summer)	117
F (winter)	71
G (high SRT)	76
G (medium SRT)	124
G (low SRT)	103

* This sampling event was excluded from further analysis.

3.2.2 TOrC Occurrence in Primary and Secondary Influents

Almost all compounds were detected in the secondary influents at concentrations above the respective reporting limit. Primidone was below the reporting limit in the plant influent in one of the 10 sampling campaigns.

The highest influent concentrations were generally observed for acetaminophen, caffeine, ibuprofen, naproxen, and the artificial sweetener sucralose (Figure 3-1). The majority of the TOrC indicators were present in the secondary influents of the seven facilities at concentrations in the same order of magnitude, regardless of facility location, size, or season during which sampling was conducted (Figures 3-1 through 3-3). The similarity in TOrC concentrations between different field sites may be related to the fact that 72-hour composite samples during the same weekdays (Monday through Thursday) were collected at all locations for this study. These results should, however, not be over interpreted, as it is known that TOrC concentrations can fluctuate significantly at different plants depending on the time of sampling.

Caffeine was typically found at higher concentrations in the wastewater influent during the winter sampling event compared to the same facility sampled in summer (Figure 3-1). DEET influent background concentrations were generally below 1 ug/L during winter months at all facilities. During summer months DEET concentrations increased up to 15 ug/L. Higher concentrations for DEET were observed at facilities located in coastal regions (Facilities B and E) compared to facilities located in inland regions (Facilities A, C, D).

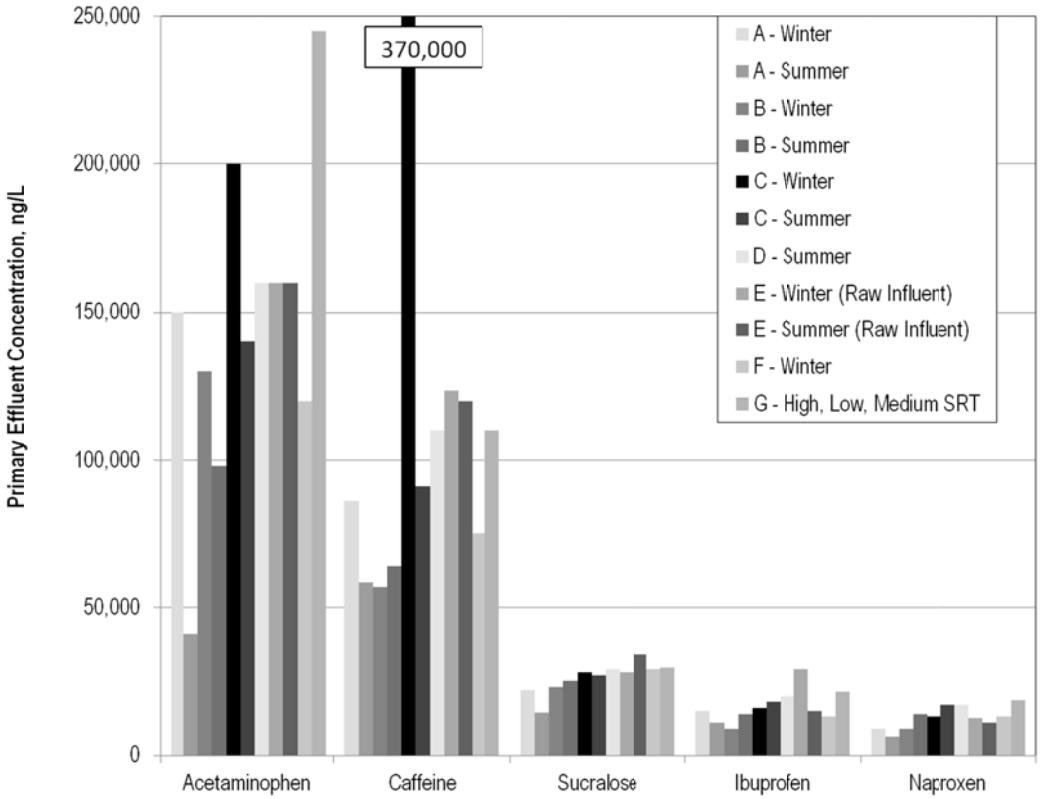


Figure 3-1. Secondary Influent TOrC Concentrations for Compounds in Excess of 10 µg/L.

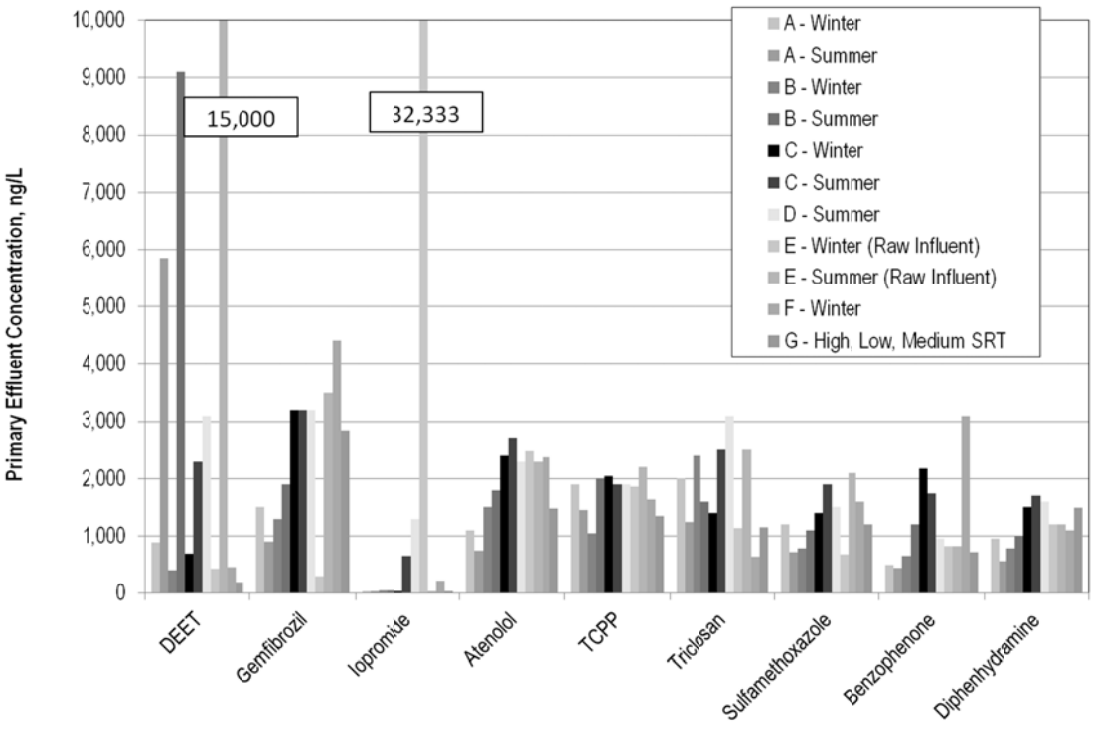


Figure 3-2. Secondary Influent TOrC Concentrations for Compounds Between 1 to 10 µg/L.

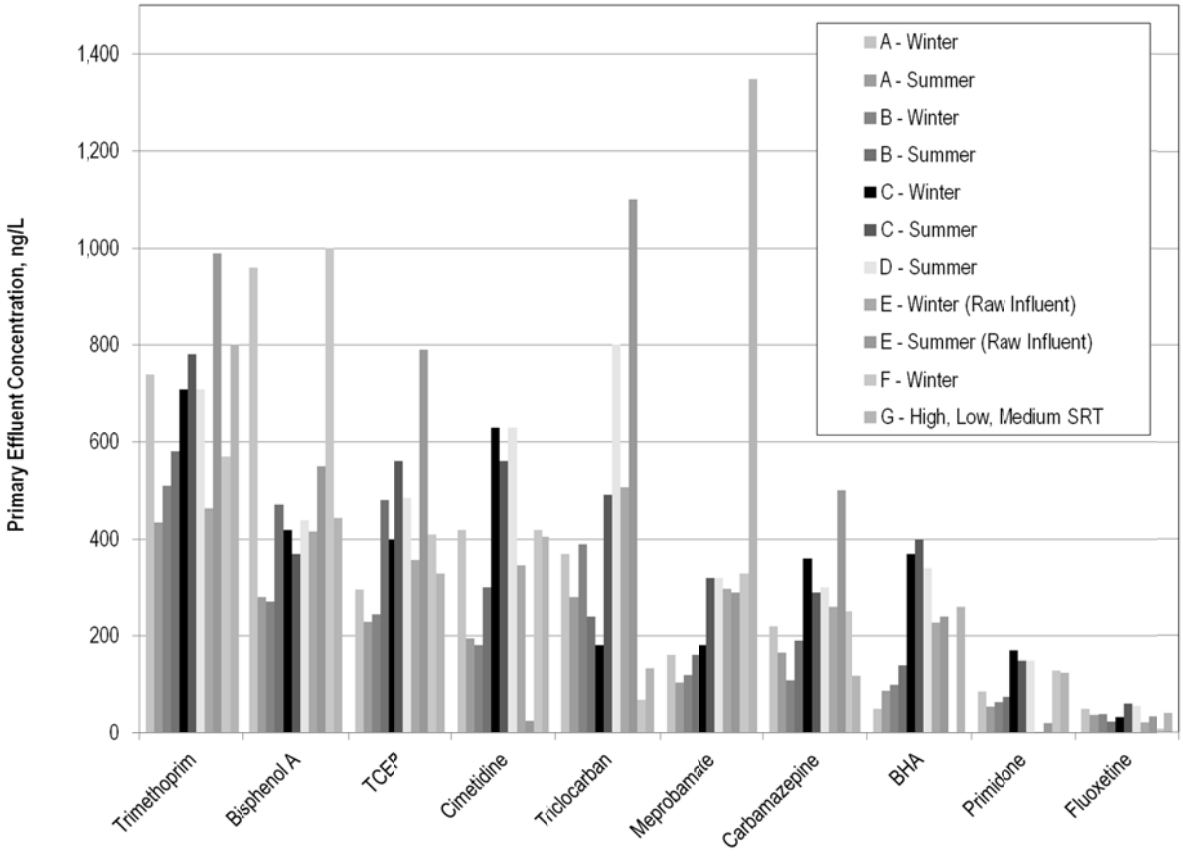


Figure 3-3. Secondary Influent TOrC Concentrations for Compounds Below 1 µg/L.

The concentration of the X-ray contrast agent iopromide was below the reporting limit in the primary or secondary influent of six of the 13 sample events conducted. Iopromide concentrations were particularly high at Facility E during the winter sampling event. This may just be a result of a natural variability in concentration of this TOrC. As Facility E is significantly smaller than any of the other facilities sampled (0.1 mgd), it is possible that the wastewater influent concentration of iopromide depends on the general usage pattern of X-ray contrast agents among the medical facilities in the service area. The concentration of a specific X-ray contrast agent in wastewater influents may be smaller in treatment plants serving a larger number of medical institutions that may be using a variety of different contrasting agents.

Influent concentrations of the tranquilizer meprobamate were about four times as high at Facility G compared to all other facilities. This may be indicating an unusual consumption pattern of this anxiolytic drug in the service area of Facility G.

The lowest secondary influent concentrations were recorded for BHA, primidone, and fluoxetine. As fluoxetine is a compound that sorbs and biotransforms well, low concentrations of this compound may result in larger errors in mass balance calculations than observed for other compounds that are recalcitrant (e.g., primidone) or generally measured at higher concentrations.

At three facilities (B, F, and G), primary influent and effluent samples were collected during four sampling events, allowing the assessment of TOrC removal during primary clarification. Facilities F and G add ferric chloride for chemically enhanced primary clarification (CEPC). For most TOrC no statistically significant difference was observed between primary influent and effluent aqueous sample concentrations. For six of the TOrC indicators the removal was significant (defined as more than 15% difference based on the typical variability of TOrC analysis for replicates (see Section 2.7.3.5), and typically higher for CEPC than for conventionally operated primary clarification (Figure 3-4). With the exception of sulfamethoxazole, the compounds that were well removed are sorbable or highly sorbable (triclocarban, TCPP, diphenhydramine, fluoxetine, and cimetidine). Primary sludge samples were not collected during these sampling campaigns.

A higher removal for TCPP, triclocarban, and fluoxetine was observed at Facility B during winter compared to summer operation. This may be attributable to differences in primary clarifier operation. In winter, the primary clarifiers were operated at lower surface overflow rate (SOR - 1,100 gpd/sf) than in summer (1500 gpd/sf) achieving higher TSS and BOD removal during the winter sampling campaign (Appendix D). The SOR at facilities F and G operating under CEPC were 650 and 750 gpd/sf, respectively.

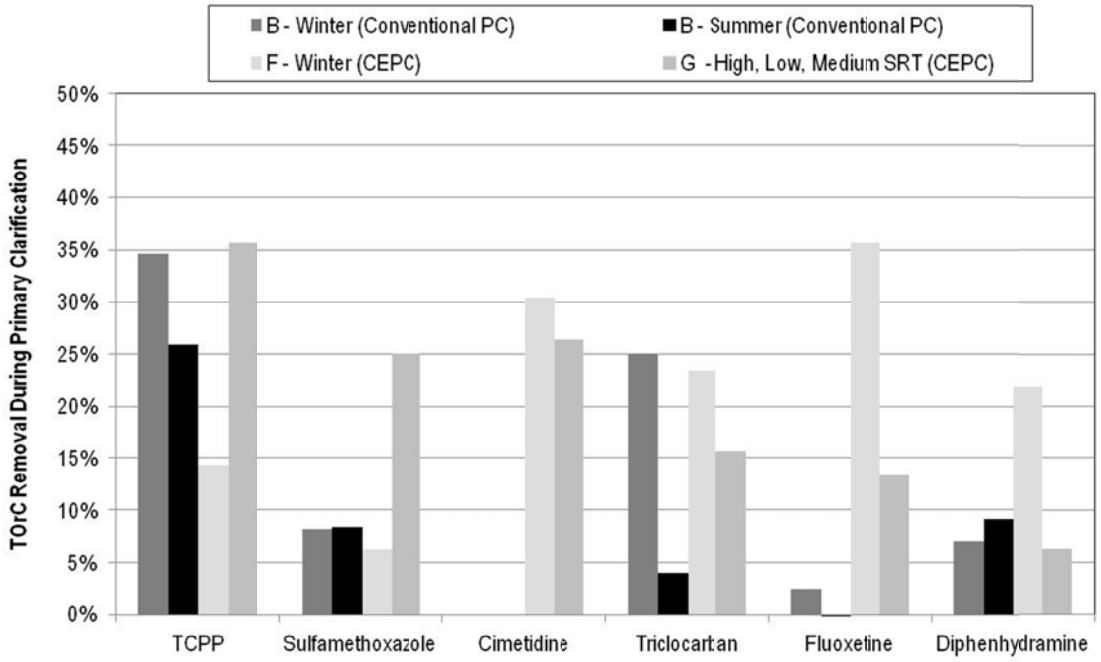


Figure 3-4. TOrC Removal During Primary Clarification.

The mass flow of TOrC associated with the solids in secondary influents was negligible in comparison to the mass flow of TOrC in liquid phase for most TOrC indicators studied. Only three TOrC (triclosan, triclocarban, and diphenhydramine) were found to have significant mass flows associated with solids in the secondary influents. All three compounds are hydrophobic in character and for two of the three compounds significant removal during primary clarification could be demonstrated (triclocarban and diphenhydramine).

Centrate streams were analyzed at Facilities A, B, and D for TOrC concentrations (Appendix E-7). Five of the TOrC indicators were present in significantly higher concentrations in centrate streams than in the respective secondary influents (carbamazepine, TCPP, gemfibrozil, bisphenol A, and ibuprofen). This result is surprising as these compounds exhibit very different biotransformation and sorption characteristics (Tables 3-2 and 3-3). It had been hypothesized that primarily compounds with high sorption could potentially accumulate in centrate recycle streams. None of the compounds detected in centrate in high concentrations was significantly removed during primary treatment at Facility B (all facilities A, B, and D use codigestion of primary and secondary sludge). For the three facilities A, B, and D it is estimated that centrate flows contributed between 10 and 65% of the TOrC mass loading for certain TOrC compounds (Appendix E). This finding indicates that TOrC may accumulate on the solids and be recycled within the treatment process to a greater extent than anticipated based on their biotransformation or sorption characteristics.

3.2.3 TOrC Removal During Secondary Treatment

Mass balances were calculated for each TOrC indicator and each sampling event. Raw data of all TOrC analysis as well as aqueous TOrC concentrations corrected for background contamination of blank results are included in Appendices E-2 and E-4. (For discussion of blank results see Chapter 2.0). The removal of TOrC during secondary treatment due to sorption and biotransformation was calculated, respectively, and compared to the overall TOrC removal between secondary influent and effluent (see Appendix F for calculations and Appendix E-5 for a complete listing of TOrC mass balance results). Mass balances errors were generally below 15% for most TOrC during all sampling campaigns.

Appendix E-8 provides an analysis of the potential sources for error and uncertainty for the TOrC mass balance calculations conducted in this study. Potential errors include contamination in the field during sample collection, incorrect or incomplete process data collection, contamination, the loss of samples during handling and shipment, analytical errors or lack of analytical precision, and errors during data transfer or calculations. Specific QA/QC measures were undertaken in this study to minimize or quantify these errors are summarized as well.

3.2.3.1 Overall TOrC Removal During Secondary Treatment

Table 3-6 provides an overview of the TOrC removal during secondary treatment for all sampling campaigns. The overall TOrC removal during secondary treatment was calculated based on the difference in TOrC mass load between secondary influent and secondary effluent.

Based on the observed removal efficiencies the TOrC indicators were categorized into four general groups. For three of the four groups, the mass balance calculations were consistent and removal by transformation and sorption could be accurately accounted for. The first group comprises compounds such as caffeine and ibuprofen that are generally very effectively removed independent of secondary treatment operation. The second group consists of compounds for which the removal varies significantly between different sites depending on the type of secondary treatment process employed, operational conditions, and season (e.g., triclosan, DEET). For some of the TOrC indicators mass balance calculations were inconsistent during some of the sampling campaigns (e.g., sulfamethoxazole, fluoxetine). In some of these cases, the calculated TOrC removal was negative indicating a net gain of TOrC mass during secondary treatment between secondary influent and effluent. These compounds were summarized in the third group.

The fourth group of TOrC is comprised of indicators that are rather refractory during secondary treatment, such as TCEP or sucralose. The maximum overall removal efficiency observed for compounds of this group remained below 30% at any field site.

Table 3-6. Overall TOrC Removal During Secondary Treatment.

	A - Winter	A - Summer	B - Winter	B - Summer	C - Winter	C - Summer	D - Summer	E - Summer	E - Winter	F – Winter	G -High SRT	G - Medium SRT	G - Low SRT	Average	Minimum	Maximum
Rapid Removal																
Caffeine	n.q.	100%	100%	100%	100%	n.q.	100%	100.0%	n.q.	99.9%	100.0%	100.0%	100.0%	100%	100%	100%
Acetaminophen	100%	99%	100%	99%	99%	100%	n.q.	100.0%	n.q.	n.q.	n.q.	100.0%	100.0%	100%	99%	100%
Ibuprofen	100%	100%	100%	100%	88%	94%	99%	99.9%	100.0%	100.0%	99.9%	100.0%	99.8%	98%	88%	100%
Naproxen	95%	99%	100%	100%	71%	89%	88%	99.8%	100.0%	98.8%	100.0%	100.0%	98.4%	95%	71%	100%
Iopromide	n.q.	n.q.	99%	99%	n.q.	n.q.	n.q.	91.1%	79.8%	64.2%	n.q.	99.6%	98.5%	90%	64%	100%
Bisphenol A	n.q.	n.q.	99%	98%	n.q.	n.q.	n.q.	99.0%	n.q.	n.q.	n.q.	n.q.	n.q.	99%	98%	99%
Moderate / Site Specific Removal																
Triclosan	94%	96%	99%	99%	56%	83%	93%	98.8%	99.2%	86.5%	97.2%	92.3%	85.7%	91%	56%	99%
Gemfibrozil	75%	89%	94%	100%	-1%	6%	49%	99.8%	99.1%	82.8%	99.5%	98.1%	83.5%	75%	-1%	100%
DEET	61%	96%	81%	100%	2%	66%	91%	99.9%	97.3%	30.3%	78.9%	62.6%	5.3%	67%	2%	100%
BHA	26%	73%	95%	100%	18%	46%	1%	90.2%	95.0%	-	99.6%	99.3%	50.0%	66%	1%	100%
Diphenhydramine	61%	70%	82%	90%	-5%	18%	62%	n.q.	96.1%	39.5%	96.3%	96.5%	41.1%	62%	-5%	96%
Atenolol	34%	42%	82%	84%	-10%	24%	31%	94.0%	93.2%	34.8%	n.q.	100.0%	52.0%	55%	-10%	100%
Trimethoprim	15%	n.q.	29%	98%	9%	n.q.	5%	94.2%	95.6%	10.8%	98.2%	97.0%	22.5%	52%	5%	98%
Benzophenone	n.q.	n.q.	22%	57%	85%	n.q.	n.q.	99.5%	91.2%	n.q.	n.q.	99.3%	n.q.	76%	22%	100%
TCPP	n.q.	n.q.	-10%	-19%	n.q.	n.q.	n.q.	48.7%	63.1%	n.q.	n.q.	n.q.	n.q.	21%	-19%	63%
Mass Balance Inconsistencies																
Sulfamethoxazole	-4%	12%	25%	45%	23%	36%	21%	61.2%	42.9%	-85.9%	-41.7%	-91.7%	-108.4%	-5%	-108%	61%
Fluoxetine	15%	33%	10%	-22%	55%	n.q.	2%	42.7%	6.5%	-117.8%	38.1%	32.9%	29.0%	10%	-118%	55%
Meprobamate	-8%	2%	-17%	-36%	2%	3%	-3%	61.2%	83.6%	-26.7%	90.4%	89.6%	11.1%	19%	-36%	90%
Cimetidine	31%	99%	57%	99%	-34%	-12%	-2%	61.8%	74.6%	38.3%	12.8%	25.5%	-16.5%	34%	-34%	99%
Triclocarban	45%	63%	96%	91%	-31%	87%	82%	79.4%	63.0%	-81.6%	74.6%	68.0%	50.5%	53%	-82%	96%
Slow / Refractory																
TCEP	n.q.	n.q.	4%	-15%	-1%	n.q.	n.q.	-3.0%	6.4%	0.4%	15.1%	12.1%	12.0%	3%	-15%	15%
Sucralose	n.q.	n.q.	21%	-12%	n.q.	n.q.	n.q.	28.7%	n.q.	n.q.	1.7%	n.q.	-22.0%	4%	-22%	29%
Carbamazepine	13%	27%	-19%	2%	7%	-13%	3%	34.2%	-4.4%	-3.6%	-17.2%	-17.2%	-8.9%	0%	-19%	34%
Primidone	9%	23%	-12%	14%	14%	-6%	8%	n.q.	n.q.	8.1%	-4.0%	-4.0%	-4.0%	4%	-12%	23%

n.q.: Removal not quantifiable.

3.2.3.2 TOrC Removal by Biotransformation and Sorption

The TOrC indicator compounds were grouped based on the observed removal efficiencies attributed to sorption and biotransformation, respectively, during full-scale sampling (Tables 3-7 and 3-8). TCPP, triclocarban, triclosan, bisphenol A, fluoxetine, and benzophenone exhibited the highest removal by sorption of all compounds (30-40% of the secondary influent TOrC mass load for some field sites). Even though sorption was significant, the total removal for most of these compounds (in particular the ones not likely to undergo biotransformation) was incomplete across secondary treatment and remained below 30-50% (Table 3-6).

A second group of TOrC indicators was removed by sorption to a lesser extent (10-20% of total TOrC mass load for some field sites). Generally, the compounds in this group were resistant to biotransformation.

All TOrC that were not sorbed during secondary treatment were hydrophilic compounds with log D_{ow} values of less than 2 (Table 3-2). Notably, diphenhydramine posed an exception to this as it was not sorbed significantly despite of its hydrophobic character. Facility E (MBR treatment) appeared to remove a higher fraction of TOrC by sorption than other CAS or MLE process configurations. Even TOrC classified as low or medium sorbable were removed onto solids between 10-20% during the summer and winter event at Facility E but not at other facilities (i.e., sulfamethoxazole, trimethoprim, cimetidine) (see Appendices E.5.8 and E.5.9). Sorption could not be reliably analyzed for all compounds at Facility E as the accuracy of the steady state mass balances was low due to accumulation of some TOrC on the solids under high SRT operation. This study did not further investigate whether the better removal of TOrC by sorption at Facility E was related to the increased MLSS concentrations, kinetic differences due to the extended HRT (the facility operates in batch mode at night when flows are low), high solid recycle rates, or other possible factors. (The sorption coefficients K_D for sulfamethoxazole, trimethoprim, and cimetidine measured in MLSS from Facility E were not significantly different compared to the K_Ds from other facilities, see Appendix G, Table G-3.)

Biotransformation led to complete removal at all field sites for acetaminophen, caffeine, and ibuprofen. These indicators represent TOrC that are very amenable to biotransformation. These compounds are of limited indicator value when attempting to compare treatment efficiencies for different biological process configurations or operational conditions.

Process configuration, operation, and seasonal conditions determined the biotransformation efficiency of a large group of compounds that underwent partial biotransformation. This group of indicators appears to be well suited for differentiating the performance of biological treatment systems for TOrC that are amenable to biotransformation.

Carbamazepine, sucralose, and primidone were confirmed to be recalcitrant in character even at field sites achieving low nutrient limits for nitrogen and phosphorus with secondary treatment.

For TCPP, triclocarban, bisphenol A, and TCEP, biotransformation efficiencies could not be quantified for enough sampling events to allow a general classification of these compounds. Mass balance results for triclocarban indicate a significant mass gain during secondary treatment (i.e., for Facility E, summer). Triclocarban is strongly hydrophobic and resistant to biotransformation. It is prone to sorb to mixed liquor solids and was found in RAS solid phase concentrations one to two orders of magnitude higher than any other TOrC indicator. The strong accumulation of triclocarban on mixed liquor solids could be a reason for the observed net

increase during secondary treatment as certain operational conditions may trigger desorption of this compound from the solids inventory into the liquid phase.

Table 3-7. TOrC Removal by Sorption During Secondary Treatment.

	% TOrC Removal by Sorption			
Indicator	n	Average	Minimum	Maximum
High Sorption				
TCPP	3	17.4%	2%	46%
Triclocarban	3	72.7%	46%	88%
Triclosan	13	12.7%	2%	33%
Bisphenol A	2	18.9%	11%	27%
Fluoxetine	10	16.4%	0%	38%
Benzophenone	6	8.1%	2%	37%
Site-Specific Efficiency / Moderate Sorption				
TCEP	9	4.0%	0%	20%
Iopromide	7	8.3%	0%	16%
Sulfamethoxazole	13	2.8%	0%	15%
Cimetidine	12	4.3%	0%	14%
BHA	13	2.2%	0%	13%
Trimethoprim	11	2.2%	0%	10%
Carbamazepine	13	1.6%	0%	9%
No / Low Sorption				
Caffeine	12	0.1%	0%	0%
Primidone	13	0.3%	0%	1%
Sucralose	5	1.2%	0%	5%
Diphenhydramine	12	1.6%	0%	3%
Meprobamate	13	0.3%	0%	2%
Atenolol	13	0.1%	0%	0%
DEET	4	0.0%	0%	0%
Gemfibrozil	13	0.3%	0%	0%
Naproxen	13	0.0%	0%	0%
Ibuprofen	13	0.0%	0%	0%
Acetaminophen	12	0.0%	0%	0%

Notes:
Average, minimum, and maximum removal percentages were calculated based on the results of 13 sampling campaigns at 7 facilities in total (Appendix E). Based on mass balance errors, certain values were excluded from this analysis.

Table 3-8. TOrC Removal by Biotransformation During Secondary Treatment.

	% TOrC Removal by Biotransformation			
Indicator	n	Average	Minimum	Maximum
Rapid Biotransformation				
Acetaminophen	7	100%	100%	100%
Caffeine	8	100%	100%	100%
Ibuprofen	13	98%	88%	100%
Moderate Biotransformation / Site Specific Efficiency				
Naproxen	13	95%	71%	100%
DEET	9	80%	30%	100%
Triclosan	13	80%	25%	98%
Gemfibrozil	12	80%	2%	100%
Diphenhydramine	12	66%	13%	96%
Atenolol	10	57%	20%	100%
BHA	12	63%	0%	99%
Trimethoprim	11	49%	2%	98%
Meprobamate	6	55%	0%	90%
Cimetidine	7	55%	14%	98%
Fluoxetine	6	23%	0%	36%
Sulfamethoxazole	8	27%	9%	45%
Benzophenone	2	76%	63%	90%
Iopromide	3	69%	55%	88%
Recalcitrant / Slow Biotransformation				
Carbamazepine	6	10%	0%	24%
Sucralose	3	12%	1%	18%
Primidone	8	11%	5%	22%
Mass Balance Uncertainties / Limited Data				
TCPP	-	NA	NA	NA
Triclocarban	-	NA	NA	NA
Bisphenol A	1	89%	89%	89%
TCEP	2	10%	9%	13%

Notes:
Averages, minimum and maximum removal percentages were calculated based on the results of 13 sampling campaigns at 7 facilities in total (Appendix E). Values excluded based on: 1) Calculated removal by biotransformation negative, and / or 2) TOrC mass balance error unacceptable (in most cases > 30%).

3.2.3.3 Seasonal Effects on TOrC Removal

Overall removal efficiencies for TOrC were consistently higher during summer sampling events compared to winter events (Table 3-6, Facilities A, B, C, and E). While several operating factors differed at each field site between summer and winter sampling events (such as SRT, HRT, or process configuration (Table 3-4) the only factor trending consistently with TOrC removal between all sites is the wastewater temperature that was between 7° and 10°C higher during summer sampling campaigns compared to the winter events. The stimulating effect of higher wastewater temperatures for TOrC removal appears to be more pronounced in treatment systems operating at low SRTs (e.g., of triclosan, DEET, or atenolol for Facility C).

3.2.3.4 TOrC Removal during Disinfection Processes

Composite samples were collected at five of the 13 sampling campaigns prior to and after final chlorination and dechlorination. Due to advanced treatment processes (i.e., flocculation, slake lime addition, carbon filtration) upstream of final disinfection at Facility B, TOrC concentrations in the chlorination influent were already low, typically close to the reporting limits (Appendix E-6). At facilities A and D, several TOrC were significantly reduced during chlorination, including bisphenol A, BHA, and cimetidine.

At Facility E samples were collected prior to and after UV disinfection. The facility uses medium pressure high output UV lamps with an effective design dosage of 80 mJ/cm^2. Primary disinfection dosages were not sufficient to reduce TOrC substantially if at all (see Appendices E.3 and E.4 for results). This study did not further investigate disinfection efficiency for TOrC removal.

3.2.3.5 TOrC Loads on Solids Leaving Secondary Treatment

The TOrC load associated with solids in secondary effluents were negligible (less than 5%) for the majority of TOrC indicators compared to the TOrC load in the liquid phase of secondary effluents at all full-scale field sites (Appendix E-8). Secondary effluent TSS concentrations were typically 5-15 mg/L at all facilities during the sampling campaigns. The highly sorbable TOrC indicators triclocarban, triclosan, and fluoxetine were an exception and TOrC loads associated with solids contributed significantly to the overall TOrC load in secondary effluents (triclocarban 10-70%, triclosan 3-30%, fluoxetine less than 10%). This finding suggests that tertiary treatment processes targeting additional solid removal (for example tertiary filtration for phosphorus reduction) will also improve effluent quality with regards to TOrC that are highly sorbable and less amenable to biotransformation.

The TOrC loads associated with the solids wasted from secondary treatment as WAS were significant for several TOrC indicators (more than 5% of the total secondary influent TOrC load) and even exceeded the total secondary influent loads for several TOrC. Again, this was the case specifically for TOrC that were highly or moderately sorbable (i.e., triclocarban, triclosan, fluoxetine, cimetidine, bisphenol A, benzophenone, etc.). This indicates that sorbable TOrC can accumulate on the solids during secondary treatment and reach much higher concentrations in recycle sludge systems than would be expected on basis of compound specific partitioning coefficients. Activated sludge systems operated at very long SRTs (specifically the MBR system, Facility E, SRT > 40 days) had a significantly higher TOrC load associated WAS solids for a higher number of compounds compared to facilities operating at lower SRTs (less than 10 days).

3.3 Fate Parameters

The sorption and biotransformation fate parameters for the indicator TOrC were measured for the full-scale activated sludge systems sampled during this study. The fate parameters measured included the TOrC mixed liquor solids partitioning coefficient and the biotransformation removal rate (rate constant). Both are critical prerequisites for TOrC mass balance modeling.

3.3.1 Sorption

Sorption isotherm tests were performed with mixed liquor activated-sludge solids collected from Facilities B, C, D, E, F, and G during the TOrC sampling campaigns. These tests were conducted to reveal whether sorption would be different in mixed liquor from different

plants and operational conditions. In addition, sorption tests were performed for laboratory-scale system assessing TOrC removal under controlled operational conditions. Appendix G lists the Freundlich isotherm model parameters (log K_F and n) for the TOrC indicators and mixed liquor solids.

Sorption coefficients could not be experimentally determined for acetaminophen, TCEP and TCPP (variability in experimental data), caffeine, iopromide (costs of isotope), and primidone and sucralose (low analytical sensitivity). The partitioning of acetaminophen (Radjenovic et al., 2009; Stevens-Garmon et al., 2011), primidone (Wick et al., 2009; Stevens-Garmon et al., 2011), TCEP (Stevens-Garmon et al., 2011), caffeine (Stevens-Garmon et al., 2011), and iopromide (Ternes et al., 2004) to sludge solids has been previously determined to be low (<65 L/kg). Therefore, sorption is not anticipated to be a critical attenuation mechanism for these compounds. This is largely supported by the results of the full-scale mass balance evaluations (Section 3.2.3.2).

To compare the sorption potential of different TOrC compounds, the sorption coefficient K_d was calculated for each TOrC using the respective Freundlich equation at a benchmark aqueous TOrC concentration of 1000 ng/L. The log K_d value was similar for a given TOrC independent of the field site and was apparently not affected by different operational conditions, such as SRT or prevalent redox conditions related to different nutrient removal regimes (Appendix G). Typically, the differences between log K_d values determined for different field sites were within 1 log unit for any given TOrC. This suggests that K_d values determined in this study will be similar for other wastewater treatment sites and can be adopted for estimating TOrC sorption for other secondary treatment systems. The range of K_d values measured for all field sites is reported in Table 3-9.

Based on the sorption coefficients determined for activated sludge, the TOrC indicators were classified by their anticipated sorption potential during activated sludge treatment (Table 3-10). For the most part, the classification based on the K_d values corresponds well to the classification based on the octanol-water partitioning coefficient (log D_{ow}), and the charge of the compounds. Compounds with a higher sorption potential (log K_d > 3) were neutral compounds, i.e., triclosan and triclocarban (with a log D_{ow} > 3), and positively ionic compounds, such as fluoxetine. This agreement suggests that the sorption coefficient specific for activated sludge could potentially be estimated through the compound's octanol-water partitioning coefficient and charge.

Table 3-9. Average, Minimum, and Maximum Log K_d for TOrC at C_w = 1000 ng/L.

	Min log K_d	Max log K_d	Avg. log K_d	Stdev. log K_d
Acetaminophen	*<1.5*	*<1.5*	*<1.5*	
Atenolol	2.35	2.87	2.58	0.21
Benzophenone	2.31	3.27	2.75	0.39
BHA	NA	NA	NA	
Bisphenol A	2.28	3.18	2.67	0.38
Caffeine	*<1.5*	*<1.5*	*<1.5*	
Carbamazepine	1.67	2.37	1.96	0.27
Cimetidine	2.19	2.79	2.48	0.22
DEET	1.77	2.14	1.96	0.15
Diphenhydramine	2.34	2.70	2.53	0.11
Fluoxetine	2.84	3.25	3.05	0.14
Gemfibrozil	1.65	2.56	2.08	0.32
Ibuprofen	1.65	2.62	2.18	0.35
Iopromide	*1.00*	*1.00*	*1.00*	
Meprobamate	1.70	2.39	2.07	0.27
Naproxen	1.41	2.39	2.03	0.33
Primidone	*<1.5*	*<1.5*	*<1.5*	
Sucralose	NA (<1.5)	NA (<1.5)	NA (<1.5)	
Sulfamethoxazole	1.94	2.93	2.40	0.33
TCEP	*<1.5*	*1.80*	*<1.5*	
TCPP	NA	NA	NA	
Triclocarban	3.21	4.41	3.87	0.55
Triclosan	3.09	3.98	3.51	0.32
Trimethoprim	2.10	2.60	2.35	0.17

NA – Not available, values in italics are estimated based on literature (Appendix G)

Table 3-10. Sorption Potential of TOrC Indicator Compounds.

Neutral or Ionic (-)				Ionic (+)	
log D at pH 7				log D at pH 7	
>4	4-3	<3		>1	<1
High Sorption	Moderate Sorption	Low Sorption		Moderate Sorption	Low Sorption
Triclosan	Benzophenone	Acetaminophen	Gemfibrozil (-)	Diphenhydramine	Cimetidine
Triclocarban	BHA	Caffeine	Meprobamate	Fluoxetine	Atenolol
Bisphenol A	TCPP	Carbamazepine	Naproxen (-)		Trimethoprim
		DEET	Primidone		Diphenhydramine
		Ibuprofen (-)	Sulfamethoxazole (-)		
		Iopromide	Sucralose		
log K_d				log K_d	
>3	3-2.5	<2.5		>3.0	3-2
Triclosan	Benzophenone	Acetaminophen	Gemfibrozil (-)	Fluoxetine	Cimetidine
Triclocarban	Bisphenol A	Caffeine	Meprobamate		Atenolol
		Carbamazepine	Naproxen (-)		Trimethoprim
		DEET	Primidone		Diphenhydramine
		Ibuprofen (-)	Sulfamethoxazole (-)		
		Iopromide			

Note: TCEP and BHA are not included, as sorption coefficients could not be determined.

As shown in Table 3-10, the sorption ability of compounds is based upon compound properties. The TOrC removal efficiencies through sorption observed during full-scale treatment (Table 3-7) support this assertion. The compounds with K_d values larger than three were effectively sorbed during activated sludge treatment achieving removal efficiencies up to 30-95%, depending on biotransformation characteristics.

3.3.2 Biotransformation

Biotransformation studies were performed to assess the degradation kinetics of the TOrC indicators in activated sludge mixed liquor collected from Facilities B, C, D, E, and F. Biotransformation kinetics were described in all cases with a pseudo first-order rate constant (Appendix G).

The TOrC indicators were categorized in relation to their biotransformation kinetics during activated sludge treatment (Table 3-11). The proposed indicator compounds span a wide range of biotransformation behavior ranging from rapid, to moderate, or slow.

Table 3-11. Biotransformation Kinetics of TOrC Indicators (Simplified).

Slow	Moderate	Rapid
<0.1 (L/g-d)	0.1-10 (L/g-d)	>10 (L/g-d)
Triclocarban	DEET	Caffeine
TCEP	Sulfamethoxazole	Naproxen
Carbamazepine	Gemfibrozil	Ibuprofen
TCPP	Cimetidine	Triclosan
Meprobamate	Trimethoprim	Fluoxetine
Sucralose	Iopromide	Diphenhydramine
Primidone		Bisphenol A
		Benzophenone
		Atenolol

Caffeine, naproxen, ibuprofen, fluoxetine and diphenhydramine generally had very fast kinetics even in mixed liquor collected from plants with a relatively low level of treatment (e.g., Facility C) (Table 3-11). Rate constants determined in this study support findings by others (Dickenson et al., 2010; Joss et al., 2006). For acetaminophen and bisphenol A removal rates of 70-120 L/g-d (Dickenson et al., 2010; Joss et al., 2006) and 13-31 L/g-d (Dickenson et al., 2010), respectively, have been previously determined suggesting that both compounds would be rapidly removed. Results from full-scale sampling indicate that TOrC with kinetic rates larger than 10 L/g-d are anticipated to be removed by at least 80% during secondary treatment based on biotransformation (Table 3-8).

Triclocarban, TCEP, and carbamazepine had very low biotransformation rate constants as these are known recalcitrant compounds (Dickenson et al., 2010; Wick et al., 2009). As TCPP and TCEP are structurally closely related (both are chlorinated aliphatic compounds), TCPP is anticipated to be similarly recalcitrant during secondary treatment. Wick et al. (2009) and Dickenson et al. (2010) reported low biotransformation rate constants for primidone (<0.1 L/g-d) in activated sludge. The results from full scale sampling support that TOrC with biotransformation rate constants below 0.1 L/g-d are not anticipated to be removed by more than 20% during secondary treatment (Table 3-8).

While TOrC sorption coefficients were generally similar between different field sites, the biotransformation rate constants differed for certain compounds between different secondary processes. These compounds included DEET, sulfamethoxazole, gemfibrozil, cimetidine, and trimethoprim and were moderately or slowly degradable with kinetic rates between 10 and 0.1 L/g-d. Similar transformation rates for DEET, gemfibrozil, and sulfamethoxazole were observed by Dickenson et al., 2010 and Joss et al., 2006.

Gemfibrozil appears to be faster biotransformed in activated sludge systems operating at a higher SRT (Figure 3-5) or low F/M ratios. Diphenhydramine, triclosan, and trimethoprim appear to follow a similar trend. In contrast, sulfamethoxazole appears to be faster biotransformed in activated sludge systems operated at younger sludge ages or higher F/M ratios. With the exception of Facility B, the biotransformation rate constants for cimetidine were consistently low for all field sites (K_b = 0.1-1 L/g-d).

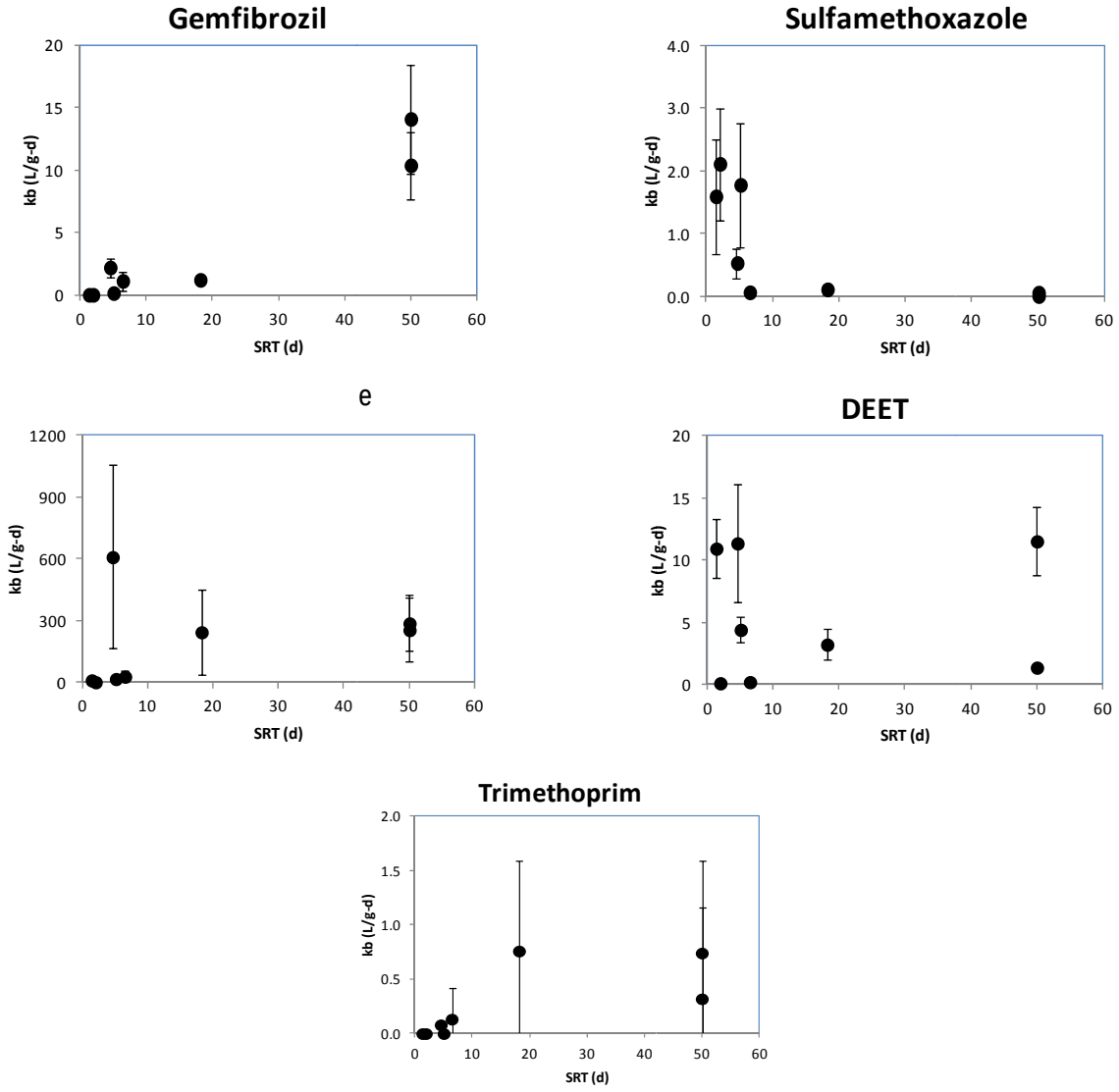


Figure 3-5. Biotransformation Rates K_b for Gemfibrozil, Sulfamethoxazole, Diphenhydramine, DEET, and Trimethoprim as a Function of SRT (K_b error bars represent the confidence interval).

The biotransformation kinetics of rapidly biotransformed compounds, such as naproxen, ibuprofen and caffeine, were faster in sludges of plants operating at very low SRTs similar to sulfamethoxazole (Appendix G). Despite the slower kinetics in high SRT activated sludge systems, these compounds were still almost completely removed. This trend could not be confirmed for fluoxetine.

Figure 3-6 compares the kinetic rates of moderately removed TOrC with the removal efficiency of the compounds quantified during full-scale mass balances. Data indicates the general trend that biotransformation removal increases abruptly when biotransformation rate constants increase above 0.2 to 1 L/g-d. Iopromide is also potentially a moderately removed compound, since Joss et al. (2006) reported a K_b of 2.0 L/g-d for iopromide.

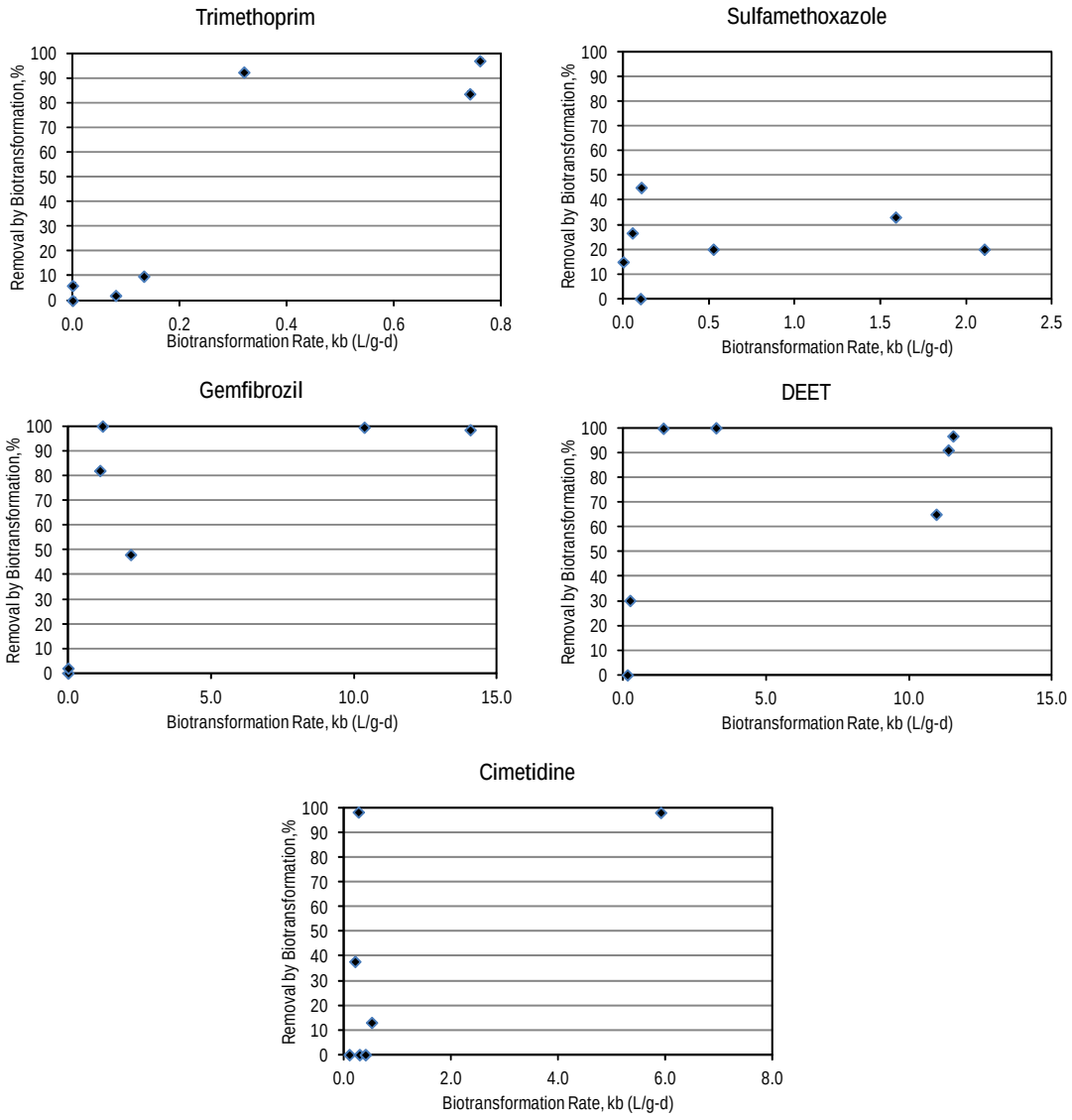


Figure 3-6. Full Scale TOrC Removal by Biotransformation in Relation to Biotransformation Rates Measured in Respective Mixed Liquor.

It is noteworthy that the biotransformation rate constants for DEET and caffeine were in general multiple times higher in mixed liquor systems that received higher concentrations of these TOrC in the aeration basin influents (Figure 3-7). The biotransformation rate constants were determined under controlled temperature conditions in the laboratory. Therefore, wastewater temperature did not affect kinetic rates measured in the laboratory. As discussed in Section 3.2.2.1, the aeration basin influent concentrations did not vary significantly for any of the other TOrC among the field sites sampled.

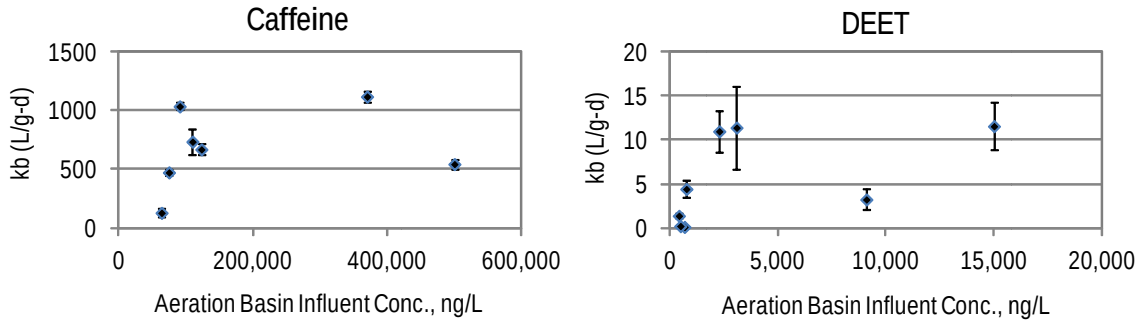


Figure 3-7. Biotransformation Rates for Caffeine and DEET as a Function of Aeration Basin Influent Concentrations. K_b error bars represent the confidence interval.

The TOrC indicators were binned according to both their measured biotransformation and sorption fate parameters (Table 3-12). Eight of the nine bins are represented by at least one indicator compound. These indicator compounds represent a wide range of sorption and biotransformation behavior. The majority of the indicators falls into the group of polar compounds with log K_d values < 2.5. Within this group, five compounds each represent the slow/ recalcitrant, moderate, and rapid biotransformation categories. The bin that is not represented is compounds with moderate biotransformation/high sorption.

Table 3-12. Summary Matrix of TOrC Indicators Based on Biotransformation and Sorption Fate Parameters.

Sorption (log K_d)	Biotransformation (K_b, L/g-d) Slow <0.1	Moderate 0.1-10	Rapid >10
Low <2.5	Carbamazepine Meprobamate Primidone TCEP Sucralose	DEET Sulfamethoxazole Gemfibrozil Iopromide Trimethoprim	Acetaminophen Caffeine Naproxen Ibuprofen Atenolol
Moderate 2.5-3	TCPP	Cimetidine	Benzophenone Diphenhydramine Bisphenol A
High >3	Triclocarban		Triclosan Fluoxetine

Note:
BHA was not included in this summary table as fate parameters could not be determined or estimated from literature.

3.4 Effect of Process Parameters on TOrC Removal

The following parameters were examined in the study: Solid retention time, temperature, redox conditions, and the differences in TOrC removal performance between fixed film and suspended growth processes.

3.4.1 Solid Retention Time

An outcome of the literature review was a resourceful electronic database that contains information for over 200 TOrC. The MS Excel™ based features make it easy to examine individual compound removal data in relation to treatment conditions. The database was used to plot the SRT and HRT against percent removal values for the target indicator compounds. These results are presented in Appendix J. For comparison purposes, the graphs display results obtained from the literature, and full- and laboratory-scale systems examined in this WERF study. Interestingly, increasing SRT and HRT increases the removal for some of the compounds. The exceptions are meprobamate, fluoxetine, TCPP, TCEP, sulfamethoxazole, trimethoprim and triclocarban, where a positive correlation is not apparent. In general, primidone, carbamazepine and sucralose are not significantly removed (less than 20%) across the range of SRTs. Table 3-13 reports the threshold SRT values for certain TOrC above which 80% or more of the compound was typically removed based on data collected in this study. The 80% threshold was selected as it allowed a comparison between a large number of indicators investigated and as it was proposed before for defining SRT boundary conditions for TOrC removal (Stephenson and Oppenheimer, 2007). Minimum SRT requirements for other removal efficiencies can be easily estimated from the graphs provided in Appendix J for the TOrC indicators.

With the exception of Facility E, the MBR treatment process, the rest of the field sites sampled in this study SRT and HRT were positively and linearly correlated ($R^2 = 0.6$) (Appendix J). Data from field investigations did therefore not allow differentiating whether SRT or HRT was limiting the biotransformation of TOrC. Whereas threshold concentrations are reported for SRT and not HRT in Table 3-13, it is recommended to further investigate the effect of HRT on the biotransformation of TOrC during full-scale treatment.

Laboratory-scale flow-through experiments were performed to systematically assess the effect of SRT on TOrC removal. As described in Chapter 2.0, three systems were operated in parallel at 5, 10, and 20 days SRT treating the same feed water. The HRT for all three systems was kept constant at ~20 hours. Four weekly sets of samples were analyzed for TOrC removal. TOrC removal was also assessed through a pilot-scale sequencing membrane bioreactor (SMBR), which treated the same wastewater source as the flow through systems. The results from both experiments generally confirm the effect on SRT on TOrC indicator removal (results not shown).

Table 3-13. Threshold SRT Values to Achieve at Least 80% TOrC Removal.

	SRT, days
Acetaminophen	2
Caffeine	2
Ibuprofen	5
Naproxen	5
Bisphenol A	10
Triclosan	10
DEET	15
Gemfibrozil	15
Atenolol	15
BHA	15
Iopromide	15
Cimetidine	15
Diphenhydramine	20
Benzophenone	20
Trimethoprim	30

Threshold SRT values could not be determined for fluoxetine, TCPP, TCEP, primidone, sulfamethoxazole, carbamazepine, triclocarban, or sucralose because compounds are recalcitrant or removal was too variable.

3.4.2 Temperature

Three pilot-scale activated sludge systems were operated in parallel at controlled temperatures of 13°, 20°, and 30°C to assess the effect of temperature on TOrC removal (see Chapter 2.0). The SRT and HRT for all three systems were kept constant at 10 days and 20 hours, respectively. One weekly set of samples was analyzed for TOrC. The experiment did not differentiate between TOrC removal in the aqueous phase by sorption or biotransformation. The results of the experiment are largely inconclusive as to the influence of temperature on TOrC removal during activated sludge treatment. It is possible that temperature effects were not noticeable in the experiment due to the high SRT and HRT and that data trends were concealed by the variability in TOrC concentration measurements (results not shown).

3.4.3 Redox Conditions

Two pilot-scale systems were operated in parallel in different reactor configurations to assess the effect of redox conditions during activated sludge treatment on TOrC removal. This process was run in an MLE configuration with an anoxic regime for nitrogen removal and the performance was compared to a fully aerated nitrifying conventional activated sludge (CAS) system. Two weekly sets of samples were analyzed for TOrC (Figure 3-8). While the aerobic and anoxic/aerobic pilot systems performed similar in terms of TOrC removal, variations in TOrC removal appeared to be lower for several compounds for the MLE system than for the nitrifying CAS system.

The two sampling events at Facility B were conducted under different secondary process conditions: Fully aerobic treatment in Summer (nitrification mode) and anoxic and aerobic

treatment in Winter (MLE, nitrification and denitrification). The aerobic SRT was comparable during both sample events (approximately 18 days). Even though the facility produces a better effluent quality during winter in terms of nitrogen removal (see Appendix D) than in summer, TOrC effluent concentrations were generally higher (Appendix E. 4.3) and removal efficiencies were generally lower in winter (Table 3-6). Whether anoxic conditions or MLE recycle reduced the TOrC removal during secondary treatment or higher temperatures in summer improved TOrC removal could not be further identified.

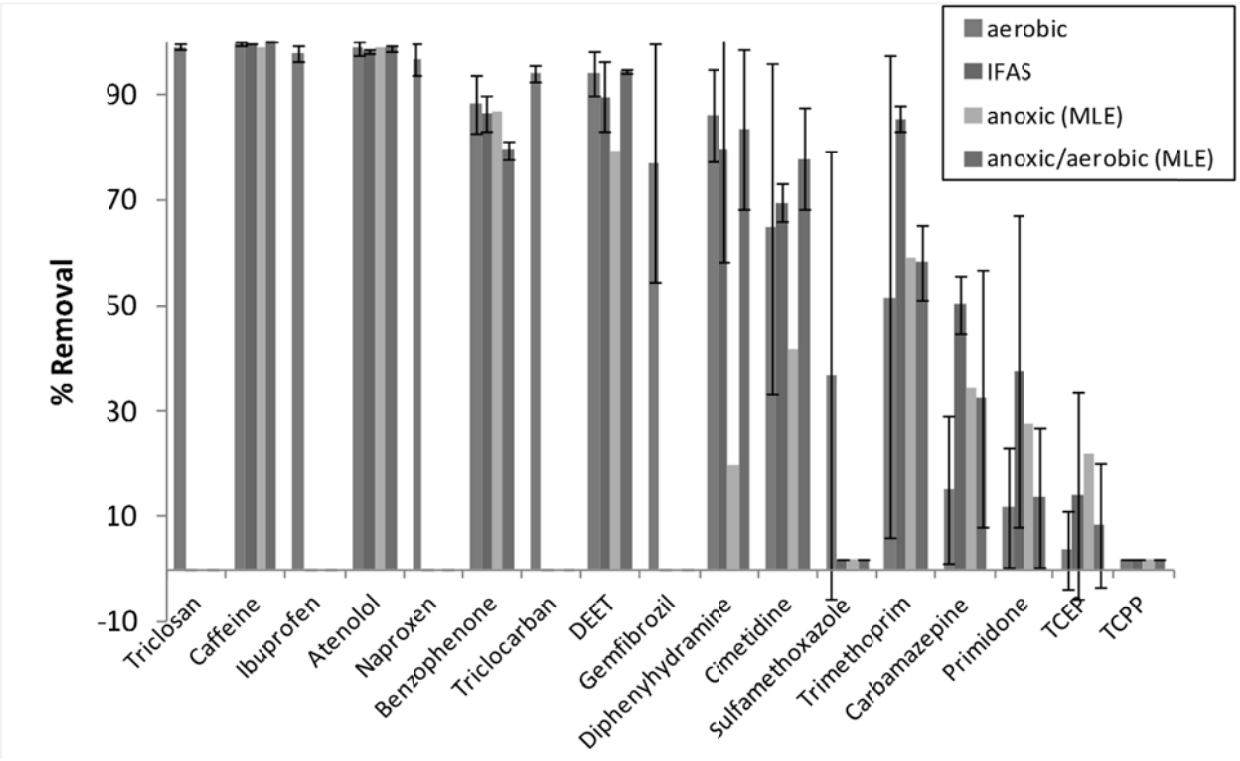
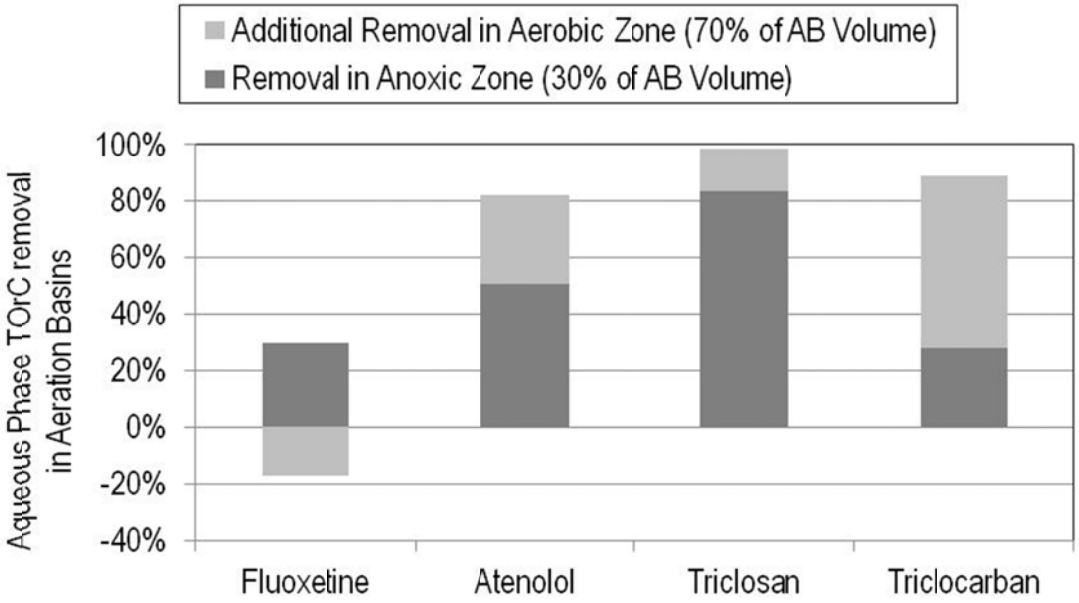


Figure 3-8.TOrC Removal During Nitrification (aerobic), IFAS, and MLE (anoxic and anoxic/aerobic) Testing.

During the full-scale testing campaign at Facility B, winter, TOrC samples were collected from the end of the anoxic zone prior to the aerobic zone in the aeration basins in addition to the secondary effluent to establish a TOrC profile through the aeration basins. Facility B operated at this time in an MLE configuration. The anoxic zone comprised 30% of the total aeration basin volume with an anoxic HRT of 2.6 hours and a MLSS concentration of 1,590 mg/L (Appendix D). The removal of TOrC indicators in the anoxic zone was calculated as the difference of the aeration basin influent liquid concentration (blend of primary effluent, MLE, and RAS) and the anoxic zone effluent liquid concentration. The removal in the subsequent aerobic zones was calculated as the difference in anoxic zone effluent and secondary effluent concentration in the liquid phase. Few TOrC indicators (i.e., fluoxetine, atenolol, triclosan, and triclocarban) were significantly removed in the anoxic zone (Figure 3-9). As triclosan, fluoxetine, and triclocarban are hydrophobic compounds it is likely that the removal observed in the anoxic zone was based on initial sorption of these compounds onto mixed liquor. With the exception of atenolol, none of the compounds amenable to biotransformation showed significant removal under anoxic conditions.

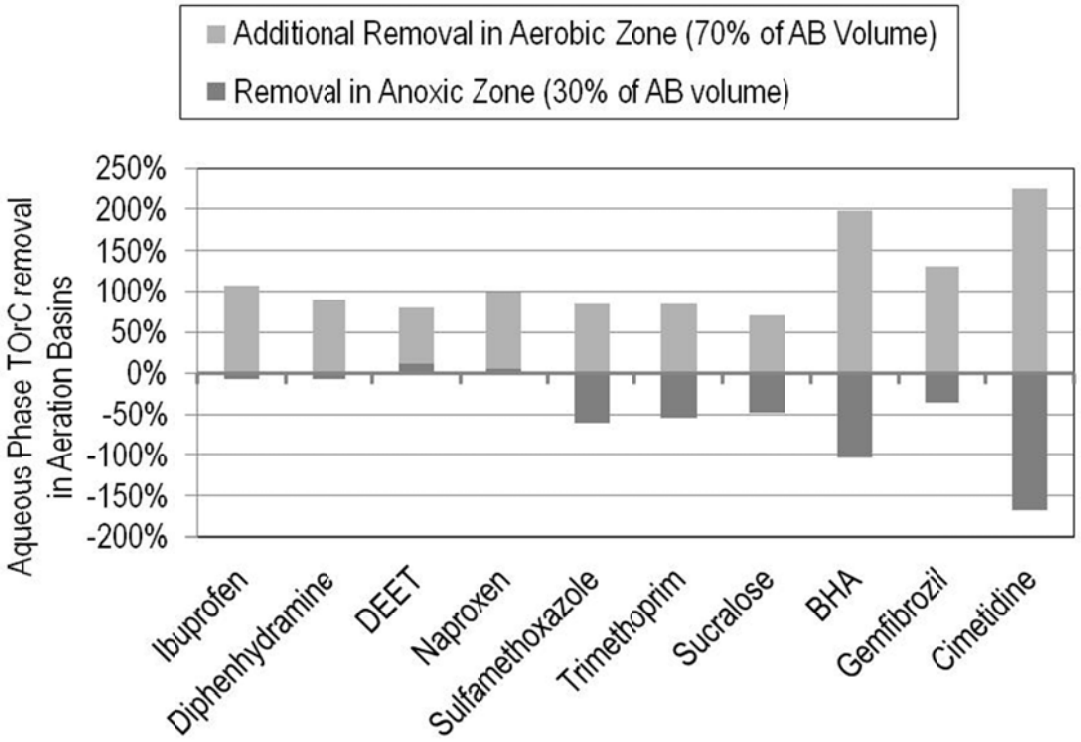


Note: Negative removal percentages indicate an increase in aqueous phase TOrC concentration.

Figure 3-9. Removal of Rapidly Biotransformed TOrC in Anoxic and Aerobic Treatment Zones of Aeration Basins at Facility B, Winter.

All other TOrC indicators, for which removal could be quantified during this profile testing, were primarily removed during aerobic treatment (

Figure 3-10). Generally, compounds that were rapidly biotransformed but not highly sorbable in accordance with Table 3-12 were nearly exclusively removed during aerobic conditions (i.e., ibuprofen, naproxen, DEET, and diphenhydramine). Several TOrC indicators that were moderately biotransformed showed an initial increase in liquid phase concentration after anoxic treatment (i.e., sulfamethoxazole, trimethoprim, gemfibrozil, and cimetidine). The reason for this increase in concentration in the aqueous phase in an anoxic environment is unclear, as these compounds are rather low in sorption potential. It is possible that anoxic conditions prompted a desorption or release of TOrC attached to the mixed liquor solids. If this effect occurs, it may be more noticeable for compounds that are comparatively slowly biotransformed. Table 3-14 illustrates that the mass of TOrC bound to mixed liquor solids in the anoxic zone was higher than the mass by which the TOrC increased in the liquid phase of the anoxic zone. This means that desorption of TOrC from solids during anoxic conditions could theoretically account for the observed increase in liquid phase concentration. It is recommended to further investigate biotransformation, sorption and desorption kinetics of TOrC on mixed liquor in different redox conditions.



Note: Negative removal percentages indicate an increase in aqueous phase TOrC concentration.

Figure 3-10. Concentration Change of Moderately Biotransformed TOrC in Anoxic and Aerobic Treatment Zones of Aeration Basins at Facility B, Winter.

Table 3-14. Comparison of Aqueous and Solid Phase TOrC Concentrations in Anoxic Zone of Facility B, Winter.

	ABI (PE, RAS, MLE), ng/L	Anox. Eff., ng/L	Aqueous Phase Increase, ng/L	(Average) Solid Concentration, ng/g	Solid phase concentration, ng/L[1)]	Percent TOrC increase of solid phase concentration
Sulfamethoxazole	685	1,100	415	127	620	67%
Trimethoprim	418	650	232	117	570	41%
Cimetidine	129	345	216	44.3	216	100%
Sucralose	22,827	34,000	11,173	<800	<3,900	-
Gemfibrozil	367	500	133	33.7	164	81%
BHA	32	65	33	<14	<68	<49%

[1)] Solid phase concentration was calculated as: (Average) aqueous solid concentrations (ng/g) * MLSS (g/L). MLSS concentration was 4.88 g/L for Facility B (winter).

3.4.4 Fixed Film Versus Suspended Growth

An integrated fix-film activated sludge (IFAS) process was operated at pilot-scale in parallel to an MLE process, in otherwise similar process configuration, to assess potential differences in TOrC removal performance between fixed film and suspended growth processes. Two weekly sets of samples were analyzed for TOrC (3.8). Due to the limited number of TOrC samples collected and the similar removal efficiency of the MLE and IFAS process for most compounds, it was not possible to identify statistically significant differences between hybrid fixed film and suspended growth processes. IFAS performed similarly well for most compounds compared to the MLE process. Trimethoprim, a moderately degradable compound, was significantly better removed in the hybrid fixed film system than in the suspended growth process.

CHAPTER 4.0

MODELING TORC REMOVAL

Evaluation and validation modeling assessments were performed with the mass balance model ASTreat.

4.1 ASTreat Background

ASTreat was selected for further evaluation based on it being a public-domain software, its success to predict compounds in a previous Canadian validation study (McAvoy et al., in prep), its simplicity of input requirements and ability to model the fate of TOrC during solid and liquid stream treatment. Other potentially viable models identified, but not further evaluated in this study were the STP Model (Clark et al., 2002), SimpleTreat (Struijs et al., 1996), TOXCHEM+ (Environmental Expert, 2002), and WATER9 (U.S. EPA, 1994). The review of these models is presented in Appendix H, which provides a comparison of the availability, source, required input parameters, and capabilities and limitations of these models.

ASTreat is a Windows-based application program with graphical interface developed by Procter & Gamble (McAvoy et al., 1999), which is designed to predict the fate of chemical compounds in a conventional activated sludge treatment plant consisting of a primary clarifier, an aeration tank, a secondary clarifier, and a digester/dewatering unit. ASTreat was used in this study to determine TOrC attenuation during secondary treatment.

ASTreat uses a concentration-based analysis approach, where compound concentrations are used in mass balance models. The secondary treatment mass balance has the general form:

Accumulation = Input – Output – (Loss to solids) – (Loss to atmosphere) – (Loss by biodegradation)

Under steady-state conditions (Accumulation = 0), the mass balance model simplifies to the following equation.

$$QC_I = QC_E + r_s + r_v + r_{bio}$$

C_I and C_E are total concentrations (g/m^3) in the secondary influent and effluent, respectively, Q is the volumetric flow rate (m^3/d), and r_s, r_v, and r_{bio} are the loss rates (g/d) by sorption partitioning, volatilization to the atmosphere and biodegradation, respectively. C_I and C_E consider the concentrations both in the aqueous phase and amount sorbed to solids. The loss by volatilization, r_v, was assumed negligible since the TOrC indicator compounds have low volatility.

ASTreat does not contain chemical databases and requires the user to define the compound in terms of biotransformation, sorption and volatilization characteristics. A first-order kinetic model was used in this study for modeling loss of the parent compound due to biotransformation, though ASTreat also has the capability to model chemical loss by using the Michaelis-Menten equation.

$$r_{bio} = k_b C\, V$$

V = volume of reactor (m^3)

K_b = first-order biodegradation rate constant (d^{-1})

C = dissolved chemical concentration in reactor (g/m^3)

The loss due to wasting from the secondary treatment process is modeled as:

$$r_s = Q_w C \; + Q_w (K_d) XC$$

Q_w = wasting flow rate from secondary treatment (m^3/d)

X = suspended solids concentration in wasting flow (kg/m^3)

C = dissolved chemical concentration in wasting flow (g/m^3)

K_d = sorption coefficient (m^3/kg)

ASTreat predicts the percent removal and effluent concentration of an organic compound. The outputs are reported as total removal and removal by sorption and biotransformation. ASTreat model predictions were previously compared with measurements for 17 nonvolatile substances sampled from a wastewater treatment plant in Ontario, Canada (McAvoy et al., in prep). The 17 substances included 10 polyaromatic hydrocarbons, five polybromodiphenyl ethers, one polybromobisphenol A compound, and one antimicrobial agent used in personal care products. The predictions from ASTreat for total removal of these highly attenuated (>75%) substances were in good agreement with the measured values. The mean absolute predicted difference (predicted % removal – measured % removal) was 3.4% for the 17 compounds studied.

4.2 ASTreat Evaluation

The ASTreat model was evaluated for its ability to simulate the removal of indicator compounds for five of the seven facilities sampled (seven of the 13 sampling campaigns: B Summer, C Winter, C Summer, D Summer, E Winter, E Summer, and F Summer). The remaining two facilities and five sampling campaigns were used in the validation of ASTreat model (Section 4.4). The processes evaluated using ASTreat represented a range of conditions based on wastewater temperature, level of nutrient removal, and operating factors (such as SRT and HRT) (Table 3-4). The model input included compound specific parameters (i.e., TOrC aeration basin influent concentrations, K_b, and K_d) and process operational parameters (i.e., influent flow rate, influent TSS, HRT, SRT (maximum 25 days), MLSS concentration, effluent TSS, and RAS TSS). Sorption (K_d) and biotransformation (K_b) fate parameters employed were measured in batch tests that used activated sludge from the same site being modeled [(Section 3.3) Table 3-4 and Appendices C and D]. TOrC secondary influent concentrations are reported in

Appendix E. A summary of the operational model input parameters for each facility is provided in Appendix H.

The simulated percent removal for each TOrC indicator modeled by ASTreat was compared to removal measured in the field (Appendix H). Table 4-1 lists the absolute predicted differences (simulated % removal – measured % removal) for each compound across the sites, as well as the mean difference (absolute value mean) and predicted bias (actual value mean). Model simulations were not performed for acetaminophen, bisphenol A, BHA, iopromide, and TCPP as their fate parameters required for modeling could not be determined.

The uncertainty associated with model parameters was determined to be on average 10% of the predicted removals. This is the mean uncertainty for compounds falling in the range of 5-95% (Appendix H). Therefore, a 20% removal difference criterion was adopted to take into account the uncertainties associated by both model (10%) and measured removals (10%).

Out of 107 total comparisons for 19 TOrC, 73% of the comparisons were within 20% of the measured removal. Based on the ability of the model to predict removals, the TOrC indicators were classified into three groups: 1) recalcitrant, 2) highly-amenable, and 3) moderately-amenable compounds. The first two compound groups comprised of compounds with 86% of predictions within 10% of the measured removal for all field sites, which were deemed excellent results. A 10% removal difference criterion can be used for compounds at the extremes, i.e., above 95% and below 5%, since the uncertainty for model predictions are lower in these ranges based on an uncertainty analysis (Appendix H). This group comprised of compounds that were either recalcitrant during secondary treatment (i.e., carbamazepine, TCEP, sucralose, primidone, and meprobamate) or very easily removed through biotransformation (i.e., caffeine, ibuprofen, and naproxen). See Figure 4-1 for example results representative for these groups.

A greater challenge for accurate TOrC fate model predictions are those compounds that show moderate removal by biotransformation or sorption in relation to site-specific operational conditions. Within this group, DEET, gemfibrozil, atenolol and triclosan (Figure 4-2) had 86%, 71%, 71%, and 100% of their percent removal values, respectively, within 20% of the observed removals, which was deemed very good (within the analytical and model uncertainty criterion). Less accurate predictions were determined for cimetidine, triclocarban (Figure 4-3, Table 4-3), sulfamethoxazole (Figure 4-3), trimethoprim (Figure 4-3), benzophenone, diphenhydramine (Figure 4-3), and fluoxetine, where 67%, 60%, 57%, 50%, 50%, 33%, and 0% of absolute differences, respectively, were assessed within 20% of the observed removals. Of these compounds, the removal for cimetidine, sulfamethoxazole, and trimethoprim was typically under-predicted and the removal for diphenhydramine and fluoxetine was typically over-predicted using ASTreat. Benzophenone and triclocarban removals had instances of over- and under-predictions.

Table 4-1. Difference Between the Simulated and Observed Percent Removals.

Compound	Difference between Modeled and Actual Removal (%)							Mean Difference (%)	Predicted Bias (%)
	B Summer	C Winter	C Summer	D Summer	E Winter	E Summer	F Summer		
Atenolol	12	17	73	48	-3	2	17	25	24
Benzophenone	38	15	NA	NA	-32	-9	NA	24	3
Caffeine	-0.1	-1	NA	-0.2	-0.1	NA	-0.5	0.3	0
Carbamazepine	-1	-6	5	-1	-34	0.7	1	7	-5
Cimetidine	-7	2	11	14	-36	NA	-31	17	-8
DEET	-14	4	15	-11	-39	-4	-22	16	-10
Diphenhydramine	10	33	63	38	NA	4	51	33	33
Fluoxetine	122	45	NA	98	NA	93	217	115	115
Gemfibrozil	-30	1	-5	-5	-8	-5	-55	15	-15
Ibuprofen	NA	-5	6	-3	0	-1	-4	3	-1
Meprobamate	9	9	11	1	NA	NA	0	6	6
Naproxen	-2	28	10	-2	-2	-5	-9	9	2
Primidone	-14	-14	0	-8	NA	NA	-8	9	-9
Sucralose	0	NA	NA	NA	-29	NA	NA	14	-14
Sulfamethoxazole	-27	10	3	-3	-60	-36	5	21	-15
TCEP	0	1	NA	NA	2	-6	0	2	-1
Triclocarban	-11	NA	-17	-31	-17	29	NA	21	-10
Triclosan	1	-10	-20	6	NA	NA	13	10	-2
Trimethoprim	-38	-7	NA	0.02	-46	-64	-4	26	-14

Note: Positive values indicate that the predicted removal was greater than the measured removal for a given compound. Negative values indicate that the predicted removal was less than the measured removal for a given compound.

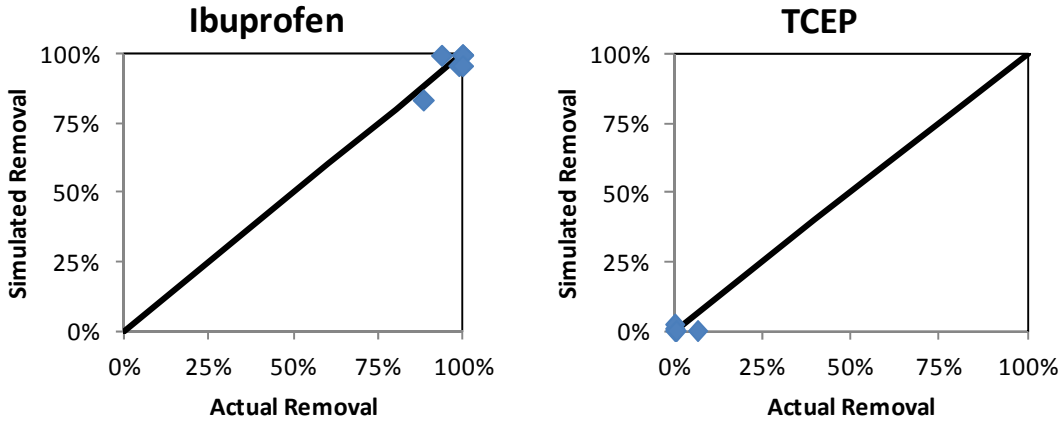


Figure 4-1. Measured Versus Simulated Removals for Ibuprofen and TCEP.

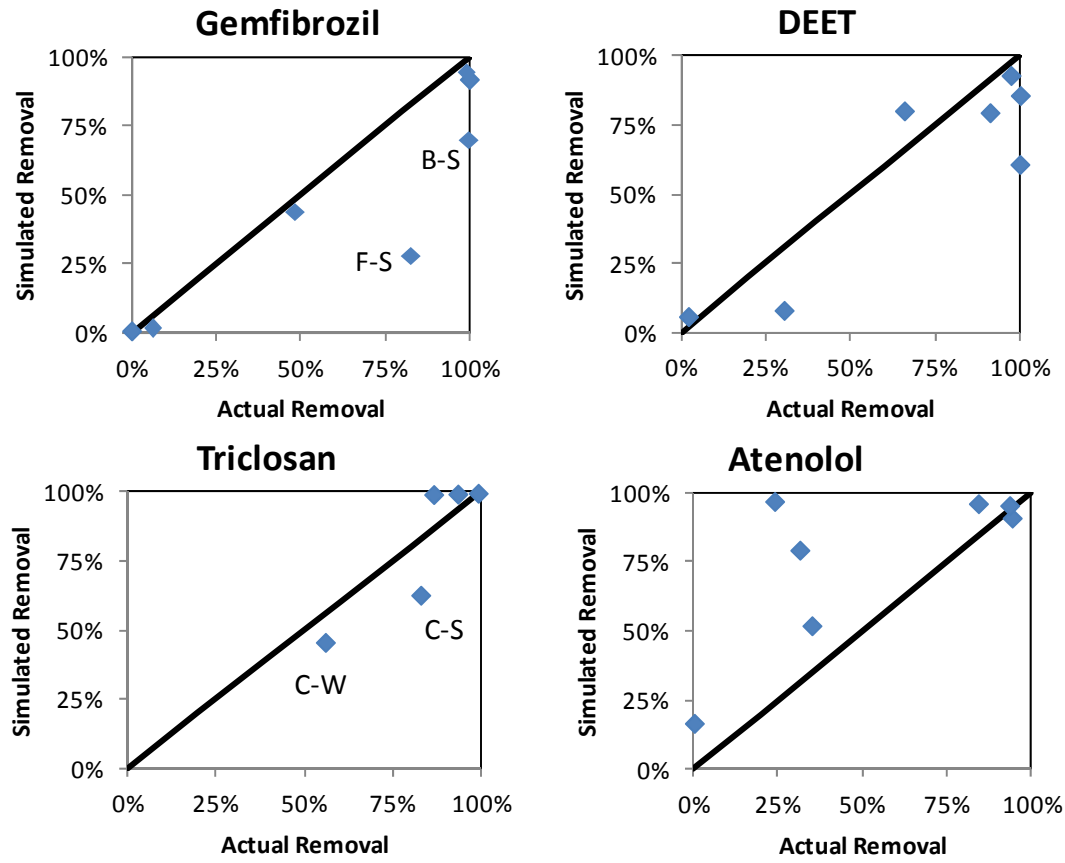


Figure 4-2. Measured Versus Simulated Removals for Gemfibrozil, DEET, Triclosan, and Atenolol.

It is worthwhile to point out the predictions for moderately to highly sorptive compounds, benzophenone, cimetidine and triclocarban, for Facility E with high SRT (>50 days) may not be properly modeled by ASTreat, since ASTreat can only handle SRTs up to 25 days. Based on the sensitivity analysis (Appendix H), SRT was found to inversely affect compound sorption, which therefore may not be captured for SRT > 25 days. Triclosan and triclocarban are highly sorptive compounds. Simulations using sorption partitioning coefficients (Kd) derived from isotherm

batch tests under-predicted the measured removal for triclocarban and triclosan for the Facility C winter and summer campaigns (data not shown). Modeling triclosan and triclocarban removal using Kd values calculated from RAS field samples resulted in a much better agreement between the simulated and measured removal for both compounds (data shown in Table 4-1 and Figure 4-3). These results suggest that the laboratory batch isotherm method may not be appropriate for determining Kd values when the compound is highly sorptive and poorly biodegradable and in treatment systems with longer SRTs.

Fluoxetine was consistently over-predicted and had the largest discrepancy between modeled and actual removals. The reason for this discrepancy is unknown. The batch tests indicated that fluoxetine is a highly sorptive and biotransformable compound, but significant attenuation is not observed in the field. Fluoxetine occurs at rather low concentrations in wastewater influents (typically below 50 ng/L); therefore errors in full-scale mass balance calculations are potentially inflated compared to the error for other compounds measured at higher concentrations. Nevertheless, the poor removal of fluoxetine during wastewater treatment is demonstrated in this study and has been reported by others (see Appendix A database).

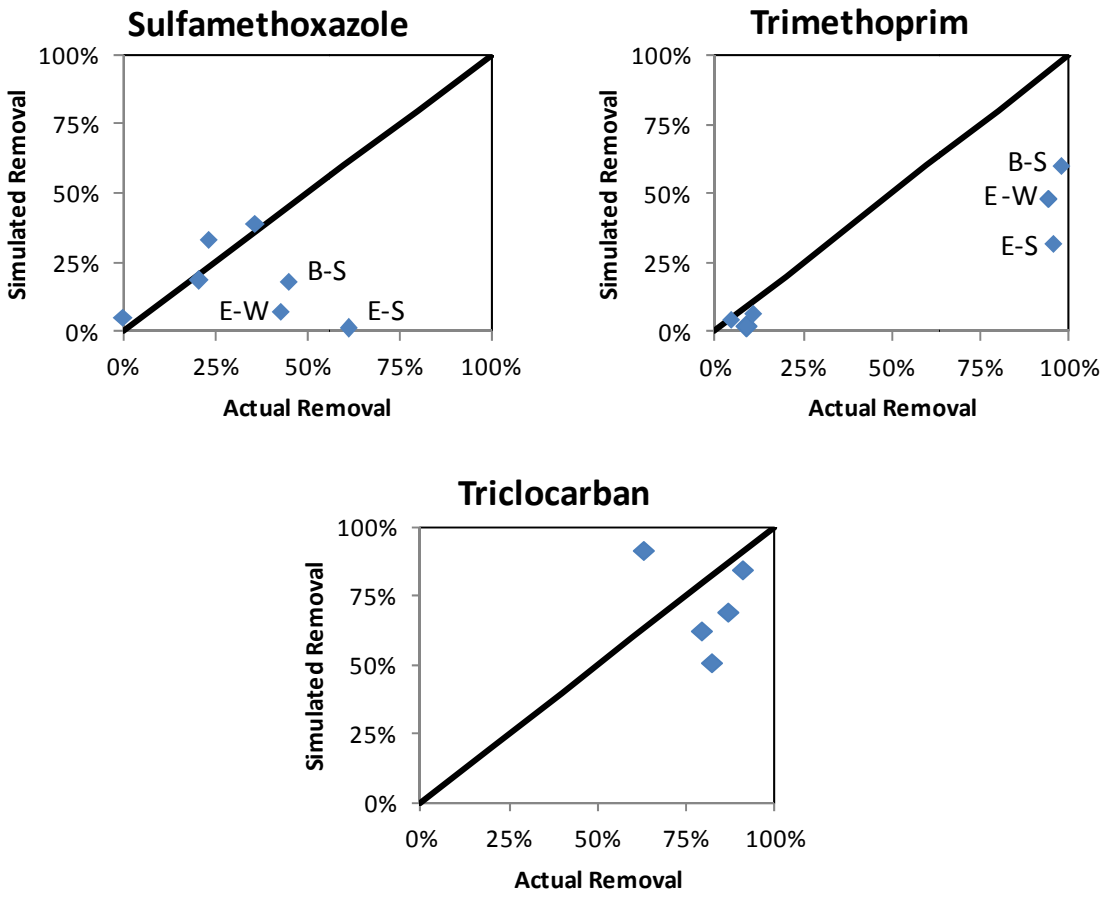


Figure 4-3. Measured Versus Simulated Removal for Sulfamethoxazole, Trimethoprim, and Triclocarban.

The measured and simulated removal efficiencies for the low sorbing antibiotics, sulfamethoxazole and trimethoprim, are depicted in

Figure 4-3 4-3. Interestingly, the only field sites for which the model predictions were inaccurate were those operated at high SRTs (Facility E winter and summer had more than 50 days and Facility B summer at 18 days). Even though >50 days at Facility E are outside of the applicability domain of ASTreat, this is probably not a factor since the sensitivity analysis demonstrated that SRT is not a factor for biotransformation removals even for SRT less than 25 days. A more likely explanation may be that the biotransformation rates measured for sulfamethoxazole in the laboratory are too low to match the actual biotransformation observed in the field. More research is needed to better understand biotransformation rates in systems that operate at longer SRTs (>25 days).

ASTreat modeling was performed for two of the most volatile compounds in this study, benzophenone and TCEP (Henry's constant (atm/m^3/mol) of 1.94E-6 and 3.29E-6, respectively), to assess the loss by volatilization as a valid assumption. The simulated removals with and without volatilization included in the model was determined for both winter and summer seasons at Facility B. Little changes (<0.3% removal) were observed for either compound, where the volatilization impact was not significant on the concentration (1 ng/L) for TCEP, which supports not including volatilization for these and the other more polar compounds in the ASTreat model.

The biotransformation (K_b) fate parameters employed were measured in batch tests at 23°C. However, the field winter temperatures at Facilities C and E were between 15-17°C. Therefore, the ASTreat model was evaluated employing the use of temperature correction equations ($k_2=k_1\theta^{(T_2-T_1)}$; θ=1.056 (20-30°C) and θ=1.135 (4-20°C)) (Metcalf & Eddy, 2003). Modeling with corrected rate constants was performed for gemfibrozil, DEET, and triclosan at sites B through F. The results indicates that for winter campaigns at utilities C (triclosan) and E (DEET, gemfibrozil) there is a 5-20% lower removal as compared to the removals using the uncorrected rate constants. However, no improvement was observed for these scenarios, where a poorer comparison with field data was observed. Correcting the effect of temperature on reaction rates would be potentially more important for those scenarios where removals were over-predicted using a higher temperature than observed (no such scenarios were observed in the evaluation assessment) or under-predicted using a lower temperature than observed in the field.

4.3 Sensitivity Analysis

A sensitivity analysis was performed for two compounds (DEET and gemfibrozil) to determine which model input parameters are most sensitive for the simulated removal for these low sorbing and moderately degradable compounds (Appendix H). The biotransformation rate Kb and HRT were found to be most and approximately equally sensitive input parameters for the predicted TOrC removal efficiency. No other input parameters, including SRT, MLSS, RAS, TSS, and influent concentration affected the predicted TOrC removal.

Field results revealed that biotransformation rates for DEET were affected by the secondary influent concentration (Figure 3-7). Also, as previously discussed, SRT was identified as one parameter affecting the biotransformation kinetics for DEET, gemfibrozil and certain other TOrC based on full- and laboratory-scale results (Section 3.4.1). These relationships are not reflected at this time by ASTreat. Instead, the model relies on the user to enter an appropriate biotransformation rate as the primary model input, which contains intrinsic information about the most relevant process conditions driving biotransformation. Biotransformation rates are not

easily determined in experiments, nor are they easily accessible in publications for model users. Moreover, biotransformation rates should be relevant to process conditions, such as SRT, TOrC influent concentrations, or temperature. It is therefore recommended to put further effort into integrating functional relationships into TOrC fate models, including multiple variable analysis, to further improve the ability of TOrC models to estimate appropriate biotransformation rates for specific treatment conditions.

A sensitivity analysis was also performed for the highly sorptive compound triclocarban (Appendix H). For this type of compound, the K_d, HRT, MLSS, and SRT input parameters were all found to be equally sensitive to predicted TOrC removal efficiency. Results from field site investigations did not reveal that TOrC sorption was limited by HRT or MLSS concentration. Interestingly, field calculated K_d values were much higher than those determined in laboratory batch isotherm experiments indicating that SRT is an important factor for highly sorptive and poorly biodegradable compounds, where accumulation of the compound on the sludge solids is likely occurring. Thus, laboratory batch isotherm experiments as they are currently being conducted may not adequately capture the sorption in systems operating at longer SRTs. In addition, there may be kinetic limitation of TOrC sorption during activated sludge treatment, particularly for treatment plants that operate at longer SRTs. ASTreat assumes instantaneous equilibrium sorption, thus future research could enhance model predictions by incorporate a kinetic expression for sorption.

4.4 ASTreat Validation

The ASTreat model was evaluated for its ability to accurately predict TOrC indicator removal at certain sites that were selected for model validation (A-summer, A-winter, G–high SRT, G–medium SRT, and G–low SRT). Operational conditions for the validation scenarios are presented in Figure 4-2 and Table 3-4. Appendix C and Appendix D provide further detail on the process operation at each facility during the time of sampling.

Model validation provided an opportunity to assess ASTreat's capability of predicting TOrC removal at facilities A and G by using biotransformation rates and sorption coefficients based on a newly developed fate parameter library based on measured fate parameters from the literature and other field sites from this study (field sites B Summer, C Winter, C Summer, D Summer, E Winter, E Summer, and F Summer). As the sorption coefficients for individual compounds did not vary much between the activated sludge systems from different operations, model validation was conducted using an average sorption coefficient for each compound. For triclocarban, an average of the K_d values from RAS analysis was used, instead of the bench-test derived K_d values, as model calibration demonstrated that field values result in better model predictions. The biotransformation rates were quite variable for some of the TOrC (Chapter 3.0). For some TOrC, biotransformation rates appeared to be a function of SRT (see Section 3.3.2). Appendix H summarizes the K_b library (Section H.3.1). For most compounds an average K_b was calculated over a specified SRT range or linear relationships were drawn for certain SRT ranges to estimate K_b values during model validation of facilities A and G. Note, the model input parameter K_b with units of g/L-d was determined by $K_b = k_b/X_{ss}$ (k_b (1/d), X_{ss} = g MLSS/L), which assumes the K_b rates is a function of the active biomass concentration.

Table 4-2. Validation Scenarios Used in ASTreat.

Validation Utility	G – low SRT	G – medium SRT	G – high SRT	A - Winter	A - Summer
Redox	Anaerobic/Anoxic/Aerobic			Anoxic/Aerobic	
SRT (d)	6	20	42	9	9
HRT (h)	5.7	8.5	11.1	10.2	6.7
MLSS (mg/L)	2256	5646	5071	1590	1740
Temp (°C)	22.6	22.6	22.6	13.8	20

The ASTreat predicted percent removals were compared to the percent removals observed during full-scale operation. These results are presented in Appendix H. Table 4-3 lists the difference between measured and predicted TOrC removals. Validation testing could not be performed for bisphenol A, BHA, and TCPP, since measured fate parameters were not available for these compounds. Out of 88 total comparisons for 21 TOrC, 66% of the comparisons were within 20% of the measured removal, where more accuracy was observed for more easily removed compounds, acetaminophen (100%), caffeine (100%), ibuprofen (100%), triclosan (100%) and naproxen (100%), recalcitrant compounds, carbamazepine (80%), meprobamate (100%), primidone (80%), TCEP (100%), and a moderately removed compound, DEET (80%). The results agree with evaluation results (Section 4.2). Accounting for the higher biotrans-formation rates for DEET in the presence of higher influent concentrations resulted in model predictions comparable to the observed removals (Figure 4-4).

Table 4-3. Difference Between the Predicted and Observed Percent Removals for ASTreat Model Validation.

Validation Utility	G	G	G	A Winter	A Summer
SRT (days)	*6*	*20*	*42*	*9*	*9*
Acetaminophen	-3	-1		-1.8	-1.9
Atenolol	21	-3	NA	50	41
Benzophenone	NA	-4	NA	NA	NA
Caffeine	-0.4	-0.1	-0.1	NA	-0.3
Carbamazepine	2	2	1	-11	-27
Cimetidine	18	17	33	11	-84
DEET	24	-2	-15	9	-11
Diphenhydramine	48	3	4	30	28
Fluoxetine	71	67	62	85	67
Gemfibrozil	-44	-20	-10	-30	-51
Ibuprofen	-1	-0.3	-0.2	-1	-1
Iopromide	-44	-22	NA	NA	NA
Meprobamate	-9	NA	NA	2	-1
Naproxen	-5	-2	-2	0.2	-6
Primidone	5	5	5	-8	-23
Sucralose	23	NA	-1	NA	NA
Sulfamethoxazole	114	104	55	5	-8
TCEP	-11	-11	-15	NA	NA
Triclocarban	25	15	-24	25	-5
Triclosan	14	8	3	6	4
Trimethoprim	-17	-42	-40	2	NA

Note: Positive values indicate that the predicted removal was greater than the measured removal for a given compound. Negative values indicate that the predicted removal was less than the measured removal for a given compound.

Model predictions were less accurate for gemfibrozil (40% of absolute differences were assessed within 20% of the observed removals), sulfamethoxazole (40%), cimetidine (60%), diphenhydramine (40%), fluoxetine (0%), atenolol (25%), diphenhydramine (40%), triclocarban (40%), and trimethoprim (40%). Interestingly, most of the deviations follow similar trends observed during the initial model evaluation (Section 4.1.1, Table 4-1). The predictions for gemfibrozil removal were more accurate for high SRT treatment (Facility G, SRT 20 and 42 days), but removal was under-predicted for lower SRT operation (Figure 4-4). In contrast, trimethoprim removal was under-predicted for the higher SRT scenarios (Figure 4-4). However, unexpectedly sulfamethoxazole was significantly over-predicted for the three SRT scenarios at Facility G. During the evaluation of the model this compound was systematically under-predicted (Section 4.2, Table 4-1). These deviations support the possibility that some of the biotransformation rates may not have been accurately measured in the batch studies.

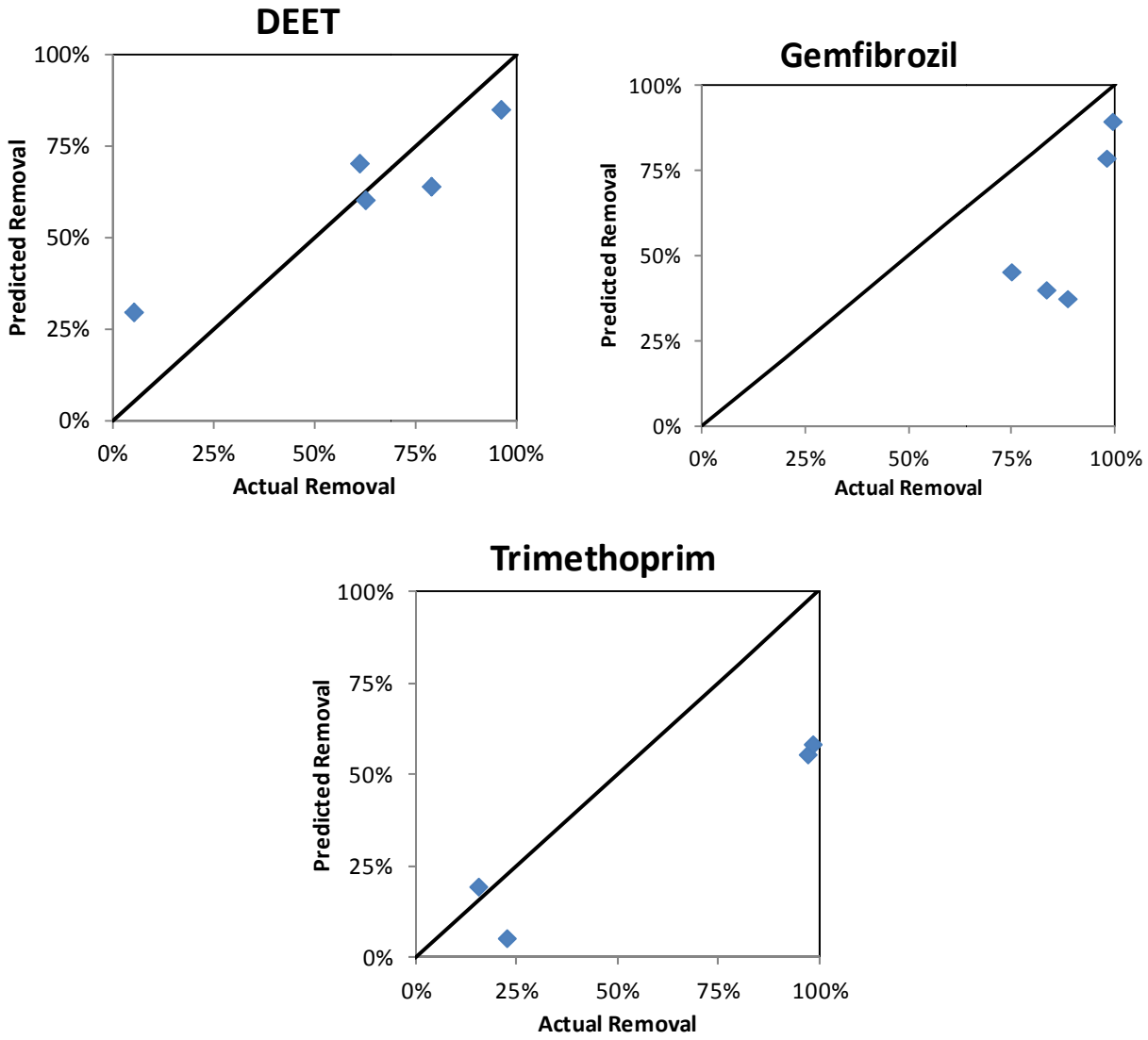


Figure 4-4. Measured Versus Simulated Removal for DEET, Gemfibrozil, and Trimethoprim.

4.5 Summary

Evaluation and validation assessments were performed on the public-domain mass balance model ASTreat. Other viable models were identified and the evaluation of these other models is recommended. The biotransformation rate, K_b, and HRT were found to be the most, and approximately equal, sensitive ASTreat input parameters for predicting removal efficiencies of TOrC attenuation by biotransformation mechanisms. The K_d, HRT, MLSS, and SRT input parameters were all found to be equally sensitive for predicting removal efficiencies of TOrC attenuation by sorption mechanisms. A 20% removal difference criterion was adopted to take into account the uncertainties associated by both model and measured removals. Note that a different criterion maybe more appropriate or valid depending on the data quality goal. The evaluation simulations revealed the classification of TOrC indicators into three groups: 1) recalcitrant, 2) highly amenable, and 3) moderately amenable compounds. The first two compound groups comprised of compounds with 86% accurate predictions. A library of sorption coefficients and biotransformation rates for target compounds was developed over an SRT range of 0-50 days and applied to the validation sites.

Table 4-4 summarizes the ability of ASTreat to predict the removal of indicator TOrC based on the evaluation and validation assessments. The assessments were for the most part in agreement, where ~70% of the comparisons were within 20% of the measured removals. ASTreat thus proved to be a useful screening tool for predicting the removal of most TOrC indicators under full-scale treatment. Higher prediction accuracy was observed for recalcitrant and highly-amenable compounds. However, lower accuracy (<60%) was observed for a majority of the moderately amenable compounds. The accuracy of predicting the removal for some TOrC that are moderately fast biotransformed was improved by recognizing that TOrC biotransformation rates are a function of the operating SRT. The fate prediction of TOrC that are sorbable and rapidly biotransformed remains a major challenge, as these compounds appear to accumulate on the solids during treatment, making a steady-state performance analysis, as attempted in this study, challenging.

Table 4-4. Predictability of ASTreat for Indicator TOrC.

Difference in % removal	Predictability *±20% > X < 20%*	Comment
Acetaminophen	High	
Atenolol	Medium	
Benzophenone	Unknown	
Bisphenol A	Unknown	
BHA	Unknown	
Caffeine	High	
Carbamazepine	High	
Cimetidine	Medium	
DEET	High	
Diphenhydramine	Medium	
Fluoxetine	Low	
Gemfibrozil	Medium	
Ibuprofen	High	
Iopromide	Medium	
Meprobamate	High (SRT < 10 d)	
Naproxen	High	
Primidone	High	
Sucralose	High	
Sulfamethoxazole	Medium	High for SRT < 10 d
TCEP	High	
TCPP	Unknown	
Triclocarban	Medium	
Triclosan	High	
Trimethoprim	Medium	High for SRT < 10 d

High – All of the scenarios was predicted with specified accuracy.
Medium – 40-60% of all scenarios could be predicted in specified accuracy.
Low – None of the scenarios was predicted accurately.

CHAPTER 5.0

COMPARATIVE COST ANALYSIS

This report has focused on better understanding the removal of TOrC through the secondary treatment processes. Process conditions that favor TOrC removal were identified and minimum operational requirements defined to achieve certain removal efficiency for TOrC indicators. This chapter is entirely different, as it looks to provide an example of how one example WWTP could reduce TOrC in their effluent by modifying their treatment process and what the costs may be for such work.

As shown in this report, the ability of existing treatment facilities to manipulate the existing secondary process conditions in favor of TOrC removal is possible, but has significant cost. For example, the capacity rating of secondary treatment systems is related to a specific SRT design criteria, above which a facility is typically not able to operate without compromising other process limitations, such as impacting the solid loading capacity on the secondary clarifiers. Operating at an SRT above the original design value to increase TOrC removal requires an expansion of the secondary treatment at most facilities in order to maintain capacity. Thus, the question we are asking in this chapter is "How does the investment into secondary treatment upgrades compare to improving TOrC removal using alternative processes from a cost standpoint?"

This chapter provides a comparative cost analysis of several treatment processes for TOrC removal and can serve as a template for any facility looking to increase TOrC treatment. Included is a summary of costs for selected membrane, oxidation, and other technologies to provide TOrC reduction in comparison to the costs of optimizing an activated sludge process.

5.1 Approach

A baseline treatment cost was defined for a hypothetical existing conventional activated sludge wastewater facility operating at an SRT of 2.5 days with a 10 mgd average daily max month design flow (ADMMF) capacity (baseline scenario). It was assumed that the secondary process is already constructed, thus the baseline construction cost for existing facilities was not part of the process cost comparison in this analysis. Construction and operational costs were estimated for upgrading this hypothetical facility to improve TOrC treatment performance. The following six technology options were included in this analysis as alternative upgrades to the baseline scenario:

- Secondary treatment expansion to maintain treatment capacity while increasing SRT operation to 6.5 days; and
- Secondary treatment expansion to maintain treatment capacity while increasing SRT operation to 9 days;

versus maintaining the baseline scenario (SRT of 2.5 days) and with the addition of:

- Ozone oxidation;
- Ultrafiltration;

- Reverse osmosis; and
- Ballasted flocculation with activated carbon addition.

Generally, the cost estimates provided for any of the six process alternatives are generic greenfield construction costs for the specific unit operation and do not consider site specific requirements that may be associated with such expansion projects, such as:

- Land acquisition.
- Major site improvement work, such as fill material or substantial clearing.
- Disinfection system (for residual or for polishing the treated effluent as needed).
- Laboratory or staff office space.
- Bringing utilities to/from the site (water, wastewater, power, communications).
- Environmental assessment of the site.
- Architectural accents to structures.
- Owner administration and legal fees.

Clearly, there are advantages beyond TOrC reduction for each of these alternative processes that could be further elucidated. Ozone, for example, will provide disinfection and thus offset disinfection costs. Reverse osmosis will reduce salts and provide quality water that can become an alternative water source. Ballasted flocculation can reduce solids and improve effluent quality, which will reduce the cost of subsequent disinfection. These potential advantages (and process limitations or disadvantages) are not detailed in this document.

5.2 TOrC Selection

The benefits of the six process alternatives regarding TOrC removal were quantified exemplarily on basis of specific TOrC indicators that span a range of sorption and biotrans-formation characteristics. The removal efficiency of the selected compounds for this analysis (DEET, naproxen, gemfibrozil, diphenhydramine, and triclosan) demonstrated sensitivity to secondary process operation, specifically to the operating SRT or HRT (see Section 3.4 and Appendix J).

Depending on the specific removal mechanism (e.g., chemical oxidation, hydrophobic interaction, size exclusions, etc.), the different processes target different groups of TOrC. For example, ozonation is able to destroy compounds such as carbamazepine that are recalcitrant during conventional wastewater treatment. While this cost analysis focuses exemplarily on five specific TOrC, more general considerations on process advantages and limitations are only partially and peripherally addressed in this chapter.

5.3 TOrC Reduction of Treatment Processes Upgrade Alternatives

The TOrC reduction for the six alternative treatment processes was evaluated based on a literature review and findings of this study.

5.3.1 Secondary Treatment Upgrades

The benefits regarding TOrC removal under a conventional activated sludge expansion were assessed using the ASTreat model and observed full-scale performance data collected in this study. Information on the secondary treatment process performance and sizing, along with ASTreat model input parameters relevant for cost estimating, are summarized in Table 5-1 for the baseline scenario (operation at an SRT of 2.5 days) and the secondary process upgrades (operation at an SRT of 6.5 (moderate) and 9 days (high), respectively). Further detail on the design basis for cost estimating purposes of these process upgrades is included in Appendix K.

Table 5-1. Secondary Treatment Assumptions for Cost Analysis.

	Low SRT (BOD Removal)	Moderate SRT (Full Nitrification)	High SRT (Full Nitrification)
Secondary Influent			
ADMMF, mgd (m^3/d)		10 (37,850)	
ADAF		8 (30,280)	
PDF		16 (60,560)	
BOD_5, mg/L		210	
TSS, mg/L		90	
Ammonia-N, mg/L		30	
TP, mg/L		5.4	
TKN, mg/L		45	
Wastewater Temperature, °C		17	
Activated Sludge Process			
HRT, hrs	6	9	12
SRT, days[1)]	2.5	6.5	9
Side Water Depth, ft (m)		16 (4.9)	
% Aerobic Volume		100	
MLSS, mg/L	2,000	3,000	3,000
DO in Aerobic Zones, mg/L	2	2	2
Secondary Clarification			
RAS Recycle Ratio	0.50	0.50	0.50
RAS TSS, mg/L	6,000	9,000	9,000
Secondary Effluent			
BOD5, mg/L	10	10	10
TSS, mg/L	15	15	15
Ammonia as N, mg/L	33	< 1	< 1

Note:
1. This assumes aerobic SRT.

The secondary process influent and anticipated removal efficiencies for the target TOrC are summarized in Table 5-2 for operation under different SRTs. Aeration basin influent concentrations were selected based on typical concentration ranges detected at full-scale facilities (Section 3.2.2.1).

Table 5-2. Anticipated TOrC Reduction for Secondary Treatment Upgrades.

TOrC	Primary Effluent TOrC Concentration, ng/L[1]	Low SRT (2.5 days)	Moderate SRT (6.5 days)	High SRT (9 days)
DEET	1,000	0-60%	60-80%	80-100%
Triclosan	1,500	0-70%	70-90%	90-100%
Diphenhydramine	1,200	0-60%	60-70%	70-90%
Naproxen	15,000	40-80%	65-100%	95-100%
Gemfibrozil	3,000	0-10%	60-80%	70-100%

Note:
1. Estimated based upon data collected during this study.

5.3.2 Ozone

Ozone (O_3) oxidation of TOrC is reviewed here. O_3 oxidation is a chemical process that targets cell membranes and nucleic acids resulting in irreversible damage to the DNA. Ozonation of water is an advanced oxidation process (AOP) because O_3 converts to oxygen (O_2) in water through a decomposition process whose intermediates include superoxide and hydroxide radicals (Glaze et al., 1987). O_3 itself is a strong oxidant, but is selective for certain chemical structures. Hydroxyl radicals that are formed during ozonation are nonselective oxidants (Snyder et al., 2003; Westerhoff et al., 2005).

Ozonation removes BOD, color, and turbidity and inactivates microorganisms proportional to dosage (Nagano et al., 1992). The presence of high concentrations of organics increases the O_3 demand in a wastewater and can decrease the feasibility of ozonation as a treatment option for TOrC removal.

O_3 reactors for wastewater disinfection were historically designed similar to drinking water O_3 reactors (with long contact time). Recent research (Ishida et al., 2008) led to California Department of Public Health (CDPH) approval of ozone CT values of 1.0 mg-min/L or less for reuse applications. The CDPH approved research demonstrated substantial disinfection at contact times of less than two minutes in pressurized ozone reactors.

Destruction of TOrC by ozone in wastewater effluents is well proven. Ozone doses greater than or equal to 2 mg/L have a removal efficiency of over 90% for a wide range of TOrC in wastewater effluent (Huber, 2004). Westerhoff et al. (2005) observed that the addition of hydrogen peroxide (H_2O_2) increased target compound oxidation by 5-15% over O_3 alone, but certain chemical constituents such as iodinated X-ray contrast media are only moderately removed by ozonation, with or without H_2O_2, even at high doses and contact times (14% removal at 15 mg/L O_3, 18 minute contact time) (Ternes et al., 2003). O_3 oxidizes more than 80% of TOrC detected in drinking water, except for compounds without aromatic groups or those with electron-withdrawing aromatic substitutions (Westerhoff et al., 2005; Benotti et al., 2009). These studies indicate that H_2O_2 addition to O_3 is expected to improve degradation in the case of some herbicides (such as atrazine) and TCEP. In other wastewater disinfection studies,

the combination of H_2O_2 and O_3 has not been shown to significantly improve TOrC oxidation over O_3 alone. A marginal increase of O_3/H_2O_2 was observed for the removal of dilantin, diazepam, DEET, iopromide, and meprobamate, but a decrease in removal efficacy was observed for pentoxifylline, caffeine, testosterone, progesterone, and androstenedione (Snyder et al., 2006). Due to the marginal benefit, H_2O_2 addition to ozonation for TOrC removal was not included in this cost study.

Particularly pertaining to this analysis, the dose/response destruction for DEET, triclosan, diphenhydramine, naproxen, and gemfibrozil was estimated based upon various publications (WateReuse Research Foundation (WRRF, 2012; Wert et al., 2009; Gerrity et al., 2011) (Table 5-3). Destruction of diphenhydramine by ozone was estimated based upon comparison with ibuprofen. Diphenhydramine was demonstrated to be slightly more resistant to hydroxyl radical oxidation compared to ibuprofen (Yuan et al., 2009), and ibuprofen was shown to be oxidized by more than 90% once the ozone to total organic carbon ratio of 1.0 was exceeded (Wert et al. 2009), which is essentially the point where the ozone demand is overcome. While the ozone demand of wastewater can vary depending upon the effluent quality, 3-5 mg/L of transferred ozone dose commonly results in >90% reduction of a wide range of TOrC (WRRF, 2012), including four of the five TOrC analyzed in this chapter.

Table 5-3. Estimated Destruction of Select TOrC with Ozone.

TOrC	Estimated % reduction following 5 mg/L of ozone
DEET	90%
Triclosan	99%
Diphenhydramine	~75%
Naproxen	95%
Gemfibrozil	99%

5.3.3 Ultrafiltration and Reverse Osmosis

Reverse osmosis (RO) and ultrafiltration (UF) reduction of TOrC is reviewed here. The key solute parameters defining membrane TOrC rejection performance for RO include molecular weight (and to a lesser degree, its aspect ratio), dissociation constant (pK_a), degree of hydrophobicity (log K_{ow}) and diffusivity (D_p). Important properties of the membrane include the molecular weight cutoff (MWCO), pore size, surface charge, roughness, and hydrophobicity (Bellona et al., 2004).

Negatively charged compounds are generally effectively rejected by NF and RO membranes, due to electrostatic repulsion of the negatively charged membranes, while non-charged organic compounds are removed based on steric exclusion (Kimura et al., 2003). In operation, rejection of nonionic organic chemical constituents is primarily related to the pore size of the membrane: smaller molecular weight compounds (such as some TOrC and chlorinated disinfection byproducts) are poorly rejected by high-pressure membrane filters. Drewes et al. (2005) found that only about

50% of influent bisphenol A was rejected during laboratory-scale RO and NF membrane experiments, while full-scale testing of the same membranes suggested that a more fully

developed fouling layer of the RO membrane in the full-scale systems provides a more robust treatment barrier for this compound.

Particulate matter plays an important role in TOrC rejection by UF membranes. Seeded TOrC were rejected at a much higher rate by UF membranes in secondary wastewater effluent compared to parallel testing of the same water but with naturally occurring particulates removed prior to seeding (WRRF, 2012). Thus, UF filtration performance for TOrC reduction is directly related to the hydrophobic (particle associated) nature of the TOrC.

Data on the rejection of the specific TOrC considered in this cost study for UF is limited and is thus less reliable than data on the other discussed technologies. The few publications focusing on UF membrane performance report a wide range of removal efficiencies likely because of different water qualities, experimental scale, and UF membrane products studied. WRRF (2012) results for DEET and triclosan are based on bench-scale investigations using wastewater effluents. Yoon et al. (2007) report removal efficiencies based on bench-scale testing of drinking water source waters. A limitation of this study was, however, that experiments were not conducted under steady-state conditions. Based on the sorption characteristics of diphenhydramine, naproxen, and gemfibrozil it is assumed that their relative removal would be higher than for DEET and less than for triclosan. Therefore, the removal of these compounds by UF is estimated to be between 95% and 99% based on WRRF (2012) findings. Yoon et al. (2007) report generally lower removal efficiencies for all compounds that have been included as lower ranges in Table 5-4. No information was found specifically for diphenhydramine. This compound is positively charged at neutral pH as the antibiotic trimethoprim and has a similar molecular weight (290 g/mol). Yoon et al. (2007) report on average 20% removal for trimethoprim during UF treatment. It is important to note that there are many TOrC which have been shown to not be well removed by UF, including TCEP (<25%reduction) and atrazine (60% reduction) (WRRF, 2012).

Table 5-4. Estimated Reduction of Select TOrC with Ultrafiltration.
(due to particle associated characteristics)

TOrC	Estimated % reduction through ultrafiltration
DEET	50-95%
Triclosan	90-99%
Diphenhydramine	20-99%
Naproxen	10-99%
Gemfibrozil	50-99%

With regard to the specific removal of the TOrC by reverse osmosis (Table 5-5), WRRF (2010) reports more than 70% reduction of DEET, more than 99% reduction of triclosan, and at least 95% reduction in gemfibrozil. Boleda et al. (2011) documented more than 99% reduction in naproxen. At this time, no literature can be found regarding rejection of diphenhydramine by RO. Due to its molecular size and charge it is anticipated that diphenhydramine will be removed by at least 90%.

Table 5-5. Estimated Reduction of Select TOrC with Reverse Osmosis.

TOrC	Estimated % reduction through reverse osmosis
DEET	>70%[1]
Triclosan	>99%[1]
Diphenhydramine	>90 (estimated)
Naproxen	>99%[1]
Gemfibrozil	>95%[1]

Note:
1. Performance greater than listed values. RO permeate concentrations below detection.

5.3.4 Ballasted Flocculation/Sedimentation with Carbon Addition

Ballasted flocculation/sedimentation with carbon addition is a process that involves addition of powdered activated carbon (PAC) and coagulant to secondary treated effluent. In the next step sand is added under rapid mixing to accelerate the settling of solids and flocs during tertiary clarification. The sludge extracted from the tertiary clarifiers is wasted while the sand and PAC contained in it can be separated out to be recycled back within the tertiary process. A fraction of the PAC is continuously wasted and replaced with fresh material. This process is commercially available under the trade name Actiflo® CARB and was originally developed for NOM and trace organic removal in the drinking water industry. It was included in this cost analysis as a possible technology for targeting TOrC removal in wastewater treatment applications. The results of pilot testing of this technology are detailed in the paragraph below along with other related research.

The removal of selected TOrC (diclofenac, ibuprofen, bezafibrate, carbamazepine and sulfamethoxazole) by chemical coagulation was studied in jar tests (Vieno et al., 2006). In Milli Q water coagulation, the TOrC were poorly removed (< 10%) with the exception of diclofenac (66%with ferric sulfate). In lake water coagulation, only diclofenac was removed (30%) with ferric sulfate. In the presence of dissolved humic matter, diclofenac as well as ibuprofen and bezafibrate could be removed by ferric sulfate coagulation. Although conditions such as high humic material content, low coagulation pH, and a small amount of ferric coagulant can increase the removal of certain ionic TOrC, it was determined that coagulation cannot effectively remove TOrC from water (Vieno et al., 2006). The removal efficiency of 13 studied TOrC was only 13% following coagulation, sedimentation, and rapid sand filtration, but ozonation at 1 mg/L removed all TOrC below detection limits except ciprofloxacin in a pilot-scale drinking water treatment plant (Vieno et al., 2007). The removal of some selected TOrC in sewage (galaxolide, tonalide, diazepam, carbamazepine, ibuprofen, naproxen, and diclofenac) by coagulation-flocculation was around 50-70%, except that carbamazepine and ibuprofen were not removed at all (Carballa et al., 2005). It is apparent that coagulation is more effective in waters with high organic content, possibly related with the coagulation removal of particles with sorbed TOrC.

Activated carbon has been found to be effective in removing TOrC. In the same study by Vieno et al., GAC adsorption effectively removed 10 TOrC except for three hydrophilic TOrC (atenolol, sotalol, and ciprofloxacin) in a pilot-scale drinking water treatment plant (Vieno et al., 2007). Activated carbon adsorption can also effectively remove estrone and 17β-estradiol in pure

water; however, the absorbability of estrone and 17β-estradiol in river water and secondary effluent fell significantly, possibly because of site competition pore blockage and the presence of surfactant and humic acid (Fukuhara et al., 2006; Zhang and Zhou, 2005). In another study at a conventional drinking water treatment plant, GAC adsorption accounted for 53% of the removal of 113 organic compounds including TOrC (Stackelberg et al., 2007).

The removal of TOrC in secondary effluent by coagulant-assisted GAC was investigated by Soliman et al. (2007), and the results showed that coagulant-assisted GAC adsorption removed most TOrC except carbamazepine, clofibric acid, gemfibrozil, ibuprofen, *p*-toluenesulfonamide, caffeine, butylated hydroxyanisole, butylated hydroxytoluene, and *N*-butyl benzenesulfonamide.

Ballasted flocculation / sedimentation with continuous addition of PAC was evaluated in pilot-scale at the Milwaukee Metropolitan Sewerage District (MMSD) as part of an ongoing study that is partially funded by WERF. In particular, the tested Actiflo® CARB process work was led by Dr. Ronan Treguer and Veolia Water Solutions and Technologies. This study MMSD study is titled "*Actiflo Carb process in the Removal of Pharmaceutical and Personal Care Products (PPCPs) and Endocrine Disrupting Compounds Within a Conventional Wastewater Treatment Line."* The operational conditions for the research at MMSD and experimental results are included in Appendix K. Within that study, different levels of polymer, ferric chloride, and powdered activated carbon (PAC) were added. Generally, TOrC removal was higher at 20 mg/L compared to 10 mg/L PAC addition and the lower doses of ferric chloride were equally effective as the higher doses of ferric chloride. Tests with relatively higher polymer doses also resulted in better performance. The data does show variability. However, in general, at the higher dosages, TOrC removal was typically higher than 80% on average for hydrophobic compounds studied (e.g., triclosan, fluoxetine, diphenhydramine, trimethoprim) while hydrophilic compounds were removed between 60 and 85% (i.e., caffeine, naproxen, sulfamethoxazole). Figures 5-1 and 5-2 illustrate the measured performance for trimethoprim and caffeine, respectively.

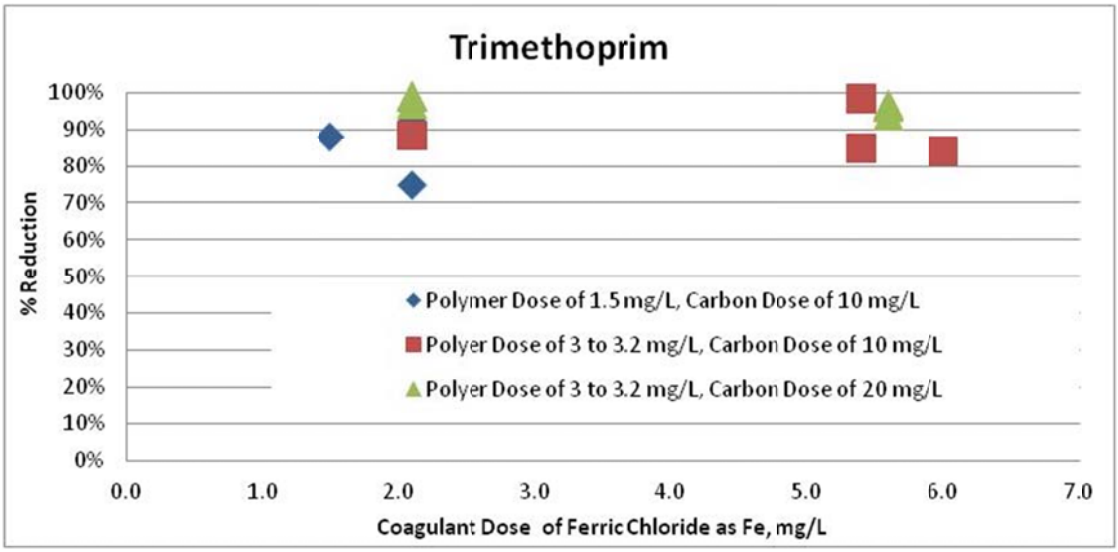


Figure 5-1. Trimethoprim Reduction Through the Actiflo™-CARB Process.

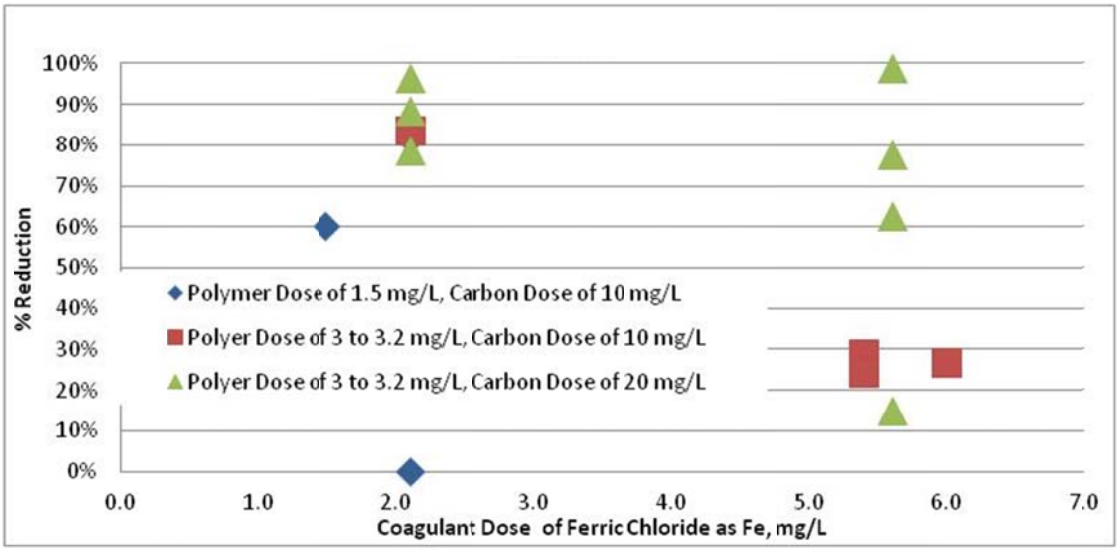


Figure 5-2. Caffeine Reduction Through the Actiflo™-CARB Process.

The range of removal performance for the five TOrC using activated carbon based processes is summarized in Table 5-6. The MMSD testing of the Actiflo™-CARB process examined three the five TOrC reviewed in this chapter (triclosan, diphenhydramine, and naproxen) and the performances for 10 and 20 mg/L carbon dosages are included in the table. Removal of DEET and gemfibrozil was not examined at MMSD and thus must be estimated from other studies. The removal of these TOrC is estimated from Snyder et al. (2007), which is not an ideal database to use as the Snyder testing was done with PAC in a single pass mode whereas the Actiflo™ -CARB process recirculates the carbon to increase removal performance. In Snyder et al. (2007) gemfibrozil and DEET removal were shown to be highly dependant upon PAC, in which PAC doses of 5 mg/L resulted in 4% and 18% reduction in DEET and gemfibrozil, respectively, whereas PAC doses of 35 mg/L resulted in 94% and 85% reduction in DEET and gemfibrozil, respectively. Based upon this information, we estimate greater than 50% removal for DEET and gemfibrozil for the conditions tested at MMSD.

Table 5-6. Reduction of Select TOrC with Actiflo®-CARB (PAC dosage 10-20 mg/L).

TOrC	% removal through Actiflo® CARB[1]
DEET	>50
Triclosan	89-91
Diphenhydramine	75-95
Naproxen	40-65
Gemfibrozil	>50

5.4 Alternative Treatment System Cost Estimates

In 1998, the Association for the Advancement of Cost Engineering (AACEI), published the "Recommended Practice 18R-97 Cost Estimate Classification System for the Process Industries." Carollo has adopted this recommended practice for estimate classification. The primary characteristic used in this practice to define the estimate class is the degree of project definition. Within the context of our design work, the most commonly used estimates are order-of-magnitude, budget, and definitive. AACEI's revised classifications include five groups, instead of the historic three-category definitions, which more accurately describe the range of potential estimates. For this project, the cost estimates are "Class 5" which are planning level estimates. Additionally, these estimates assume "greenfield" construction without any significant site, regulatory, or geotechnical issues. The costs for the alternative secondary treatment upgrades were estimated on basis of design assumptions laid out in Table 5-1.

The expansion requirements for the secondary treatment were developed using process modeling. The costs for amending the secondary treatment process from the baseline scenario to operating at a moderate and high SRT included expansion of aeration basins, secondary clarifiers, blowers and other process appurtenances. The operational costs included operating power for aeration blowers, process pumps, and other process equipment. Annual maintenance costs were estimated as $10,000 for each secondary clarifier and $20,000 for each aeration basin.

The costs for the alternative tertiary treatment systems (ozone oxidation, UF, RO, and high rate settling with PAC addition) were estimated based on the flow assumptions and secondary effluent quality of the baseline treatment scenario (low SRT, 2.5 days, BOD removal only) as summarized in Table 5-1.

Ozone treatment was costed based on side stream injection methods. The major components for the ozone system are feed gas to ozone generators, ozone generation unit, ozone dissolution and contacting unit, dissolved ozone quenching and degasifying unit, and ozone destruct unit. The operational costs included gas supply and energy. The annual maintenance costs included repair and replacement.

The basis for the cost development of UF and RO treatment are detailed in Appendix K. As is well acknowledged in the industry, RO treatment is preceded by MF treatment for protection of the RO membranes. The costs for MF pre-treatment have not been included in the RO costs presented herein and must be added to understand the true cost of RO treatment..

The equipment costs for the ballasted flocculation/PAC addition process were estimated on basis of the Actiflo® CARB system. Equipment costs included coagulation, maturation, and settling tank, microsand recycle circuits, and PAC contact tanks. Project costs included equipment and instrumentation, tankage, and all necessary components for operation. The operation and maintenance costs consider chemical consumption of sand, polymer, coagulant, and PAC as well as labor, energy, and replacement costs of the system.

Tables 5-7 and 5-8 summarize the TOrC treatment expectations for DEET, triclosan, diphenhydramine, naproxen, and gemfibrozil. Based on this comparison RO provides the most robust treatment for the TOrC assessed in this analysis.

Table 5-7. Anticipated TOrC Reduction for Secondary Treatment Upgrades.

Estimated % TOrC Reduction	Low SRT (2.6 days)	Moderate SRT (6.5 days)	High SRT (9 days)
DEET	0-60%	60-80%	80-100%
Triclosan	0-70%	70-90%	90-100%
Diphenhydramine	0-60%	60-70%	70-90%
Naproxen	40-80%	65-100%	95-100%
Gemfibrozil	0-10%	60-80%	70-100%

Table 5-8. Anticipated TOrC Reduction for Alternative Treatment Processes.

Estimated % TOrC Reduction	Ozone (5 mg/L)	Ultrafiltration	Reverse osmosis	Actiflo® CARB (10-20 mg/L PAC)
DEET	90%	50-95%	>70%	~50
Triclosan	99%	90-99%	>99%	89-91
Diphenhydramine	~75%	20-99%	NA	75-95
Naproxen	95%	10-99%	>99%	40-65
Gemfibrozil	99%	50-99%	>95%	~50

The project costs for each process scenario are summarized in Figure 5-3. For comparison purposes, the project and O&M costs of all treatment options were translated into net present worth costs (Table 5-9 and Figure 5-4). Based on this overall cost analysis RO provides the highest level of treatment, but costs are about three to six times higher than for other process alternatives. UF, high rate settling with PAC addition, and high SRT activated-sludge treatment remove a wide range of TOrC compounds at lower costs (Table 5-8 and Table 5-9).

Table 5-9. Cost Summary for all Treatment Scenarios.

Treatment	Project Costs	Annual Costs	Net Present Worth[2]
Low SRT Activated Sludge	Sunk Cost	$490,000	$6,200,000
Moderate SRT Activated Sludge	$11,400,000	$890,000	$22,500,000
High SRT Activated Sludge	$14,300,000	$940,000	$26,100,000
Ozone	$7,263,000	$164,000	$9,400,000
UF	$23,245,000	$1,588,000	$43,100,000
RO[1]	$34,868,000	$2,330,000	$63,900,000
Actiflo® CARB	$4,826,250	$696,000	$13,500,000

Notes:

1. *RO costs shown are for RO only. RO will require MF or UF filtration as pretreatment and those costs must be accounted for.*
2. Net present worth is the combination of project cost and annual cost once the annual cost is converted to a present value (calculated based upon 20 years of operation at an interest rate of 5%, which is a 12.46 times multiplication of the annual cost).

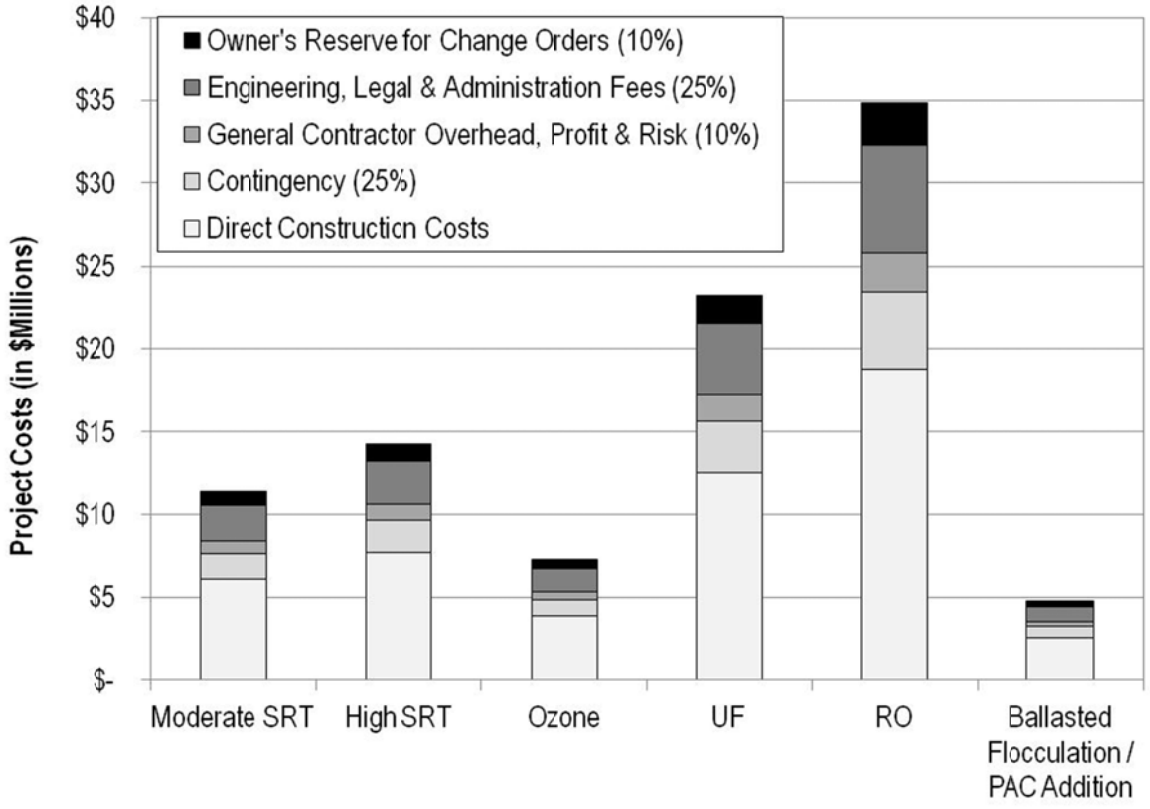


Figure 5-3. Project Cost Summary for All Treatment Scenarios.

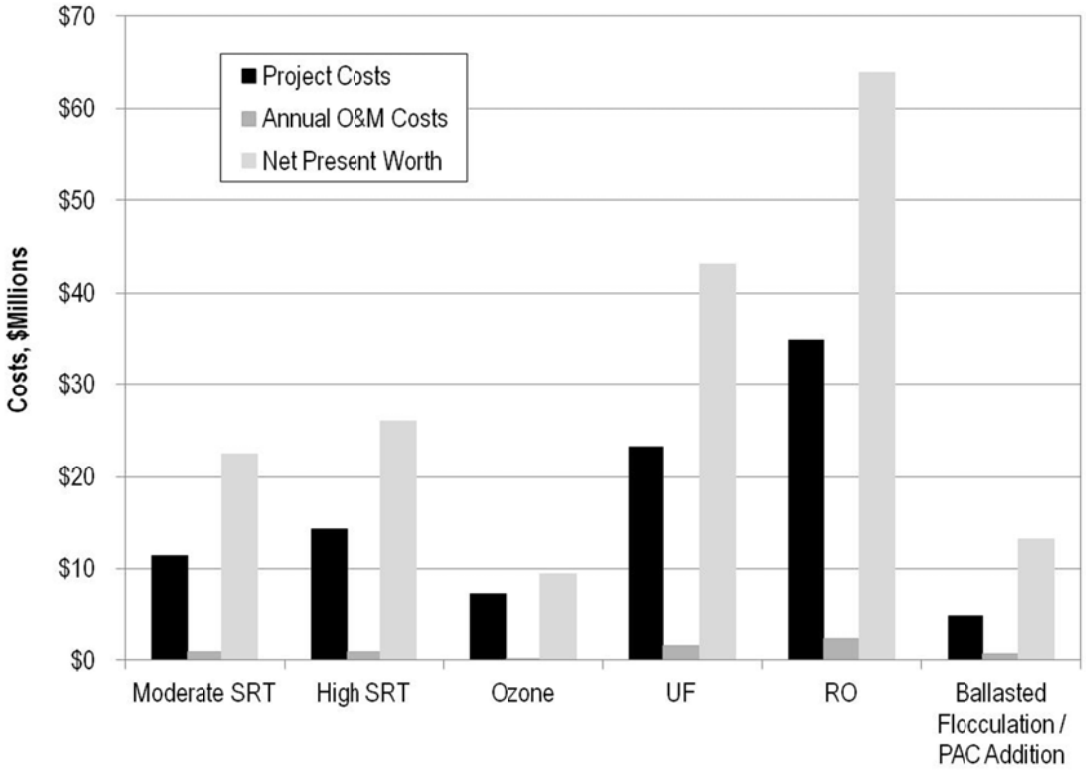


Figure 5-4. Net Present Worth Summary for All Treatment Scenarios.

The net present worth analysis conducted in this cost analysis is generic and based on a number of hypothetical assumptions. Specific case study scenarios may differ from relative cost ratios presented herein. Findings of this cost analysis suggest ozonation and high rate sedimentation with PAC addition (such as the Actiflo™-CARB process) as cost competitive options for TOrC reduction in comparison to activated sludge treatment at high SRT. Additional process options or a combination of processes may be preferable depending on site-specific treatment goals. Depending on the specific TOrC of concern in a given watershed, certain treatment strategies may be more suitable than others due to high and consistent removal efficiencies. Other treatment goals beside TOrC removal may shift the benefit assessment towards other technologies, such as high quality effluent for reuse applications, increased water quality resulting in more efficient downstream treatment (e.g., increased UV transmittance making UV disinfection less expensive), enhanced solids removal, footprint availability, or reduction of nutrients.

CHAPTER 6.0

RESULTS AND DISCUSSION – ANAEROBIC DIGESTION

6.1 Indicator Selection

A subset of the indicator list used for the liquid process stream evaluation previously described was used for assessing the removal of TOrC during anaerobic digestion (Table 6-1). Past studies indicate that these selected candidates frequently occur at quantifiable concentrations in biosolids. Their sorptive and biotransformation properties (see Tables 3-2 and 3-3) also suggest that they should be present in biosolids.

Table 6-1. Selected Indicator TOrC Short-List for Anaerobic Digestion Study (Lab- and Full-Scale).

Compound	
Atenolol*	Gemfibrozil*
Benzophenone^	Ibuprofen^
Bisphenol A*	Meprobamate*
Caffeine*^	Naproxen^
Carbamazepine*	Sulfamethoxazole^
Cimetidine^	TCEP*^
DEET*^	TCPP*
Diphenhydramine^	Triclocarban*^
Fluoxetine*^	Triclosan^
	Trimethoprim*^

* Compounds Used in Full-Scale Investigations at Facility A.
^ Compounds Used in Lab-Scale Investigations.

6.2 TOrC Mass Balances at a Full-Scale Facility

The selected indicator compounds were used to assess the removal efficiency of TOrC in a full-scale anaerobic digestion process at Facility A. A schematic of the treatment processes and the sampling locations is provided in Appendix I. The sampling campaign focusing on anaerobic digestion was conducted at the same time that the Facility A – Winter sampling campaign was conducted that focused on the liquid stream secondary treatment performance (see Chapter 3.0).

6.2.1 Operational Conditions During Sampling Period

Operational conditions for the anaerobic digestion process at Facility A during the sampling period are summarized in Table 6-2. More detailed information on the process operation at the time of sampling is presented in Appendix I.

Flow rates from the primary sludge gravity thickener (GT) underflow to the anaerobic digester averaged 1065 ± 289 gph (785 gph to 1,468 gph), whereas overflow flow rates from the waste activated sludge dissolved air flotation thickener (DAFT) to the anaerobic digester averaged 842 ± 46 gph (794 gph to 834 gph). The corresponding combined flow rates of both process streams to the first stage anaerobic digester averaged 1907 ± 296 gph (1,618 gph to 2,303 gph). The flow rates from the second stage digester to the sludge storage prior to

centrifugation averaged 5446 ± 495 gph (4,904 gph to 6,092 gph), though this flow rate only occurred for 8 h per day. The HRT in the first- and second-stage digesters during the study period were 20 and 15 days, respectively. The pH of the thickened primary and secondary sludges ranged from 5.9 to 6.6, while the pH in the anaerobic digesters ranged from 7.3 to 7.4. The alkalinity in the first and second stage anaerobic digesters were 5,300 mg/L and 5,640 mg/L (as $CaCO_3$), respectively. These pH and alkalinity values stayed within the optimum range for controlling an anaerobic digestion process (Metcalf and Eddy, 2003). Total solids (TS) of the thickened sludges ranged from 5.0% to 5.5%, while TS in the anaerobic digesters ranged from 2.3% in the first stage digester to 2.1% in the second stage digester. More than 50% TS reduction was observed in the digestion process, which is typical for a two-stage anaerobic digestion process.

Table 6-2. Operational Conditions During Sampling Campaign at Facility A.

Operation Parameter	GT Underflow	DAFT Overflow	AD-1st Stage	AD-2nd Stage
Flow (gph)				
3/28/2011	1,468	834	2,303	6,092*
3/29/2011	1,039	905	1,944	5,493*
3/30/2011	968	794	1,762	5,297*
3/31/2011	785	834	1,618	4,904*
pH				
3/28/2011	-	6.7	-	-
3/29/2011	6.2	6.6	7.4	7.4
3/30/2011	6.2	6.5	7.4	7.4
3/31/2011	6.1	6.7	7.5	7.5
Temperature (ºC)				
3/28/2011	14.4	14.5	30.4	32.9
3/29/2011	13.9	14.5	30.0	32.4
3/30/2011	14.6	15.4	29.3	32.2
3/31/2011	14.9	15.2	32.2	32.2
TSS (mg/L)				
3/28/2011	29,100	36,750	19,050	17,000
3/29/2011	57,800	35,250	18,600	17,700
3/30/2011	41,400	33,250	19,800	-
3/31/2011	28,200	36,250	18,450	16,350
TS (%)				
3/29/2011	5.55	4.99	2.27	2.06
3/31/2011	5.32	5.23	2.28	2.10
VS (% TS)				
3/29	89	88	76	74
Alk (mg/L as $CaCO_3$)				
3/29/2011	-	-	5,300	5,640

GT = Gravity Thickener (fed by primary sludge)
DAFT = Dissolved Air Floatation Thickener (fed by secondary sludge)
AD = Anaerobic Digester
* Flow rates occur over 8 h per d (from storage to centrifuge)

Daily grab samples of GT underflow, DAFT overflow, first- and second-stage anaerobic digester effluent, and dewatered biosolids cake were analyzed for pH, temperature, and total suspended solids (Table 6-2). Temperatures of the thickened sludges ranged from 13.9ºC to 15.4ºC, whereas temperatures of the anaerobic digester biosolids ranged from 29.3ºC to 32.9ºC. TSS concentrations averaged 39,125 ± 13,829 mg/L for the primary thickened sludge (GT underflow) and 35,375 ± 1,548 mg/L for the secondary thickened waste activated sludge (DAFT overflow). While the average TSS concentrations of the sludge streams were similar, the primary thickened sludge was more variable from day to day. The average TSS concentration in the first and second stage anaerobic digesters were 18,975 ± 606 mg/L and 17,017 ± 675 mg/L, respectively. These values result in a TSS reduction of 48 ± 9% in the first-stage digester and an additional 9 ± 4% reduction in the second-stage digester.

6.2.2 TOrC Occurrence During the Sampling Period

Daily grab samples of sludge and biosolids were composited to form a four-day composite sample (see Appendix I for sampling locations). Concentrations of the indicator compounds for all composite samples are summarized in Table 6-3.

6.2.2.1 TOrC Occurrence in Sludge and Biosolids

The highest concentrations in the gravity thickened primary sludge (TPS) were observed for caffeine and triclocarban. Caffeine was among the TOrC indicators with the highest wastewater influent concentrations (Section 3.2.2). Caffeine was not among the compounds that showed statistically significant reductions in the liquid process stream during primary clarification at other facilities (Section 3.2.2.1). The detection of caffeine in thickened primary sludge samples indicates, however, that even hydrophilic TOrC present in high concentrations in the wastewater influent can be present in significant concentrations in primary sludge samples.

Triclocarban was among the TOrC indicators with the lowest wastewater influent concentrations, however, this compound is hydrophobic and highly sorbable and was among the compounds that demonstrated a significant reduction in liquid stream concentration during primary clarification at other facilities (Section 3.2.2.1). While the concentration of triclocarban was also enriched in the thickened waste activated sludge (TWAS), the concentration of caffeine was an order of magnitude lower in TWAS compared to TPS. This difference in sludge concentrations is presumable due to the amenability of caffeine to microbial attack under aerobic conditions, whereas triclocarban was shown to be recalcitrant in the activated sludge process (see Table 3-8).

Several of the indicator compounds increased in concentration through anaerobic digestion resulting in significantly higher solid concentrations in the dewatered biosolids compared to the primary or secondary sludges (i.e., bisphenol A, TCPP, cabamazepine, fluoxetine, and triclocarban). All these compounds have in common a hydrophobic character and a demonstrated moderate to high sorption potential to activated sludge (Table 3-7). Such enrichment would be expected for compounds that are highly sorbable and/or poorly biodegradable under anaerobic conditions due to a reduction in the solids concentration during anaerobic digestion (e.g., in absence of any removal a 50% reduction in TSS would cause a 100% increase in TOrC concentration during digestion when reported on a mass of solids basis).

With the exception of atenolol, caffeine, and trimethoprim (rapidly and moderately biotransformed during secondary treatment) none of the TOrC indicators of the short-list used in the

anaerobic digestion study demonstrated a relevant reduction in TOrC concentration on the solids during anaerobic digestion.

Table 6-3. Sludge and Biosolids TOrC Concentrations During Sampling Campaign at Facility A.

TOrC	TPS (ng/g)	TWAS (ng/g)	AD-1st Stage (ng/g)	AD-2nd Stage (ng/g)	Dewatered Biosolids Cake (ng/g)	Dewatered Biosolids Cake Flux g/d	Cake Flux as % of ABI Flux
Atenolol	118	22	28	9.4	n.q.	NA	NA
Bisphenol A	811	508	1,473	1,532	1,585	5.4	10
Caffeine	3,271	391	179	204	220	0.8	0
Cabamazepine	90	26	317	308	170	0.6	5
DEET	141	165	181	203	159	0.5	1
Fluoxetine	171	303	516	446	601	2.1	73
Gemfibrozil	37	86	194	158	75	0.3	0
Meprobamate	4.5	19	48	4.9	n.q.	NA	NA
TCEP	134	111	442	370	150	0.5	3
TCPP	158	279	1,245	691	365	1.2	1
Triclocarban	6,129	8,912	12,193	8,319	10,673	35.5	175
Trimethoprim	150	297	75	36	26	0.1	0

TPS = Thickened Primary Sludge / Gravity Thickener Underflow
TWAS = Thickened Waste Activated Sludge / Dissolved Air Floatation Thickener Overflow
n.q.= not quantified (Below Signal to Noise Criterion for Quantitation)

The mass flux of highly sorbable TOrC indicators in the dewatered biosolids cake can constitute a significant portion of the TOrC mass flux in the aeration basin influent. For fluoxetine, the dewatered biosolids carried approximately 70% of the TOrC flux entering the secondary treatment during the sampling campaign at Facility A. The mass flux of triclocarban in the biosolids cake was higher than the average mass flux in the secondary influent during the sampling campaign (175%). A portion of this mass flux likely derived from primary sludge which was not separately sampled during this sampling event.

6.2.3 TOrC Removal During Anaerobic Digestion

Mass flux calculations were performed for each TOrC indicator through the solids handling process at Facility A (Table 6-4). Details of these calculations maybe found in Appendix I.

Based on observed removal efficiencies, the TOrC indicators were categorized into three general groups. The first group comprises compounds with significant attenuation (> 90% removal) such as atenolol, caffeine, and trimethoprim. These results are supported by the laboratory anaerobic bioreactor and batch biotransformation rate studies (see Sections 6.3.3 and 6.4.2). The second group consists of compounds that had moderate attenuation during anaerobic digestion (removals between 15 and 90%) such as DEET, and triclocarban. However, these results are not supported by the laboratory anaerobic bioreactor and batch biotransformation rate studies (see Sections 6.3.3 and 6.4.2). The third group of compounds are rather refractory during anaerobic digestion (removals < 15%) consisting of bisphenol A, carbamazepine, fluoxetine, gemfibrozil, TCEP, and TCPP. These results are in agreement with the laboratory anaerobic bioreactor and batch biotransformation rate studies (see Sections 6.3.3 and 6.4.2), with the exception of TCEP, for which biotransformation was observed (see Section 6.4.2).

For some of the TOrC indicators, the mass balance calculations were inconsistent between the first- and second-stage digesters. For example, the calculated TOrC removals were negative for bisphenol A, cabamazepine, fluoxetine, gemfibrozil, meprobamate, TCEP, and TCPP in the first-stage digester, but positive in the second-stage digester. The increase in calculated mass flux across the first stage digester could have been caused by a sampling artifact due to the collection of four-day manual composite samples for the TPS and TWAS, whereas the first-stage digester had an HRT of 20 days. The duration of the composite sampling for influent flows to the first-stage digester may thus not have been long enough to represent potential flux variations over the complete duration of first-stage anaerobic digestion.

Table 6-4. Mass Flux of TOrC Indicators During Anaerobic Digestion at Facility A.

TOrC	TPS (mg/h)	TWAS (mg/h)	AD-1st Stage (mg/h)	AD-2nd Stage (mg/h)	AD-1st Stage % Removal	AD-2nd Stage % Removal	Overall % Removal
Significant Removal (>90%)							
Atenolol	18.5	2.5	3.8	1.1	82.1	70.8	94.8
Caffeine	515.9	44.0	24.5	23.9	95.6	2.5	95.7
Trimethoprim	23.6	33.5	10.3	4.2	81.9	59.1	92.6
Moderate Removal (15-90%)							
DEET	22.3	18.6	24.8	23.7	39.4	4.4	42.0
Meprobamate	0.7	2.1	6.6	0.6	-130.5	91.3	79.9
Triclocarban	966.7	1004.7	1669.9	972.5	15.3	41.8	50.7
Refractory (<15%)							
Bisphenol A	127.9	57.3	201.7	179.1	-8.9	11.2	3.3
Fluoxetine	27.0	34.1	70.7	52.1	-15.6	26.2	14.7
Gemfibrozil	6.0	9.7	26.5	18.5	-68.8	30.2	-17.7
TCEP	21.1	12.5	60.6	43.3	-80.2	28.5	-28.7
TCPP	24.9	31.4	170.5	80.8	-202.9	52.6	-43.5
Cabamazepine	14.2	2.9	43.5	35.9	-154.3	17.3	-110.3

6.3 Laboratory-Scale Anaerobic Bioreactor

A detailed summary of the laboratory-scale anaerobic bioreactor study is provided in Appendix I.

6.3.1 Feed Source

Raw wastewater was collected from a student housing complex located on the Colorado School of Mines campus, Colorado. The wastewater solids were settled in a laboratory-scale primary clarifier for use as a feed to the bioreactor. The characteristics of the raw wastewater during the study are summarized in Table 6-5. The primary clarifier was drained on a daily basis so that only fresh sludge solids were fed to the anaerobic bioreactor.

Table 6-5. Raw Wastewater Analysis from the Housing Complex at Colorado School of Mines.

Parameter	Value (mean ± st.dev.; n=5)
Total Solids (TS), mg/L	527 ± 63
Volatile Solids (VS), mg/L	255 ± 55
Total Suspended Solids (TSS), mg/L	144 ± 46
Total Dissolved Solids (TDS), mg/L	383 ± 35
Volatile Suspended Solids (VSS), mg/L	115 ± 65
Chemical Oxygen Demand (COD), mg/L	476 ± 101
Alkalinity, mg/L as $CaCO_3$	155 ± 26
pH	6.96 ± 0.3
Nitrate (NO_3), mg/L-N	0.13 ± 0.05
Ammonia (NH_3), mg/L-N	29.6 ± 6.3
Ortho Phosphates (Ortho-P), mg/L PO_4-P	10.8 ± 3.0

6.3.2 Operational Conditions of Laboratory-Scale Bioreactor

The laboratory-scale bioreactor was operated for a total of 87 days. The first 60 days were used to achieve steady-state conditions, whereas the remaining 27 days were used to evaluate TOrC removal. Based on a feed rate of 665 mL/d, the bioreactor had an average HRT of 22 days over the study period.

A summary of the operational conditions for the anaerobic bioreactor are provided in Table 6-6. The destruction of volatile solids (51%), total suspended solids (39%), and chemical oxygen demand (50%) were with the typical range of an anaerobic digester being operated with an HRT of 20-25 days. The bioreactor pH (7.5) and alkalinity (3,348 mg/L as CaCO3) were within the optimal range for operating an anaerobic digester (pH = 6.6 – 7.6; Alk = 2000 – 5000 mg/L). Since the feed had minimal alkalinity (Table 6-6), soda ash (Na_2CO_3) was added to the bioreactor to maintain optimal pH and alkalinity conditions. These results suggest that the bioreactor was operated properly over the course of study.

6.3.3 TOrC Removal in Laboratory-Scale Bioreactor

Weekly composite samples of bioreactor influent and effluent were collected during the last three weeks of the study and analyzed for the TOrC indicators (Table 6-7). The indicator compounds were already present in the raw wastewater, so no additional TOrC were added to the influent feed. The influent feed TOrC concentrations were similar to the gravity thickened primary sludge concentrations at Facility A, though some of the laboratory-scale bioreactor values were slightly higher and some slightly lower than those measured in the full-scale system (Table 6-3). The negative removal values for fluoxetine and triclocarban could have been due to the presence of these highly sorptive compounds the anaerobic digester sludge from Facility A, which was used to start up the laboratory anaerobic bioreactor.

Table 6-6. Operational Parameters for Laboratory-Scale Anaerobic Bioreactor.

	Value (mean ± st.dev.; n=8)		
Parameter	Influent	Effluent	Difference
TS, mg/L	16,105 ± 4575	10,878 ± 1834	-32%
VS, mg/L	14,630 ± 3708	7204 ± 2015	-51%
VS, % of TS	91 ± 2	66 ± 12	-27%
TSS, mg/L	12,909 ± 5950	7847 ± 5149	-39%
VSS, mg/L	11,703 ± 4730	5731 ± 3043	-51%
COD, mg/L	25,919 ± 10,824	12,881 ± 3138	-50%
Alk, mg/L as $CaCO_3$	155 ± 151	3348 ± 932	2060%
pH	4.9 ± 0.4	7.5 ± 0.2	53%
NO_3-N, mg/L	1.4 ± 0.9	4.2 ± 1.1	200%
NH_3-N, mg/L	25.6 ± 16.3	496.9 ± 395	1841%
Ortho- P, mg/L	26.6 ± 18.7	145.9 ± 59	448%

Table 6-7. TOrC Concentrations in Laboratory-Scale Bioreactor Study.

TOrC	Influent (ng/g)	Influent (µg/L)	Effluent (ng/g)	Effluent (µg/L)	Removal (%)
Trimethoprim	475 ± 119	6.1	36 ± 4	0.3	95%
Caffeine	8566 ± 745	110.6	3990 ± 1510	31.3	72%
Sulfamethoxazole	517 ± 451	6.7	298	2.3	65%
Naproxen	498 ± 174	6.4	300 ± 208	2.4	63%
Ibuprofen	1143 ± 229	14.8	738 ± 534	5.8	61%
Cimetidine	551 ± 55	7.1	445 ± 131	3.5	51%
Benzophenone	3238 ± 1830	41.8	3781 ± 1381	29.7	29%
Triclosan	125613 ± 20210	1621.7	216369 ± 127610	1698.5	-5%
DEET	133 ± 39	1.7	297 ± 124	2.3	-35%
TCEP	495 ± 151	6.4	1162 ± 297	9.1	-43%
Diphenhydramine	127 ± 11	1.6	353 ± 171	2.8	-69%
Triclocarban	8862 ± 2529	114.4	50523 ± 5440	346.6	-247%
Fluoxetine	53 ± 7	0.7	677 ± 56	5.3	-670%

6.4 Fate Parameters

Sorption and biotransformation fate parameters for the indicator compounds were measured using anaerobic digester sludge collected from Facility A. The fate parameters include sorption distribution coefficients (K_d) and biotransformation rate constants (K_b). Both are critical for determining TOrC fate and transport through the sludge digestion process.

6.4.1 Sorption

Sorption isotherm tests were performed with anaerobic digester sludge collected from the first- and second -stage digesters at Facility A. The Freundlich isotherm model parameters (log K_F and n) for the TOrC indicators are provided in Appendix I. Sorption distribution coefficients (K_d) were also determined for the TOrC indicators.

To compare the sorption potential of different TOrC indicators, the K_d was calculated for each TOrC using their respective Freundlich equation at a benchmark aqueous TOrC concentration of 1000 ng/L. The log K_d values were then compared to the previously determined log K_d values for activated sludge solids from different facilities (Table 6-8). The difference between log K_d values determined for anaerobic digester sludge and activated sludge were within 1 log unit for any given TOrC. This suggests that K_d values for anaerobic digester sludge will be similar to K_d values for activated sludge.

Table 6-8. Log K_d for TOrC at C_w = 1000 ng/L.

	AD-1 log K_d	AD-2 log K_d	AS-Avg log K_d	AS-St Dev log K_d
Low sorption (K_d<2)				
DEET	1.21	1.12	1.96	0.15
Carbamazepine	1.51	1.36	1.96	0.27
Trimethoprim	1.53	1.48	2.35	0.17
Sulfamethoxazole	1.68	1.33	2.40	0.33
Bisphenol A	1.89	1.89	2.67	0.38
Ibuprofen	-	1.98	2.18	0.35
Moderate Sorption (K_d 2-3)				
Atenolol	2.10	1.87	2.58	0.21
Benzophenone	2.12	2.29	2.75	0.39
Cimetidine	2.17	1.79	2.48	0.22
Diphenhydramine	2.43	2.10	2.53	0.11
High Sorption (K_d>3)				
Triclocarban	3.99	3.99	3.87	0.55
Triclosan	3.54	3.54	3.51	0.32
Fluoxetine	3.47	3.40	3.05	0.14
Not Determined				
Caffeine	-	-	*<1.5*	-
Naproxen	-	-	2.03	0.33
TCEP	-	-	*<1.5*	-
Meprobamate	-	-	2.07	0.27
Gemfibrozil	-	-	2.08	0.32

AD-1 = First-Stage Anaerobic Digester
AD-2 = Second-Stage Anaerobic Digester
AS-Ave = Average Value for Activated Sludge
AS-St Dev = Standard Deviation for Activated Sludge

Based on the sorption distribution coefficients determined for anaerobic digester sludge, the TOrC indicators were classified into three groups. The first group comprises compounds with log K_d values > 3 such as triclocarban, triclosan, and fluoxetine. The second group consists of compounds that had moderate sorption potential with log K_d values between 2 and 3. Compounds that fell into this group include atenolol, benzophenone, cimetidine, and diphenhydramine. The third group of compounds are rather non-sorptive with log K_d values < 2 such as bisphenol A, carbamazepine, DEET, sulfamethoxazole, and trimethoprim.

For the most part, the classification based on K_d values correspond well to the classification based on the octanol-water partitioning coefficient (K_{ow}) and the charge of the compounds (see Table 3-2). TOrC with a higher sorption potential (log K_d > 3) tend to be neutral compounds, i.e., triclosan and triclocarban, with a log D_{ow} > 3 or positively charged compounds such as fluoxetine. This suggests that the octanol-water partitioning coefficient and charge of a TOrC can give guidance for estimating the sorption coefficient for anaerobic digester sludge.

In general, compounds with the highest sorption potential (log K_d > 3) are expected to have the highest sludge concentrations. However, even compounds with low sorption potential (log K_d < 2) such as bisphenol A, caffeine, carbamazepine, DEET, and trimethoprim had measurable quantities in the sludge and biosolids at Facility A. This indicates that low sorptive TOrC can be transferred at relevant loads to the digestion process with primary and waste activated sludges. This appears to be particularly the case for high usage TOrC like caffeine and recalcitrant TOrC like bisphenol A, carbamazepine, and trimethoprim.

6.4.2 Biotransformation

Biotransformation experiments were performed to assess the degradation kinetics of the TOrC indicators in anaerobic digester sludge. The compounds investigated were atenolol, benzophenone, bisphenol A, caffeine, carbamazepine, cimetidine, DEET, diphenhydramine, fluoxetine, gemfibrozil, ibuprofen, meprobamate, naproxen, sulfamethoxazole, TCEP, TCPP, triclocarban, triclosan, and trimethoprim. Biotransformation kinetic rates are described with a pseudo first-order rate constant (Appendix I).

The TOrC indicators were categorized by their biotransformation kinetic rates (Table 6-9). Most of the TOrC indicators exhibited little to no degradation under anaerobic conditions. Exceptions were atenolol (K_b = 0.15 d^{-1}), caffeine (K_b = 0.028 d^{-1}), meprobamate (K_b = 0.012 d^{-1}), and TCEP (K_b = 0.024 d^{-1}), which had moderate biotransformation kinetic rates (here defined as 0.01-0.1 d^{-1}), and naproxen (K_b = 1.51 d^{-1}), sulfamethoxazole (K_b = 3.27 d^{-1}), and trimethoprim (K_b = 9.53 d^{-1}), which had rapid biotransformation kinetic rates (here defined as > 1 d^{-1}).

Theoretically, TOrC with a first order rate constant K_b of more than 0.07 d^{-1} are anticipated to achieve a removal of at least 90% during anaerobic digestion at an HRT of 35 days. The results from Facility A support this prediction for the moderately and rapidly biotransformed TOrC that were included in the full-scale evaluation (i.e., atenolol, caffeine, and trimetroprim) (see Appendix I.6.3).

The basis for biotransformation rate classification of TOrC indicators in anaerobic digester sludge (i.e., rapid, moderate, slow) differed from that used for activated sludge (Table 3-11). The biotransformation rates listed in Table 6-9 were not normalized on the basis of the TSS concentration of the digester sludge sample as was done for the activated sludge samples in order to compare values from samples originating different facilities. When normalized by the TSS concentration in the anaerobic digester (ca. 18 g/L TSS), the kinetic rates measured during conditions simulating anaerobic digester environments were for all compounds slower than under activated sludge conditions.

It was found that the classification of TOrC indicators into the three categories was not always consistent with the classification observed in activated sludge. In activated sludge, atenolol, benzophenone, bisphenol A, caffeine, diphenhydramine, fluoxetine, ibuprofen, and triclosan showed rapid kinetics, while these compounds demonstrated slow to moderate

biotransformation kinetics in anaerobic digester sludge. DEET, cimetidine, and gemfibrozil had moderate kinetics in activated sludge but slow biotransformation kinetics in anaerobic digester sludge (Table 3-11).

Table 6-9. Biotransformation Kinetic Rates in Anaerobic Digester Sludge.

Slow	Moderate	Rapid
<0.01 (d^{-1})	1-0.01 (d^{-1})	>1 (d^{-1})
Benzophenone	Atenolol (0.15)	Naproxen (1.5)
Bisphenol A	Caffeine (0.96)	Sulfamethoxazole (3.3)
Carbamazepine	Meprobamate (0.01)	Trimethoprim (9.7)
Cimetidine	TCEP (0.02)	
DEET		
Diphenhydramine		
Fluoxetine		
Gemfibrozil		
Ibuprofen		
TCPP		
Triclocarban		
Triclosan		

Similar to the bin groups developed in an activated sludge environment, the TOrC indicators were binned according to their measured biotransformation and sorption fate parameters in anaerobic digester sludge (Table 6-10). Seven of the nine bins are represented by at least one indicator compound. These indicator compounds represent a broad range of sorption and biotransformation behavior. The majority of the indicators fall into the slow/recalcitrant biotransformation group ($K_b < 0.01\ d^{-1}$). The bins that are not represented in the summary matrix include moderate biotransformation/high sorption and rapid biotransformation/high sorption.

Table 6-10. Summary Matrix of TOrC Indicators Based on Biotransformation and Sorption Fate Parameters.

		Biotransformation (K_b, d^{-1})		
		Slow	Moderate	Rapid
		<0.01	0.01-1	>1
Sorption (log K_d)	Low <2	Bisphenol A Carbamazepine DEET Ibuprofen Trimethoprim	Caffeine* TCEP*	Sulfamethoxazole Trimethoprim
	Moderate 2-3	Benzophenone Cimetidine Diphenhydramine Gemfibrozil*	Atenolol Meprobamate*	Naproxen*
	High >3	Fluoxetine Triclocarban Triclosan		

* Activated sludge Kd values were used because Kd values were not determined for anaerobic digester sludge.

CHAPTER 7.0

SUMMARY, CONCLUSIONS, AND RECOMMENDATIONS

7.1 Indicator Compound Selection

This study focused on investigating the reduction of TOrC during conventional wastewater treatment with an emphasis on activated sludge treatment. The TOrC assessed in this study were non-volatile and removed primarily by biotransformation and sorption allowing for more accurate mass balances and fate analysis. Only the removal of the parent compound was assessed. The study identified a group of TOrC indicator compounds that can be used to assess the performance efficiency of secondary wastewater treatment. The proposed indicator compounds fall into the four general categories of pharmaceuticals (acetaminophen, atenolol, carbamazepine, cimetidine, diphenhydramine, fluoxetine, gemfibrozil, ibuprofen, iopromide, meprobamate, naproxen, sufamethoxazole, trimethoprim), food additives (caffeine, sucralose), personal care products (benzophenone, DEET, triclocarban, and triclosan), and other high production volume (HPV) chemicals (bisphenol A, TCEP, TCPP).

The indicators were selected to represent a range of properties that are relevant for predicting the removal of TOrC during conventional wastewater treatment. A secondary factor for selection was their toxicological relevance to humans and aquatic organisms. The indicators were selected based on a high detection ratio (>10) and detection frequency in wastewater influents, the availability of robust and sensitive analytical methods suitable for their quantification in different wastewater matrices, and a range of biotransformation and sorption characteristics. Compounds that are known to be generated during wastewater treatment from metabolites of parent compounds were excluded from the indicator candidate list.

Findings of this study support that in most cases the overall attenuation of a TOrC indicator during activated sludge treatment can be reasonably well estimated if basic compound properties, process parameters, such as SRT, HRT, temperature, and redox conditions are known. This suggests that the removal of other TOrC compounds of interest can also be estimated by matching compound to the indicators from this study based on similar properties in terms of biotransformation and sorption characteristics.

7.1.1 Indicator Compound Occurrence

During 13 independent sampling campaigns, the TOrC indicators were quantified in the primary effluents / secondary influents of all seven municipal wastewater facilities sampled in this study, regardless of service area size, geographical location, and season (with the exception of iopromide and primidone). The highest concentrations (10-370 µg/L) were observed for acetaminophen, caffeine, ibuprofen, naproxen, and sucralose. The lowest concentrations (below100 ng/L) were observed for primidone and fluoxetine.

TOrC indicators occurring at very low concentrations in wastewater influents posed a challenge for establishing reliable mass balances across treatment processes in particular for compounds that are not recalcitrant (i.e., fluoxetine). Depending on the sample matrix, analytical reporting limits may be higher than the concentrations of these compounds. The propagation of

error during mass balance calculations is increased for such compounds compared to the uncertainty associated with compounds occurring at high concentrations.

The X-ray contrast agent iopromide occurred below the reporting limit in the primary or secondary influent of six of the 13 sample events. Iopromide concentrations may vary drastically in the influents of wastewater treatment facilities as a result of the use patterns of particular agents used in medical facilities in the service area. In this study, the secondary influent concentrations of the TOrC indicators were generally very similar and within an order of magnitude between different plant sites. Exceptions to this observation were caffeine and DEET for which influent concentrations exhibited a seasonal and geographical dependency. Even though influent concentrations for most compounds were surprisingly similar between different plants in this study, it should not be considered unusual if larger concentration fluctuations are observed at other facilities during future sampling events.

7.1.2 Analytical Amenability and QA/QC During Field Sampling

All proposed indicators can be measured in solid and aqueous samples with one single analytical method (LC/MS-MS) using isotope dilution. This method provides the most accurate and reliable results to date for quantifying TOrC in challenging matrices, such as raw wastewater. This method was recently evaluated in a "Round Robin" test between different laboratories (Vanderford et al., 2012). Costs per sample among various laboratories are estimated as $500-3,000 and there are currently at least 10 commercial laboratories in the U.S. offering this analysis to the industry.

Detailed sampling and QA/QC procedures were established for conducting TOrC sampling campaigns at wastewater facilities. Contamination of blanks in the field was significantly reduced for all compounds and resulted in remaining concentrations close to the level of detection in field blanks by preventing airborne sample contamination. Benzophenone was the only compound exhibiting consistent contamination in field blanks with concentrations below 500 ng/L.

The potential sources for error and uncertainty for mass balance calculations were identified and quantified during field sampling campaigns through:

- Preservation studies for MLSS samples used in laboratory biotransformation tests.
- Preservation studies for 72-hour TOrC composite samples.
- Analysis of different types of blanks (DI water, sample container, sample equipment, sample handling).
- Selected sample replicates.
- Laboratory blanks spiked (fortified) with target TOrC.
- Laboratory fortified sample matrices.
- Mass balance checks using conservative process parameters.

Of the parameters required for establishing TOrC mass balances during secondary treatment, the RAS TSS concentration had the highest variability (commonly up to 15%) and thus impacted the mass balance calculations the most.

7.2 Removal During Conventional Treatment

The efficiency and mechanisms of TOrC removal were evaluated during activated sludge treatment under steady-state process conditions characterized by stable flows and loads, process performance and operation prior and during the sampling event. TOrC removal efficiencies may vary significantly during abnormal treatment conditions, such as biological process upsets, or wet weather flow events and may temporarily even lead to higher effluent than influent concentrations for certain TOrC.

TOrC removal by sorption can occur at different locations during conventional treatment, primary clarification, secondary treatment, tertiary filtration, or activated carbon treatment. In this study, the observed removal during primary clarification was limited to compounds that were moderately or highly sorbable. Removal of these compounds during primary clarification typically ranged between 5% and 35%. Limited data collected indicated that the removal of certain TOrC during primary clarification is enhanced by coagulant addition and potentially by operation at SORs in the range of 600-1,000 gpd/sf as opposed to higher SORs.

The mass of target TOrC associated with the solids in secondary influents was typically insignificant compared to the mass in the aqueous phase. The mass of strongly hydrophobic compounds (log K_d > 3) associated with primary effluent solids should be considered in future TOrC mass balance calculations. Triclocarban accumulated strongly on mixed liquor solids. This may be an explanation for the fact that triclocarban concentrations were at some facilities higher in the secondary effluent compared to the influent. Certain operational conditions may trigger desorption of this compound from the solids inventory into the liquid phase.

Centrate return streams from anaerobic digestion can contribute a significant fraction of certain TOrC to the overall secondary influent load. For the compounds, carbamazepine, TCPP, ibuprofen, bisphenol A, and gemfibrozil, the contribution amounted to 5-65%. Surprisingly, the compounds found in elevated concentrations in centrate streams were not directly related to sorption or biotransformation characteristics of the compounds or respective plant influent concentrations.

Seasonal sampling revealed consistently higher TOrC removal efficiencies during activated sludge treatment with wastewater temperatures being 7-10°C higher during summer (20-26°C) than in winter (14-17°C) sampling events. The stimulating effect of higher wastewater temperatures for TOrC removal appeared to be more pronounced in treatment systems operating at low SRTs (< 5 days). This may be the reason why the same trend could not be demonstrated in controlled pilot-scale experiments that were conducted at an SRT of 10 days.

Based on the biotransformation kinetics quantified in this study the TOrC indicators were classified into three groups:

- Rapid (K_b > 10 L/g-d)
- Moderate (K_b = 0.1 to 10 L/g-d)
- Slow (K_b < 0.1 L/g-d)

Based on the sorption partitioning between aqueous and solid phase (mixed liquor) the TOrC indicators were classified into three groups:

- High (log K_d > 3)
- Moderate (K_d = 2.5 to 3)
- Low (K_d < 2.5)

Table 7-1 summarizes the anticipated removal efficiencies of TOrC indicators during activated sludge treatment based on the three groups for biotransformation and sorption. While these performance estimates were generated on the basis of the observed removal in this study, it is expected that similar efficiencies will be achieved for other TOrC that fall into the respective grouping based on their biotransformation and sorption characteristics.

Table 7-1. Anticipated Overall Removal of TOrC Based on Biotransformation and Sorption Characteristics.

Sorption (log K_d)	Biotransformation (k_b, L/g-d) Slow <0.1	Moderate 0.1-10	Rapid >10
Low <2.5	0-30% (Typical: 5%)	0-100%[1)] (Typical: 70-90%)	70-100% (Typical: 95%)
Moderate 2.5-3	0-60% (Typical 20%)	0-100%[1)] (Typical 30-50%)	60-100% (Typical: 70%)
High >3	0-95% (Typical 50%)*	n.a.	0-100%*

Note:
* Data basis weak to estimate removal for this group.
[1)]The anticipated removal can be narrowed for a specific compound and process operation by using the threshold $SRT_{80\%}$ identified in this study.

This summary suggests that the removal for compounds with rapid biotransformation *and* high sorption is not necessarily better than for compounds with rapid biotransformation but low sorption. Compounds with high sorption were typically still not more than 50% removed during conventional treatment if these compounds were biologically recalcitrant. TOrC indicators that are rapidly biotransformed in accordance with Table 7-1 were almost completely removed in the first 30% (HRT = 2.6 hours) of the aeration basin volume at one field side where profile testing was conducted after the anoxic zone. TOrC indicators that are moderately biotransformed in accordance with Table 7-1 ranged in removal anywhere from 0 to 100% removal depending on activated sludge operation.

In narrowing the estimated removal further for moderately biotransformed compounds, we defined a threshold SRT at which 80% removal is anticipated to occur. Threshold SRT values could be identified for all bioamenable TOrC indicators ranging from 2-30 days. Operation above the threshold SRT is anticipated to result in at least 80% removal of the respective TOrC during secondary treatment. Field investigations could not reveal whether HRT is limiting sorption of

TOrC during secondary treatment. The relevance of HRT could ultimately not be defined, as SRT and HRT were positively correlated for the full-scale facilities and thus both parameters were linked.

The concentration of moderately biotransformed compounds was found to increase in the aqueous phase of the anoxic zone before being partially removed during subsequent aerobic treatment. It is possible that anoxic conditions prompted the desorption or release of TOrC attached to the mixed liquor solids. If this effect indeed occurs, it may explain why this was more noticeable for compounds that are slowly biotransformed.

Activated sludge process configuration, operation, and seasonal conditions determined the biotransformation rate of a large group of compounds that are slow or moderate in biotransformation. Some of these indicators appeared to be well suited for differentiating the performance of different biological treatment systems (i.e., DEET, atenolol, trimethoprim, gemfibrozil).

The biotransformation kinetics measured in different mixed liquor samples varied as a function of SRT for most TOrC. Gemfibrozil appeared to biotransform faster in activated sludge systems operating at longer SRTs. Diphenhydramine, triclosan, and trimethoprim appear to follow a similar trend. In contrast, sulfamethoxazole appeared to biotransform more rapidly in activated sludge systems operated at shorter sludge ages. The fact that many rapidly biotransformed compounds were greater removed under shorter SRT operation may be related to the fact that the microbial community in the mixed liquor of these treatment plants is essentially adapted to consuming easily degradable carbon food. Microbial strains that specialize in breaking down more recalcitrant carbon substrates would be expected to be prevalent under low F/M ratios associated with longer SRT operation. Despite the slower kinetics in longer SRT activated sludge systems, rapidly biotransformed compounds were almost completely removed in all facilities indicating that the HRT during activated sludge treatment is not limiting the biotransformation of these compounds.

The relationship between TOrC removal by biotransformation and kinetic rates is not necessarily linear. The removal of moderately biotransformed TOrC drastically increased in mixed liquor when biotransformation rates exceeded 0.2 to 1 L/g-d. The biotransformation rates for DEET and caffeine were generally multiple times greater in mixed liquor systems that received higher concentrations of these TOrC in the aeration basin influents.

It was not possible to determine a significant difference in performance between hybrid fixed film and suspended growth processes. It was hypothesized that hybrid systems may harbor a wider range of microbial strains that may be better suited to break down a variety of TOrC compounds. In laboratory experiments IFAS performed similarly well for most compounds compared to the MLE process under comparable SRT and HRT conditions. Trimethoprim, a moderately biotransformed compound, was significantly better removed in the hybrid fixed film system than in the suspended growth process.

7.3 Model Predictions

Several TOrC fate models were evaluated for their ability to predict the removal of different TOrC indicators during full-scale treatment. Of these fate models, ASTreat was selected for further evaluation because of its simplicity of input requirements and ability to model the fate of TOrC during solid and liquid stream treatment. Given the current level of understanding on the mechanisms driving TOrC removal during conventional treatment and the current

sophistication of TOrC fate models, the goal of the model evaluation was to assess the usefulness of such tools as screening approaches for estimating the fate of TOrC during treatment.

One of the biggest limitations with existing mass balance models is the lack of appropriate fate parameter values (i.e., biotransformation rate constants, partitioning coefficients) that are needed as model inputs. While sorption properties for most compounds are often already published or can be easily quantified, biotransformation rates are not easily measured and are system specific.

This study evaluated the model predictions by measuring site-specific fate parameters for a suite of TOrC indicators. These parameters were determined in the presence of fresh mixed liquor samples collected from various facilities using spiked target TOrC at ambient concentrations. Considering the library of fate parameters collected in this study, guidelines were developed to help select appropriate biotransformation rates and sorption coefficients for a given TOrC based on general activated sludge process conditions. For biotransformation rates, these guidelines are based on observed relationships with SRT.

The ability of ASTreat to predict TOrC indicator removal accurately and reliably depended on the type of TOrC compound. Generally recalcitrant compound removed primarily by sorption were accurately predicted. Likewise, hydrophilic compounds with rapid biotransformation were successfully modeled. Compounds with moderate or slow biotransformation kinetics removal efficiencies, were difficult to predict. The most challenging compounds were those with both high biotransformation rates and sorption coefficients
(Table 7-2).

Table 7-2. Anticipated Modeling Accuracy for TOrC Using ASTreat.

Sorption (log K_d)	Biotransformation (k_b, L/g-d) Slow <0.1	Moderate 0.1-10	Rapid >10
Low <2.5	High accuracy, reliable	Medium accuracy, partially reliable	High accuracy, reliable
Moderate 2.5-3	n.a.	Medium accuracy, partially reliable	Low accuracy
High >3	High accuracy, reliable	n.a.	Variable[1] (Low for certain compounds, High and reliable for others)

Notes:
High accuracy: Anticipated model prediction generally within 10% of actual removal (light gray shading)
Medium accuracy: Anticipated model prediction within 20% of actual removal for approximately half of attempted field sites (medium gray shading).
Low accuracy: Anticipated model prediction poor and generally not within 30% of actual removal.
1) The accuracy and reliability of TOrC in the group of rapidly degradable and highly sorptive compounds was very compound specific.
n.a. Modeling of representative TOrC Indicators in this group was not conducted in this study.

Improving model predictions for these challenging compound groups hinges on the ability to better predict biotransformation in the field, and the possible dynamics of TOrC accumulation on solids in the activated sludge system. Data collected in this study suggests that sorptive compounds may undergo desorption from solids recycled in activated sludge systems. This would mean that even under process conditions that appear on the macro-scale to be in equilibrium, TOrC may be subject to process dynamics that are not adequately described by an instantaneous equilibrium sorption assumption. Moreover, the model does not currently take into account anoxic zones during activated sludge treatment. This lack of modeling capability may also contribute to variable results for the moderately sorptive and biodegradable compounds.

Specific inaccuracies with model predictions identified in this study were three-fold:

- Biotransformation rate measurements in the laboratory were inconsistent for a few of the investigated compounds. Thus, the reliability for model outputs was low because this input parameter significantly affects model predictions for bioamenable compounds.
- Desorption kinetics, which are currently not being modeled, could play an important role in the overall removal of moderately sorptive and biodegradable compounds.
- Other process parameters, like anoxic zones, may affect sorption or biotransformation and are currently not sufficiently understood to quantify the effect of redox conditions in a mass balance model.

7.4 Cost Analysis

The findings of this study for secondary treatment were put into a broader context by comparing the performance and cost of modifying and operating a secondary process for TOrC reduction to that of alternative treatment processes targeting TOrC removal. The cost analysis was conducted for five process alternatives and the benefits were evaluated for removing a specific small group of TOrC. Processes considered were activated sludge treatment at different SRT levels, ozonation, UF and RO treatment, and balasted flocculation/ sedimentation with PAC addition. For the selected compounds, RO had the highest and most consistent removal performance, however, net present worth cost was multiple times higher than for other treatment alternatives.

Considering only the removal of the specific TOrC indicators, ozonation and PAC treatment in combination with ballasted flocculation/sedimentation were the most cost competitive processes at similar treatment efficiencies. However, none of the advanced treatment processes investigated offers a 100% barrier against TOrC.

In practical applications, cost analyses may be more complex than demonstrated in this study. The assessment will be driven in the first instance by the specific reason for evaluating TOrC reduction at a given facility, such as protection of an endangered species, or potable reuse. Implementation of TOrC reduction strategies, where required, may be staged over time, implemented in increments, or be subject to the integration of process modifications into other treatment goals unrelated to TOrC removal, such as disinfection upgrades, general water quality improvements, etc.

7.5 Anaerobic Digestion

Removal of TOrC during anaerobic digestion was investigated at one facility. The mass balance calculations for some of the TOrC indicators were inconsistent between the first and second stage digesters. For example, the calculated TOrC removals were negative for bisphenol A, carbamazepine, fluoxetine, gemfibrozil, meprobamate, TCEP, and TCPP in the first stage digester, but positive in the second stage digester. These negative removal values in the first stage digester could be due to the collection of a 4-day composite sample for primary and secondary sludges, whereas the first stage digester had an HRT of 20 days. Thus, the amount of these compounds measured for the influent to the first stage digester could have been less than what actually entered the first stage digester over its 20-d hydraulic retention time.

7.6 Recommendations for Future Investigations

TOrC indicator compounds become useful as "performance indicators" if they share general properties with a larger group of compounds that result in similar behavior during wastewater treatment. There is little benefit if these general properties are not easily identified for TOrC of interest and associated with respective indicators whose fate has been studied and is understood in detail. In this study, biotransformation and sorption properties were evaluated as the basis for linking TOrC to removal during wastewater treatment. To support this effort, tools are needed to quickly predict biotransformation characteristics of different TOrC compounds. A promising development in this regard is ongoing research efforts using structural properties of compounds as a method to predict the biotransformation likelihood of a compound without having to conduct actual kinetic studies.

To improve modeling accuracy it is recommended that future studies focus on compounds with moderate biotransformation rates and sorption potential because these TOrC were the most difficult to model accurately under a variety of treatment operating conditions (medium gray shaded cells in Table 7-2). Equal attention should be given to better understanding the factors driving the fate of compounds that are highly sorptive and biotransformable (diagonally shaded cell in Table 7-2). For this group it may be necessary to assess sorption and desorption kinetics under different operational conditions to better understand why at times aqueous phase concentrations were found to increase during treatment. In addition, it is recommended that future modeling efforts include the ability to model anoxic or anaerobic zones in the activated sludge process. Future modeling efforts should also include the ability to model the fate of TOrC during anaerobic digestion.

Further recommendations on future work relevant to the industry that resulted from this study were:

- Evaluate the feasibility for side stream treatment of centrate or filtrate from solid treatment for removing TOrC cost-effectively during wastewater treatment.
- Assess the fate of TOrC on solids after digestion and the feasibility of solid pre-treatment prior to digestion for increasing TOrC removal during liquid and solid stream treatment.
- Conduct a long-term mass balance study for the anaerobic digestion process to obtain better influx data to digesters so that more accurate removals of TOrC could be determined.
- Conduct further testing on comparing the performance of fixed film hybrid activated sludge systems and suspended growth systems for TOrC removal.

- Assess the relationship between TOrC indicator removal and effluent toxicity (e.g., WET testing).
- Identify whether HRT may be limiting sorption for certain compounds during full-scale secondary treatment. This could be accomplished in controlled laboratory experiments under constant SRT conditions.
- Focus on the role of different redox conditions (anoxic and anaerobic) for TOrC removal, and assess the importance of sorption/desorption dynamics for moderately to highly sorptive compounds.

APPENDIX A

LITERATURE REVIEW: INDICATOR DATABASE

A.1 Literature Review of TOrC Indicator Candidates

A.2 Literature Review of Fate of TOrC During Conventional Wastewater Treatment

Appendix A.1

Literature Review of TOrC Indicator Candidates

WERF CEC4R08
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Name	Application	Category	Plant Influent (ng/L)	Influent Standard Deviation (ng/L)	DR > 10 Conc/100	Plant Effluent (ng/)	Effluent Standard Deviation (ng/L)	Sludge Detects (%)	Sludge Conc Mean (ug/kg)	Sludge Conc Std. Dev. (ug/kg)
NDMA	DBP	Nitrosamine	138-158			17-50				
			27-470		no	17-58				
Acriflavine	HHC	Antiseptic	<100		no	<10				
Butylated hydroxytoluene	HHC	Antioxidant	385	280	no	70	50			
Butylated hydroxyanisole	HHC	Antioxidant	175	60	no	80	115			
			ND		no	ND				
			<11-790		no					
Hydrocortisone	HHC	Corticosteroid hormone	270	80	no	6	15			
TCEP	HHC	Flame retardent	<180-1200							
			574-1324			168-711				
			244-535		no					
			ND, 405 (mean detected)	130	no					
			ND-1010			880-1730				
			ND (<400)-81		no	108-124				
TCPP	HHC	Flame retardent	1050-1989		yes	490-1339				
DEET	HHC	Insecticide	570	445	no	150	170			
			<86-1300							
			792		no	278				
			154-700		no					
			ND, 271 (mean detected)	192	no					
			ND-360		no	ND-1310				
			350-7500			160-960				
			285		no	211				
Indolebutyric acid (3-)	HHC	Plant growth regulator	870	620	no	170	115			
Bisphenol A	HHC	Plasticizer	514-747		no	<5-33				
			700-6100			100-1500				
Dibutyl phthalate	HHC	Plasticizer	2850	1950	yes	590	410			
			1700-4400		yes	28-350				
			7540-14600		yes	ND-3710				
Butylbenzylphthalate	HHC	Plasticizer	2700-6400		yes	20-98				
Diethylphthalate	HHC	Plasticizer	4000-13200		yes	70-280				
Caffeine	HHC	Psychoactive stimulant	<53-31000							
			DET-68200		yes					
			71600		yes	<10				
			1260-49479		yes	41-156				
			51100		yes	26.8				
			32500-64500		yes					
			48948	23690	yes					
			42000	6300	yes	15200	4400			
			49000-69000		yes	40-9300				
									39.57	
								46	10-4600	
Paraxanthine		Caffeine derivative	55000	34000	yes	25000	14000			
			DET-62600		yes					
Nicotine			17000	12000	yes	2100	1700			
Cotinine		metabolite of nicotine	NQ(490)-DET-2980							
			7800	550	yes	4000	240			
			5550		yes	5.9				

Name	Application	Category	Plant Influent (ng/L)	Influent Standard Deviation (ng/L)	DR > 10 Conc/100	Plant Effluent (ng/)	Effluent Standard Deviation (ng/L)	Sludge Detects (%)	Sludge Conc Mean (ug/kg)	Sludge Conc Std. Dev. (ug/kg)
								46	11-690	
Sucralose		artificial sweetner	39100		yes	34200				
Acesulfame		artificial sweetner								
Saccharin		artificial sweetner								
Nonylphenol	HHC	Surfactant	39984000		yes	1300-11500				
Octylphenol	HHC	Surfactant	<4-510		no					
			c.a. 200			c.a. 200				
									937	
PFOA	HHC/PCP	Surfactant, emulsifier								
PFOS	HHC									
Oxybenzone	HHC	UV stabilizer	1440	70	yes	40	60			
			420-11000							
			6240-6870		yes	ND-840				
			657-924							
			ND, 2325 (mean detected)	2106	yes					
			190-630		no	60-1100				
			5740		yes	35.6				
1,4 Dioxane			2300-16800		yes	460-180				
Testosterone	Hormone	Androgen	ND-115		no					
			95		no	<20				
								20	31-2040	
Estradiol (17β-)	Hormone	Estrogen	<100		no					
			<20		no	<20				
								13	22-355	
Estriol	Hormone	Estrogen	DET							
			ND, 309 (mean detected)	13	no					
			414		no	<40				
			200-300		no	20				
								21	8-232	
Estrone	Hormone	Estrogen	DET							
			<100		no					
			50-100		no	20-230				
			72		no	21				
Ethinylestradiol	Hormone	Estrogen	<100		no					
			<40		no	<40				
								6	16-49	
Progesterone	Hormone	Progestogen	<100		no					
			30-200		no	20				
Androstenedione	Hormone		276		no	<10				
			ND, 150 (mean detected)	11	no					
Androsterone	Hormone		1800		yes	<20				
Isobutylparaben	PCP	Antimicrobial	250	140	no	3	3			
Phenoxyethanol	PCP	Antimicrobial	14300	6730	yes	240	350			
Phenylphenol (o-)	PCP	Antimicrobial	1800	1850	yes	75	110			
			271		no	<20				
Propylparaben	PCP	Antimicrobial	1300	490	yes	4	3			
Methylparaben	PCP	Antimicrobial	<300-13000							
			18600-46000		yes	ND-2210				

Name	Application	Category	Plant Influent (ng/L)	Influent Standard Deviation (ng/L)	DR > 10 Conc/100	Plant Effluent (ng/)	Effluent Standard Deviation (ng/L)	Sludge Detects (%)	Sludge Conc Mean (ug/kg)	Sludge Conc Std. Dev. (ug/kg)
Chloroxylenol	PCP	Antimicrobial	<15-2300							
			1610-3550		yes	ND-1700				
Triclocarban	PCP	Antimicrobial	215	160		70	42			
			625			138				
			187-13700							
								100	39,433	59,924
Triclosan	PCP	Antimicrobial	1300	630	yes	220	240			
			<350-34000							
			996-12000							
			480-1690			47-78				
			180-1247			516-596				
			300-450			280-2000				
			564-3780							
			ND, 1138 (mean detected)	1426	yes					
			3180		yes	50.1				
			100-630		no	20-370				
									2,997	
								94	16,097	65,135
Acetyl cedrene	PCP	Fragrance	4970	2270	yes	176	150			
Benzyl acetate	PCP	Fragrance	3740	3460	yes	49	34			
Benzyl salicylate	PCP	Fragrance	<22-3200							
			19500	10800	yes	91	50			
Bucinal	PCP	Fragrance	1610	731	yes	35	10			
Camphor	PCP	Fragrance	1650	309	yes	13	35			
Galaxolide	PCP	Fragrance	<610-4500							
			408-797							
			16600	10400	yes	2053	1314			
									1100	
Hexyl salicylate	PCP	Fragrance	5480	3560	yes	9	4			
Hexylcinnamaldehyde	PCP	Fragrance	15300	12100	yes	10	5			
Isobornyl acetate	PCP	Fragrance	6470	8530	yes	17	7			
Menthol	PCP	Fragrance	10300	6800	yes	115	250			
Methyl dihydrojasmonate	PCP	Fragrance	7210	4190	yes	107	18			
Methyl ionone	PCP	Fragrance	3370	2560	yes	66	109			
Methyl salicylate	PCP	Fragrance	10200	9690	yes	21	17			
Musk ketone	PCP	Fragrance	<34-580		no					
			23-104		no					
			640	395	no	58	28			
Musk xylene	PCP	Fragrance	386	299	no	10	4			
OTNE	PCP	Fragrance	3550	1930	yes	159	117			
Terpineol	PCP	Fragrance	63700	36400	yes	51	54			
Tonalide	PCP	Fragrance	12500	7350	yes	1326	270			
									4070	
Vanillin	PCP	Fragrance	3211	3120	yes	2665	160			
3-Phenylpropionate butylbenzyl phthalate	PCP	Fragrance	<11000-1380000		yes					
Hydrocinnamic acid		hydroxy derivatives of cinnamic acid	14700-25700		yes	ND-22300				
Benzophenone	PCP	UV Blocker	1500	480	yes	220	200			
			1390-2430		yes	960-1030				

Name	Application	Category	Plant Influent (ng/L)	Influent Standard Deviation (ng/L)	DR > 10 Conc/100	Plant Effluent (ng/)	Effluent Standard Deviation (ng/L)	Sludge Detects (%)	Sludge Conc Mean (ug/kg)	Sludge Conc Std. Dev. (ug/kg)
			<43-6700							
									220	
Atrazine	Pesticide	Herbicide	1	2	no	1	2			
			NQ(13.2)-DET-87.7		no					
			<100		no					
			<100		no	<20				
Linuron	Pesticide	Herbicide								
Simazine	Pesticide	Herbicide	4	7	no	5	8			
			NQ(3.32)-DET-6.65		no					
4,4'-DDE	Pesticide		<1.5-DET-4.58		no					
Alpha-chlordane	Pesticide		<1.76-DET-12.3		no					
Dieldrin	Pesticide		NQ(1.44)-DET-7.09		no					
Gamma-chlordane	Pesticide		<2.26-DET-11.8		no					
Trans-nonachlor	Pesticide		NQ(1.8)-7.86		no					
Chlorpyriphos	Pesticide		NQ(3.61)-DET-262		no					
Diazinon	Pesticide		NQ(3.61)-DET-71.9		no					
Cis-permethrin	Pesticide		NQ(9.59)-306		no					
Cypermethrins	Pesticide		NQ(9.00)-DET-70.5		no					
Permethrin	Pesticide		NQ(19.1)-DET-689		no					
Trans- Permethrin	Pesticide		9.26-383		no					
Desethyl atrazine	Pesticide		NQ(1.83)-DET-58		no					
Enalapril	PhAC	ACE inhibitor	19-31		no	0.7-0.82				
			<100		no	<100				
Acetaminophen	PhAC	Analgesic	DET-340000							
			61000	19000	yes	860	710			
			75200	87844	yes					
			14200-23500		yes					
			444000		yes	0				
			9900-130000		yes	20-400				
								2	1120-1300	
Diclofenac	PhAC	Analgesic	63-83		no	62-58				
			544-1480			635-1120				
			ND, 157 (mean detected)		no					
			458		no	274				
Hydrocodone	PhAC	Analgesic	113		no	38.3				
			ND-35		no					
			ND, 138 (mean of detects)	45	no					
			70	31	no	8.6	3.5			
Ibuprofen	PhAC	Analgesic	<1400-32000							
			DET-20500							
			7616-43533		yes	<4-743				
			272-24740			92-966				
			2270-68700		yes					
			16680	22652	yes					
			7500-22700		yes	ND				
			7000		yes	0				
			9400-12400		yes	500-610				
								64	100-11900	

Name	Application	Category	Plant Influent (ng/L)	Influent Standard Deviation (ng/L)	DR > 10 Conc/100	Plant Effluent (ng/)	Effluent Standard Deviation (ng/L)	Sludge Detects (%)	Sludge Conc Mean (ug/kg)	Sludge Conc Std. Dev. (ug/kg)
Ketoprofen	PhAC	Analgesic	<200		no	<40				
			1000	1300	no	nd				
Naproxen	PhAC	Analgesic	DET-18800							
			4923-26600		yes	67-337				
			1272-28646		yes	156-302				
			ND-23210			ND-24600				
			4480-17200		yes					
			10710	8385	yes					
			23200		yes	18.7				
								52	21-1020	
Salicylic acid	PhAC	Analgesic	37467-150932		yes	65-503				
			66000-181000		yes	250-1000				
Ciprofloxacin	PhAC	Antibiotic	NQ-DET-15100							
			300-400			20				
								100	10,501	17,658
Erythromycin-H_2O	PhAC	Antibiotic	NQ-DET-2330							
			440		no	<1				
			79-628		no					
			ND, 436 (mean detected)	346	no					
			332		no	85.7				
			2000-3000		yes	50				
									16.6	
								92	36	58
Ofloxacin	PhAC	Antibiotic	DET-3240							
								99	8,573	21,998
Clarithromycin	PhAC	Antibiotic	DET-784			NQ(12.5)-89.7-DET				
								54	9-617	
Azithromycin	PhAC	Antibiotic	DET-669			NQ(12.5)-DET				
								95	831	2342
Sulfamethoxazole	PhAC	Antibiotic	DET-2620							
			421-4060			820-1580				
			1549-10000		yes	1089-1340				
			360	210	no	140	94			
			320-360		no					
			642	469	no					
			1780		yes	3430				
Trimethoprim	PhAC	Antibiotic	DET-498		no					
			335-1190			387-520				
			568-5600			363-1332				
			300	100	no	120	71			
			213-716		no					
			ND, 469 (mean of detects)	242	no					
			788		no	222				
									4.4	
								29	12-204	
4-Epitetracycline		Antibiotic	DET-475							
								95	1135	1741
Tetracycline		Antibiotic	NQ-DET-490							

Name	Application	Category	Plant Influent (ng/L)	Influent Standard Deviation (ng/L)	DR > 10 Conc/100	Plant Effluent (ng/)	Effluent Standard Deviation (ng/L)	Sludge Detects (%)	Sludge Conc Mean (ug/kg)	Sludge Conc Std. Dev. (ug/kg)
								96	1278	2255
Chlorotetracycline (CTC)	PhaC	Antibiotic								
Doxycycline	PhaC	Antibiotic								
								90	877	17658
Minocycline	PhaC	Antibiotic								
Sulfadiazine	PhaC	Antibiotic								
Sulfadimethoxine	PhaC	Antibiotic								
Sulfamerazine	PhaC	Antibiotic								
Sulfamethazine	PhaC	Antibiotic								
Sulfamethizole	PhaC	Antibiotic								
Sulfathiazole	PhaC	Antibiotic								
Tylosin	PhaC	Antibiotic								
Cefotaxime	PhaC	Antibiotic								
Cloxacillin	PhaC	Antibiotic								
Lincomycin	PhaC	Antibiotic								
Penicillin V	PhaC	Antibiotic								
Virginiamycin	PhaC	Antibiotic								
Carbamazepine	PhAC	Anticonvulsant	DET-163							
			124-444		no	196-409				
			391		no	512				
			1100		yes	1100				
			ND, 187 (mean detected)	82	no					
			78-274		no					
			100	78	no	65	15			
			170-390			110-330				
									68	
								95	135	298
Dilantin	PhAC	Anticonvulsant	40-252		no	103-243				
			<100-266		no	317-332				
			ND, 184 (mean detected)	78	no					
			51-170		no					
			109		no	228				
Primidone	PhAC	Anticonvulsant	157		no	177				
			250-1500			60-790				
			604		no	342				
Fluoxetine	PhAC	Antidepressant	NQ(15.0)-DET-58.7		no					
			1992		yes	904				
			600	280	no	560	250			
			ND-168		no					
			ND-10		no					
			ND		no	262				
			100-200		no	20				
									237	
								94	245	329
Amitriptyline	PhAC	Antidepressant	146		no	128				
Miconazole	PhAC	Antifugal Agent	DET-114							
									186	
								95	1239	7311

Name	Application	Category	Plant Influent (ng/L)	Influent Standard Deviation (ng/L)	DR > 10 Conc/100	Plant Effluent (ng/)	Effluent Standard Deviation (ng/L)	Sludge Detects (%)	Sludge Conc Mean (ug/kg)	Sludge Conc Std. Dev. (ug/kg)
Thiabendazole	PhAC	Fungicide	NQ(13.0)-DET-34							
									913	
								69	8-239	
Albuterol	PhAC	Antiasthmatic	NQ(24.2)-DET-75.6							
			13000	4000	yes	8100	3400			
									168	
								1	23	
Cimetidine	PhAC	Anti-acid reflux	DET-11700							
			14	7.3	no	12	6.9			
								88	1332	10314
Metformin	PhAC	Antidiabetic	NQ(326)-DET-248000							
			26000	17000		11000	7100			
								7	550-1160	
Ranitidine	PhAC	Anti-acid reflux	DET-16800							
								55	4-2250	
			330	260	no	62	24			
Atorvastatin	PhAC	Antilipidemic	174-198		no	32-65				
			<100-170		no	96-168				
Gemfibrozil	PhAC	Antilipidemic	DET-6630							
			1787-3810		yes	20-839				
			ND-1220							
			ND, 2037 (mean detected)	1185	yes					
			256-2469			1060-1768				
			2900-8200		yes	2100-8200				
									210	
								90	12-2650	
Simvastatin	PhAC	Antilipidemic	<2.5-12		no	<0.25				
			<20		no	<20				
Risperidone	PhAC	Antipsychotic	<80		no	<80				
Clozapine	PhAC	Antipsychotic	51		no	50				
Diazepam	PhAC	Anxiolytic	2.7		no	3.2				
			<20		no	<20				
			<100		no					
			ND		no					
Hydroxyzine	PhAC	Anxiolytic	21		no	<20				
Meprobamate	PhAC	Anxiolytic	188-345		no	294-353				
			563		no	607				
			124-560		no					
			ND, 653 (mean detected)	529	no					
			1330		yes	477				
Atenolol	PhAC	Beta-blocker	2490-3090		yes	944-779				
			112-2318			1460-1526				
Omeprazole	PhAC	proton pump inhibitor	<20		no	<20				
Metoprolol	PhAC	Beta-blocker								
Propranolol	PhAC	Beta-blocker	13-250		no	3-58				
Pentoxifylline	PhAC	PDE inhibitor	ND		no					
			ND-138		no					
Dehydronifedipine	PhAC	Metabolite of nifedipine (dihydropyridine calcium channel blocker)	NQ(5.6)-DET							

Name	Application	Category	Plant Influent (ng/L)	Influent Standard Deviation (ng/L)	DR > 10 Conc/100	Plant Effluent (ng/)	Effluent Standard Deviation (ng/L)	Sludge Detects (%)	Sludge Conc Mean (ug/kg)	Sludge Conc Std. Dev. (ug/kg)
Diphenhydramine	PhAC	Antihistamine	NQ(7.7)-DET-1490							
									943	
								100	877	1588
Iopromide	PhAC	X-ray contrast media	ND-17		no					
			ND-121		no					
Triamterene	PhAC	Antihypertensive	235		no	341				
Verapamil	PhAC	Antihypertensive	84		no	90				
Diltiazem	PhAC	Antihypertensive	DET-1490							
			57	13	no	53	25			
									13.4	
								82	1-225	
Codeine			NQ(664)-DET-345							
									6.42	
								24	10-328	
Warfarin			NQ(10.6)-DET							
Beta sitosterol	Sterol		DET-239000							
Beta Stigmastanol	Sterol		DET-46000							
								99	168,079	419,232
Campesterol	Sterol		DET-46600							
								100	100879	193694
Cholestanol	Sterol		DET-45700							
								100	680,046	2,374,369
Cholesterol	Sterol		DET-745000							
									55,200	
								96	1,129,268	4,171,366
Coprostanol	Sterol	Carbon stanol	DET-496000							
									96,220	
								100	4,366,714	22,636,715
Desmosterol	Sterol		DET-11100							
Epicoprostanol	Sterol		DET-21400							
								99	1,702,708	26783520
Ergosterol	Sterol		NQ-DET-4490							
Stigmasterol	Sterol	Plant sterol	DET-37200							
									15,669	
								90	321,199	2464383

PhAC - Pharmaceutical Active Compound
HHC - Household Chemical
HVP - High Volume Production Chemical
PCP - Personal Care Product
DBP - Disinfection Byproduct
EDC - Endocrine disrupting compound or suspected EDC
CCL3 - Listed in the current Contamnaint Candidate List
REG - Currently regulated by EPA
NM - No method established by the team to date
CHEMID - ChemIDPlus Advanced by United States National Libaray of Medicein (http://chem.sis.nlm.nih.gov/chemidplus/)

Name	Measured by Isotopic Dilution	Study		# of POTWs	Influent Notes	Influent Detection Frequency >80%	Effluent Notes	MW (g/mol)	log D (pH 7) CHEMID
NDMA		Drewes et al. 2008	WRF	1					
		OCSD		1					
Acriflavine		Drewes et al. 2009	WERF	6					0.83
Butylated hydroxytoluene		Drewes et al. 2009	WERF	6		yes			
Butylated hydroxyanisole		Drewes et al. 2009	WERF	6		yes		180.25	3.5
		Loraine and Pettigrove 2006		1					
		Stephenson and Oppenheimer 2007	WERF	8	Intermediate frequency (25-75%)	no	Poor removal (<50%)		
Hydrocortisone		Drewes et al. 2009	WERF	6					
TCEP		Stephenson and Oppenheimer 2007	WERF	8	Infrequent (<25%)	no	Poor removal (<50%)	285.5	2.11
	Yes	Drewes et al. 2008	WRF	2	2 of 2	yes			
		Trenholm et al. 2006		2		yes			
		SNWA		6	Inf: 50% (3of 6)	no			
		Loraine and Pettigrove 2006		1					
	Yes	Dickenson et al.	WERF	1	1 of 2	no			
TCPP	Yes (uses TCEP)	Drewes et al. 2008	WRF	2	2 of 2	yes	Poor removal	327.6	3.36
DEET		Drewes et al. 2009	WERF	6		yes		191.3	2.5
		Stephenson and Oppenheimer 2007	WERF	8	Intermediate frequency (25-75%)	no	Poor removal (<50%)		
	Yes	Dickenson et al.	WERF	1	1 of 1	yes	some removal		
		Trenholm et al. 2006		2		yes			
		SNWA		8	7 of 8	yes			
		Loraine and Pettigrove 2006		1					
		OCSD		1		yes			
		Westerhoff	ASW RWQ	1		yes			
Indolebutyric acid (3-)		Drewes et al. 2009	WERF	6		yes			
Bisphenol A	Yes	Drewes et al. 2008	WRF	1		yes		228.3	4.04
		OCSD		1		yes			
Dibutyl phthalate		Drewes et al. 2009	WERF	6		yes			
		OCSD		1		yes			
		Loraine and Pettigrove 2006		1		yes			
Butylbenzylphthalate		OCSD		1		yes			
Diethylphthalate		OCSD		1		yes			
Caffeine		Stephenson and Oppenheimer 2007	WERF	8	frequent (>75%)	yes	Good removal (>80%)	194.2	-0.79
	Yes	USEPA 2009a		9	Inf: 100% (9 of 9)	yes	Effl: 0% (0 of 9)		
	Yes	Drewes et al. 2008	WRF	1		yes			
	Yes	Dickenson et al.	WERF	1	2 of 2	yes	well removed		
		Westerhoff	ASU RWQ	1		yes			
		Trenholm et al. 2006		2		yes			
		SNWA		8	Inf: 100% (8 of 8)	yes			
		Benotti and Brownawell 2007		1		yes	64% removal		
		OCSD		1		yes			
		Kinney et al. 2006							
		USEPA 2009b				no (sludge)			
Paraxanthine		Benotti and Brownawell 2007		1		yes	54% removal	180.2	0.24
		USEPA 2009a		9	Inf: 100% (9 of 9)	yes	Effl: 0% (0 of 9)		
Nicotine		Benotti and Brownawell 2007		1		yes	59% removal	162.2	-0.7
Cotinine	Yes	USEPA 2009a		9	Inf: 89% (8 of 9)	yes	Effl: 33% (3 of 9)	176.2	0.21
		Benotti and Brownawell 2007		1		yes	49% removal		
		Westerhoff	ASU RWQ	1		yes			

Name	Measured by Isotopic Dilution	Study		# of POTWs	Influent Notes	Influent Detection Frequency >80%	Effluent Notes	MW (g/mol)	log D (pH 7) CHEMID
		USEPA 2009b				no (sludge)			
Sucralose		Westerhoff	ASU RWQ	1	not removed	yes		397.6	-0.47
Acesulfame					not removed (Buerge et al 2009)				
Saccharin					removed (Buerge et al 2009)				
Nonylphenol		OCSD		1		yes			
Octylphenol		Stephenson and Oppenheimer 2007	WERF	8	infrequent (<25%)	no	Moderate removal (50-80%)	206.32	
		OCSD		1					
		Kinney et al. 2006							
PFOA									
PFOS									
Oxybenzone		Drewes et al. 2009	WERF	6		yes		228.247	3.55
		Stephenson and Oppenheimer 2007	WERF	8	frequent (>75%)	yes	Good removal (>80%)		
		Loraine and Pettigrove 2006		1		yes			
		Trenholm et al. 2006		2		yes			
		SNWA		8	5 of 8	no			
		OCSD		1		yes			
		Westerhoff	ASU RWQ	1		yes			
1,4 Dioxane		OCSD		1		yes			
Testosterone		SNWA unpublished		8	1 of 8	no		288.4	3.77
	Yes	Dickenson et al.	WERF	1	1 of 8	no			
		USEPA 2009b				no (sludge)			
Estradiol (17β-)		SNWA unpublished		8	Inf: 0% (0 of 8)	no		272.4	3.75
	Yes	Dickenson et al.	WERF	1	0 of 1	no			
		USEPA 2009b				no (sludge)			
Estriol		USEPA 2009a		5	Inf: 100% (5 of 5)	yes	Effl: 0% (0 of 5)	288.4	2.67
		SNWA unpublished		7	2 of 7	no			
	Yes	Dickenson et al.	WERF	1		yes			
		OCSD		1		yes			
		USEPA 2009b				no (sludge)			
Estrone		USEPA 2009a		9	Inf: 56% (5 of 9)	no	Effl: 0% (0 of 9)	270.4	4.31
		SNWA unpublished		8	Inf: 0% (0 of 8)	no			
		OCSD		1		yes			
	Yes	Dickenson et al.	WERF	1	1 of 1	yes			
Ethinylestradiol		SNWA unpublished		8	Inf: 0% (0 of 8)	no		296.4	3.81
	Yes	Dickenson et al.	WERF	1		no			
		USEPA 2009b				no (sludge)			
Progesterone		SNWA unpublished		8	Inf: 0% (0 of 8)	no		314.5	4.15
		OCSD		1		yes			
Androstenedione	Yes	Dickenson et al.	WERF	1	1 of 1	yes		286.4	3.93
		SNWA		8	3 of 8	no			
Androsterone	Yes	Dickenson et al.	WERF	1	1 of 1	yes		290.4	3.77
Isobutylparaben		Drewes et al. 2009	WERF	6		yes			
Phenoxyethanol		Drewes et al. 2009	WERF	6		yes		138.2	1.16
Phenylphenol (o-)		Drewes et al. 2009	WERF	6		yes		170.21	3.32
	Yes	Dickenson et al.	WERF	1	1 of 1	yes	well removed		
Propylparaben		Drewes et al. 2009	WERF	6		yes		180.2	2.54
Methylparaben		Stephenson and Oppenheimer 2007	WERF	8	frequent (>75%)	yes	Good removal (>80%)	152.1	1.66
		Loraine and Pettigrove 2006		1		yes			

Name	Measured by Isotopic Dilution	Study		# of POTWs	Influent Notes	Influent Detection Frequency >80%	Effluent Notes	MW (g/mol)	log D (pH 7) CHEMID	
Chloroxylenol		Stephenson and Oppenheimer 2007	WERF	8	frequent (>75%)	yes	Good removal (>80%)	156.6	3.3	
		Loraine and Pettigrove 2006		1		yes				
Triclocarban		Drewes et al. 2009	WERF	6		yes		315.6	4.93	
	Yes	Dickenson et al	WERF	1	1 of 1	yes				
		USEPA 2009a		5	Inf: 100% (5 of 5)	yes	Effl: 80% (4 of 5)			
		USEPA 2009b				yes (sludge)				
Triclosan		Drewes et al. 2009	WERF	6		yes		289.54	4.9	
		Stephenson and Oppenheimer 2007	WERF	8	frequent (>75%)	yes	Moderate removal (50-80%)			
	Yes	USEPA 2009a		5	Inf: 100% (5 of 5)	yes	Effl: 0% (0 of 5)			
	Yes	Drewes et al. 2008	WRF	2		yes				
	Yes	Dickenson et al.	WERF	1	2 of 2	yes				
		Loraine and Pettigrove 2006		1		yes				
		Trenholm et al. 2006		2		yes				
		SNWA		8	7 of 8	yes				
		Westerhoff	ASU RWQ	1		yes				
		OCSD		1		yes				
		Kinney et al. 2006								
		USEPA 2009b				yes (sludge)				
Acetyl cedrene		Simonich et al. 2002	Proctor and Gamble	12		yes	>95% removal (AS)	246.4	3.87	
Benzyl acetate		Simonich et al. 2002	Proctor and Gamble	12		yes	>95% removal (AS)	150.2	1.65	
Benzyl salicylate		Stephenson and Oppenheimer 2007	WERF	8	frequent (>75%)	yes	Good removal (>80%)	228.2	4.05	
		Simonich et al. 2002	Proctor and Gamble	12		yes	>99% removal (AS)			
Bucinal		Simonich et al. 2002	Proctor and Gamble	12		yes	>95% removal (AS)	204.3	3.73	
Camphor		Drewes et al. 2009	WERF	6		yes		152.2	2.55	
Galaxolide		Stephenson and Oppenheimer 2007	WERF	8	frequent (>75%)	yes	Poor removal (<50%)	258.4	4.72	
		Trenholm et al. 2006		2		yes				
		Simonich et al. 2002	Proctor and Gamble	12		yes	>80% removal (AS)			
		Kinney et al. 2006								
Hexyl salicylate		Simonich et al. 2002	Proctor and Gamble	12		yes	>99% removal (AS)	222.3	4.54	
Hexylcinnamaldehyde		Simonich et al. 2002	Proctor and Gamble	12		yes	>99% removal (AS)	216.3224	4.6	
Isobornyl acetate		Simonich et al. 2002	Proctor and Gamble	12		yes	>99% removal (AS)	196.3	2.43	
Menthol		Drewes et al. 2009	WERF	6		yes		156.3	2.66	
Methyl dihydrojasmonate		Simonich et al. 2002	Proctor and Gamble	12		yes	>98% removal (AS)	226.3	2.5	(ACD)
Methyl ionone		Simonich et al. 2002	Proctor and Gamble	12		yes	>96% removal (AS)	206.3	3.71	
Methyl salicylate		Simonich et al. 2002	Proctor and Gamble	12		yes	>99% removal (AS)	152.1	2.32	
Musk ketone		Stephenson and Oppenheimer 2007	WERF	8	frequent (>75%)	yes	Poor removal (<50%)	294.3	3.98	
		Trenholm et al. 2006		2		yes				
		Simonich et al. 2002	Proctor and Gamble	12		yes	>90% removal (AS)			
Musk xylene		Simonich et al. 2002	Proctor and Gamble	12		yes	>97% removal (AS)			
OTNE		Simonich et al. 2002	Proctor and Gamble	12		yes	>90% removal (AS)	234.2	4.2	
Terpineol		Simonich et al. 2002	Proctor and Gamble	12		yes	>99% removal (AS)	154.3	2.17	
Tonalide		Simonich et al. 2002	Proctor and Gamble	12		yes	>88% removal (AS)	258.4	4.96	
		Kinney et al. 2006								
Vanillin		Drewes et al. 2009	WERF	6		yes		152.1	1.16	
3-Phenylpropionate butylbenzyl phthalate		Stephenson and Oppenheimer 2007	WERF	8	frequent (>75%)	yes	Good removal (>80%)			
Hydrocinnamic acid		Loraine and Pettigrove 2006		1		yes		150.2	-0.19	
Benzophenone		Drewes et al. 2009	WERF	6		yes		182.2	3.43	
		Loraine and Pettigrove 2006		1		yes				

Name	Measured by Isotopic Dilution	Study		# of POTWs	Influent Notes	Influent Detection Frequency >80%	Effluent Notes	MW (g/mol)	log D (pH 7) CHEMID
		Stephenson and Oppenheimer 2007	WERF	8	frequent (>75%)	yes	Moderate removal (50-80%)		
		Kinney et al. 2006							
Atrazine		Drewes et al. 2009	WERF	6		yes		215.7	2.2
		USEPA 2009a		9	Inf: 89% (8 of 9)	yes	Effl: 100% (9 of 9)		
		SNWA		8	Inf: 0% (0 of 8)	no			
	Yes	Dickenson et al.	WERF	1	2 of 2	no			
Linuron									
Simazine		Drewes et al. 2009	WERF	6		yes			
		USEPA 2009a		9	Inf: 44% (4 of 9)	no	Effl: 56% (5 of 9)		
4,4'-DDE		USEPA 2009a		9	Inf: 89% (8 of 9)	yes	Effl: 0% (0 of 9)		
Alpha-chlordane		USEPA 2009a		9	Inf: 89% (8 of 9)	yes	Effl: 0% (0 of 9)		
Dieldrin		USEPA 2009a		9	Inf: 89% (8 of 9)	yes	Effl: 56% (5 of 9)		
Gamma-chlordane		USEPA 2009a		9	Inf: 89% (8 of 9)	yes	Effl: 11% (1 of 9)		
Trans-nonachlor		USEPA 2009a		9	Inf: 78% (7 of 9)	no	Effl: 0% (0 of 9)		
Chlorpyriphos		USEPA 2009a		9	Inf: 67% (6 of 9)	no	Effl: 0% (0 of 8)		
Diazinon		USEPA 2009a		9	Inf: 67% (6 of 9)	np	Effl: 56% (5 of 9)		
Cis-permethrin		USEPA 2009a		5	Inf: 80% (4 of 5)	yes	Effl: 0% (0 of 5)		
Cypermethrins		USEPA 2009a		9	Inf: 78% (7 of 9)	no	Effl: 0% (0 of 9)		
Permethrin		USEPA 2009a		9	Inf: 89% (8 of 9)	yes	Effl: 22% (2 of 9)		
Trans- Permethrin		USEPA 2009a		5	Inf: 100% (5 of 5)	yes	Effl: 0% (0 of 5)		
Desethyl atrazine		USEPA 2009a		9	Inf: 89% (8 of 9)	yes	Effl: 89% (8 of 9)		
Enalapril	Yes	Drewes et al. 2008	WRF	1		yes		376.5	-1.1
	Yes	Dickenson et al.	WERF	1		no			
Acetaminophen	Yes	USEPA 2009a		9	Inf: 100% (9 of 9)	yes	Effl: 0% (0 of 9)	151.2	0.91
		Benotti and Brownawell 2007		1		yes	99% removal		
		SNWA		8	8 of 8	yes			
		Trenholm et al. 2006		2		yes			
		Westerhoff	ASU RWQ	1		yes			
		OCSD		1		yes			
		USEPA 2009b				no (sludge)			
Diclofenac	Yes	Drewes et al. 2008	WRF	1	not removed	yes		296.16	1.37
	Yes	Dickenson et al.	WERF	1	2 of 2	yes	not well removed		
		SNWA		8	Inf: 25% (2 of 8)	no			
		Westerhoff	ASU RWQ	1		yes			
Hydrocodone		Westerhoff	ASU RWQ	1		yes		299.4	0.35
		Trenholm et al. 2006		2		no			
		SNWA		8	3 of 8	no			
		Benotti and Brownawell 2007		1		yes	88% removal		
Ibuprofen		Stephenson and Oppenheimer 2007	WERF	8	frequent (>75%)	yes	Good removal (>80%)	206.3	1.71
	Yes	USEPA 2009a		9	Inf: 100% (9 of 9)	yes	Effl: 0% (0 of 9)		
	Yes	Drewes et al. 2008	WRF	2		yes			
	Yes	Dickenson et al.	WERF	1	2 of 2	yes	well removed		
		Trenholm et al. 2006		2		yes			
		SNWA		8	8 of 8	yes			
		Loraine and Pettigrove 2006		1		yes			
		Westerhoff	ASU RWQ	1		yes			
		OCSD		1		yes			
		USEPA 2009b				no (sludge)			

Name	Measured by Isotopic Dilution	Study		# of POTWs	Influent Notes	Influent Detection Frequency >80%	Effluent Notes	MW (g/mol)	log D (pH 7) CHEMID
Ketoprofen	Yes	Dickenson et al.	WERF	1		no			
		Benotti and Brownawell 2007		1		yes			
Naproxen	Yes	USEPA 2009a		9	Inf: 100% (9 of 9)	yes	Effl: 20% (1 of 5)	230.26	0.25
	Yes	Drewes et al. 2008	WRF	2		yes			
	Yes	Dickenson et al.	WERF	1	2 of 2	yes	well removed		
		Loraine and Pettigrove 2006		1		yes			
		Trenholm et al. 2006		2		yes			
		SNWA		8	Inf: 100% (8 of 8)	yes			
		Westerhoff	ASU RWQ	1		yes			
		USEPA 2009b				no (sludge)			
Salicylic acid	Yes	Drewes et al. 2008	WRF	2		yes			
		OCSD		1		yes			
Ciprofloxacin	Yes	USEPA 2009a		9	Inf: 78% (7 of 9)	no	Effl: 44% (4 of 9)	331.3	-1.38
		OCSD		1		yes			
		USEPA 2009b				yes (sludge)			
Erythromycin-H_2O	Yes	USEPA 2009a		9	Inf: 89% (8 of 9)	yes	Effl: 56% (5 of 9)	733.9	1.2
	Yes	Drewes et al. 2008	WRF	1		yes			
		Trenholm et al. 2006		2		yes			
		SNWA		8	6 of 8	no			
		Westerhoff	ASU RWQ	1		yes			
		OCSD		1		yes			
		Kinney et al. 2006							
		USEPA 2009b				yes (sludge)			
Ofloxacin		USEPA 2009a		5	Inf: 100% (5 of 5)	yes	Effl: 20% (1 of 5)	361.4	0.07
		USEPA 2009b				yes (sludge)			
Clarithromycin		USEPA 2009a		5	Inf: 100% (5of 5)	yes	Effl: 60% (3 of 5)	748.0	1.84
		USEPA 2009b				yes (sludge)			
Azithromycin		USEPA 2009a		5	Inf: 100% (5of 5)	yes	Effl: 40% (2 of 5)	749.0	-1.99
		USEPA 2009b				yes (sludge)			
Sulfamethoxazole	Yes	USEPA 2009a		8	Inf: 100% (8 of 8)	yes	Effl: 88% (7 of 8)	253.4	0.14
	Yes	Drewes et al. 2008	WRF	2	not removed	yes			
	Yes	Dickenson et al.	WERF	1	2 of 2	yes	not well removed		
		Benotti and Brownawell 2007		1	62% removal	yes			
		Trenholm et al. 2006		2		yes			
		SNWA		8	8 of 8	yes			
		Westerhoff	ASU RWQ	1		yes			
Trimethoprim	Yes	USEPA 2009a		9	Inf: 100% (9 of 9)	yes	Effl: 33% (3 of 9)	290.3212	0.92
	Yes	Drewes et al. 2008	WRF	2		yes			
	Yes	Dickenson et al.	WERF	1	2 of 2	yes	not well removed		
		Benotti and Brownawell 2007		1	60% removal	yes			
		Trenholm et al. 2006		2		yes			
		SNWA		8	7 of 8	yes			
		Westerhoff	ASU RWQ	1		yes			
		Kinney et al. 2006							
		USEPA 2009b				no (sludge)			
4-Epitetracycline		USEPA 2009a		5	Inf: 100% (5 of 5)	yes	Effl: 0% (0 of 5)	444.4	-6.19
		USEPA 2009b				yes (sludge)			
Tetracycline		USEPA 2009a		9	Inf: 78% (7of 9)	no	Effl: 11% (1 of 9)	444.4	-6.19

Name	Measured by Isotopic Dilution	Study		# of POTWs	Influent Notes	Influent Detection Frequency >80%	Effluent Notes	MW (g/mol)	log D (pH 7) CHEMID
		USEPA 2009b				yes (sludge)			
Chlorotetracycline (CTC)		USEPA 2009a		9	11% (1 of 9)		11% (1 of 9)		
Doxycycline		USEPA 2009a		9	67% (6 of 9)	no	11% (1 of 9)	444.4376	-6.00
		USEPA 2009b				yes (sludge)			
Minocycline		USEPA 2009a		5	20% (1 of 5)	no	0% (0 of 5)		
Sulfadiazine		USEPA 2009a		5	20% (1 of 5)	no	20% (1 of 5)		
Sulfadimethoxine		USEPA 2009a		8	25% (2 of 8)	no	13% (1 of 8)		
Sulfamerazine		USEPA 2009a		8	50% (4 of 8)	no	0% (0 of 8)		
Sulfamethazine	Yes	USEPA 2009a		8	38% (3 of 8)	no	13% (1 of 8)		
Sulfamethizole		USEPA 2009a		8	13% (1 of 8)	no	13% (1 of 8)		
Sulfathiazole		USEPA 2009a		8	25% (2 of 8)	no	0% (0 of 8)		
Tylosin		USEPA 2009a		9	0% (0 of 9)	no	11% (1 of 9)		
Cefotaxime		USEPA 2009a		5	0% (0 of 5)	no	20% (1 of 5)		
Cloxacillin		USEPA 2009a		5	20% (1 of 5)	no	0% (0 of 5)		
Lincomycin		USEPA 2009a		9	56% (5 of 9)	no	22% (2 of 9)		
Penicillin V		USEPA 2009a		5	40% (2 of 5)	no	0% (0 of 5)		
Virginiamycin		USEPA 2009a		9	22% (2 of 9)	no	0% (0 of 9)		
Carbamazepine		USEPA 2009a		5	Inf: 100% (5 of 5)	yes	Effl: 80% (4 of 5)	236.26	2.77
	Yes	Drewes et al. 2008	WRF	2	not removed	yes			
	Yes	Dickenson et al.	WERF	1	1 of 1	yes	not well removed		
		Westerhoff	ASU RWQ	1		yes			
		SNWA		8	5 of 8	no			
		Trenholm et al. 2006		2		yes			
		Benotti and Brownawell 2007		1		yes	37% removal		
		OCWD				yes			
		Kinney et al. 2006							
		USEPA 2009b				yes (sludge)			
Dilantin	Yes	Drewes et al. 2008	WRF	2	not removed	yes		252.272	2.13
	Yes	Dickenson et al.	WERF	1	2 of 2	yes	not well removed		
		SNWA		8	Inf: 50% (4 of 8)	no			
		Trenholm et al. 2006		2		yes			
		Westerhoff	ASU RWQ	1		yes			
Primidone	Yes	Dickenson et al.	WERF	1	1 of 1	yes	not well removed	218.25	1.49
		OCSD		1		yes			
		Westerhoff	ASU RWQ	1		yes			
Fluoxetine	Yes	USEPA 2009a		9	Inf: 78% (7 of 9)	no	Effl: 56% (5 of 9)	309.3305	1.5
	Yes	Dickenson et al.	WERF	1		yes			
		Benotti and Brownawell 2007		1		yes	7.5% removal		
		SNWA		8	1 of 8	no			
		Trenholm et al. 2006		2		no			
		Westerhoff	ASU RWQ	1		no			
		OCSD		1		yes			
		Kinney et al. 2006							
		USEPA 2009b				yes (sludge)			
Amitriptyline	Yes	Dickenson et al.	WERF	1		yes		313.87	1.82
Miconazole		USEPA 2009a		5	Inf: 100% (5 of 5)	yes	Effl 0% (0 of 5)	416.134	5.82
		Kinney et al. 2006							
		USEPA 2009b				yes (sludge)			

Name	Measured by Isotopic Dilution	Study		# of POTWs	Influent Notes	Influent Detection Frequency >80%	Effluent Notes	MW (g/mol)	log D (pH 7) CHEMID
Thiabendazole	Yes	USEPA 2009a		5	Inf: 80% (4 of 5)	yes	Effl 80% (4 of 5)		
		Kinney et al. 2006							
						no (sludge)			
Albuterol	Yes	USEPA 2009a		9	Inf: 67% (6 of 9)	no	Effl: 22% (2 of 9)	239.313	-1.68
		Benotti and Brownawell 2007		1		yes	36% removal		
		Kinney et al. 2006							
		USEPA 2009b				no (sludge)			
Cimetidine		USEPA 2009a		9	Inf: 100% (9 of 9)	yes	Effl: 22% (2 of 9)	252.3	-0.34
		Benotti and Brownawell 2007		1		yes			
		USEPA 2009b				yes (sludge)			
Metformin	Yes	USEPA 2009a		8	Inf: 88% (7 of 8)	yes	Effl: 88% (7 of 8)	129.17	-4.93
		Benotti and Brownawell 2007		1		yes	59% removal		
		USEPA 2009b				no (sludge)			
Ranitidine		USEPA 2009a		8	Inf: 100% (8 of 8)	yes	Effl: 25% (2 of 8)	314.4	-0.13
		USEPA 2009b				no (sludge)			
		Benotti and Brownawell 2007		1		yes	81% removal		
Atorvastatin	Yes	Drewes et al. 2008	WRF	2		yes		558.6	2.77
	Yes	Dickenson et al.	WERF	1		no			
Gemfibrozil	Yes	USEPA 2009a		9	Inf: 100% (9 of 9)	yes	Effl: 78% (7 of 9)	250.337	1.85
	Yes	Drewes et al. 2008	WRF	2		yes			
		Trenholm et al. 2006		2		no			
		SNWA		8	Inf: 75% (6 of 8)	no			
	Yes	Dickenson et al.	WERF	1	2 of 2	yes			
		OCSD		1		yes			
		Kinney et al. 2006							
		USEPA 2009b				yes (sludge)			
Simvastatin	Yes	Drewes et al. 2008	WRF	2		no			
	Yes	Dickenson et al.	WERF	1	1 of 1	no			
Risperidone	Yes	Dickenson et al.	WERF	1		no		410.5	0.86
Clozapine	Yes	Dickenson et al.	WERF	1	1 of 1	yes		326.8	2.88
Diazepam		Westerhoff	ASU RWQ	1		yes		284.7	3.01
	Yes	Dickenson et al.	WERF	1		no			
		SNWA		8	Inf: 0% (0 of8)	no			
		Trenholm et al. 2006		2		no			
Hydroxyzine	Yes	Dickenson et al.	WERF	1 of 1		yes		447.8	2.31
Meprobamate	Yes	Drewes et al. 2008	WRF	2	not removed	yes		218.3	0.93
	Yes	Dickenson et al.	WERF	1	1 of 1	yes	not well removed		
		Trenholm et al. 2006		2		yes			
		SNWA		8	7 of 8	yes			
		Westerhoff	ASU RWQ	1		yes			
Atenolol	Yes	Drewes et al. 2008	WRF	2		yes		266.3	-2.23
	Yes	Dickenson et al.	WERF	1	2 of 2	yes	not well removed		
Omeprazole	Yes	Dickenson et al.	WERF	1		no		345.4	1.96
Metoprolol									
Propranolol		Fono and Sedlak 2005		6		yes			
Pentoxifylline		Trenholm et al. 2006		2		no			
		SNWA		8	1 of 8	no			
Dehydronifedipine		USEPA 2009a		5	Inf: 80% (4 of 5)	yes	Effl: 60% (3 of 5)		

Name	Measured by Isotopic Dilution	Study		# of POTWs	Influent Notes	Influent Detection Frequency >80%	Effluent Notes	MW (g/mol)	log D (pH 7) CHEMID
Diphenhydramine		USEPA 2009a		5	Inf: 60% (3 of 5)	no	Effl: 40% (2 of 5)	255.359	1.79
		Kinney et al. 2006							
		USEPA 2009b				yes (sludge)			
Iopromide		Trenholm et al. 2006		2		no		791	
		SNWA		8	1 of 8	no			
Triamterene	Yes	Dickenson et al.	WERF	1 of 1		yes		253.3	1.37
Verapamil	Yes	Dickenson et al.	WERF	1	Inf: 100% (1 of 1)	yes		491.1	1.91
Diltiazem		USEPA 2009a		9	Inf: 100% (9 of 9)	yes	Effl: 44% (4 of 9)	414.5	1.53
		Benotti and Brownawell 2007		1		yes			
		Kinney et al. 2006							
		USEPA 2009b				yes (sludge)			
Codeine		USEPA 2009a		5	63% (5 of 8)	no	13% (1 of 8)	299.368	-0.83
		Kinney et al. 2006							
		USEPA 2009b				no (sludge)			
Warfarin	Yes	USEPA 2009a		9	44% (4 of 9)	no (sludge)	0% (0 of 9)		
Beta sitosterol		USEPA 2009a		9	Inf: 100% (9 of 9)	yes	Effl: 44% (4 of 9)	414.7	7.84
Beta Stigmastanol		USEPA 2009a		5	Inf: 100% (5 of 5)	yes	Effl: 40% (2 of 5)		
		USEPA 2009b				yes (sludge)			
Campesterol		USEPA 2009a		5	Inf: 100% (5 of 5)	yes	Effl: 40% (2 of 5)	400.7	7.4
		USEPA 2009b				yes (sludge)			
Cholestanol		USEPA 2009a		9	Inf: 100% (9 of 9)	yes	Effl: 78% (7 of 9)	388.675	7.52
		USEPA 2009b				yes (sludge)			
Cholesterol		USEPA 2009a		9	Inf: 100% (9 of 9)	yes	Effl: 67% (6 of 9)	386.659	7.11
		Kinney et al. 2006							
		USEPA 2009b				yes (sludge)			
Coprostanol		USEPA 2009a		9	Inf: 100% (9 of 9)	yes (sludge)	Effl: 89% (8 of 9)	389	7.52
		Kinney et al. 2006							
		USEPA 2009b				yes (sludge)			
Desmosterol		USEPA 2009a		9	Inf: 100% (9 of 9)	yes	Effl: 44% (4 of 9)	384.644	6.71
Epicoprostanol		USEPA 2009a		9	Inf: 100% (9 of 9)	yes	Effl: 67% (6 of 9)		
		USEPA 2009b				yes (sludge)			
Ergosterol		USEPA 2009a		8	Inf: 88% (7 of 8)	yes	Effl: 50% (4 of 8)		
Stigmasterol		USEPA 2009a		9	Inf: 100% (9 of 9)	yes	Effl: 67% (6 of 9)	412.7	7.48
		Kinney et al. 2006							
		USEPA 2009b				yes (sludge)			

PhAC - Pharmaceutical Active Compound
HHC - Household Chemical
HVP - High Volume Production Chemical
PCP - Personal Care Product
DBP - Disinfection Byproduct
EDC - Endocrine disrupting compound or suspected EDC
CCL3 - Listed in the current Contamnaint Candidate List
REG - Currently regulated by EPA
NM - No method established by the team to date
CHEMID - ChemIDPlus Advanced by United States National Libaray of Medicein (http://chem.sis.nlm.nih.gov/chemidplus/)

Name	pkA CHEMID	Charged/ Uncharged	(pH 7)	CAS #	LC-MS/MS Method	Isotopic Dilution SNWA	Isotopic Dilution CSM	Isotopic Dilution UNSW	Isotopic Dilution USEPA (2007) (Method 1693)	Health Relevance
NDMA										CCL3
Acriflavine	0.56, 1.71, 8.82 (CHEMID)	charged (+)		8048-52-0	Yes					
Butylated hydroxytoluene										
Butylated hydroxyanisole	11.19 (SPARC)	uncharged		25013-16-5	Yes	Yes				EDC, CCL3
Hydrocortisone					Yes					
TCEP	n.a.	uncharged		115-96-8	Yes	Yes	Yes	Yes		
TCPP	n.a.	uncharged		13674-84-5	Yes	Yes (uses TCEP)				
DEET	n.a.	uncharged		134-62-3	Yes	Yes	Yes	Yes		EDC
Indolebutyric acid (3-)					Yes					EDC
Bisphenol A	9.78 acidic	uncharged		80-05-7	Yes	Yes	Yes			EDC
Dibutyl phthalate										
Butylbenzylphthalate										
Diethylphthalate										
Caffeine	1.5 basic	uncharged		58-08-2	Yes	Yes	Yes	Yes	Yes	
Paraxanthine	10.76 acidic	uncharged		611-59-6	Yes					
Nicotine	8.86 basic 2.27 basic	charged (+)		54-11-5						
Cotinine	4.79 basic	uncharged		486-56-6	Yes				Yes	

Name	pkA CHEMID	Charged/ Uncharged	(pH 7)	CAS #	LC-MS/MS Method	Isotopic Dilution SNWA	Isotopic Dilution CSM	Isotopic Dilution UNSW	Isotopic Dilution USEPA (2007) (Method 1693)	Health Relevance
Sucralose	11.91 acidic	uncharged		56038-13-2						
Acesulfame										
Saccharin										
Nonylphenol										EDC
Octylphenol		uncharged		27193-28-9	Yes					EDC
PFOA					Yes					CCL3
PFOS					Yes					CCL3
Oxybenzone	7.77	charged (-) & uncharged		131-57-7	Yes					
1,4 Dioxane										
Testosterone	19.4 acidic	uncharged		58-22-0	Yes	Yes	Yes	Yes		EDC
Estradiol (17β-)	10.3 acidic	uncharged		50-28-2	Yes	Yes	Yes	Yes		EDC, CCL3
Estriol	10.3 acidic	uncharged		50-27-1	Yes		Yes	Yes		EDC, CCL3
Estrone	10.3 acidic	uncharged		53-16-7	Yes	Yes	Yes	Yes		EDC, CCL3
Ethinylestradiol	10.3 acidic	uncharged		57-63-6	Yes	Yes	Yes	Yes		EDC, CCL3
Progesterone	n.a.	uncharged		57-83-0	Yes	Yes	Yes			EDC
Androstenedione	n.a.	uncharged		63-05-8	Yes			Yes		EDC
Androsterone	18.3 acidic	uncharged		53-41-8	Yes			Yes		
Isobutylparaben					Yes					
Phenoxyethanol	15.1	uncharged		122-99-6						
Phenylphenol (o-)	9.69 acidic	uncharged		90-43-7	Yes			Yes		
Propylparaben	8.5 acidic	uncharged	charged (-)	94-13-3	Yes		Yes			
Methylparaben	8.5 acidic	uncharged	charged (-)	99-76-3						

Name	pkA CHEMID	Charged/ Uncharged	(pH 7)	CAS #	LC-MS/MS Method	Isotopic Dilution SNWA	Isotopic Dilution CSM	Isotopic Dilution UNSW	Isotopic Dilution USEPA (2007) (Method 1693)	Health Relevance
Chloroxylenol	9.21	uncharged		88-04-0						
Triclocarban	11.42 acidic	uncharged		101-20-2	Yes		Yes	Yes	Yes	
Triclosan	7.68	uncharged	charged (-)	3380-34-5	Yes	Yes	Yes	Yes	Yes	
Acetyl cedrene	n.a.	uncharged		32388-55-9						
Benzyl acetate	n.a.	uncharged		140-11-4						
Benzyl salicylate	9.72	uncharged		118-58-1						
Bucinal	n.a.	uncharged		80-54-6						
Camphor	n.a.	uncharged		76-22-2						
Galaxolide	n.a.	uncharged		1222-05-5						
Hexyl salicylate	9.72	uncharged		6259-76-3						
Hexylcinnamaldehyde	n.a.	uncharged		101-86-0						
Isobornyl acetate	n.a.	uncharged		125-12-2						
Menthol	-0.81 basic	uncharged		89-78-1						
Methyl dihydrojasmonate	n.a.	uncharged		24851-98-7						
Methyl ionone	n.a.	uncharged		127-51-5						
Methyl salicylate	9.72	uncharged		119-36-8						
Musk ketone	n.a.	uncharged		81-14-1	Yes	Yes				EDC
Musk xylene										
OTNE	n.a.	uncharged		54464-57-2						
Terpineol	-0.87 basic	uncharged		8000-41-7 562-74-3						
Tonalide	n.a.	uncharged		21145-77-7						
Vanillin	7.81	uncharged	charged (-)	121-33-5						
3-Phenylpropionate butylbenzyl phthalate										
Hydrocinnamic acid	4.73	charged (-)		501-52-0						
Benzophenone	n.a.	uncharged		119-61-9	Yes	Yes				EDC

Name	pkA CHEMID	Charged/ Uncharged	(pH 7)	CAS #	LC-MS/MS Method	Isotopic Dilution SNWA	Isotopic Dilution CSM	Isotopic Dilution UNSW	Isotopic Dilution USEPA (2007) (Method 1693)	Health Relevance
Atrazine	2.0 basic	uncharged		1912-24-9	Yes	Yes	Yes	Yes		REG, EDC
Linuron					Yes	Yes	Yes	Yes		
Simazine					Yes					REG
4,4'-DDE										
Alpha-chlordane										
Dieldrin										
Gamma-chlordane										
Trans-nonachlor										
Chlorpyriphos										
Diazinon										
Cis-permethrin										
Cypermethrins										
Permethrin										
Trans- Permethrin										
Desethyl atrazine										
Enalapril	5.19 basic 3.18 acidic	charged (-)		75847-73-3	Yes	Yes		Yes		
Acetaminophen	9.46 acidic	uncharged		103-90-2	Yes		Yes	Yes	Yes	
Diclofenac	4.0	charged (-)		15307-86-5	Yes	Yes	Yes	Yes		
Hydrocodone	8.61	charged (+)		125-29-1	Yes		Yes			
Ibuprofen	4.85	charged (-)		15687-27-1	Yes	Yes	Yes	Yes	Yes	

Name	pkA CHEMID	Charged/ Uncharged	(pH 7)	CAS #	LC-MS/MS Method	Isotopic Dilution SNWA	Isotopic Dilution CSM	Isotopic Dilution UNSW	Isotopic Dilution USEPA (2007) (Method 1693)	Health Relevance
Ketoprofen					Yes		Yes	Yes		
Naproxen	4.19	charged (-)		22204-53-1	Yes	Yes	Yes	Yes	Yes	
Salicylic acid										
Ciprofloxacin	5.76 acidic 8.76 basic	charged	(- and +)	85721-33-1	Yes				Yes	
Erythromycin-H_2O	12.91 acidic 8.38 basic	charged (+)		114-07-8	Yes				Yes	CCL3
Ofloxacin	5.45 acidic 6.2 basic	charged	(- and +)	83380-47-6	Yes					
Clarithromycin	8.38 basic	charged (+)		81103-11-9	Yes					
Azithromycin	8.91, 9.57 basic	charged (+)		83905-01-5	Yes					
Sulfamethoxazole	6.16 acidic	charged (-)		723-46-6	Yes	Yes	Yes	Yes	Yes	
Trimethoprim	7.16 basic	Uncharged	charged (+)	738-70-5	Yes	Yes	Yes	Yes	Yes	
4-Epitetracycline	4.15 acidic 8.36 basic	charged	(- and +)	79-85-6	Yes					
Tetracycline	4.15 acidic 8.36 basic	charged	(- and +)	60-54-8	Yes					

Name	pkA CHEMID	Charged/ Uncharged	(pH 7)	CAS #	LC-MS/MS Method	Isotopic Dilution SNWA	Isotopic Dilution CSM	Isotopic Dilution UNSW	Isotopic Dilution USEPA (2007) (Method 1693)	Health Relevance
Chlorotetracycline (CTC)					Yes					
Doxycycline	4.15 acidic 3.67 acidic 7.82 bascic	charged	(- and +)	564-25-0	Yes					
Minocycline					Yes					
Sulfadiazine					Yes					
Sulfadimethoxine					Yes					
Sulfamerazine					Yes					
Sulfamethazine					Yes				Yes	
Sulfamethizole					Yes					
Sulfathiazole					Yes					
Tylosin					Yes					
Cefotaxime					Yes					
Cloxacillin					Yes					
Lincomycin					Yes					
Penicillin V					Yes					
Virginiamycin					Yes					
Carbamazepine	0.31 basic	uncharged		298-46-4	Yes	Yes	Yes	Yes		
Dilantin	8.46 acidic	Uncharged charged (-)		57-41-0	Yes	Yes	Yes	Yes		
Primidone	13, 14 (acid)	uncharged		125-33-7	Yes	Yes	Yes	Yes		
Fluoxetine	9.8 basic	charged (+)		54910-89-3	Yes	Yes	Yes	Yes	Yes	
Amitriptyline	9.76 (base)	charge (+)		549-18-8	Yes			Yes		HVP
Miconazole	6.77 (base)	charge (+)		22916-47-8	Yes					

Name	pkA CHEMID	Charged/ Uncharged	(pH 7)	CAS #	LC-MS/MS Method	Isotopic Dilution SNWA	Isotopic Dilution CSM	Isotopic Dilution UNSW	Isotopic Dilution USEPA (2007) (Method 1693)	Health Relevance
Thiabendazole					Yes				Yes	
Albuterol	9.87 basic 8.87 acidic	charge (- & +)		18559-94-9	Yes				Yes	
Cimetidine	6.9 basic	uncharged charge (+)		51481-61-9	Yes					
Metformin	10.3,12.3 (base)	charge (+)		1115-70-4	Yes			Yes	Yes	HVP
Ranitidine	8.08 basic	uncharged charge (+)		66357-35-5	Yes					
Atorvastatin	4.3 & 11.8 acidic	charge (-)		134523-00-5	Yes	Yes		Yes		
Gemfibrozil	4.42 acidic	charged (-)		25812-30-0	Yes	Yes	Yes	Yes	Yes	
Simvastatin					Yes	Yes old	Yes	Yes		
Risperidone	1.16 & 9.76 basic	charged (+)		106266-06-2	Yes	Yes old		Yes		
Clozapine	3.9,7.4 (base)	uncharged charged (+)		5786-21-0	Yes			Yes		Top ten deadliest drug
Diazepam	2.92 (base)	uncharged		439-14-5	Yes	Yes	Yes	Yes		
Hydroxyzine	2.1 & 7.8 (base) 15.3(acid)	charge (+) & uncharged		2192-20-3	Yes			Yes		
Meprobamate	15.2 acidic	uncharged		57-53-4	Yes	Yes	Yes	Yes		
Atenolol	9.87 basic	Charged (+)		29122-68-7	Yes	Yes	Yes	Yes		
Omeprazole	1.59, 4.77 (base) 9.68 (acid)	uncharged charged (+) (slight)		73590-58-6	Yes			Yes		
Metoprolol										
Propranolol										
Pentoxifylline					Yes					
Dehydronifedipine					Yes					

Name	pkA CHEMID	Charged/ Uncharged	(pH 7)	CAS #	LC-MS/MS Method	Isotopic Dilution SNWA	Isotopic Dilution CSM	Isotopic Dilution UNSW	Isotopic Dilution USEPA (2007) (Method 1693)	Health Relevance
Diphenhydramine	8.87 (base)	charge (+) uncharged		58-73-1	Yes					
Iopromide		uncharged		73334-07-3	Yes	Yes				
Triamterene	4.57 (base)	uncharged		396-01-0	Yes			Yes		HVP
Verapamil	9.68 (base)	charge (+)		152-11-4	Yes			Yes		HVP
Diltiazem	8.18 basic	uncharged charge (+)		42399-41-7	Yes					
Codeine	9.19 basic	charge (+)		76-57-3	Yes					
Warfarin					Yes				Yes	
Beta sitosterol	18.2 acidic	uncharged		83-46-5						
Beta Stigmastanol										
Campesterol	18.2 acidic	uncharged		474-62-4						
Cholestanol				80-97-7						
Cholesterol	18.2 acidic	uncharged		57-88-5					Yes	
Coprostanol	18.2 acidic	uncharged		360-68-9						Biomarker of human fecal matter
Desmosterol				313-04-2						
Epicoprostanol										
Ergosterol										
Stigmasterol	-1.4 basic	Uncharged		83-48-7						

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Name	Sorption Fate	Biodegradation	Team's Established Analytical Method Reference	TRC	CDN	Cambridge
NDMA			EPA 1625M			
Acriflavine			Trenholm et al. (2008)			
Butylated hydroxytoluene			Trenholm et al. (2008)			
Butylated hydroxyanisole			Trenholm et al. (2008)			
Hydrocortisone			Trenholm et al. (2008)			
TCEP	some sorption		Trenholm et al. (2006)			
TCPP	Some sorption	Recalcitrant	Snyder (unpublished)			
DEET	Low sorption	biotransforms	Trenholm et al. (2008)			
Indolebutyric acid (3-)			Trenholm et al. (2008)			
Bisphenol A	High sorption	biotransforms	Vanderford and Snyder (2006)			
Dibutyl phthalate			Trenholm et al. (2008)			
Butylbenzylphthalate						
Diethylphthalate						
Caffeine	low sorption	biotransforms	Trenholm et al. (2006)			
Paraxanthine	low sorption					
Nicotine	some sorption			yes		
Cotinine	low sorption					

Name	Sorption Fate	Biodegradation	Team's Established Analytical Method Reference	TRC	CDN	Cambridge
Sucralose	low sorption			yes		
Acesulfame						
Saccharin						
Nonylphenol			NM			
Octylphenol	high sorption		Snyder (unpublished)			
PFOA			Higgins et al. (2005)			
PFOS						
Oxybenzone	some sorption		Trenholm et al. (2006)	no	yes	yes
1,4 Dioxane						
Testosterone	some sorption		Trenholm et al. (2006)			
Estradiol (17β-)	some sorption		Trenholm et al. (2006)			
Estriol	low sorption	biotransforms	Trenholm et al. (2006)			
Estrone	high sorption		Trenholm et al. (2006)			
Ethinylestradiol	some sorption		Trenholm et al. (2006)			
Progesterone	high sorption		Trenholm et al. (2006)			
Androstenedione	some sorption		Trenholm et al. (2006)			
Androsterone	some sorption					
Isobutylparaben			Trenholm et al. (2008)			
Phenoxyethanol	low sorption		Trenholm et al. (2008)	no	yes	
Phenylphenol (o-)	some sorption	Biotransforms	Trenholm et al. (2008)			
Propylparaben	low sorption		Trenholm et al. (2008)			
Methylparaben	low sorption			no	yes	

Name	Sorption Fate	Biodegradation	Team's Established Analytical Method Reference	TRC	CDN	Cambridge
Chloroxylenol				no	no	no
Triclocarban	high sorption	recalcitrant	Trenholm et al. (2008)			
Triclosan	high soprtion	biotransforms	Vanderford and Snyder (2006)			
Acetyl cedrene	some sorption		NM	no	no	
Benzyl acetate	low sorption		NM	no	no	
Benzyl salicylate	high sorption		NM		yes	
Bucinal	some sorption		NM	no	no	
Camphor	low sorption		Trenholm et al. (2008)	no	no	
Galaxolide	high sorption		Trenholm et al. (2008)	no	no	yes
Hexyl salicylate	high sorption		NM	no	no	
Hexylcinnamaldehyde	high sorption		NM	no	no	
Isobornyl acetate	low sorption		NM	no	no	
Menthol	low sorption		Trenholm et al. (2008)	yes	no	
Methyl dihydrojasmonate	low sorption		NM	no	no	
Methyl ionone	some sorption		NM	no	no	
Methyl salicylate	low sorption		NM	no	yes	
Musk ketone	some sorption		Snyder (unpublished)			
Musk xylene			NM			
OTNE	high sorption		NM	no	no	
Terpineol	low sorption		NM	yes		
Tonalide	high sorption		NM	no	no	no
Vanillin	low sorption		Trenholm et al. (2008)	no	no	
3-Phenylpropionate butylbenzyl phthalate						
Hydrocinnamic acid	low sorption					
Benzophenone	some sorption		Snyder (unpublished)			

Name	Sorption Fate	Biodegradation	Team's Established Analytical Method Reference	TRC	CDN	Cambridge
Atrazine	low sorption	recalcitrant	Vanderford and Snyder (2006)			
Linuron			Vanderford and Snyder (2006)			
Simazine			Trenholm et al. (2008)			
4,4'-DDE						
Alpha-chlordane						
Dieldrin						
Gamma-chlordane						
Trans-nonachlor						
Chlorpyriphos						
Diazinon						
Cis-permethrin						
Cypermethrins						
Permethrin						
Trans- Permethrin						
Desethyl atrazine						
Enalapril	low sorption	biotranforms	Vanderford and Snyder (2006)			
Acetaminophen	low sorption	biotransforms	Trenholm et al. (2006)			
Diclofenac	low sorption	recalcitrant	Vanderford and Snyder (2006)			
Hydrocodone	some sorption		Trenholm et al. (2006)			
Ibuprofen	low sorption	biotransforms	Trenholm et al. (2006)			

Name	Sorption Fate	Biodegradation	Team's Established Analytical Method Reference	TRC	CDN	Cambridge
Ketoprofen	low sorption	biotransforms	Reddersen et al. (2003)			
Naproxen	low sorption		Vanderford and Snyder (2006)			
Salicylic acid	low sorption	biotransforms	Drewes (unpublished)			
Ciprofloxacin	high sorption		NM			
Erythromycin-H_2O	some sorption		Trenholm et al. (2006)			
Ofloxacin	high sorption		NM			
Clarithromycin	some sorption					
Azithromycin	some sorption			no	no	no
Sulfamethoxazole	low sorption	biotransforms	Vanderford and Snyder (2006)			
Trimethoprim	some sorption		Vanderford and Snyder (2006)			
4-Epitetracycline	some sorption					
Tetracycline	some sorption			yes		

Name	Sorption Fate	Biodegradation	Team's Established Analytical Method Reference	TRC	CDN	Cambridge
Chlorotetracycline (CTC)						
Doxycycline	some sorption					
Minocycline						
Sulfadiazine						
Sulfadimethoxine						
Sulfamerazine						
Sulfamethazine						
Sulfamethizole						
Sulfathiazole						
Tylosin						
Cefotaxime						
Cloxacillin						
Lincomycin						
Penicillin V						
Virginiamycin						
Carbamazepine	low sorption	recalcitrant	Vanderford and Snyder (2006)			
Dilantin	low sorption	recalcitrant	Vanderford and Snyder (2006)			
Primidone	low sorption	recalcitrant	Snyder (unpublished)			
Fluoxetine	some sorption		Vanderford and Snyder (2006)			
Amitriptyline	some sorption					
Miconazole	some sorption			no	no	no

Name	Sorption Fate	Biodegradation	Team's Established Analytical Method Reference	TRC	CDN	Cambridge
Thiabendazole	some sorption					
Albuterol	some sorption					
Cimetidine	some sorption			yes		
Metformin	some sorption					
Ranitidine	some sorption					
Atorvastatin	low sorption		Vanderford and Snyder (2006)			
Gemfibrozil	low sorption	biotransforms	Vanderford and Snyder (2006)			
Simvastatin			Vanderford and Snyder (2006)			
Risperidone	some sorption		Vanderford and Snyder (2006)			
Clozapine	some sorption					
Diazepam	low sorption		Vanderford and Snyder (2006)			
Hydroxyzine	some sorption					
Meprobamate	low sorption	recalictrant	Vanderford and Snyder (2006)			
Atenolol	low sorption	biotransforms	Vanderford and Snyder (2006)			
Omeprazole	some sorption					
Metoprolol			NM			
Propranolol			NM			
Pentoxifylline			Trenholm et al. (2006)			
Dehydronifedipine						

Name	Sorption Fate	Biodegradation	Team's Established Analytical Method Reference	TRC	CDN	Cambridge
Diphenhydramine	some sorption			yes		
Iopromide	low sorption		Trenholm et al. (2006)			
Triamterene						
Verapamil	some sorption					
Diltiazem	some sorption			yes	no	no
Codeine	some sorption					
Warfarin						
Beta sitosterol	high sorption					
Beta Stigmastanol	high sorption					
Campesterol	high sorption					
Cholestanol	high sorption					
Cholesterol	high sorption					
Coprostanol	high sorption			no	no	
Desmosterol	high sorption					
Epicoprostanol	high sorption					
Ergosterol	high sorption					
Stigmasterol	high sorption					

PhAC - Pharmaceutical Active Compound
HHC - Household Chemical
HVP - High Volume Production Chemical
PCP - Personal Care Product
DBP - Disinfection Byproduct
EDC - Endocrine disrupting compound or suspected EDC
CCL3 - Listed in the current Contamnaint Candidate List
REG - Currently regulated by EPA
NM - No method established by the team to date
CHEMID - ChemIDPlus Advanced by United States National Libaray of Medicein (http://chem.sis.nlm.nih.gov/chemidplus/)

Appendix A.2

Literature Review of Fate of TOrC During Conventional Wastewater Treatment

NR - not reported	EDC - Endocrine-disrupting compound	SYN- synthetic	MBR - Membrane bio-reactor	AS - activated sludge
NA - not applicable	PCM - polycylic musk	BR - Batch reactor	CAS - conventional activated sludge	'--' - not in study

Compound	Abbr. in paper	PPCP Category	Analytical Method	Mol. Weight	log K_{ow}	Author	Year	Publication	Scale	Container	Volume
17α-ethynylestradiol	EE2	Hormone	GC/MS SPE	296.41	3.67	Urase	2005	Water Research	Lab	BR	4L
17α-ethynylestradiol	EE2	Hormone	GC/MS SPE	296.41	3.67	Urase	2005	Water Research	Lab	BR	4L
17α-ethynylestradiol	EE2	Hormone	GC/MS SPE	296.41	3.67	Urase	2005	Water Research	Lab	BR	4L
17α-ethynylestradiol	EE2	Hormone	GC/MS SPE	296.41	3.67	Urase	2005	Water Research	Lab	BR	4L
17α-ethynylestradiol	EE2	Hormone	GC/MS SPE	296.41	3.67	Urase	2005	Water Research	Lab	BR	4L
17α-ethynylestradiol	EE2	Hormone	GC/MS SPE	296.41	3.67	Urase	2005	Water Research	Lab	BR	4L
17β -estradiol	E2	Hormone	GC/MS SPE	272.39	4.01	Urase	2005	Water Research	Lab	BR	4L
17β -estradiol	E2	Hormone	GC/MS SPE	272.39	4.01	Urase	2005	Water Research	Lab	BR	4L
17β -estradiol	E2	Hormone	GC/MS SPE	272.39	4.01	Urase	2005	Water Research	Lab	BR	4L
17β -estradiol	E2	Hormone	GC/MS SPE	272.39	4.01	Urase	2005	Water Research	Lab	BR	4L
17β -estradiol	E2	Hormone	GC/MS SPE	272.39	4.01	Urase	2005	Water Research	Lab	BR	4L
17β -estradiol	E2	Hormone	GC/MS SPE	272.39	4.01	Urase	2005	Water Research	Lab	BR	4L
benzophenone	BZP	EDC	GC/MS SPE	182.22	3.18	Urase	2005	Water Research	Lab	BR	4L
benzophenone	BZP	EDC	GC/MS SPE	182.22	3.18	Urase	2005	Water Research	Lab	BR	4L
benzophenone	BZP	EDC	GC/MS SPE	182.22	3.18	Urase	2005	Water Research	Lab	BR	4L
benzophenone	BZP	EDC	GC/MS SPE	182.22	3.18	Urase	2005	Water Research	Lab	BR	4L
benzophenone	BZP	EDC	GC/MS SPE	182.22	3.18	Urase	2005	Water Research	Lab	BR	4L
benzophenone	BZP	EDC	GC/MS SPE	182.22	3.18	Urase	2005	Water Research	Lab	BR	4L
bisphenol A	BPA	EDC	GC/MS SPE	228.29	3.32	Urase	2005	Water Research	Lab	BR	4L
bisphenol A	BPA	EDC	GC/MS SPE	228.29	3.32	Urase	2005	Water Research	Lab	BR	4L
bisphenol A	BPA	EDC	GC/MS SPE	228.29	3.32	Urase	2005	Water Research	Lab	BR	4L
bisphenol A	BPA	EDC	GC/MS SPE	228.29	3.32	Urase	2005	Water Research	Lab	BR	4L
bisphenol A	BPA	EDC	GC/MS SPE	228.29	3.32	Urase	2005	Water Research	Lab	BR	4L
bisphenol A	BPA	EDC	GC/MS SPE	228.29	3.32	Urase	2005	Water Research	Lab	BR	4L
carbamazepine	CBZ	pharmaceutical	GC/MS SPE	236.38	2.45	Urase	2005	Water Research	Lab	BR	4L
carbamazepine	CBZ	pharmaceutical	GC/MS SPE	236.38	2.45	Urase	2005	Water Research	Lab	BR	4L
carbamazepine	CBZ	pharmaceutical	GC/MS SPE	236.38	2.45	Urase	2005	Water Research	Lab	BR	4L

Appendix A.2

Literature Review of Fate of TOrC During Conventional Wastewater Treatment

carbamazepine	CBZ	pharmaceutical	GC/MS	SPE	236.38	2.45	Urase	2005	Water Research	Lab	BR	4L
carbamazepine	CBZ	pharmaceutical	GC/MS	SPE	236.38	2.45	Urase	2005	Water Research	Lab	BR	4L
carbamazepine	CBZ	pharmaceutical	GC/MS	SPE	236.38	2.45	Urase	2005	Water Research	Lab	BR	4L
clofibric Acid	CA	pharmaceutical	GC/MS	SPE	214.65	2.57	Urase	2005	Water Research	Lab	BR	4L
clofibric Acid	CA	pharmaceutical	GC/MS	SPE	214.65	2.57	Urase	2005	Water Research	Lab	BR	4L
clofibric Acid	CA	pharmaceutical	GC/MS	SPE	214.65	2.57	Urase	2005	Water Research	Lab	BR	4L
clofibric Acid	CA	pharmaceutical	GC/MS	SPE	214.65	2.57	Urase	2005	Water Research	Lab	BR	4L
clofibric Acid	CA	pharmaceutical	GC/MS	SPE	214.65	2.57	Urase	2005	Water Research	Lab	BR	4L
clofibric Acid	CA	pharmaceutical	GC/MS	SPE	214.65	2.57	Urase	2005	Water Research	Lab	BR	4L
diclofenac	DCF	pharmaceutical	GC/MS	SPE	296.16	4.51	Urase	2005	Water Research	Lab	BR	4L
diclofenac	DCF	pharmaceutical	GC/MS	SPE	296.16	4.51	Urase	2005	Water Research	Lab	BR	4L
diclofenac	DCF	pharmaceutical	GC/MS	SPE	296.16	4.51	Urase	2005	Water Research	Lab	BR	4L
diclofenac	DCF	pharmaceutical	GC/MS	SPE	296.16	4.51	Urase	2005	Water Research	Lab	BR	4L
diclofenac	DCF	pharmaceutical	GC/MS	SPE	296.16	4.51	Urase	2005	Water Research	Lab	BR	4L
diclofenac	DCF	pharmaceutical	GC/MS	SPE	296.16	4.51	Urase	2005	Water Research	Lab	BR	4L
esterone	E1	Hormone	GC/MS	SPE	270.39	3.13	Urase	2005	Water Research	Lab	BR	4L
esterone	E1	Hormone	GC/MS	SPE	270.39	3.13	Urase	2005	Water Research	Lab	BR	4L
esterone	E1	Hormone	GC/MS	SPE	270.39	3.13	Urase	2005	Water Research	Lab	BR	4L
esterone	E1	Hormone	GC/MS	SPE	270.39	3.13	Urase	2005	Water Research	Lab	BR	4L
esterone	E1	Hormone	GC/MS	SPE	270.39	3.13	Urase	2005	Water Research	Lab	BR	4L
esterone	E1	Hormone	GC/MS	SPE	270.39	3.13	Urase	2005	Water Research	Lab	BR	4L
fenoprofen	FEP	pharmaceutical	GC/MS	SPE	242.28	3.90	Urase	2005	Water Research	Lab	BR	4L
fenoprofen	FEP	pharmaceutical	GC/MS	SPE	242.28	3.90	Urase	2005	Water Research	Lab	BR	4L
fenoprofen	FEP	pharmaceutical	GC/MS	SPE	242.28	3.90	Urase	2005	Water Research	Lab	BR	4L
fenoprofen	FEP	pharmaceutical	GC/MS	SPE	242.28	3.90	Urase	2005	Water Research	Lab	BR	4L
fenoprofen	FEP	pharmaceutical	GC/MS	SPE	242.28	3.90	Urase	2005	Water Research	Lab	BR	4L
fenoprofen	FEP	pharmaceutical	GC/MS	SPE	242.28	3.90	Urase	2005	Water Research	Lab	BR	4L
gemfibrozil	GFZ	pharmaceutical	GC/MS	SPE	250.34	4.77	Urase	2005	Water Research	Lab	BR	4L
gemfibrozil	GFZ	pharmaceutical	GC/MS	SPE	250.34	4.77	Urase	2005	Water Research	Lab	BR	4L
gemfibrozil	GFZ	pharmaceutical	GC/MS	SPE	250.34	4.77	Urase	2005	Water Research	Lab	BR	4L
gemfibrozil	GFZ	pharmaceutical	GC/MS	SPE	250.34	4.77	Urase	2005	Water Research	Lab	BR	4L
gemfibrozil	GFZ	pharmaceutical	GC/MS	SPE	250.34	4.77	Urase	2005	Water Research	Lab	BR	4L
gemfibrozil	GFZ	pharmaceutical	GC/MS	SPE	250.34	4.77	Urase	2005	Water Research	Lab	BR	4L
ibuprofen	IBP	pharmaceutical	GC/MS	SPE	206.29	3.97	Urase	2005	Water Research	Lab	BR	4L

ibuprofen	IBP	pharmaceutical	GC/MS	SPE	206.29	3.97	Urase	2005	Water Research	Lab	BR	4L
ibuprofen	IBP	pharmaceutical	GC/MS	SPE	206.29	3.97	Urase	2005	Water Research	Lab	BR	4L
ibuprofen	IBP	pharmaceutical	GC/MS	SPE	206.29	3.97	Urase	2005	Water Research	Lab	BR	4L
ibuprofen	IBP	pharmaceutical	GC/MS	SPE	206.29	3.97	Urase	2005	Water Research	Lab	BR	4L
ibuprofen	IBP	pharmaceutical	GC/MS	SPE	206.29	3.97	Urase	2005	Water Research	Lab	BR	4L
indomethicin	IDM	pharmaceutical	GC/MS	SPE	357.80	4.27	Urase	2005	Water Research	Lab	BR	4L
indomethicin	IDM	pharmaceutical	GC/MS	SPE	357.80	4.27	Urase	2005	Water Research	Lab	BR	4L
indomethicin	IDM	pharmaceutical	GC/MS	SPE	357.80	4.27	Urase	2005	Water Research	Lab	BR	4L
indomethicin	IDM	pharmaceutical	GC/MS	SPE	357.80	4.27	Urase	2005	Water Research	Lab	BR	4L
indomethicin	IDM	pharmaceutical	GC/MS	SPE	357.80	4.27	Urase	2005	Water Research	Lab	BR	4L
indomethicin	IDM	pharmaceutical	GC/MS	SPE	357.80	4.27	Urase	2005	Water Research	Lab	BR	4L
ketoprofen	KEP	pharmaceutical	GC/MS	SPE	254.29	3.12	Urase	2005	Water Research	Lab	BR	4L
ketoprofen	KEP	pharmaceutical	GC/MS	SPE	254.29	3.12	Urase	2005	Water Research	Lab	BR	4L
ketoprofen	KEP	pharmaceutical	GC/MS	SPE	254.29	3.12	Urase	2005	Water Research	Lab	BR	4L
ketoprofen	KEP	pharmaceutical	GC/MS	SPE	254.29	3.12	Urase	2005	Water Research	Lab	BR	4L
ketoprofen	KEP	pharmaceutical	GC/MS	SPE	254.29	3.12	Urase	2005	Water Research	Lab	BR	4L
ketoprofen	KEP	pharmaceutical	GC/MS	SPE	254.29	3.12	Urase	2005	Water Research	Lab	BR	4L
naproxen	NPX	pharmaceutical	GC/MS	SPE	230.27	3.18	Urase	2005	Water Research	Lab	BR	4L
naproxen	NPX	pharmaceutical	GC/MS	SPE	230.27	3.18	Urase	2005	Water Research	Lab	BR	4L
naproxen	NPX	pharmaceutical	GC/MS	SPE	230.27	3.18	Urase	2005	Water Research	Lab	BR	4L
naproxen	NPX	pharmaceutical	GC/MS	SPE	230.27	3.18	Urase	2005	Water Research	Lab	BR	4L
naproxen	NPX	pharmaceutical	GC/MS	SPE	230.27	3.18	Urase	2005	Water Research	Lab	BR	4L
naproxen	NPX	pharmaceutical	GC/MS	SPE	230.27	3.18	Urase	2005	Water Research	Lab	BR	4L
propyphenazone	PPZ	pharmaceutical	GC/MS	SPE	230.31	1.94	Urase	2005	Water Research	Lab	BR	4L
propyphenazone	PPZ	pharmaceutical	GC/MS	SPE	230.31	1.94	Urase	2005	Water Research	Lab	BR	4L
propyphenazone	PPZ	pharmaceutical	GC/MS	SPE	230.31	1.94	Urase	2005	Water Research	Lab	BR	4L
propyphenazone	PPZ	pharmaceutical	GC/MS	SPE	230.31	1.94	Urase	2005	Water Research	Lab	BR	4L
propyphenazone	PPZ	pharmaceutical	GC/MS	SPE	230.31	1.94	Urase	2005	Water Research	Lab	BR	4L
propyphenazone	PPZ	pharmaceutical	GC/MS	SPE	230.31	1.94	Urase	2005	Water Research	Lab	BR	4L

calculated from study values

Process	Wastewater	WWTP	Redox Cond.	No. of Runs	Run Number	Gen. Cond.	Duration (h)	Temp (°C)	MLSS (g MLSS/L)	DOC (mg/L)	Initial pH
AS	synthetic		aerobic	6	A-1	Normal	96	20	2.663	144	6.7
AS	synthetic		aerobic	6	A-2	Normal	120	20	2.701	155	7.0
AS	synthetic		aerobic	6	B-1	Lower pH	96	20	2.77	145	5.6
AS	synthetic		aerobic	6	B-2	Lower pH	48	20	2.189	138	4.4
AS	synthetic		aerobic	6	C-1	Lower DOC	48	20	1.711	40	7.2
AS	synthetic		aerobic	6	C-2	Higher DOC	48	20	2.41	242	7.0
AS	synthetic		aerobic	6	A-1	Normal	96	20	2.663	144	6.7
AS	synthetic		aerobic	6	A-2	Normal	120	20	2.701	155	7.0
AS	synthetic		aerobic	6	B-1	Lower pH	96	20	2.77	145	5.6
AS	synthetic		aerobic	6	B-2	Lower pH	48	20	2.189	138	4.4
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AS	synthetic		aerobic	6	C-2	Higher DOC	48	20	2.41	242	7.0
AS	synthetic		aerobic	6	A-1	Normal	96	20	2.663	144	6.7
AS	synthetic		aerobic	6	A-2	Normal	120	20	2.701	155	7.0
AS	synthetic		aerobic	6	B-1	Lower pH	96	20	2.77	145	5.6
AS	synthetic		aerobic	6	B-2	Lower pH	48	20	2.189	138	4.4
AS	synthetic		aerobic	6	C-1	Lower DOC	48	20	1.711	40	7.2
AS	synthetic		aerobic	6	C-2	Higher DOC	48	20	2.41	242	7.0
AS	synthetic		aerobic	6	A-1	Normal	96	20	2.663	144	6.7
AS	synthetic		aerobic	6	A-2	Normal	120	20	2.701	155	7.0
AS	synthetic		aerobic	6	B-1	Lower pH	96	20	2.77	145	5.6
AS	synthetic		aerobic	6	B-2	Lower pH	48	20	2.189	138	4.4
AS	synthetic		aerobic	6	C-1	Lower DOC	48	20	1.711	40	7.2
AS	synthetic		aerobic	6	C-2	Higher DOC	48	20	2.41	242	7.0
AS	synthetic		aerobic	6	A-1	Normal	96	20	2.663	144	6.7
AS	synthetic		aerobic	6	A-2	Normal	120	20	2.701	155	7.0
AS	synthetic		aerobic	6	B-1	Lower pH	96	20	2.77	145	5.6

AS	synthetic	aerobic	6	B-2	Lower pH	48	20	2.189	138	4.4
AS	synthetic	aerobic	6	C-1	Lower DOC	48	20	1.711	40	7.2
AS	synthetic	aerobic	6	C-2	Higher DOC	48	20	2.41	242	7.0
AS	synthetic	aerobic	6	A-1	Normal	96	20	2.663	144	6.7
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AS	synthetic	aerobic	6	B-1	Lower pH	96	20	2.77	145	5.6
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AS	synthetic	aerobic	6	B-1	Lower pH	96	20	2.77	145	5.6
AS	synthetic	aerobic	6	B-2	Lower pH	48	20	2.189	138	4.4
AS	synthetic	aerobic	6	C-1	Lower DOC	48	20	1.711	40	7.2
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AS	synthetic	aerobic	6	A-2	Normal	120	20	2.701	155	7.0
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AS	synthetic	aerobic	6	A-2	Normal	120	20	2.701	155	7.0
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AS	synthetic	aerobic	6	C-1	Lower DOC	48	20	1.711	40	7.2
AS	synthetic	aerobic	6	C-2	Higher DOC	48	20	2.41	242	7.0

Reaction Order	MLSS (g SS/L)	k_b (h^{-1}) sorption	k_p (L/gMLSS) water/sludge mass transfer	$k_1 + k_2$ (h^{-1})	k_1(h^{-1}) biodegradation	k_1 (L/gSS d) biodegredation	k_{E1-E2} (h^{-1}) biodegredation of E1-E2	Influent Conc. (ng/L)	Mixed Liqour Conc.	Effluent Conc.
1st	2.5	2.000	0.438	NA	0.013	0.125	NA	10000.000	NR	NR
1st	2.5	5.361	0.505	NA	0.140	1.344	NA	10000.000	NR	NR
1st	2.5	1.684	0.547	NA	0.105	1.008	NA	10000.000	NR	NR
1st	2.5	4.968	0.554	NA	0.088	0.845	NA	10000.000	NR	NR
1st	2.5	>10	0.434	NA	0.059	0.566	NA	10000.000	NR	NR
1st	2.5	1.413	0.757	NA	0.016	0.154	NA	10000.000	NR	NR
1st	2.5	>10	1.506	6.839	0.000	65.654	6.839	10000.000	NR	NR
1st	2.5	>10	NR	2.423	0.000	23.261	2.432	10000.000	NR	NR
1st	2.5	>10	0.713	8.390	0.000	80.544	8.390	10000.000	NR	NR
1st	2.5	>10	0.426	13.329	0.000	127.958	13.329	10000.000	NR	NR
1st	2.5	>10	0.529	19.997	0.000	191.971	19.997	10000.000	NR	NR
1st	2.5	>10	2.003	4.695	0.000	45.072	4.695	10000.000	NR	NR
1st	2.5	3.542	0.161	NA	0.363	3.485	NA	10000.000	NR	NR
1st	2.5	NR	NR	NA	NR	NR	NA	10000.000	NR	NR
1st	2.5	>10	0.168	NA	0.091	0.874	NA	10000.000	NR	NR
1st	2.5	3.965	0.177	NA	0.081	0.778	NA	10000.000	NR	NR
1st	2.5	>10	0.154	NA	0.521	5.002	NA	10000.000	NR	NR
1st	2.5	>10	0.136	NA	0.265	2.544	NA	10000.000	NR	NR
1st	2.5	2.278	0.217	NA	0.028	0.269	NA	10000.000	NR	NR
1st	2.5	0.369	0.273	NA	0.049	0.470	NA	10000.000	NR	NR
1st	2.5	2.934	0.304	NA	0.225	2.160	NA	10000.000	NR	NR
1st	2.5	6.027	0.378	NA	0.130	1.248	NA	10000.000	NR	NR
1st	2.5	>10	0.263	NA	0.132	1.267	NA	10000.000	NR	NR
1st	2.5	0.928	0.651	NA	0.028	0.269	NA	10000.000	NR	NR
1st	2.5	>10	0.066	NA	0.030	0.288	NA	10000.000	NR	NR
1st	2.5	NR	NR	NA	NR	NR	NA	10000.000	NR	NR
1st	2.5	>10	0.028	NA	0.000	0.000	NA	10000.000	NR	NR

1st	2.5	3.281	0.035	NA	0.000	0.000	NA	10000.000	NR	NR
1st	2.5	>10	0.034	NA	0.011	0.106	NA	10000.000	NR	NR
1st	2.5	NR	NR	NA	NR	NR	NA	10000.000	NR	NR
1st	2.5	>10	0.029	NA	0.017	0.163	NA	10000.000	NR	NR
1st	2.5	NR	NR	NA	NR	NR	NA	10000.000	NR	NR
1st	2.5	>10	0.162	NA	0.000	0.000	NA	10000.000	NR	NR
1st	2.5	>10	0.554	NA	0.025	0.240	NA	10000.000	NR	NR
1st	2.5	3.161	0.024	NA	0.115	1.104	NA	10000.000	NR	NR
1st	2.5	NR	NR	NA	NR	NR	NA	10000.000	NR	NR
1st	2.5	3.795	0.032	NA	0.000	0.000	NA	10000.000	NR	NR
1st	2.5	NR	NR	NA	NR	NR	NA	10000.000	NR	NR
1st	2.5	>10	0.159	NA	0.260	2.496	NA	10000.000	NR	NR
1st	2.5	>10	0.701	NA	0.052	0.499	NA	10000.000	NR	NR
1st	2.5	2.025	0.016	NA	0.493	4.733	NA	10000.000	NR	NR
1st	2.5	NR	NR	NA	NR	NR	NA	10000.000	NR	NR
1st	2.5	>10	0.170	NA	0.109	1.046	NA	10000.000	NR	NR
1st	2.5	>10	0.236	NA	0.121	1.162	NA	10000.000	NR	NR
1st	2.5	>10	0.218	NA	0.263	2.525	NA	10000.000	NR	NR
1st	2.5	>10	0.303	NA	0.167	1.603	NA	10000.000	NR	NR
1st	2.5	>10	0.250	NA	0.123	1.181	NA	10000.000	NR	NR
1st	2.5	>10	0.364	NA	0.046	0.442	NA	10000.000	NR	NR
1st	2.5	0.178	0.057	NA	0.160	1.536	NA	10000.000	NR	NR
1st	2.5	NR	NR	NA	NR	NR	NA	10000.000	NR	NR
1st	2.5	0.296	0.306	NA	0.400	3.840	NA	10000.000	NR	NR
1st	2.5	1.311	0.515	NA	0.141	1.354	NA	10000.000	NR	NR
1st	2.5	0.611	0.926	NA	0.675	6.480	NA	10000.000	NR	NR
1st	2.5	NR	NR	NA	NR	NR	NA	10000.000	NR	NR
1st	2.5	0.448	0.100	NA	0.052	0.499	NA	10000.000	NR	NR
1st	2.5	NR	NR	NA	NR	NR	NA	10000.000	NR	NR
1st	2.5	0.401	0.327	NA	0.434	4.166	NA	10000.000	NR	NR
1st	2.5	0.403	1.106	NA	0.210	2.016	NA	10000.000	NR	NR
1st	2.5	0.434	0.075	NA	0.178	1.709	NA	10000.000	NR	NR
1st	2.5	NR	NR	NA	NR	NR	NA	10000.000	NR	NR
1st	2.5	0.199	0.080	NA	0.201	1.930	NA	10000.000	NR	NR

1st	2.5	NR	NR	NA	NR	NR	NA	10000.000	NR	NR
1st	2.5	0.054	1.265	NA	0.186	1.786	NA	10000.000	NR	NR
1st	2.5	1.061	0.470	NA	0.352	3.379	NA	10000.000	NR	NR
1st	2.5	0.374	0.072	NA	0.348	3.341	NA	10000.000	NR	NR
1st	2.5	NR	NR	NA	NR	NR	NA	10000.000	NR	NR
1st	2.5	7.225	0.039	NA	0.541	5.194	NA	10000.000	NR	NR
1st	2.5	NR	NR	NA	NR	NR	NA	10000.000	NR	NR
1st	2.5	0.125	1.158	NA	0.253	2.429	NA	10000.000	NR	NR
1st	2.5	1.540	2.851	NA	0.112	1.075	NA	10000.000	NR	NR
1st	2.5	4.106	0.028	NA	0.281	2.698	NA	10000.000	NR	NR
1st	2.5	NR	NR	NA	NR	NR	NA	10000.000	NR	NR
1st	2.5	0.337	0.029	NA	0.061	0.586	NA	10000.000	NR	NR
1st	2.5	NR	NR	NA	NR	NR	NA	10000.000	NR	NR
1st	2.5	2.271	0.072	NA	0.078	0.749	NA	10000.000	NR	NR
1st	2.5	>10	0.429	NA	0.028	0.269	NA	10000.000	NR	NR
1st	2.5	2.592	0.016	NA	0.389	3.734	NA	10000.000	NR	NR
1st	2.5	NR	NR	NA	NR	NR	NA	10000.000	NR	NR
1st	2.5	0.464	0.024	NA	0.013	0.125	NA	10000.000	NR	NR
1st	2.5	NR	NR	NA	NR	NR	NA	10000.000	NR	NR
1st	2.5	1.184	0.093	NA	0.079	0.758	NA	10000.000	NR	NR
1st	2.5	1.916	0.444	NA	0.041	0.394	NA	10000.000	NR	NR
1st	2.5	1.727	0.013	NA	0.389	3.734	NA	10000.000	NR	NR
1st	2.5	NR	NR	NA	NR	NR	NA	10000.000	NR	NR
1st	2.5	4.098	0.015	NA	0.030	0.288	NA	10000.000	NR	NR
1st	2.5	NR	NR	NA	NR	NR	NA	10000.000	NR	NR
1st	2.5	1.003	0.015	NA	0.000	0.000	NA	10000.000	NR	NR
1st	2.5	6.216	0.019	NA	0.090	0.864	NA	10000.000	NR	NR
1st	2.5	6.829	0.023	NA	0.126	1.210	NA	10000.000	NR	NR
1st	2.5	NR	NR	NA	NR	NR	NA	10000.000	NR	NR

Gen Info

APPENDIX B

ANALYTICAL METHOD PARAMETER AND REPORTING LIMITS

B.1 Preservation Study

A preservation study was performed on three different wastewater matrices from Facility G to determine the suitability of sodium azide (NaN_3) for reducing biotransformation during sampling, storage, and shipping. NaN_3 is a bacteriostatic agent that disrupts a variety of enzymes but is commonly linked to enzymes essential to cellular respiration (i.e., leading to bacterial asphyxiation). Specifically, NaN_3 inhibits the cytochrome oxidase enzyme, which disrupts electron transfer and ATP production during cellular respiration. With respect to water and wastewater samples, NaN_3 is commonly used to inhibit aerobic degradation of target compounds.

Grab samples were collected from the primary clarifier influent, mixed liquor, and secondary clarifier effluent to encompass some of the most challenging matrices that would be encountered during the full-scale sampling phase. Although mixed liquor will not be tested frequently during the full-scale sampling phase, this matrix was targeted due to its high degree of biological activity, thereby significantly challenging the preservative.

On the sampling day (Day 0), 5 L of each wastewater matrix were collected in 1-L silanized, amber glass bottles. Some of the bottles contained preservative according to the test protocol (see Table B-1). One bottle of each wastewater matrix (not preserved) was designated as a time-zero (T_0) control. Each of the bottles was then spiked with the target compounds to supplement the ambient concentrations, and the bottles were stored as indicated in Table B-1. The samples were not mixed or agitated during the storage period. The T_0 control was processed, spiked with isotopes, and extracted immediately. The "4ºC for 3 days" samples were intended to represent full-scale samples that were either refrigerated or cooled with ice packs during the 72-hour composite period. The "20ºC for 3 days" samples were intended to represent samples that were not cooled properly during the 72-hour composite period. After three days, all of the samples were stored at 4ºC for an additional 11 days (total of 14 days) to mimic a worse-case scenario in which the samples had to be shipped and stored for an extended period prior to the solid phase extractions.

Following the 14-day holding period, the experimental samples were processed, spiked with isotopes, and extracted. All of the samples, including the T_0 control, were then analyzed with liquid chromatography/tandem mass spectrometry (LC-MS/MS) with isotope dilution (see TOrC analysis section). Table B-2 provides the target compound concentrations in the primary clarifier influent, mixed liquor, and secondary clarifier effluent, respectively, at the end of the holding study. Notable differences between the T_0 and experimental sample concentrations are indicated by blue (30% higher than T_0) or yellow (30% lower than T_0) highlighting. The sorption and biotransformation columns also illustrate which compounds are susceptible/resistant to these mechanisms, thereby providing potential explanations for the notable differences.

Table B-1. Experimental Conditions for Holding Study.

Wastewater matrix	Preservative	Storage temperature
Primary Clarifier Influent	0 g/L NaN_3	4ºC for 3 days, 4ºC for 11 days
	0 g/L NaN_3	20ºC for 3 days, 4ºC for 11 days
	1 g/L NaN_3	4ºC for 3 days, 4ºC for 11 days
	1 g/L NaN_3	20ºC for 3 days, 4ºC for 11 days
Mixed Liquor	0 g/L NaN_3	4ºC for 3 days, 4ºC for 11 days
	0 g/L NaN_3	20ºC for 3 days, 4ºC for 11 days
	1 g/L NaN_3	4ºC for 3 days, 4ºC for 11 days
	1 g/L NaN_3	20ºC for 3 days, 4ºC for 11 days
Secondary Clarifier Effluent	0 g/L NaN_3	4ºC for 3 days, 4ºC for 11 days
	0 g/L NaN_3	20ºC for 3 days, 4ºC for 11 days
	1 g/L NaN_3	4ºC for 3 days, 4ºC for 11 days
	1 g/L NaN_3	20ºC for 3 days, 4ºC for 11 days

For the primary clarifier influent, caffeine was the only compound for which the concentration of the preserved 4ºC sample was 30% less than the T_0 control. For the high-sorption/high-biotransformation compounds, only the 20ºC bisphenol A samples differed by more than 30%. Since the 20ºC bisphenol A sample containing preservative showed a significant difference but the 20ºC sample without preservative did not, the deviation can likely be attributed to sorption rather than biotransformation. Sorption also appears to be the dominant mechanism since most of the 30% deviations were linked to compounds with high sorption potentials. In fact, the greatest number of deviations occurred in the high-sorption/low-biotransformation category. Caffeine and acetaminophen (high-biotransformation) were the only low-sorption compounds to demonstrate a significant deviation. However, the acetaminophen outlier did not contain preservative and was held at 20ºC for the initial three-day "sampling" period. All of the low-sorption/low-biotransformation compounds satisfied the 30% requirement.

There were a number of fully preserved (i.e., 4ºC with 1 g/L of NaN_3) mixed liquor samples with notable deviations from the T_0 control. However, all of the 30% deviations for the fully preserved samples were linked to high-sorption compounds and most were linked to high-sorption/low-biotransformation compounds. Therefore, despite the high biological activity in the mixed liquor samples prior to preservation, the significant deviations appear to be dominated by sorption. Four low-sorption/high-biotransformation compounds had concentrations that were 30% lower than the T_0 control, but they were unpreserved samples in all cases. These compounds may have been affected by a combination of sorption and biotransformation, but at both temperatures, the preservative was sufficient to prevent significant biotransformation of these compounds. The low-sorption/low-biotransformation compounds all satisfied the 30% benchmark.

Table B-2. Holding Study Results for Three Wastewater Matrices.

				Primary influent					Mixed liquor					Secondary effluent				
					4ºC		20ºC			4ºC		20ºC				4ºC		20ºC	
Compound	Sorp.	Bio.	Spike ng/L	T_0 ng/L	w/o ng/L	w ng/L	w/o ng/L	w ng/L	T_0 ng/L	w/o ng/L	w ng/L	w/o ng/L	w ng/L	T_0 ng/L	w/o ng/L	w ng/L	w/o ng/L	w ng/L
Cimetidine				1770	1790	2190	1930	2020	967	1260	1480	1270	1810	997	1100	1210	1040	1340
BHA				1170	1270	1180	1460	1310	699	495	474	459	558	931	979	963	857	1010
Bisphenol A				2230	1530	1720	1880	1500	1430	335	402	743	751	2060	1410	1670	1070	2070
Benzophenone				6580	5950	5960	5700	5660	3990	2470	2240	2630	2510	5580	5890	5760	3930	5240
Trimethoprim				2020	1930	1980	1650	1920	815	355	707	150	749	1090	1070	1090	1020	1220
Fluoxetine				427	255	376	239	344	243	61.1	85.9	7.84	109	1030	1050	1000	1090	1380
TCPP				7150	7780	8610	10300	6100	9130	4810	5550	5230	5950	9460	8590	13300	12500	1100
Diphenhydrami				2920	3170	3670	2780	3470	923	539	770	166	856	1120	1200	1170	1090	1320
Musk Ketone				1860	1230	1670	356	994	933	<RL	468	<RL	<RL	4160	4370	5280	4910	3570
Triclocarbon				614	297	476	247	206	167	<RL	<RL	<RL	74	936	886	720	387	1050
Triclosan				1890	1500	1590	1860	1380	106	47.5	71.4	50.1	88.3	857	877	1050	379	1550
Sulfamethoxaz				2810	4150	3620	3790	4020	2040	1780	3100	1230	3330	2260	2450	2820	1910	3320
Atenolol				3990	4460	4150	4050	4130	1330	788	1030	615	1200	1470	1470	1520	1410	1650
Caffeine				17200	95000	98600	85800	103000	772	323	580	225	556	1300	876	1090	389	1270
DEET				1190	1250	1220	1150	1170	1130	1020	1080	1010	1180	1100	1150	1120	1220	1270
Gemfibrozil				6510	5710	5730	5410	5520	874	717	838	786	961	995	1050	969	625	1020
Naproxen				24000	24600	22600	23800	23000	975	753	1220	1100	1320	947	716	947	524	1040
Ibuprofen				30200	28300	27200	27900	27200	723	760	1510	1240	1650	1040	638	1020	525	1180
Acetaminophen				33900	289000	274000	185000	249000	1150	295	947	493	825	1940	840	2020	162	2200
Iopromide				925	1140	923	1020	948	979	931	900	797	903	1030	832	961	1280	1050
Meprobamate				2530	2640	2720	2950	2670	1620	1320	1640	1310	1760	1580	1680	1630	1580	1790
Primidone				1310	1330	1260	1160	1160	1120	1030	1080	1020	1110	1040	1160	1200	1180	1290
Carbamazepin				1290	1210	1150	1090	1220	1190	1020	1120	1020	1120	1190	1190	1230	1240	1270
TCEP				4440	4330	4270	4160	4030	4480	3770	4220	3590	4470	4690	4730	4740	5110	4980
Sucralose				38100	35900	42300	36300	41200	31200	32100	29000	28300	33400	31400	32500	31900	34100	3510

"W/o" indicates samples with no preservative, and "w" indicates samples with 1 g/L NaN_3. Blue shading indicates that a concentration was 30% higher than the corresponding T_0 concentration. Yellow shading indicates that a concentration was 30% lower than the corresponding T_0 concentration. Green shading indicates compounds with low sorption or biotransformation potentials, whereas red shading indicates compounds with high sorption or biotransformation potentials.

In contrast to the primary influent and mixed liquor samples, the only secondary effluent samples with concentrations that were 30% lower than the T_0 control were unpreserved. For those compounds with significant deviations, the unpreserved 20ºC samples always had lower concentrations than the unpreserved 4ºC samples. Furthermore, a majority of the deviations occurred for low-sorption/high-biotransformation compounds. These observations indicate that biotransformation may have been the dominant mechanism in the secondary effluent matrix. However, the preservative was sufficient for reducing biotransformation at both temperatures and for all of the target compounds. Once again, the low-sorption/low-biotransformation compounds all satisfied the 30% benchmark.

Throughout the experiment, there were also several compounds with concentrations that were 30% higher than the T_0 control (e.g., cimetidine, fluoxetine, TCPP, triclosan, sulfamethoxazole, naproxen, and ibuprofen). For some of these compounds, the increases were consistent for each of the matrices and experimental samples, thereby indicating that some degree of desorption was occurring during the holding time. However, it is unclear whether this desorption is related to the ambient or spiked concentrations of the target compounds. It is possible that the spiked compounds in the T_0 control quickly adsorbed to the solids in each matrix and were subsequently filtered out prior to the solid phase extraction.

With the exception of caffeine, which is highly amenable to biotransformation, the data suggested that the proposed preservation protocol (i.e., 1 g/L of NaN_3 with sampling and storage at 4ºC) was sufficient for the full-scale sampling phase. Most of the significant deviations for the fully preserved samples were connected to high-sorption compounds in a high-solids matrix (i.e., mixed liquor) and this was addressed with the Accelerated Solvent Extraction (ASE) protocol for solids. The holding study also assessed a worse-case scenario in which the time from sampling to extraction was 14 days. This holding study indicates that the full-scale samples will not experience significant biotransformation assuming the samples are collected, preserved, shipped, and processed according to the proposed protocols.

B.2 Sampling Protocols

A sampling protocol was customized for each facility to guide the full-scale field sampling campaigns. Along with the sample bottle shipment a Sample Information Sheet was included that contained Chain of Custody information for the samples. The Sample Inventory Sheet defined each sample to be collected, exact location of each same, type of sample (composite or grab), all water quality parameters to be collected by the respective utility, and lab location to which the sample should be shipped for analysis. The general content of the sampling protocols is provided in the following.

Sampling Protocol for WERF Project CEC4R08
Liquid Stream Sampling
Trace Organic Compound Removal during Wastewater Treatment – Categorizing Wastewater Treatment Processes by their Efficacy in Reduction of a Suite of Indicator TOrCs

Site: [x]
Sampling Event: [x]

Shipments

1. You will receive the following shipments with sampling bottles.
    - The shipment from [*institution*] will contain the 1-Liter pre-cleaned, pre-labeled amber glass sampling bottles that contain preservatives (sodium azide and ascorbic acid for chlorine quenching). 72-hour composite samples from [*number*] locations in the treatment process will be transferred into these 1-Liter bottles prior to shipping for Trace Organic analysis by [*institution*]. The grab sample of [*sample locations*], will be directly sampled into the dedicated 1-Liter sampling bottles. The shipment from [*institution*] includes [*number*] 1-L bottles filled with DI water for [*rinse and field blank*] and 1 gallon container filled with DI water for the [*equipment blank sample*]. This water should be processed as described in these instructions.
      As requested, two unlabeled sample bottles have been added to the shipment in case of breakage.
    - The shipment from [*institution*] will contain
        a) Small bottles containing preservatives for composite sample collection. [*number*] 5-gallon sampling containers are to be used for collecting 72-hour composite samples with time or flow based autosamplers. [*number*] of the 5-gallon sampling containers is to be used for generating a Rinse Blank as described in these instructions.
        The containers are to be stored in the dark to avoid light penetration and the bottle mouth should be covered with parafilm during sampling. The small bottles containing preservatives are dedicated for each 5-gallon sampling container. MSDS datasheets for the preservatives are included in shipments. Avoid inhalation or direct contact with the preservative when in powder form! The correct amounts of preservatives are already filled into the small sample vials. (The 5-gallon container dedicated for the rinse blank will receive less preservative than the other bottles (about 1-2 g).)
        b) Two smaller sized bottles should be filled with (a split of) the RAS grab sample to be send back to [*institution*] for TSS analysis.
    - Return shipment labels and Chain of Custody forms are included in each shipment.

Sampling Preparations

1. Place all ice packs (for shipping purposes) in freezer upon arrival.
2. Sampling should start on [*Date*], a Monday morning and continue through Thursday morning [*Date*]. Samples to be shipped for ToRC analysis should then be refrigerated over the weekend and shipped out the following Monday [*Date*] to arrive by Tuesday next day at the receiving lab. Make sure the samples do not freeze as this can lead to

bottle breakage. The [*RAS*] sample should be collected on the last day of the 72-h sample collection [*Date*] and needs to be stored on site refrigerated to be shipped out with other TOrC samples on the following Monday to [*institution*]. A split sample of [*RAS*] should be sampled and filled in the two smaller bottles provided by [*institution*]. Ship ASAP to [*institution*] on same day [*Date*] per overnight delivery.

3. If possible, refrigerate composite sampling containers to 4ºC during the entire 72 hours of sample collection. Where refrigeration is not possible, place ice, or ice packs around sampling containers in composite sampler shacks prior to sampling. Replace ice/ice packs periodically during the 72-hour collection period to keep the sample cooled for the entire sampling period.
4. Collect 72-hour, time-based composite samples in the dedicated 5-gallon glass containers as indicated on the Sample Inventory Sheet. The preservatives from the smaller bottles should be transferred to each 5-gallon glass container immediately prior to sampling. The personnel handling the preservative should be familiar with the accompanying MSDS datasheets. Avoid inhalation or direct contact with the preservative when in powder form! Please use the dedicated preservative bottle labeled "[*RB*]" for the container receiving the rinse blank as the mass contained for it is lower. The 5-gallon sampling containers are pre-cleaned and should not be pre-rinsed.
5. If the composite samplers used for sampling need to be borrowed from another location or purpose (e.g., from pre-industry monitoring programs), possible sources of trace organic contamination must be avoided by cleaning the equipment that will be in contact with the sample (e.g., tubing). We ask that new tubing is rinsed for about 1 week with tap water. Please collect after this rinse the equipment blank as described below. The autosamplers with pre-rinsed tubing should then be hooked up to the actual sample location and be exposed to the actual sample for 1 week prior to sample collection. If plastic tubing is used, well-conditioned tubing is preferred as opposed to brand new tubing where leaching potential of plasticizers (i.e., Bisphenol A) is higher or sorption of TOrC to the tubing can occur if instructions for tubing conditioning as described above are not followed. If the autosamplers used are permanent samplers and dedicated to the specific sampling location they are acclimated to the sample water to be collected, and the equipment does not need to be cleaned or conditioned.

Sampling

1. Refer to the Sample Inventory Sheet for sampling locations and types of samples to be collected.
2. All personnel handling samples and containers need to wear nitrile gloves at all times and avoid touching or breathing on the samples. Also, people collecting or handling samples need to avoid the use of sunscreen, lotion, perfume, cologne, DEET, and antimicrobial soaps before and during sampling. Samples are prone to contamination due to trace concentrations of compounds.
3. Collect 72-hour, time-weighted composite samples from locations [*sample locations*], as indicated on the Sample Inventory Sheet. To avoid the loss of preservatives from the 5-gallon sampling containers, do not rinse and avoid overfilling any sample containers. Adjust the flow to the containers during sampling collection to collect at least 8-10 L during the 72-hour period but avoid overfilling the containers.
4. Equipment Blank: Since new tubing will be used for this sampling campaign, we will add an equipment blank to this sample site. Please follow the instructions above for tubing

conditioning. After the new tubing has been rinsed for about a week with tap water, please process the DI water shipped in a 1 gallon container labeled "[*bottle label*]" through one of the autosamplers equipped with the new tubing. Discard the first 2 Liters and collect the following 1 Liter in the sample bottle labeled "[*bottle label]*". Avoid overfilling the bottle as it contains the preservative. Cap and seal with no headspace. Then continue to hook up the autosampler to the actual sample location at least a week prior to the sample event to condition the tubing to the sample matrix to be collected.

5. Rinse Blank: Place the 5-gallon container labeled "Rinse Blank" next to the sample container in the Secondary Effluent composite sampler and fill with dedicated preservative and the 1 L DI water contained in sample bottle labeled "[*bottle label]*". Leave the "Rinse Blank" container next to Secondary Effluent sampling container for the complete duration of the 72-hour sampling period and cool with ice. Process the content of this container as all other composite samples and as described in "Sample Handling and Shipment" when sampling period is completed.
6. The preservatives interfere with certain analyses that your facility may be required to conduct as part of monitoring and reporting requirements (e.g., nitrate, BOD, DOC, TOC). If such parameter testing is required for the composite location sampled, a parallel sampling connection needs to be temporarily installed that allows a parallel sample collection for routine monitoring in a container in parallel to the 5-gallon container containing the preservative. Please refer to the Sample Information Sheet (will be included with shipment) and Sample Inventory Sheet for sample parameters needed for this project that should be analyzed for by the utility and be submitted to the project team.
7. [*Sample locations*] are the only samples for TOrC analysis that will not be collected with a composite sampler. All [*number*] samples can be collected as grab samples directly into the 1-L sampling bottles. RAS samples should be collected on the last day of the 72-h sample collection [*Date*] and need to be stored on site refrigerated to be shipped out with other TOrC samples on the following Monday. Collect a RAS sample at the same time and location in the smaller bottles provided by [*institution*] and ship to [*institution*] same day overnight. Cool the sample until and during shipment.
   Transferring samples from the 5-gallon sampling containers into the 1-L sampling bottles using secondary sampling containers or other equipment (e.g., funnels) should be avoided to minimize the risk for sample contamination. Fill the 1-L bottles as close to the top as possible, slightly overflowing the bottles to avoid headspace. Avoid overflowing the bottles heavily as the preservative in the bottles may be lost. The bottles should not be rinsed!

Sample Handling and Shipment

1. Immediately after sample collection, mix each composite sample thoroughly and distribute to the appropriate 1-L glass sample bottles (see Sample Inventory Sheet for number of samples required and sample labeling conventions for the sampling site). Sample transfers from the 5-gallon containers into the 1-L sample bottles can be made in the field or in the laboratory. If possible, avoid the use of funnels or other equipment that may contaminate the samples. If a funnel is necessary to transfer the samples the funnel needs to be cleaned followed by three rinses with methanol before use for a different sample location. Fill the 1-L bottles as close to the top as possible, slightly overflowing the bottles to avoid headspace. Avoid overflowing the bottles heavily as the preservative in the bottles may be lost. The bottles should not be rinsed!

2. Please follow the labeling instructions provided for your field site to assure that samples match all sample bottle labels. (The samples will be distributed into several bottles to allow for analytical repetitions. This will be indicated on the Sample Inventory Sheet for each field site.)
3. Field Blank: One field blank will be provided for each sampling event. Please transfer the water provided into the field blank sample bottle at the same location and at the same time that composite bottles are transferred into 1-L sampling bottles.
4. Rinse Blank: Transfer the rinse blank from the 5-gal sample container into the dedicated 1-L sample bottle at the same location and time that composite bottles are transferred into 1-L sampling bottles.
5. Make sure all caps are tightly closed.
6. Immediately after sampling, conduct all parameter testing and analysis for each composite / grab sample collected as indicated on the Sample Inventory Sheet. Record the results and analytical methods used and send to: [*Contact*]
7. Fill out the Sample Information Sheet.

Shipping Trace Organic Samples

1. After transferring composite samples, place all 1-Liter sample bottles in refrigerator at ≤4°C. Cool samples prior to shipping until following Monday.
2. When ready to ship, place 1 Liter sample bottles into blue coolers between foam and include ice packs.
3. Make sure the Sample Information Sheet is filled out. Be sure to double-check sample ID, name, and sampling dates.
4. Make a copy of the Sample Information Sheet for yourself.
5. Finally, place the Sample Information Sheet into a plastic bag and inside the cooler.
6. Place the cooler lid on and close the cooler box and shake it gently to verify that the bottles cannot move.
7. Seal the cooler with packing tape.
8. Ship coolers Priority 10AM Next Day delivery on the following Monday using the return labels provided with the initial shipments. The samples must arrive at the [*Institution*] laboratory by Tuesday. Please insure cases for a minimum of [*$ amount*] in case of loss or damage due to shipper and note no signature needed upon arrival. Send to:

   [*Contact*]

9. Send confirmation e-mail/tracking number to [*Contact*].

B.3 TOrC Analysis

B.3.1 Standards and Reagents

Certified standard solutions for each target compound were purchased commercially along with corresponding isotopically-labeled versions (Table B-3). Trace analysis grade methanol was obtained from Burdick and Jackson (Muskegon, MI). Methyl-t-butyl ether (MTBE) was purchased from EM Science (Gibbstown, NJ) and ammonium acetate was obtained from J.T. Baker (Phillipsburg, NJ).

B.3.2 Solid-Phase Extraction

Solid phase extraction protocols were based on work by Vanderford and Snyder 2006. Analytes were extracted from aqueous samples in batches of six using 6 mL, 200 mg hydrophilic-lipophilic balance (HLB) cartridges from Waters Corporation (Millford, MA). Extractions were performed on an AutoTrace™ automated SPE system (Dionex Corporation, Sunnyvale, CA). The SPE cartridges were sequentially preconditioned with 5 mL of MTBE, 5 mL of methanol, and 5 mL of reagent water. As dictated by sample matrix and projected analyte concentration levels, sample aliquots of 500 mL, 50 mL or 5 mL (diluted to 50 mL in reagent water) were spiked with a solution of isotopically labeled standards that contained a stable isotope of each analyte, then loaded onto the cartridges at 15 mL/min. Cartridges were then rinsed with 5 mL of reagent water and subsequently dried under a nitrogen stream for 30 min. Each cartridge was then eluted with 5 mL methanol followed by 5mL of 10/90 (v/v) methanol/MTBE, and both fractions collected in a single 15 mL calibrated centrifuge tube. The resulting extract was concentrated with a gentle stream of nitrogen to volume just below 500 µL, then brought to a final volume of 500 µL using methanol.

Analyte concentrations, in specific instances, exceeded calibration ranges and prevented practical dilution of isotopically labeled standards in extracts from 5 mL sample volumes. In such cases, solid-phase extraction was not conducted. Rather, isotopically labeled standards were spiked directly into 1:2 reagent water dilutions of sample prior to analysis. Sample aliquots were extracted and analyzed as separate samples; however, best-available results were reported for each analyte in a sample. In each case, reporting limits for individual analytes were adjusted to account for concentration and dilution factors.

B.3.3 Return Activated Sludge Samples

All return activated sludge (RAS) samples were prepared in triplicate to account for heterogeneity in the solids sampled. The RAS samples were shaken vigorously to disperse any solids that had settled during shipping and storage. An aliquot was poured into a glass beaker and stirred using stir-plate in order to prevent settling of the solids. 10 mL of this solution was then filtered using a 1 µm glass fiber filter and a vacuum filter apparatus. The solids remained on the vacuum filter apparatus for a minimum of 30 minutes in order to remove residual liquid.

Filtrate. A 5 mL portion of the resulting filtrate was diluted to 50 mL using laboratory reagent water and spiked with the internal standard solution. This solution was extracted using the solid phase extraction procedure employed for aqueous samples described previously.

Solids. Solid extraction was performed using a method based on work by Radjenovic et al., 2009. The accelerated solvent extraction (ASE) was performed on a Dionex 200 ASE unit. A 22 mL ASE cell was partially filled with 25-mesh Ottawa Sand (Fisher Scientific, Pittsburgh, PA), which had been previously baked at 400°C for 4 hours to help eliminate contamination.

The solids and glass fiber filter were transferred to the cell and spiked with the internal standard solution. The cell was then filled with sand, compacted, capped and loaded into the ASE apparatus. The extraction was performed using three cycles, 33% methanol/ water as the solvent, a temperature of 100°C and a pressure of 1500 psi. The preheating and static periods were set to 5 minutes, and the flush was set to 100%. The resulting extract (~35 mL) was diluted to 1 L with laboratory reagent water and subjected to the SPE method as described above, with the exception of using a 500 mg SPE cartridge in order to account for any effects from the methanol present.

B.3.4 Oher Solid-Containing Samples

In addition to RAS samples, other samples that contained a significant amount of suspended solids (e.g., primary influent) were also extracted according to the protocol discussed above for RAS.

B.3.5 Instrumental Analysis

An Agilent (Palo Alto, CA) G1312A binary pump and an HTC-PAL autosampler (CTC Analytics, Zwingen, Switzerland) were used for all analyses. All analytes were separated using a 100 X 4.6 mm Onyx Monolithic C18 column (Phenomenex, Torrance, CA). Chromatographic separation was accomplished using a binary gradient of 5mM ammonium acetate (v/v) in water (A) and 100% methanol (B) and a flow rate of 800 µL/min. The gradient range was 10% B to 100% over 12 min, with a 2 min equilibration step at 10% B. An injection volume of 10 µL was used for all analyses. Tandem mass spectrometry was performed using an API 4000 triple-quadrupole mass spectrometer (Applied Biosystems, Foster City, CA). The process of optimization of the mass spectrometer has been previously published (Vanderford, 2003). Briefly, analytes were grouped into negative electrospray ionization (ESI) or positive ESI based on sensitivity and selectivity for each compound. Once this was established, the optimal compound-dependent parameters were determined and source-dependent parameters optimized for each compound group. Data was collected in two separate acquisition periods for ESI negative mode and two acquisition periods for ESI positive to allow for a minimum acquisition time of 25 msec for each transition monitored (Table B-3).

Table B-3. Target Compound List and Analytical Method Parameters.

MS/MS acquisition period	Compound	Isotope dilution standard (Manufacturer)	Precursor ion	Product ion	Aqueous method reporting limit (ng/L)	Solids method reporting limit (ng/L)
Positive Electrospray Ionization						
1	Sulfamethoxazole	Sulfamethoxazole-d_4 (TRC)	254	156	0.25	Various
1	Atenolol	Atenolol-d_7 (CDN[a])	267	145	0.25	Various
1	Trimethoprim	Trimethoprim-d_9 (TRC)	291	261	0.25	Various
1	Iopromide	Iopromide-d_3 (IsoSciences[b])	792	573	10	Various
1	Caffeine	Caffeine- d_9 (CDN)	195	138	5.0	Various
1	Meprobamate	Meprobamate-d_3 (TRC[c])	219	158	0.25	Various
1	Primidone	Primidone- d_5 (CDN)	219	162	0.50	Various
2	Fluoxetine	Fluoxetine-d_5 (CDN)	310	44	0.50	Various
2	Carbamazepine	Carbamazepine-d_{10} (CDN)	237	165	0.50	Various
2	Benzophenone	Benzophenone-d_{10} (CDN)	183	105	0.50	Various
2	TCPP	* TCEP- d_{12} (Isotec)	327	99	100	Various
2	DEET	DEET- d_6 (CDN)	192	119	1.0	Various
2	TCEP	TCEP- d_{12} (Isotec[d])	285	99	10	Various
2	Diphenhydramine (HCl)	Diphenhydramine-d_5 (CDN)	256	167	0.50	Various
Negative Electrospray Ionization						
1	Acetaminophen	Acetaminophen-d_4 (CDN)	150	107	5.0	Various
1	Cimetidine	Cimetidine-d_3 (CDN)	251	157	2.0	Various
1	Sucralose	Sucralose-d_6 (CDN)	395	35	25	Various
1	Naproxen	Naproxen-d_3 (CDN)	229	169	0.50	Various
1	Bisphenol A	Bisphenol A-d_{16} (CIL[e])	227	212	5.0	Various
1	Ibuprofen	Ibuprofen- d_3 (CDN)	205	161	1.0	Various
1	BHA	BHA- d_3 (Isotec)	179	164	1.0	Various
2	Gemfibrozil	Gemfibrozil-d_6 (TRC)	249	121	0.25	Various
2	Musk Ketone	Musk Ketone-d_9 (CIL)	293	251	25	Various
2	Triclocarban	Triclocarban-d_4 (CDN)	313	160	2.0	Various
2	Triclosan	Triclosan-d_3 (CDN)	287	35	1.0	Various

B.4 Quality Control

While an extensive quality control plan is advisable for any environmental analysis method, it is especially critical for the analysis of TOrCs due to the lack of standardized methods.

B.5 Calibration

An isotopically labeled version of each analyte, corresponding to the isotopes added to each sample prior to extraction, was added to each calibration point to generate a relative response ratio. Recoveries of the isotopes were compared with the relative response ratio and a concentration of the unlabeled analyte was calculated. The only exception was TCPP, which was calibrated externally. Linear or quadratic regression with 1/x weighting was used and regression coefficients typically exceeded 0.995. Calibration curve verifications were analyzed at least every six samples and were generally between 80% and 120% of the expected concentration.

B.6 Method Detection and Reporting Limits

Aqueous method reporting limits (MRL) were based on method detection limits (MDL) calculated from 12 replicate measurements of deionized water samples fortified with analytes at their expected detection limits and extracted as previously described. The MDL was calculated by multiplying the standard deviation of the replicate measurements by the appropriate student's T value for n – 1 degrees of freedom. MRLs for each analyte were set at greater than three times the MDL (Table B-3). If the MDL fell below the level that was spiked by more than a factor of 10, the procedure was repeated at a lower level. If the MDL was above the level of the spike, the procedure was repeated at a higher concentration.

The MDL for solid samples was determined from the analysis of a least eight samples processed through the procedure described above. The samples consisted of filter paper spiked with analytes at levels approaching the predicted MDL and internal standards from a methanol solution. The spiked filter papers were handled in exactly the same manner as filtered solids throughout the rest of the process. The MDL was calculated in the manner of the aqueous MDLs.

The MRL of each analyte in the solids method was calculated by multiplying the MDL value by a minimum factor of 5. A second criterium applied was that the MRL for each analyte could not fall below the MRL used for the well-established liquid method. The MRLs employed for this method take into account background contamination issues from historical data and have additional factors applied for problematic compounds. The MRLs were then adjusted for each sample by dividing the MRL by the mass of the solids calculated to be present on the filter paper from TSS measurements performed on samples taken during the same sampling event. It should be noted that background contamination prevented a meaningful MRL from being established for DEET and pushed the MRL for trimethoprim to values significantly higher than that established in the liquid method.

B.7 Blanks

Twelve (12) field blanks were analyzed during the study to quantify the degree of contamination present during sampling. Of those, one had a detection of benzophenone at 99 ng/L (MRL = 50 ng/L), one had a detection of TCEP at 48 ng/L (MRL = 10 ng/L), two had detections for gemfibrozil at 0.98 and 1.1 ng/L (MRL = 0.25 ng/L), one had a detection of

naproxen at 1.9 ng/L (MRL = 0.50 ng/L), and one had a detection of ibuprofen at 1.1 ng/L (MRL = 1.0 ng/L). All of the detections were in separate field blanks with the exception of one of the gemfibrozil detections (1.1 ng/L) and the detection of naproxen (1.9 ng/L) which were detected in the same sample.

Twelve (12) rinse blanks were conducted to determine the degree of contamination introduced by the sampling equipment. Detections are shown in Table B-4. All other analytes were <MRL for all samples.

Table B-4. Summary of Rinse Blank Detections.

Analyte	# of detections in rinse blanks (n = 12)	Concentration range of detects (ng/L)
Atenolol	2	220 – 270
Benzophenone	8	53 – 480
Caffeine	3	10 – 68
DEET	7	1.5 – 20
Diphenhydramine	1	34
Fluoxetine	1	1.3
Gemfibrozil	1	0.98
Ibuprofen	5	1.3 – 8.1
Naproxen	5	1.1 – 11
TCEP	3	10 – 25
TCPP	1	100
Triclocarban	1	140
Triclosan	1	80

Laboratory deionized (DI) water blanks were also extracted alongside project samples quantify the degree of blank contamination during extraction and analysis. Thirty-three (33) DI blanks were analyzed during the project and the majority of analytes were not detected in any of the blanks. Exceptions to this are shown in Table B-5.

Table B-5. Summary of DI Blank Detections.

Analyte	# of detections in DI blanks (n = 33)	Concentration range of detects (ng/L)
Atenolol	2	1.7 – 4.0
Benzophenone	1	73
DEET	3	2.2 – 9.9
Diphenhydramine	1	0.55
Triclosan	1	1.3
Trimethoprim	1	1.5

In addition, blanks were performed on the ASE during solids extraction (Table B-6). Most compounds were not detected in the ASE blanks; however, four compounds showed varying degrees of blank contamination. Triclocarban was also found in five of the 12 blanks at levels between 4.7 and 58 ng/L.

Table B-6. Summary of ASE Blank Detections.

Analyte	# of detections in DI blanks (n = 12)	Concentration range of detects (ng/L)
Carbamazepine	1	3.3
Naproxen	1	2.0
TCEP	1	49
Triclocarban	5	4.7 – 58
Triclosan	1	4.7

B.8 Laboratory Fortified Blanks

A total of 27 laboratory fortified SPE blanks (LFBs-SPE) and 12 LFBs-ASE were extracted and analyzed to determine and monitor the accuracy of the analytical method without matrix interference. Results of the spiked samples are shown in Table B-7. All mean SPE recoveries were between 98-118% and %RSDs were all ≤ 12% with one exception (bisphenol A = 22%). ASE recoveries ranged from 88-112% and %RSDs were ≤ 15% with three exceptions (benzophenone = 27%, BHA = 36%, diphenhydramine = 18%).

Table B-7. Summary of LFBs.

Analyte	Mean % Recovery LFBs-SPE	%RSD LFBs-SPE	Mean % Recovery LFBs-ASE	%RSD LFBs-ASE
Sulfamethoxazole	112	3.5	111	3.9
Atenolol	111	5.0	112	5.2
Trimethoprim	108	3.5	110	4.9
Iopromide	110	12	112	8.3
Caffeine	110	4.5	110	5.7
Fluoxetine	99	6.7	96	10
Meprobamate	112	6.2	108	7.0
Carbamazepine	104	4.1	103	5.5
Benzophenone	98	5.7	106	27
Primidone	106	6.7	105	7.8
TCPP	98	9.7	113	10
DEET	118	3.4	N/A	N/A
TCEP	112	4.2	111	5.6
Gemfibrozil	105	5.4	105	8.2
Bisphenol A	112	22	102	8.5
Naproxen	111	4.7	109	8.5
Triclosan	107	11	108	9.7
BHA	103	7.0	88	36
Musk Ketone	106	10	102	15
Ibuprofen	110	6.6	108	8.0
Diphenhydramine	104	5.2	99	18
Cimetidine	100	7.3	99	8.5
Triclocarban	105	5.1	104	9.2
Acetaminophen	102	8.5	103	13
Sucralose	103	12	100	7.0

B.8.1 Laboratory Fortified Sample Matrices (LFSMs)

Twelve LFSMs were conducted over the course of the project to determine the accuracy of the method in the sample matrices and its susceptibility to matrix interferences. The following matrices were represented in the 12 LFSM samples: primary influent, aeration basin influent, centrate, mixed liquor, secondary effluent, and post-CaRRB basin. A summary of the LFSMs is presented in Table B-8.

Table B-8. Summary of LFSMs.

Analyte	Mean % Recovery	%RSD
Acetaminophen	112	10.9
Atenolol	102	10.7
Benzophenone	103	16.0
BHA	117	12.9
Bisphenol A	114	13.9
Caffeine	103	6.0
Carbamazepine	103	7.4
Cimetidine	110	16.4
DEET	125	13.1
Diphenhydramine	109	14.2
Fluoxetine	93	4.6
Gemfibrozil	102	11.8
Ibuprofen	105	10.3
Iopromide	94	23.7
Meprobamate	96	19.4
Musk Ketone	107	9.9
Naproxen	114	10.4
Primidone	108	13.8
Sucralose	104	11.7
Sulfamethoxazole	110	4.1
TCEP	111	5.3
TCPP	115	20.0
Triclocarban	107	10.0
Triclosan	111	8.2
Trimethoprim	108	8.4

B.8.2 Replicates

Overall, 30 sets of aqueous replicate samples (either duplicates or triplicates) were analyzed to assess and monitor analytical precision during extraction and analysis of aqueous matrices. Percent relative standard deviations (%RSDs) were calculated for each analyte on each set of duplicates/triplicates and the averages of those %RSDs are shown in Table B-9. For a given analyte, sample sets in which two or more samples were non-detect were not used in the calculation.

High degrees of precision were observed for most of the compounds. Musk ketone (16%), detected in only one sample set, was the only compound with an average %RSD > 15%; the remaining compounds had average %RSDs ≤ 10%. Solid replicates were also relatively precise with all analytes having %RSDs ≤ 17%, with one exception (caffeine = 49%).

Table B-9. Summary of Aqueous and Solid Replicates.

	Aqueous		Solid	
Analyte	Average %RSD	# of sets	Average %RSD	# of sets
Sulfamethoxazole	4.0	30	8.3	14
Atenolol	4.4	25	17	6
Trimethoprim	4.0	27	7.7	4
Iopromide	8.5	10	N/A	0
Caffeine	3.7	14	49	13
Fluoxetine	6.8	15	16	11
Meprobamate	4.6	30	9.7	4
Carbamazepine	7.1	30	14	10
Benzophenone	4.4	13	11	3
Primidone	7.6	22	N/A	0
TCPP	5.7	15	9.9	1
DEET	4.3	21	N/A	N/A
TCEP	2.8	15	N/A	0
Gemfibrozil	5.1	27	13	14
Bisphenol A	6.6	12	8.3	11
Naproxen	8.4	28	N/A	0
Triclosan	10	20	10	8
BHA	5.8	14	10	14
Musk Ketone	16	1	2.4	1
Ibuprofen	6.3	23	N/A	0
Diphenhydramine	5.4	30	9.5	10
Cimetidine	7.9	24	8.5	12
Triclocarban	7.9	19	15	14
Acetaminophen	7.9	9	N/A	0
Sucralose	6.5	30	13	3

N/A = not applicable

B.8.3 Data Reporting

Sample extracts with compound concentrations greater than the calibration range were diluted and reanalyzed. All reported aqueous values accounted for sample-specific dilution or concentration. The calculation of analyte concentration for the solid samples required that two factors be applied to the value obtained by the LC-MS/MS method. The first factor was applied to relate the obtained value to the mass of solids that were present on the filter paper at the beginning of the extraction. The second factor applied was a concentration factor needed to relate the final extract (0.5 mL methanol) to the calibration curve, which was in units of ng/mL. Therefore, the following calculation was used to convert the obtained values into final values in ng/g:

$$Final\ concentration\ \left(\frac{ng}{g}\right) = \frac{Measured\ value}{2 * solids\ mass\ (g)}$$

Due to contamination problems, meaningful MRLs were unable to be calculated for DEET and therefore it was not reported for solid samples.

APPENDIX C

WWTP PROCESS FLOW SCHEMATICS

C.1 Facility A

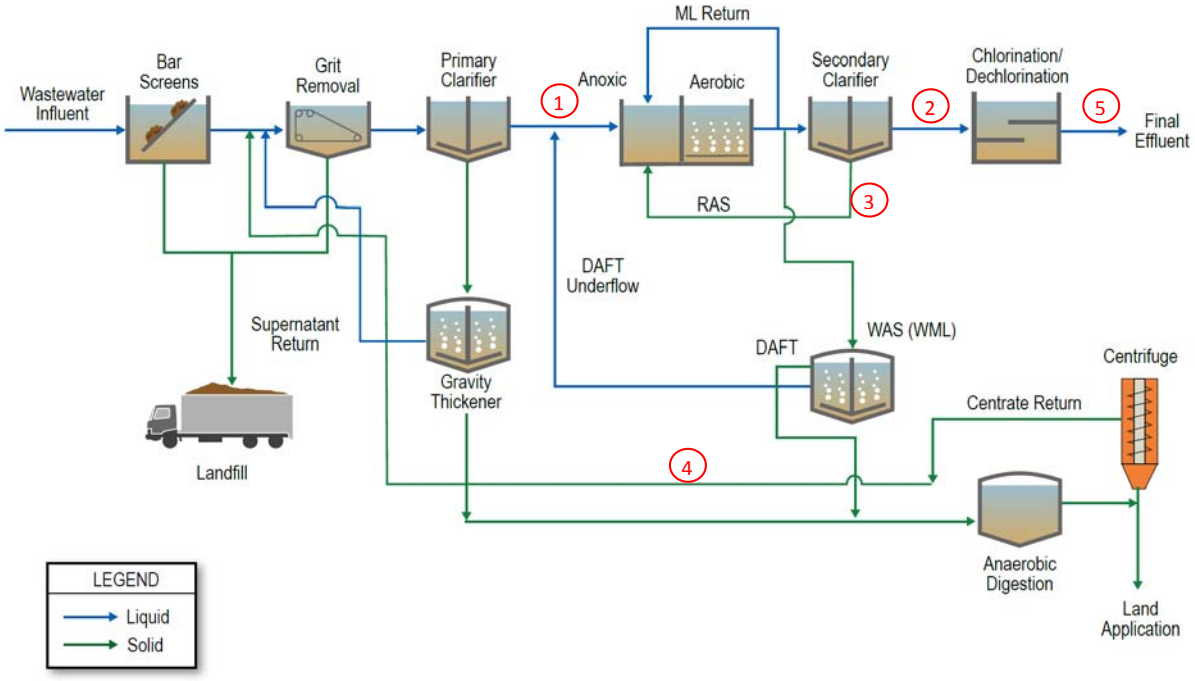


Figure C-1. Process Flow Schematic for Facility A.

Sampling locations for Facility A for TOrC mass balances around the secondary treatment:

1. Primary effluent including recycle streams (liquid) (composite)
2. Secondary clarifier effluent (liquid) (composite)
3. RAS (solid) (grab sample)
4. Centrate (liquid) (anaerobic digester return) (grab sample)
5. Final Plant Effluent after dechlorination (liquid) (composite)

C.2 Facility B

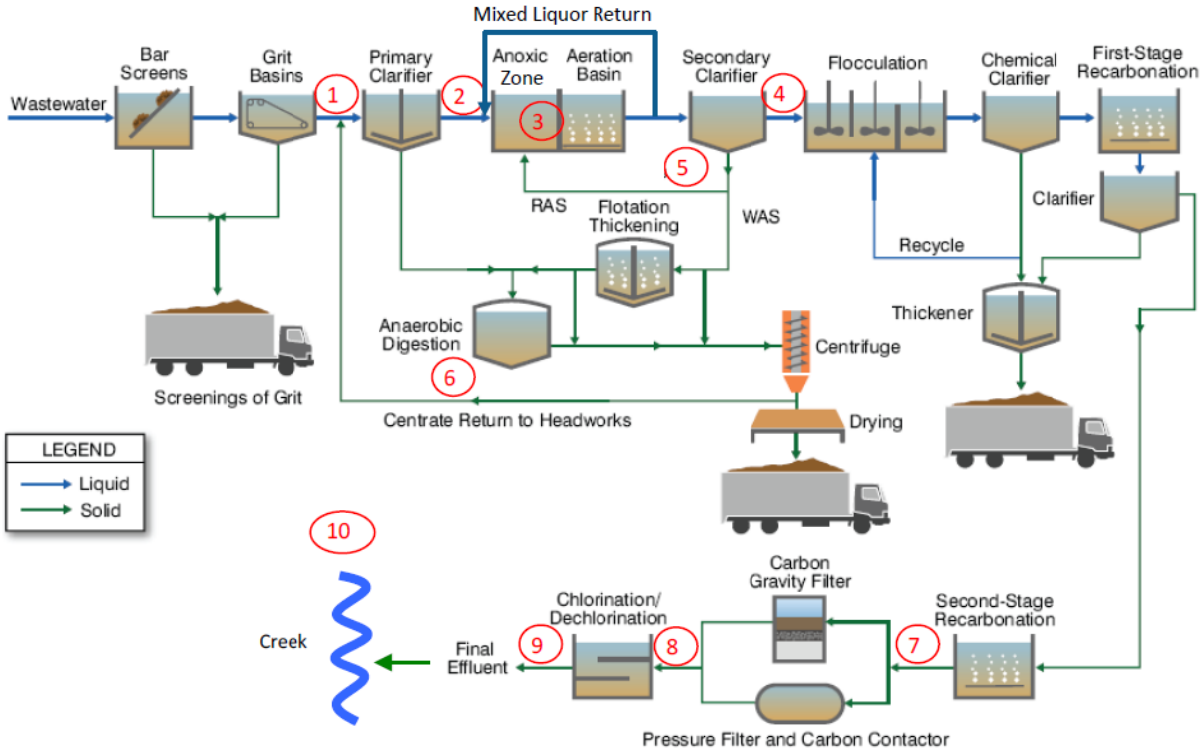


Figure C-2. Process Flow Schematic for Facility B.

Sampling locations for Facility B:

1. Primary Influent (liquid) (manual grab or short composite)
2. Primary effluent (liquid) (fixed auto sampler)
3. Anoxic zone effluent (liquid) (portable auto sampler) (sample only collected during denitrification operation in winter)
4. Secondary Clarifier Effluent (liquid) (fixed auto sampler)
5. RAS (solid) (manual grab or short composite)
6. Centrate (liquid)(manual grab or short composite)
7. Carbon Filter Influent (liquid) (funded by utility) (fixed auto sampler)
8. Carbon Filter Effluent (liquid) (funded by utility) (portable auto sampler)
9. Final Plant Effluent after dechlorination (fixed auto sampler or manual grab/short composite)
10. Creek upstream of discharge (funded by utility) (manual grab or short composite)

C.3 Facility C

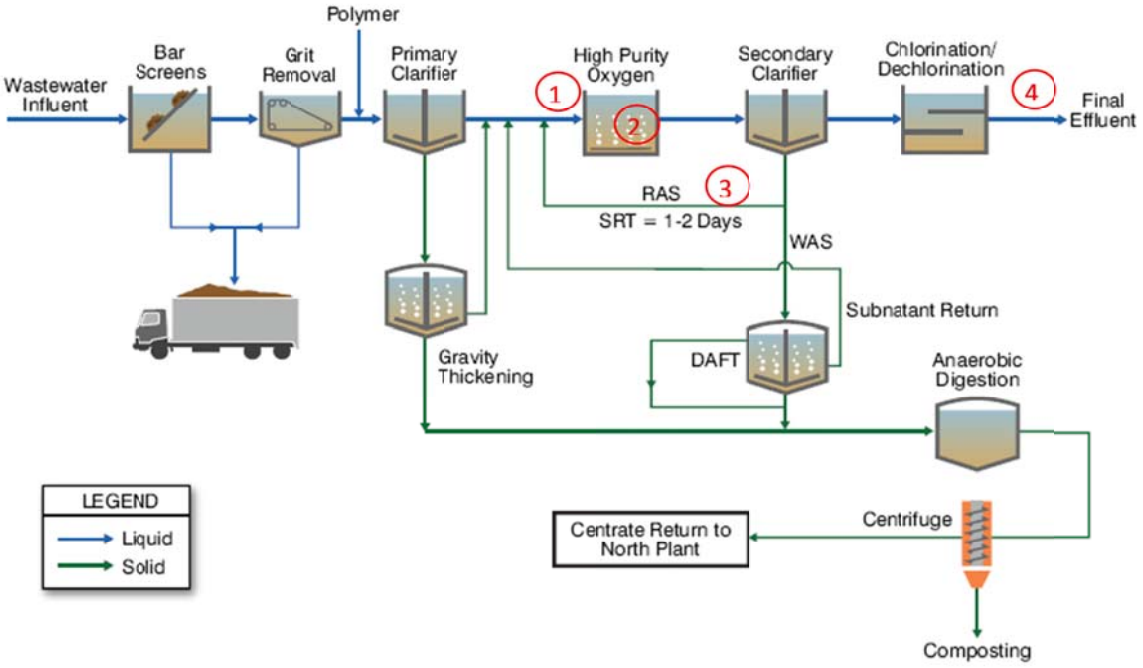


Figure C-3. Process Flow Schematic for Facility C.

Sampling locations for Facility C:

1. Secondary Influent (liquid) (fixed composite sampler)
2. Mixed liquor (liquid) *(*fixed composite sampler)
3. RAS (solid) *(*fixed composite sampler at either West or East side)
4. Final Effluent (fixed composite sampler)

C.4 Facility D

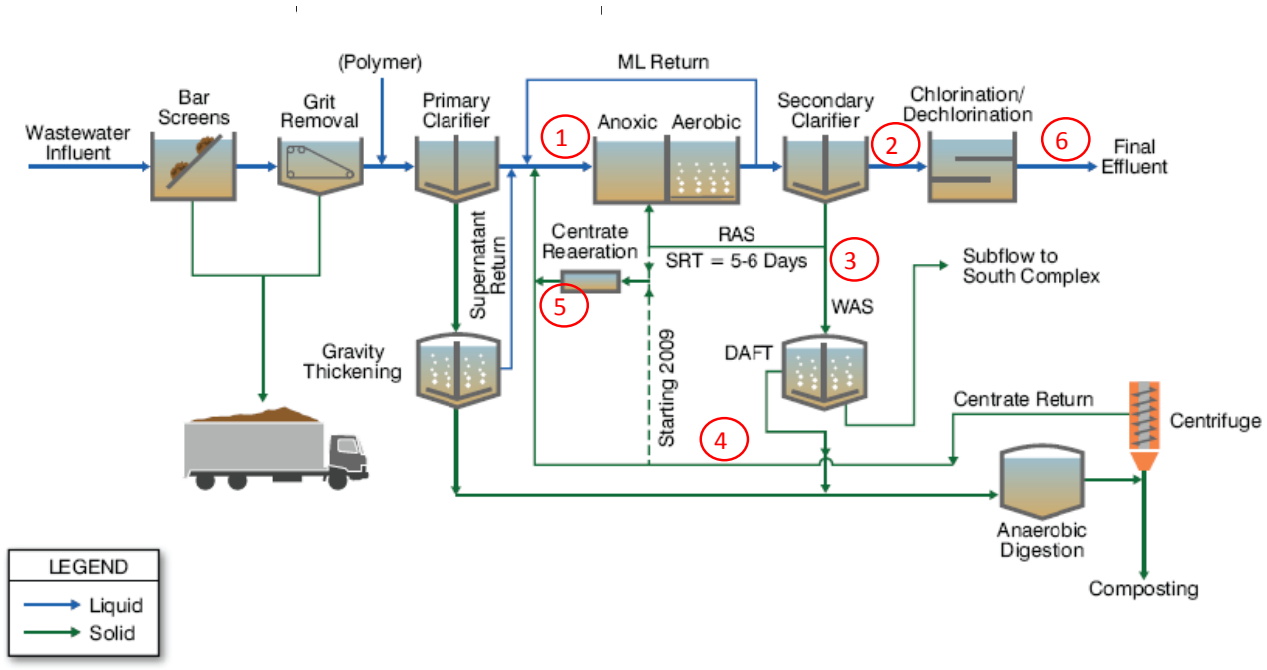


Figure C-4. Process Flow Schematic for Facility D.

Sampling locations for Facility D:

1. Secondary Influent (liquid) (fixed composite sampler)
2. Secondary Effluent (liquid) (fixed composite sampler)
3. RAS (solid) (fixed composite sampler at either West or East side)
4. Centrate (grab sample)
5. Post CaRRB Basins (fixed composite sampler)
6. Final Effluent (fixed composite sampler)

C.5 Facility E

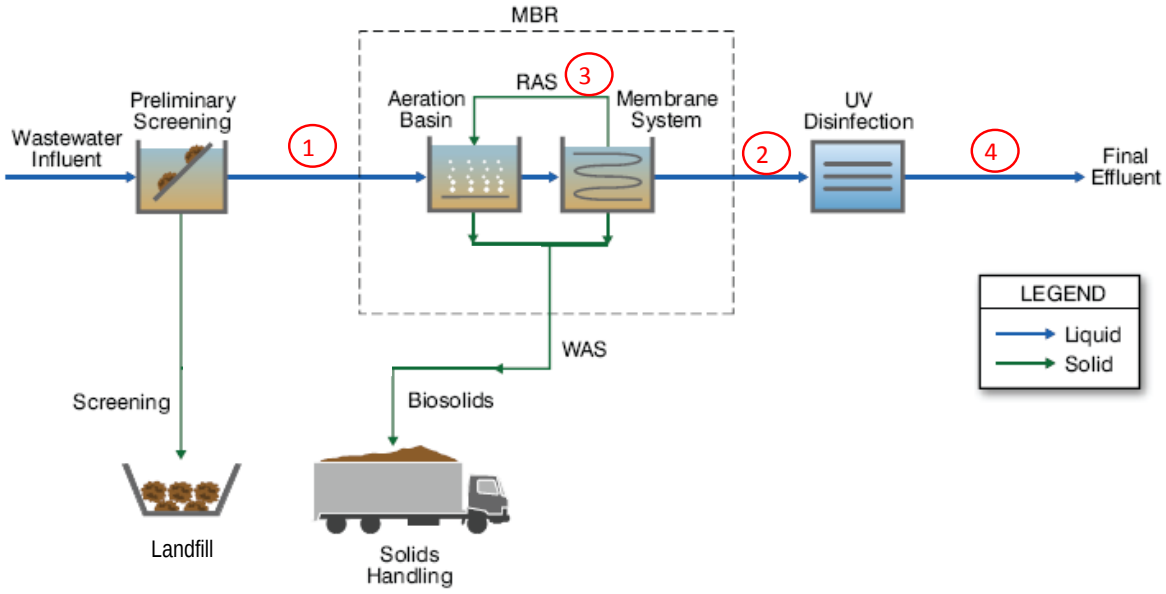


Figure C-5. Process Flow Schematic for Facility E.

Sampling locations for Facility E:

1. Aeration Basin Influent (liquid) (temporary composite sampler)
2. Membrane Effluent (liquid) (temporary composite sampler)
3. RAS (solid) (grab sample)
4. Final Plant Effluent after Disinfection (fixed composite sampler)

C.6 Facility F

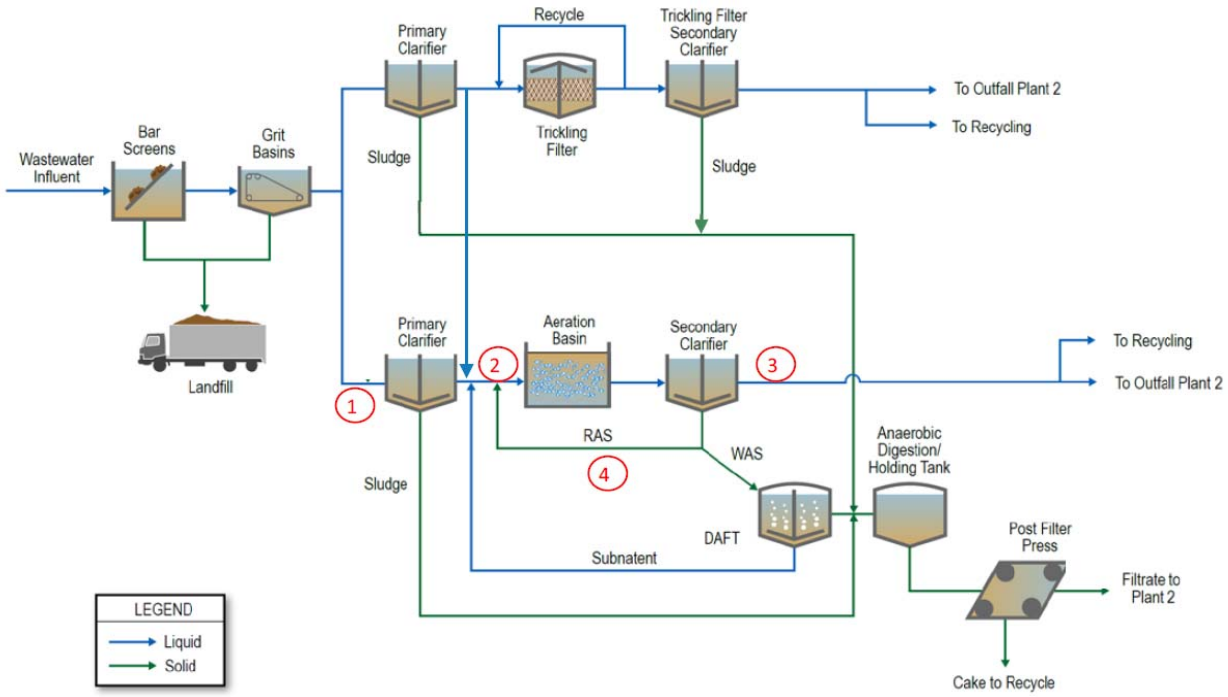


Figure C-6. Process Flow Schematic for Facility F.

Sampling locations for Facility F:

1. Primary Clarifier Influent after Recycle Streams (liquid)
2. Aeration Basin Influent after Recycle Streams (liquid)
3. Secondary Effluent (liquid)
4. RAS (solid)

C.7 Facility G

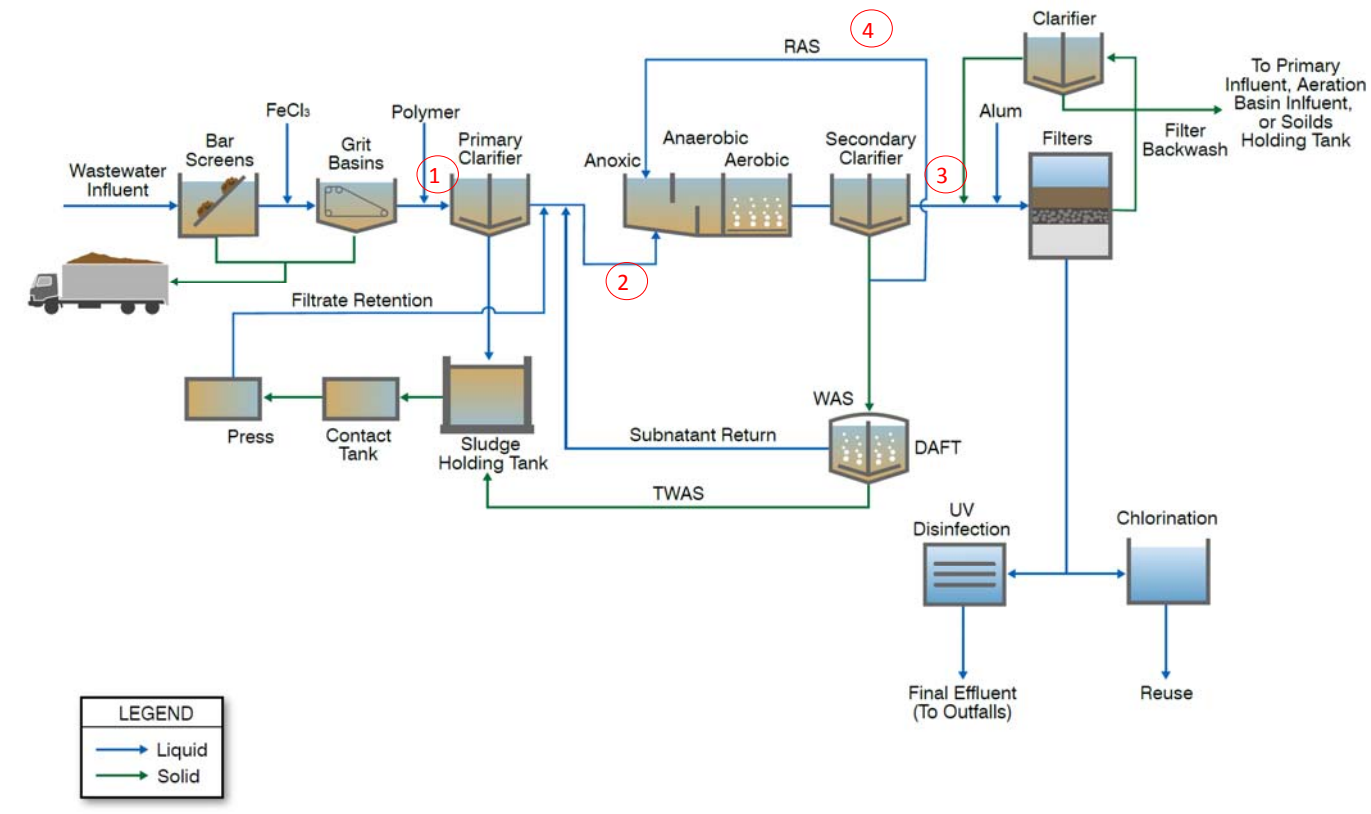


Figure C-7. Process Flow Schematic for Facility G.

Sampling locations for Facility G:

1. Primary Clarifier Influent
2. Aeration Basin Influent (liquid)
3. Secondary Effluent (liquid)
4. RAS (solid)

APPENDIX D

CONVENTIONAL WASTEWATER TREATMENT OVERVIEW DURING TORC SAMPLING

Note: Values provided in figures of this appendix are typically the averages of three 24-hour composite sample data points recorded by the utilities during the 72-hour sampling period.

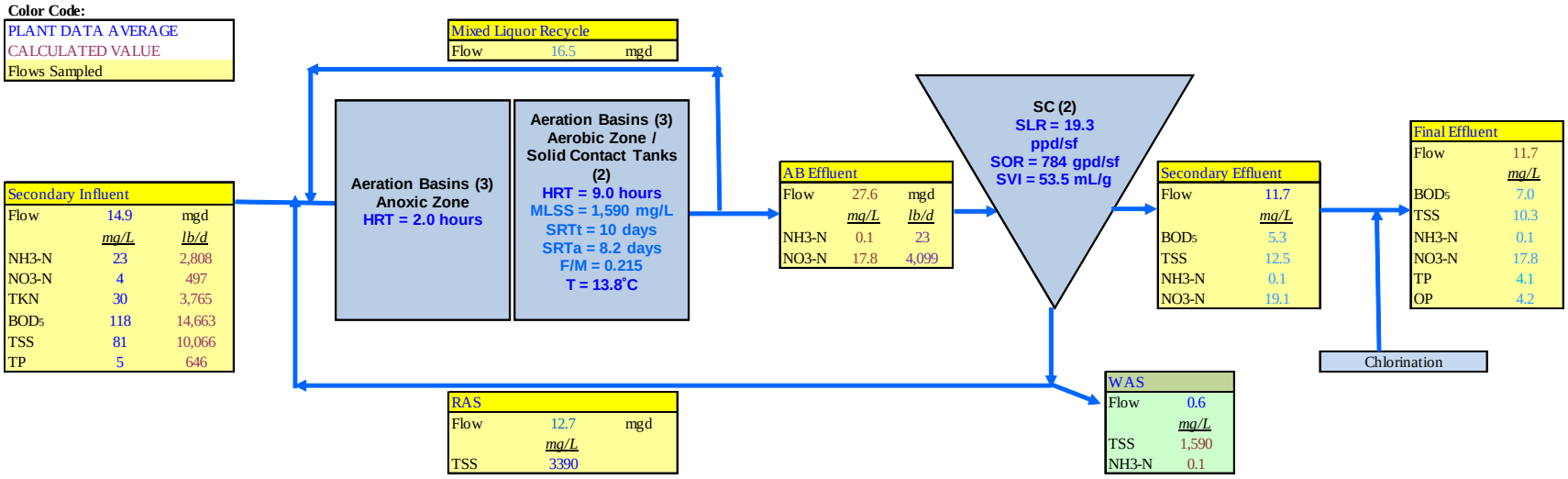


Figure D-1. Facility A (Winter): Conventional Wastewater Treatment Overview During TOrC Sampling Campaign.

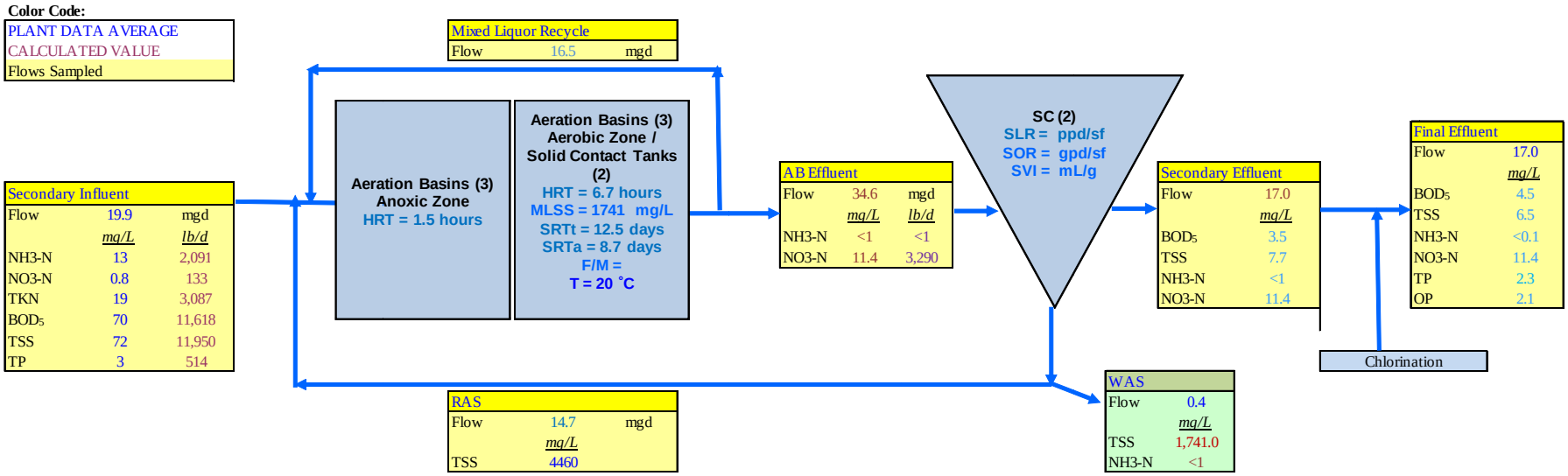
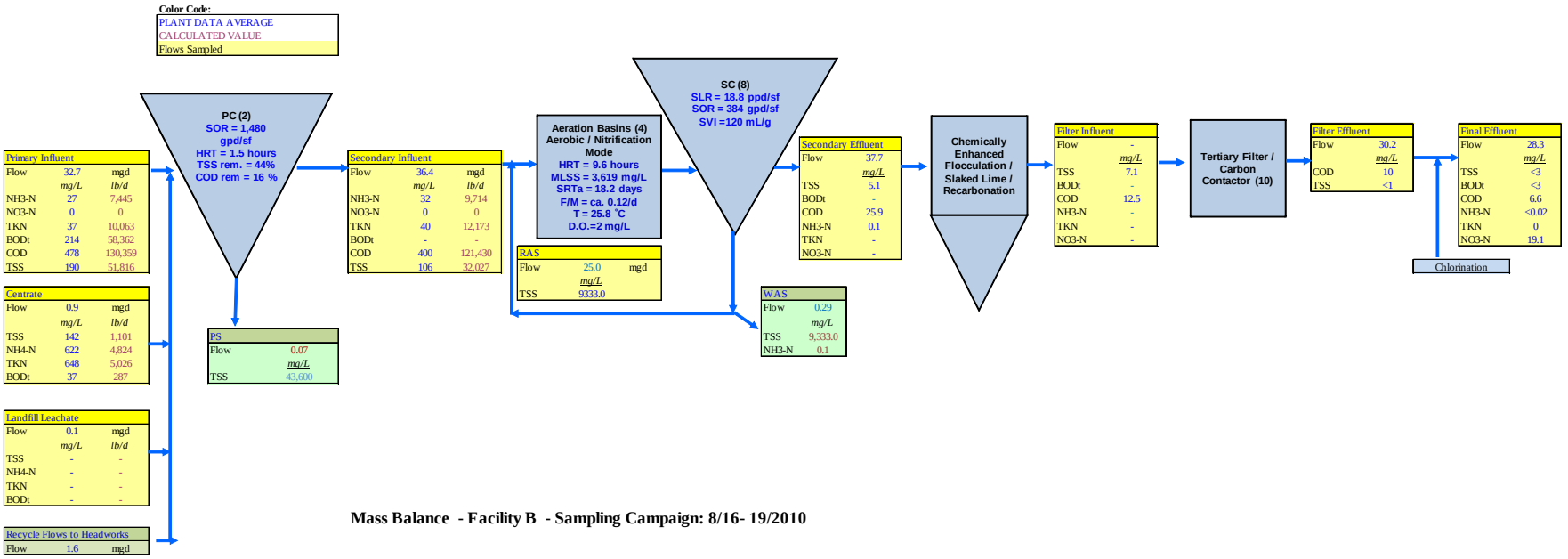


Figure D-2. Facility A (Summer): Conventional Wastewater Treatment Overview During TOrC Sampling Campaign.



Mass Balance - Facility B - Sampling Campaign: 8/16- 19/2010

Figure D-3. Facility B (Summer): Conventional Wastewater Treatment Overview During TOrC Sampling Campaign.

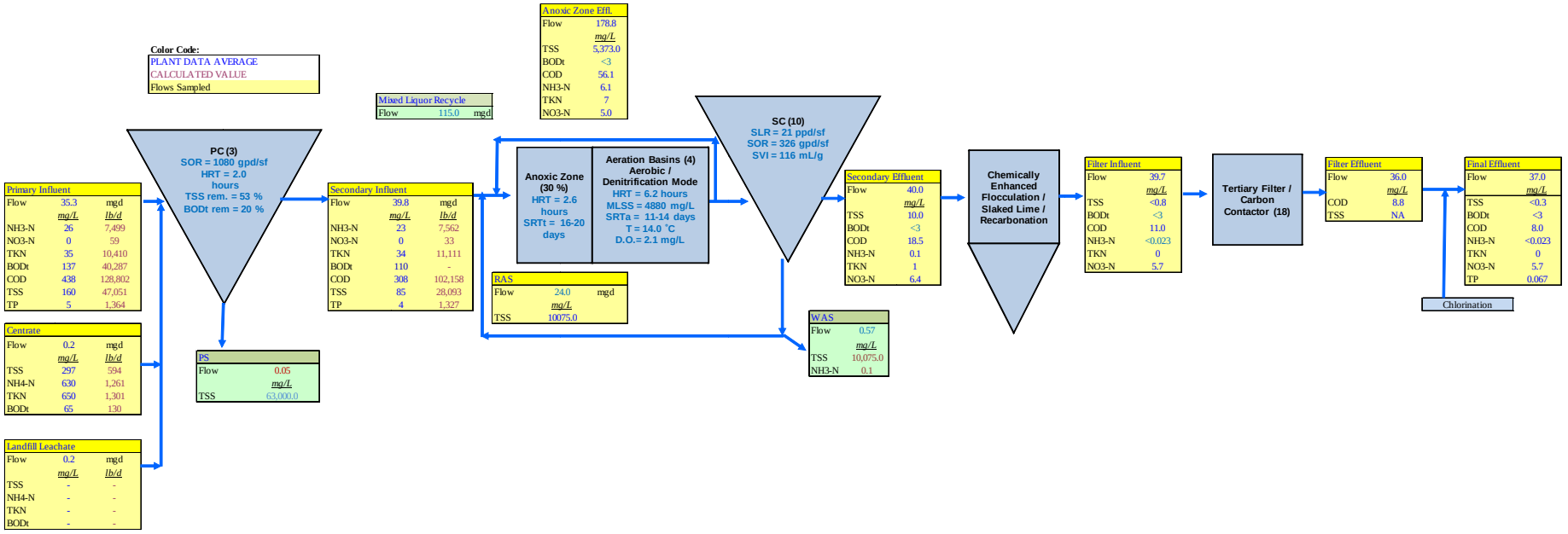


Figure D-4. Facility B (Winter): Conventional Wastewater Treatment Overview During TOrC Sampling Campaign.

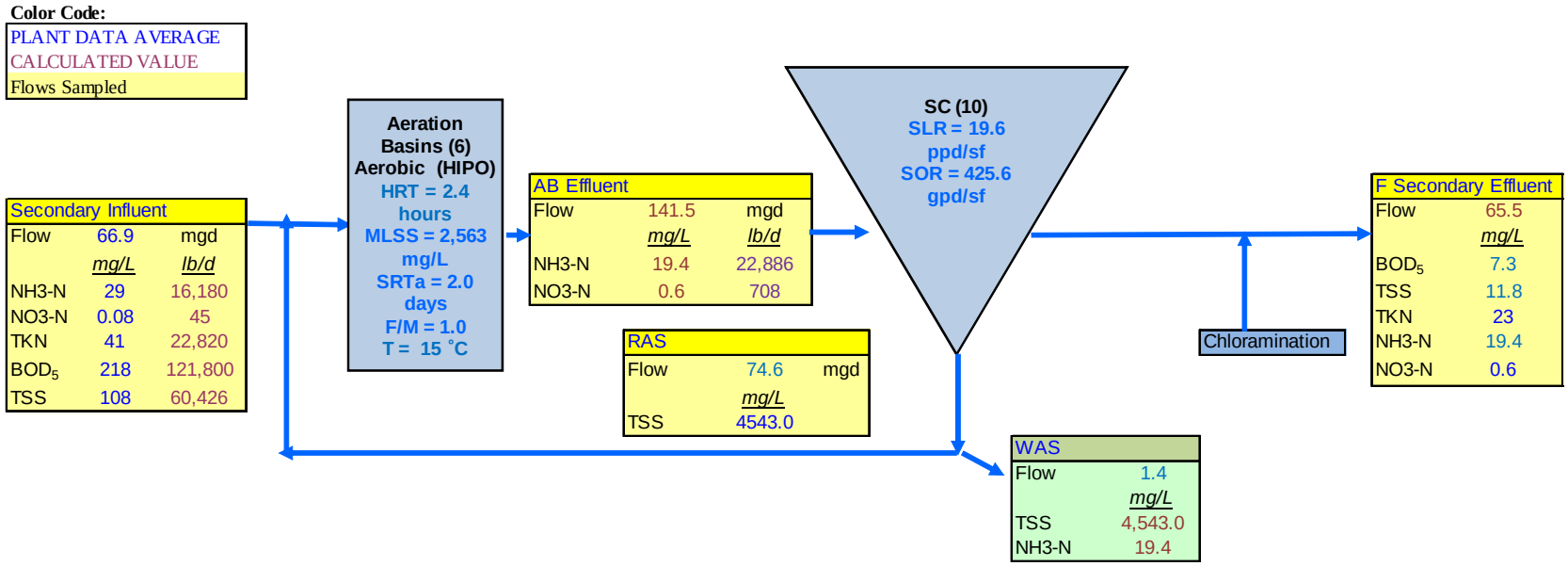


Figure D-5. Facility C (Winter): Conventional Wastewater Treatment Overview During TOrC Sampling Campaign.

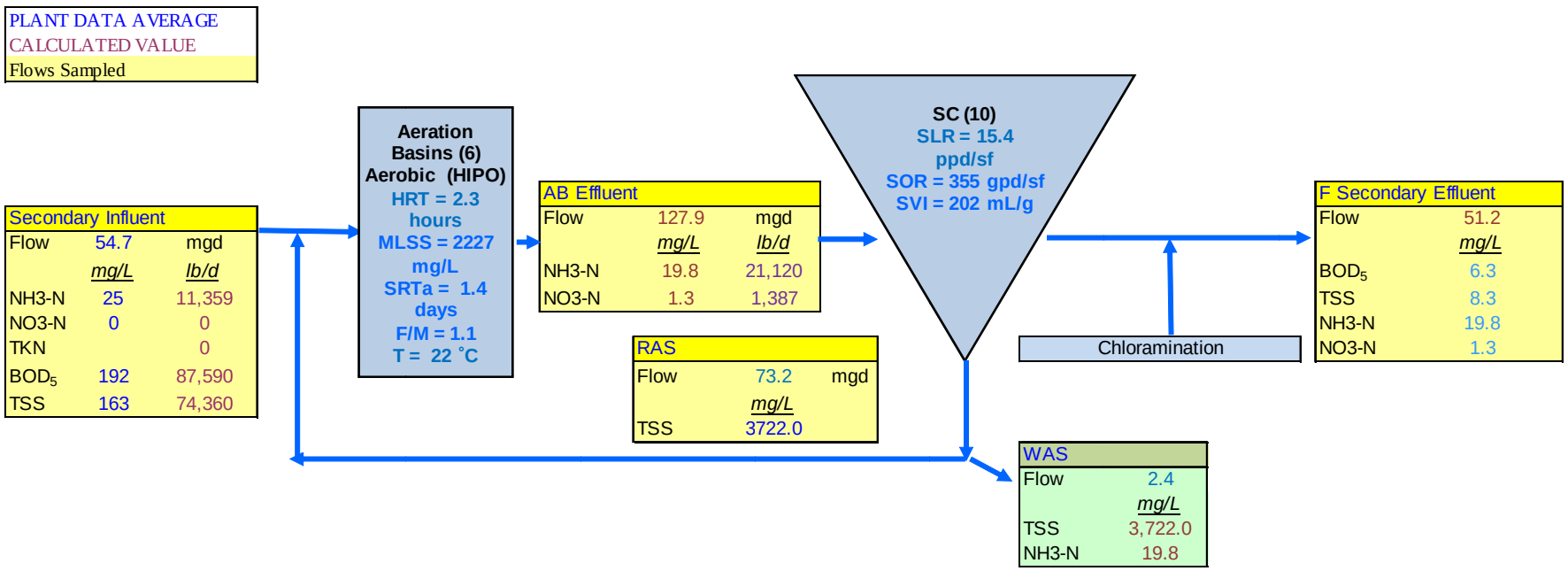


Figure D-6. Facility C (Summer): Conventional Wastewater Treatment Overview During TOrC Sampling Campaign.

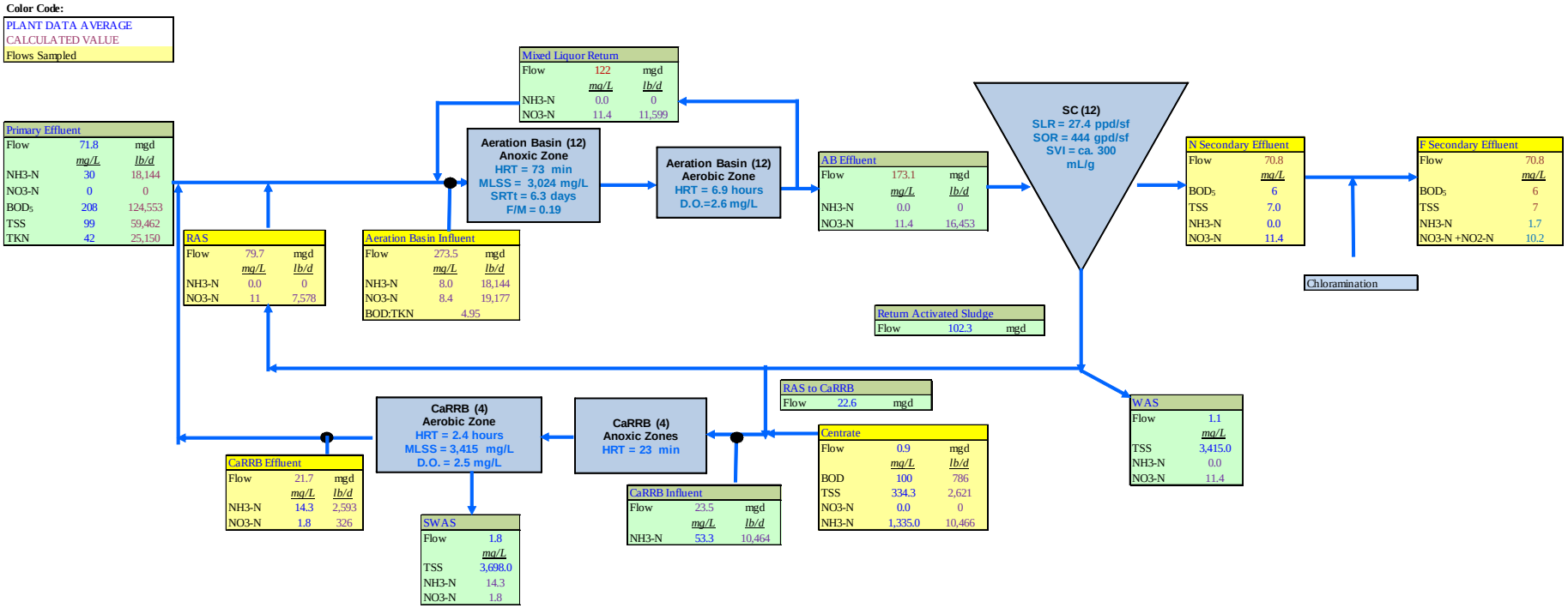


Figure D-7. Facility D (Winter): Conventional Wastewater Treatment Overview During TOrC Sampling Campaign.

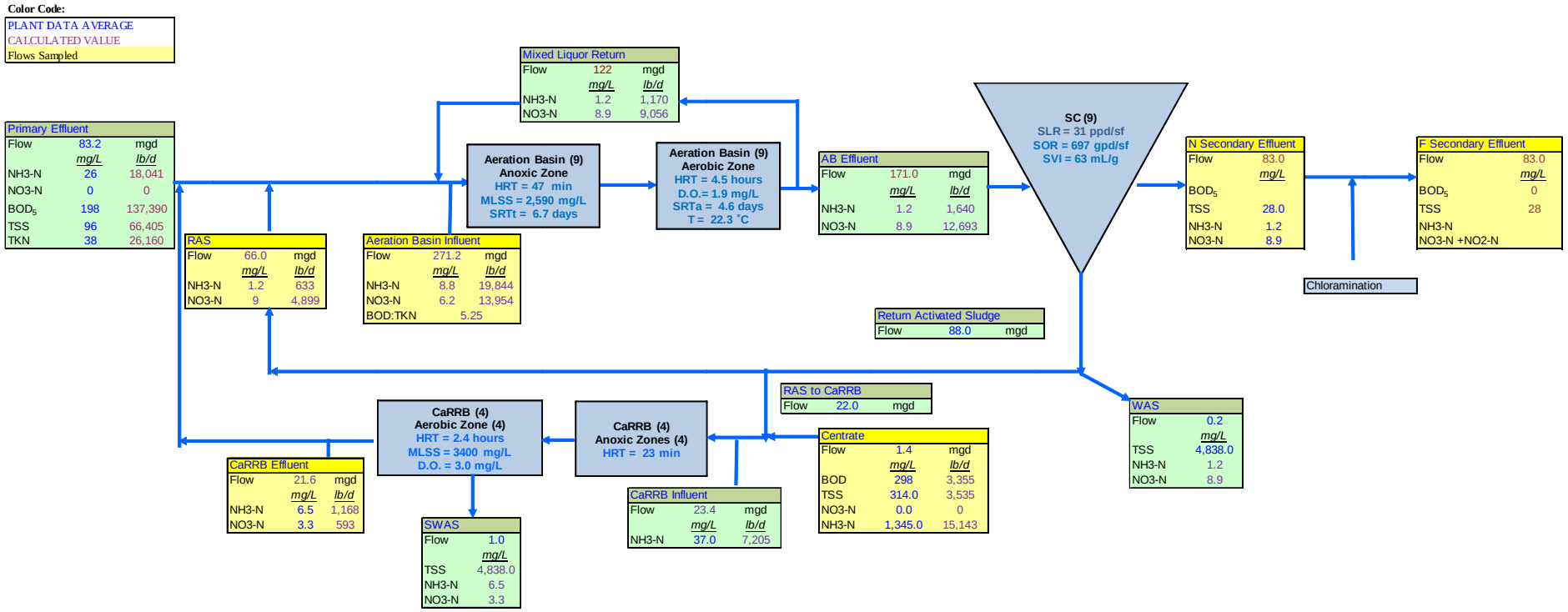


Figure D-8. Facility D (Summer): Conventional Wastewater Treatment Overview During TOrC Sampling Campaign.

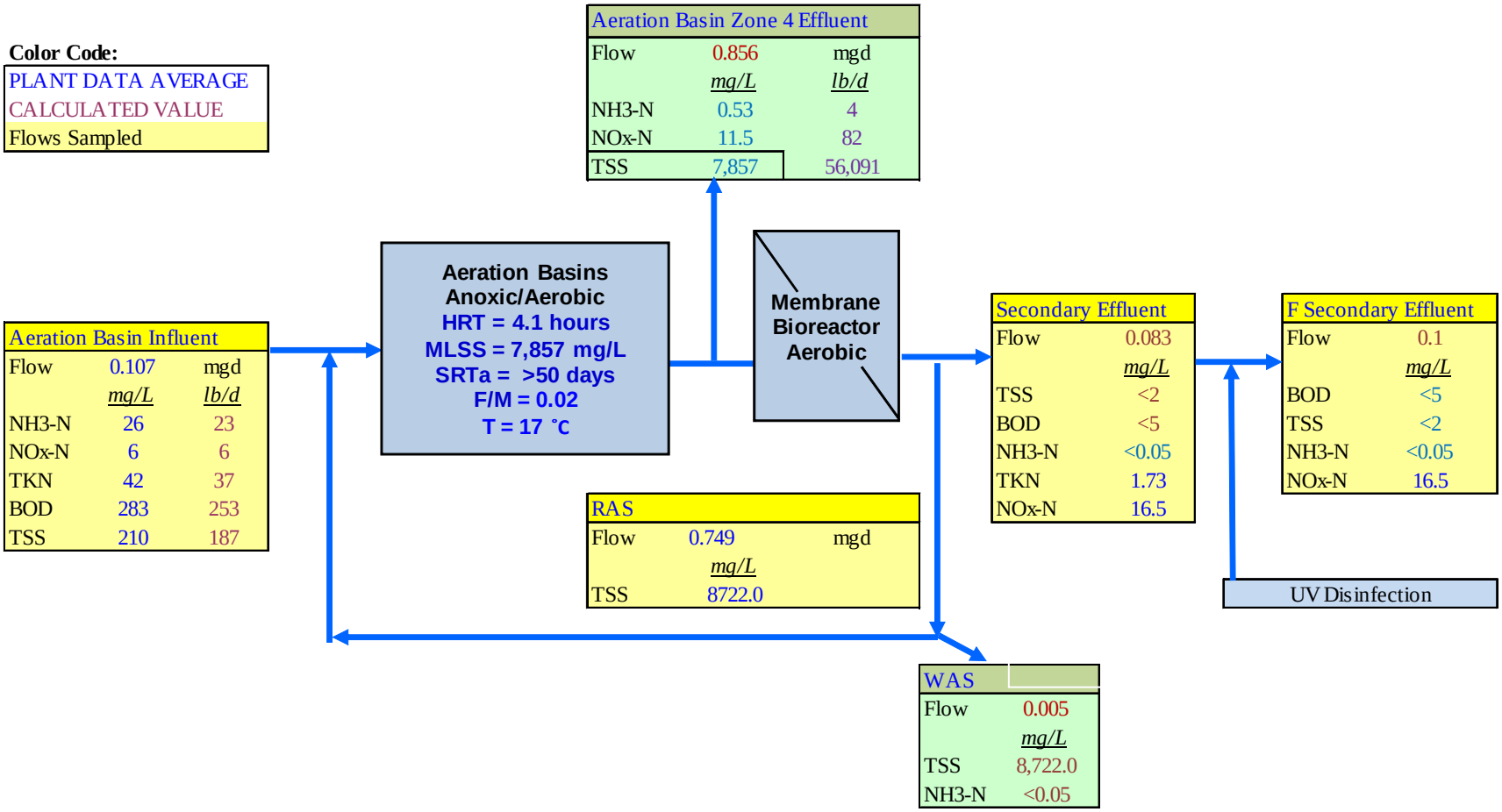


Figure D-9. Facility E (Winter): Conventional Wastewater Treatment Overview During TOrC Sampling Campaign.

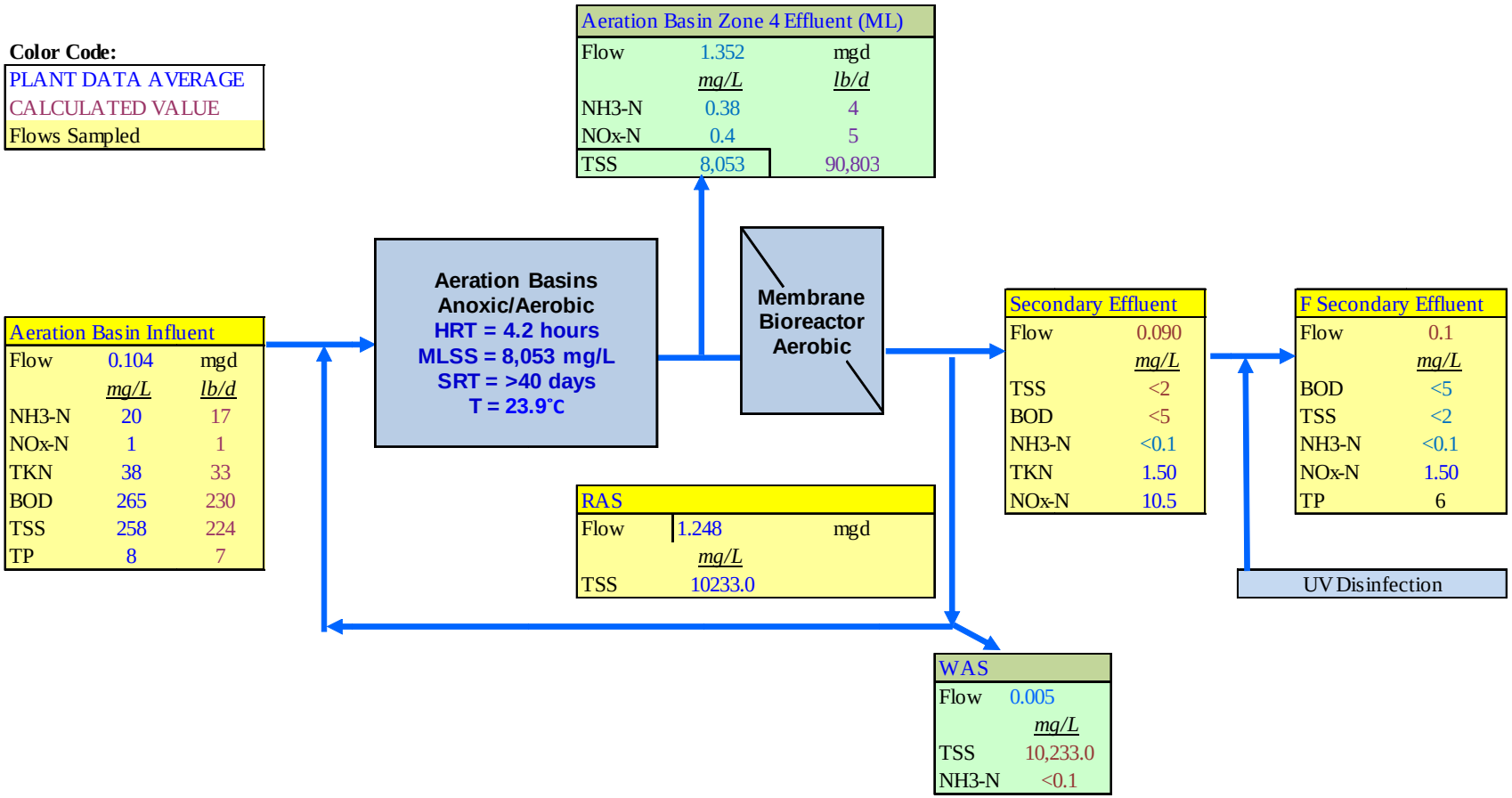


Figure D-10. Facility E (Summer): Conventional Wastewater Treatment Overview During TOrC Sampling Campaign.

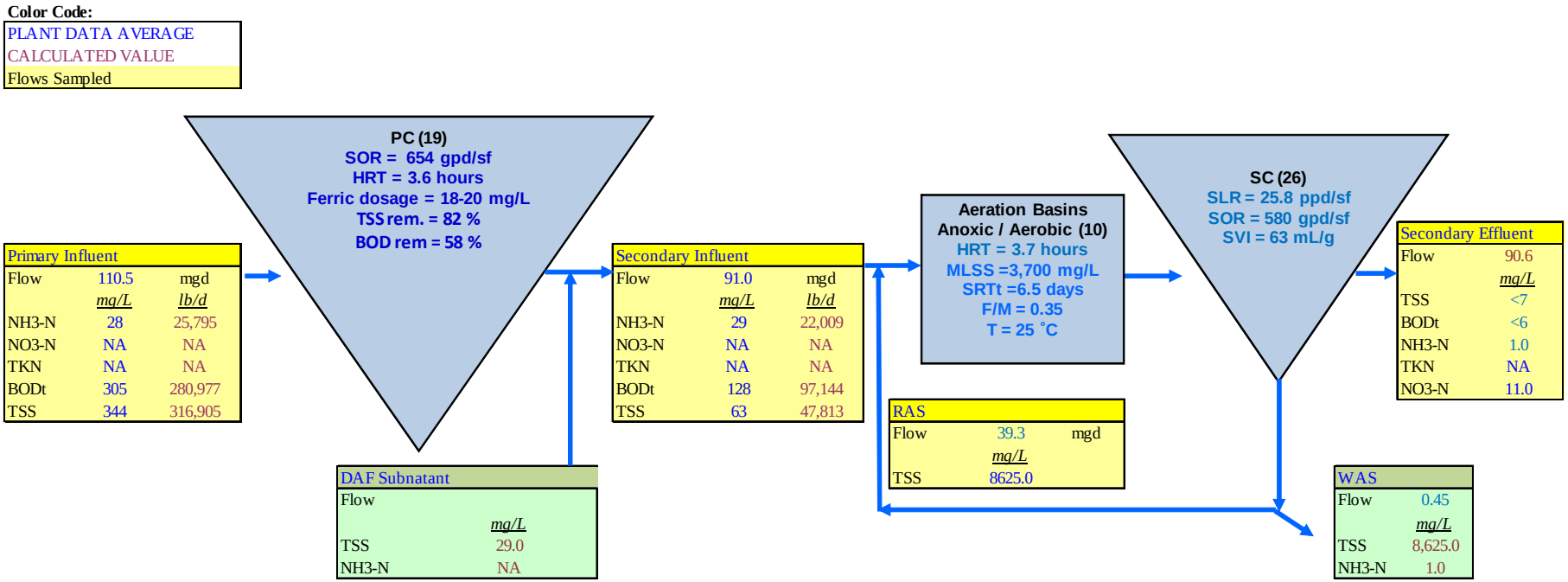


Figure D-11. Facility F (Winter): Conventional Wastewater Treatment Overview During TOrC Sampling Campaign.

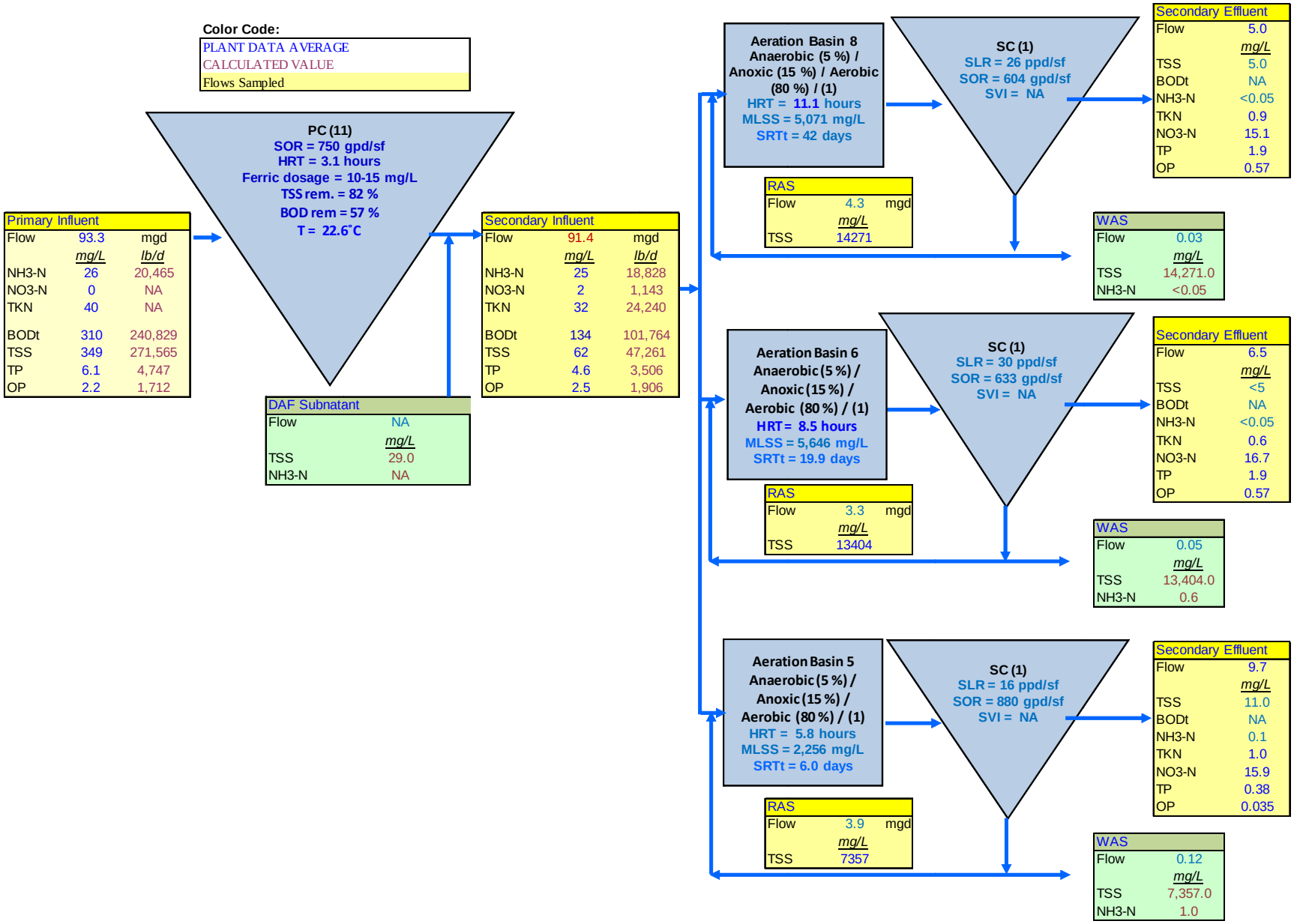


Figure D-12. Facility G (Winter): Conventional Wastewater Treatment Overview During TOrC Sampling Campaign.

APPENDIX E

TOrC Results and Mass Balances

E.1 Sample Container and DI Blank Results

All blank results for rinse blanks field blanks and equipment blanks are reported for each facility as part of the raw TOrC data results in Section E.2 of this Appendix. All results highlighted in yellow in this appendix were higher than the respective analytical level of quantification.

Table E-1. Sample Container and DI Water Blank Results (units in ppt).

Sample ID	10070435-001	QC100804-089	QC100804-090
Location	Rinse Blank	In-house DI Blank	In-house DI Blank
	ng/L	ng/L	ng/L
Sulfamethoxazole	<0.25	<0.25	<0.25
Atenolol	<1.0	<1.0	<1.0
Trimethoprim	<0.25	<0.25	<0.25
Iopromide	<10	<10	<10
Caffeine	10	<5.0	<5.0
Fluoxetine	<0.50	<0.50	<0.50
Meprobamate	<0.25	<0.25	<0.25
Carbamazepine	<0.50	<0.50	<0.50
Benzophenone	69	73	<50
Primidone	<0.50	<0.50	<0.50
TCPP	<100	<100	<100
DEET	20	9.9	<1.0
TCEP	25	<10	<10
Gemfibrozil	<0.25	<0.25	<0.25
Bisphenol A	<5.0	<5.0	<5.0
Naproxen	<0.50	<0.50	<0.50
Triclosan	<1.0	<1.0	<1.0
BHA	<1.0	<1.0	<1.0
Musk Ketone	<25	<25	<25
Ibuprofen	<1.0	<1.0	1.1
Diphenhydramine	<0.50	<0.50	<0.50
Cimetidine	<0.50	<0.50	<0.50
Triclocarban	<1.0	<1.0	<1.0
Acetaminophen	<5.0	<5.0	<5.0
Sucralose	<5.0	<5.0	<5.0

Note: "<" indicates that concentrations were below the reporting limit.

E.2 Raw TOrC Results

E.2.1 Facility A, Winter

Table E-2. Facility A, Winter (Aqueous Phase) Raw TOrC Results.

Date Collected		3/31/2011	3/31/2011	3/31/2011	3/31/2011	3/31/2011	3/31/2011	3/31/2011	3/31/2011	3/31/2011	3/31/2011	3/31/2011
A - Winter Sub Location		Aeration Basin Influent	Secondary Effluent	RAS liquid	RAS liquid - Duplicate	RAS liquid - Triplicate	Centrate	Centrate Duplicate	Centrate Matrix Spike	Final Effluent	Rinse Blank	Field Blank
Sulfamethoxazole	ng/L	1200	1300	1300	1300	1300	150	140	111%	190	<0.25	<0.25
Atenolol	ng/L	1100	760	690	730	730	560	560	99%	670	<1.0	<1.0
Trimethoprim	ng/L	740	650	710	740	750	91	91	117%	120	<0.25	<0.25
Iopromide	ng/L	<100	11	<1000	<1000	<1000	<100	<100	112%	<10	<10	<10
Caffeine	ng/L	86000	<5.0	<500	<500	<500	<50	<50	104%	<5.0	<5.0	<5.0
Fluoxetine	ng/L	50	43	<50	<50	<50	29	28	98%	48	<0.50	<0.50
Meprobamate	ng/L	160	180	160	180	160	170	170	113%	180	<0.25	<0.25
Carbamazepine	ng/L	220	200	200	240	220	1400	1400	102%	180	<0.50	<0.50
Benzophenone	ng/L	540	120	<5000	<5000	<5000	680	560	81%	180	<50	<50
Primidone	ng/L	86	82	65	73	72	75	77	94%	72	<0.50	<0.50
TCPP	ng/L	2000	2200	<10000	<10000	<10000	3800	2800	79%	1800	<100	<100
DEET	ng/L	890	360	250	270	260	290	290	123%	350	1.8	<1.0
TCEP	ng/L	310	310	<1000	<1000	<1000	220	220	112%	300	10	<10
Gemfibrozil	ng/L	1500	390	550	610	570	1000	1100	114%	230	<0.25	<0.25
Bisphenol A	ng/L	960	220	<500	<500	<500	1100	1700	102%	<50	<5.0	<5.0
Naproxen	ng/L	9000	510	480	580	590	120	120	109%	160	<0.50	<0.50
Triclosan	ng/L	2000	100	120	110	100	880	860	110%	29	<1.0	<1.0
BHA	ng/L	<100	38	<100	<100	<100	<10	<10	102%	<10	<1.0	<1.0
Musk Ketone	ng/L	<250	<25	<2500	<2500	<2500	<250	<250	115%	<25	<25	<25
Ibuprofen	ng/L	15000	<10	430	520	420	3100	3200	124%	<10	<1.0	<1.0
Diphenhydramine	ng/L	950	380	470	530	500	150	150	116%	190	<0.50	<0.50
Cimetidine	ng/L	420	300	470	490	460	540	630	129%	<0.50	<0.50	<0.50
Triclocarban	ng/L	370	120	<100	<100	<100	100	100	120%	130	<1.0	<1.0
Acetaminophen	ng/L	150000	<5.0	<500	<500	<500	<500	<500	125%	<5.0	<5.0	<5.0
Sucralose	ng/L	22000	20000	24000	23000	21000	22000	22000	116%	23000	<5.0	<5.0

Table E-3. Facility A, Winter (Solid Phase) Raw TOrC Results.

Date Collected		3/31/2011	3/31/2011	3/31/2011
A - Winter Sub Location		RAS Solid	RAS Solid Duplicate	RAS Solid Triplicate
Sulfamethoxazole	ng/g	120	110	110
Atenolol	ng/g	24	21	22
Trimethoprim	ng/g	190	180	190
Iopromide	ng/g	<300	<300	<300
Caffeine	ng/g	580	300	420
Fluoxetine	ng/g	110	90	110
Meprobamate	ng/g	<9.4	<9.4	<9.4
Carbamazepine	ng/g	<19	<19	<19
Benzophenone	ng/g	<940	<940	<940
Primidone	ng/g	<9.4	<9.4	<9.4
TCPP	ng/g	<1900	<1900	<1900
TCEP	ng/g	<190	<190	<190
Diphenhydramine	ng/g	260	220	230
Gemfibrozil	ng/g	54	45	44
Bisphenol A	ng/g	<1400	<1400	<1400
Naproxen	ng/g	78	81	95
Triclosan	ng/g	2200	1900	2400
BHA	ng/g	<55	<55	<55
Musk Ketone	ng/g	<6600	<6600	<6600
Ibuprofen	ng/g	80	72	86
Cimetidine	ng/g	100	88	120
Triclocarban	ng/g	8500	5800	7800
Acetaminophen	ng/g	<64	<64	<64
Sucralose	ng/g	<3000	<3000	<3000

E.2.2 Facility A, Summer

Table E-4. Facility A, Summer (Aqueous Phase) Raw TOrC Results.

Date Collected		7/14/2011	7/14/2011	7/14/2011	7/14/2011	7/14/2011	7/14/2011	7/14/2011	7/14/2011	7/14/2011	7/14/2011	7/14/2011
A - Summer Sub Location		Aeration Basin Influent	Aeration Basin Influent Duplicate	Aeration Basin Influent Matrix Spike	Secondary Effluent	RAS liquid	RAS liquid - Duplicate	RAS liquid - Triplicate	Centrate	Final Effluent	Rinse Blank	Field Blank
Sulfamethoxazole	ng/L	700	730	117%	740	720	690	680	120	220	<0.25	<0.25
Atenolol	ng/L	760	720	94%	500	270	240	260	290	510	<1.0	<1.0
Trimethoprim	ng/L	440	430	115%	380	310	330	300	15	130	<0.25	<0.25
Iopromide	ng/L	<100	<100	112%	<10	<1000	<1000	<1000	<100	<10	<10	<10
Caffeine	ng/L	57000	60000	104%	46	<500	<500	<500	<50	<5.0	<5.0	<5.0
Fluoxetine	ng/L	39	37	88%	30	<50	<50	<50	13	38	<0.50	<0.50
Meprobamate	ng/L	110	100	112%	120	100	100	110	120	120	<0.25	<0.25
Carbamazepine	ng/L	170	160	112%	140	590	140	150	3700	140	<0.50	<0.50
Benzophenone	ng/L	480	500	97%	170	<5000	<5000	<5000	1900	180	<50	<50
Primidone	ng/L	56	55	92%	50	<50	<50	<50	56	52	<0.50	<0.50
TCPP	ng/L	1600	1500	159%	1700	<10000	<10000	<10000	4400	1500	<100	<100
DEET	ng/L	5900	5800	109%	260	<100	<100	<100	440	270	2.2	<1.0
TCEP	ng/L	270	260	123%	340	<1000	<1000	<1000	160	310	<10	<10
Gemfibrozil	ng/L	900	900	108%	120	83	80	75	1600	100	<0.25	<0.25
Bisphenol A	ng/L	270	290	124%	2200	<500	<500	<500	3000	<50	<5.0	<5.0
Naproxen	ng/L	6500	6000	100%	78	280	300	250	<50	36	<0.50	<0.50
Triclosan	ng/L	1300	1200	109%	57	150	130	160	690	12	<1.0	<1.0
BHA	ng/L	87	88	117%	28	<100	<100	<100	<10	2.5	<1.0	<1.0
Musk Ketone	ng/L	<250	<250	95%	<25	<2500	<2500	<2500	290	<25	<25	<25
Ibuprofen	ng/L	11000	11000	95%	15	460	520	530	17000	<10	<1.0	<1.0
Diphenhydramine	ng/L	570	560	113%	200	390	350	320	170	100	<0.50	<0.50
Cimetidine	ng/L	180	210	111%	<5.0	<50	<50	<50	720	<0.50	<0.50	<0.50
Triclocarban	ng/L	290	270	111%	76	<100	<100	<100	55	79	<1.0	<1.0
Acetaminophen	ng/L	41000	41000	96%	<500	<500	<500	<500	<2000	<10	<5.0	<5.0
Sucralose	ng/L	14000	15000	105%	14000	14000	14000	13000	18000	8900	<5.0	<5.0

Table E-5. Facility A, Summer (Solid Phase) Raw TOrC Results.

Date Collected		7/14/2011	7/14/2011	7/14/2011
A - Summer Sub Location		RAS Solid	RAS Solid Duplicate	RAS Solid Triplicate
Sulfamethoxazole	ng/g	65	67	62
Atenolol	ng/g	<12	<12	<12
Trimethoprim	ng/g	<120	<120	<120
Iopromide	ng/g	<200	<200	<200
Caffeine	ng/g	230	320	700
Fluoxetine	ng/g	99	100	130
Meprobamate	ng/g	<6.2	<6.2	<6.2
Carbamazepine	ng/g	<12	<12	<12
Benzophenone	ng/g	<620	<620	<620
Primidone	ng/g	<6.2	<6.2	<6.2
TCPP	ng/g	<1200	<1200	<1200
TCEP	ng/g	<120	<120	<120
Diphenhydramine	ng/g	220	280	350
Gemfibrozil	ng/g	<11	11	<11
Bisphenol A	ng/g	<920	<920	<920
Naproxen	ng/g	37	37	35
Triclosan	ng/g	1100	1500	1900
BHA	ng/g	<36	<36	<36
Musk Ketone	ng/g	<4300	<4300	<4300
Ibuprofen	ng/g	57	58	56
Cimetidine	ng/g	<22	<22	<22
Triclocarban	ng/g	4400	5100	6200
Acetaminophen	ng/g	<42	<42	<42
Sucralose	ng/g	<2000	<2000	<2000

E.2.3 Facility B, Winter

Table E-6. Facility B, Winter (Aqueous Phase) Raw TOrC Results.

Date Collected		2/7/2011	2/7/2011	2/7/2011	2/7/2011	2/7/2011	2/7/2011	2/10/2011	2/10/2011	2/10/2011	2/10/2011	2/7/2011	2/7/2011	2/7/2011	2/10/2011	2/7/2011	2/10/2011	1/31/2011
B - Winter Sub Location		Primary Influent	Aeration Basin Influent	Anoxic Zone	Anoxic Zone Duplicate	Anoxic Zone Matrix Spike	Secondary Effluent	RAS liquid	RAS liquid - Duplicate	RAS liquid - Triplicate	Centrate	Filter Influent	Filter Effluent	Final Effluent	Creek Above Discharge	Rinse Blank	Field Blank	Equipment Blank
Sulfamethoxazole	ng/L	860	790	1100	1100	110%	590	950	1000	950	620	640	230	4.5	3.5	<0.25	<0.25	<0.25
Atenolol	ng/L	1800	1500	260	250	90%	270	<100	<100	<100	<10	150	29	30	<1.0	<1.0	<1.0	<1.0
Trimethoprim	ng/L	550	510	660	640	105%	360	540	550	550	10	200	9.4	0.68	<0.25	<0.25	<0.25	<0.25
Iopromide	ng/L	110	<100	<100	<100	108%	<10	<1000	<1000	<1000	<100	<10	<10	<10	<10	<10	<10	<10
Caffeine	ng/L	66000	57000	110	120	104%	21	<500	<500	<500	150	36	24	17	37	<5.0	<5.0	<5.0
Fluoxetine	ng/L	41	40	26	23	89%	35	<50	<50	<50	42	30	0.85	0.81	<0.50	<0.50	<0.50	<0.50
Meprobamate	ng/L	120	120	140	140	99%	140	150	160	160	210	140	150	140	0.49	<0.25	<0.25	<0.25
Carbamazepine	ng/L	110	110	140	140	98%	130	140	130	140	1600	130	69	61	<0.50	<0.50	<0.50	<0.50
Benzophenone	ng/L	660	680	<500	<500	103%	<50	<5000	<5000	<5000	630	<50	<50	<50	<50	<50	<50	100
Primidone	ng/L	67	64	74	66	97%	71	72	67	69	84	61	45	41	0.51	<0.50	<0.50	<0.50
TCPP	ng/L	1600	1100	1300	1300	141%	1200	<10000	<10000	<10000	3000	970	650	830	1700	<100	<100	<100
DEET	ng/L	600	410	140	140	117%	79	<100	<100	<100	220	86	48	46	8.0	<1.0	<1.0	5.1
TCEP	ng/L	240	250	180	200	110%	240	<1000	<1000	<1000	97	240	230	230	<10	<10	48	17
Gemfibrozil	ng/L	1500	1300	500	<10000	85%	74	220	230	230	2000	41	9.3	6.0	0.88	<0.25	<0.25	<0.25
Bisphenol A	ng/L	260	270	<50	<50	123%	<5.0	<500	<500	<500	<10000	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0
Naproxen	ng/L	11000	9000	2000	1900	113%	13	210	220	190	330	16	<0.50	<0.50	5.9	<0.50	<0.50	<0.50
Triclosan	ng/L	2800	2400	88	95	105%	32	<100	<100	<100	550	19	<1.0	<1.0	<1.0	<1.0	<1.0	2.0
BHA	ng/L	<100	100	66	63	122%	<10	<100	<100	<100	<100	<10	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0
Musk Ketone	ng/L	<2500	<2500	<250	<250	114%	<25	<2500	<2500	<2500	<250	<25	<25	<25	<25	<25	<25	<25
Ibuprofen	ng/L	11000	9000	2200	2100	106%	2.4	<100	<100	<100	20000	<10	<10	2.1	7.0	<1.0	<1.0	<1.0
Diphenhydramine	ng/L	850	790	320	320	104%	150	170	180	170	450	65	4.4	3.4	<0.50	<0.50	<0.50	<0.50
Cimetidine	ng/L	170	180	340	350	138%	76	280	320	300	1200	71	<0.50	<0.50	<0.50	<0.50	<0.50	<0.50
Triclocarban	ng/L	520	390	89	88	103%	43	<100	<100	<100	52	32	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0
Acetaminophen	ng/L	140000	130000	<10000	<10000	104%	<5.0	<500	<500	<500	<50	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0
Sucralose	ng/L	25000	23000	34000	34000	94%	18000	44000	49000	44000	56000	19000	16000	21000	170	<5.0	<5.0	<5.0

Table E-7. Facility B, Winter (Solid Phase) Raw TOrC Results.

Date Collected		2/7/2011	2/7/2011	2/10/2011	2/10/2011	2/10/2011
B - Winter Sub Location		Primary Influent Solids	Aeration Basin Influent Solids	RAS Solid	RAS Solid Duplicate	RAS Solid Triplicate
Sulfamethoxazole	ng/g	<16	<27	130	120	130
Atenolol	ng/g	<63	<110	<5.0	<5.0	<5.0
Trimethoprim	ng/g	<630	<1100	120	120	110
Iopromide	ng/g	<1000	<1700	<80	<80	<80
Caffeine	ng/g	620	16000	690	740	730
Fluoxetine	ng/g	<320	<540	65	65	58
Meprobamate	ng/g	<32	<54	<2.5	<2.5	<2.5
Carbamazepine	ng/g	<63	<110	9.8	10	8.3
Benzophenone	ng/g	<3200	<5400	320	260	280
Primidone	ng/g	<32	<54	<2.5	<2.5	<2.5
TCPP	ng/g	<6300	<11000	<500	<500	<500
TCEP	ng/g	<630	<1100	<50	<50	<50
Diphenhydramine	ng/g	320	440	110	100	100
Gemfibrozil	ng/g	<55	<95	35	34	32
Bisphenol a	ng/g	<4700	<8200	<375	<375	<375
Naproxen	ng/g	77	<130	70	73	60
Triclosan	ng/g	14000	22000	770	720	710
BHA	ng/g	<180	<320	<14	<14	<14
Musk ketone	ng/g	<22000	<38000	<1800	<1800	<1800
Ibuprofen	ng/g	<130	<220	<10	<10	<10
Cimetidine	ng/g	<110	<200	53	41	39
Triclocarban	ng/g	19000	17000	2900	2900	2900
Acetaminophen	ng/g	<210	<370	<17	<17	<17
Sucralose	ng/g	<10000	<17000	<800	<800	<800

E.2.4 Facility B, Summer

Table E-8. Facility B, Summer (Aqueous Phase) Raw TOrC Results.

Date Collected		8/19/2010	8/19/2010	8/19/2010	8/19/2010	8/19/2010	8/19/2010	8/19/2010	8/19/2010	8/19/2010	8/19/2010	8/19/2010	8/19/2010	8/19/2010	8/23/2010	8/19/2010	8/19/2010	8/19/2010
B - Summer Sub Location		Primary Influent	Landfill Leachate	Aeration Basin Influent	Secondary Effluent	Secondary Effluent Duplicate	Secondary Effluent Matrix Spike	RAS liquid	RAS liquid - Duplicate	RAS liquid - Triplicate	Filter Influent	Filter Effluent	Final Effluent	Centrate	Creek Above Discharge	Rinse blank	Field blank	Equipment blank
Sulfamethoxazole	ng/L	1200	670	1100	580	580	108%	530	490	560	670	98	3.3	210	0.96	< 0.25	< 0.25	< 0.25
Atenolol	ng/L	1800	< 10	1800	280	280	107%	160	170	150	110	2.6	2.0	< 10	< 1.0	< 1.0	< 1.0	< 1.0
Trimethoprim	ng/L	640	< 2.5	580	10	9.2	112%	< 25	26	< 25	3.6	< 0.25	< 0.25	9.6	< 0.25	< 0.25	< 0.25	< 0.25
Iopromide	ng/L	< 100	< 100	< 100	< 10	< 10	65%	< 1000	< 1000	< 1000	< 10	< 10	< 10	< 100	< 10	< 10	< 10	< 10
Caffeine	ng/L	66000	< 50	64000	12	11	106%	< 500	< 500	< 500	29	19	19	250	34	< 5.0	< 5.0	< 5.0
Fluoxetine	ng/L	20	< 5.0	24	28	29	91%	< 50	< 50	< 50	27	< 0.50	0.53	12	< 0.50	< 0.50	< 0.50	< 0.50
Meprobamate	ng/L	150	3.1	160	210	210	108%	150	160	160	200	190	180	190	< 0.25	< 0.25	< 0.25	< 0.25
Carbamazepine	ng/L	230	95	190	180	190	99%	210	210	230	200	54	56	1600	< 0.50	< 0.50	< 0.50	< 0.50
Benzophenone	ng/L	1200	< 500	1200	110	110	82%	< 5000	< 5000	< 5000	68	95	96	1100	< 50	53	< 50	150
Primidone	ng/L	68	< 5.0	76	63	65	100%	< 50	< 50	< 50	78	38	43	76	< 0.50	< 0.50	< 0.50	< 0.50
TCPP	ng/L	2700	< 1000	2000	2300	2100	90%	< 10000	< 10000	< 10000	1600	1300	1400	4200	410	< 100	< 100	< 100
DEET	ng/L	8600	12	9100	10	10	119%	< 100	< 100	< 100	1.9	9.1	8.6	3200	62	1.5	< 1.0	6.4
TCEP	ng/L	510	< 100	480	540	540	105%	< 1000	< 1000	< 1000	490	340	330	230	23	< 10	< 10	< 10
Gemfibrozil	ng/L	1800	39	1900	2.7	2.7	107%	< 25	< 25	< 25	1.3	1.7	1.2	2600	< 0.25	< 0.25	< 0.25	< 0.25
Bisphenol A	ng/L	480	760	470	< 5.0	< 5.0	116%	< 500	< 500	< 500	< 5.0	< 5.0	< 5.0	1600	< 5.0	< 5.0	< 5.0	< 5.0
Naproxen	ng/L	13000	74	14000	< 0.50	< 0.50	110%	< 50	< 50	< 50	< 0.50	< 0.50	< 0.50	170	< 0.50	< 0.50	< 0.50	< 0.50
Triclosan	ng/L	1500	< 10	1600	20	21	114%	< 100	270	< 100	7.9	< 1.0	1.0	670	< 1.0	< 1.0	< 1.0	< 1.0
BHA	ng/L	140	< 10	140	< 1.0	< 1.0	104%	< 100	< 100	< 100	< 1.0	< 1.0	< 1.0	< 10	< 1.0	< 1.0	< 1.0	< 1.0
Musk Ketone	ng/L	< 250	< 250	< 250	< 25	< 25	105%	< 2500	< 2500	< 2500	< 25	< 25	< 25	< 250	< 25	< 25	< 25	< 25
Ibuprofen	ng/L	12000	< 10	14000	< 10	< 10	109%	250	270	250	< 1.0	< 1.0	3.1	16000	1.7	2.2	< 1.0	1.1
Diphenhydramine	ng/L	1100	< 5.0	1000	99	99	97%	120	140	120	73	1.5	0.87	190	< 0.50	< 0.50	< 0.50	< 0.50
Cimetidine	ng/L	290	< 5.0	300	< 5.0	< 5.0	115%	< 50	< 50	< 50	< 0.50	< 0.50	< 0.50	640	< 0.50	< 0.50	< 0.50	< 0.50
Triclocarban	ng/L	250	< 10	240	180	180	96%	< 100	< 100	< 100	160	2.3	< 1.0	200	< 1.0	< 1.0	< 1.0	< 1.0
Acetaminophen	ng/L	91000	< 50	98000	< 5.0	< 5.0	112%	< 500	< 500	< 500	< 5.0	< 5.0	< 5.0	< 50	< 5.0	< 5.0	< 5.0	< 5.0
Sucralose	ng/L	25000	260	25000	27000	26000	88%	22000	23000	22000	23000	24000	25000	36000	120	< 5.0	< 5.0	< 5.0

Table E-9. Facility B, Summer (Solid Phase) Raw TOrC Results.

Date Collected		8/19/2010	8/19/2010	8/19/2010	8/19/2010
B - Summer Sub Location		Aeration Basin Influent Solids	RAS Solid	RAS Solid Duplicate	RAS Solid Triplicate
Sulfamethoxazole	ng/g	<24	67	70	60
Atenolol	ng/g	<94	<12	<12	<12
Trimethoprim	ng/g	<940	<120	<120	<120
Iopromide	ng/g	<1500	<200	<200	<200
Caffeine	ng/g	570	160	140	110
Fluoxetine	ng/g	<470	<61	<61	<61
Meprobamate	ng/g	<47	<6.1	<6.1	<6.1
Carbamazepine	ng/g	<94	<12	13	<12
Benzophenone	ng/g	<4700	<610	<610	<610
Primidone	ng/g	<47	<6.1	<6.1	<6.1
TCPP	ng/g	<9400	<1200	<1200	<1200
TCEP	ng/g	<940	<120	<120	<120
Diphenhydramine	ng/g	600	78	83	59
Gemfibrozil	ng/g	82	20	23	20
Bisphenol A	ng/g	<24000	<3200	<3200	<3200
Naproxen	ng/g	<110	<14	<14	<14
Triclosan	ng/g	20000	520	610	650
BHA	ng/g	<270	<36	<36	<36
Musk Ketone	ng/g	<33000	<4300	<4300	<4300
Ibuprofen	ng/g	<190	<24	24	<24
Cimetidine	ng/g	<170	33	33	34
Triclocarban	ng/g	21000	6500	6700	4500
Acetaminophen	ng/g	<320	<42	<42	<42
Sucralose	ng/g	<15000	<2000	<2000	<2000

E.2.5 Facility C, Winter

Table E-10. Facility C, Winter (Aqueous Phase) Raw TOrC Results.

Date Collected		3/15/2010 9:40	3/15/2010 8:45	3/16/2010 8:45	3/17/2010 8:45	3/15/2010 9:17	3/15/2010 9:17	3/15/2010 9:17	3/15/2010 8:20	3/15/2010 10:58	3/15/2010 9:40
C - Winter Sub Location		Secondary Influent	Mixed Liquor	Mixed Liquor Sample Duplicate	Mixed Liquor Matrix Spike	RAS Aqueous Phase	RAS Aqueous Phase Analytical Duplicate	RAS Aqueous Phase Analytical Triplicate	Final Effluent	Field Blank	Rinse blank
Sulfamethoxazole	ng/L	1400	1100	1100	107%	1700	1400	1700	640	<0.25	<0.25
Atenolol	ng/L	2400	2700	2800	105%	3100	2400	2900	3400	<1.0	<1.0
Trimethoprim	ng/L	710	660	740	100%	830	770	830	710	<0.25	<0.25
Iopromide	ng/L	1200	820	810	105%	1100	<1000	<1000	930	<10	<10
Caffeine	ng/L	370000	140	150	96%	<500	<500	<500	1200	<5.0	15
Fluoxetine	ng/L	34	15	16	100%	<50	<50	<50	48	<0.50	<0.50
Meprobamate	ng/L	180	180	180	59%	230	190	220	180	<0.25	<0.25
Carbamazepine	ng/L	360	340	360	98%	380	340	370	350	<0.50	<0.50
Benzophenone	ng/L	2400	560	560	100%	<5000	<5000	<5000	750	<50	400
Primidone	ng/L	170	150	160	122%	150	120	160	140	<0.50	<0.50
TCPP	ng/L	2200	1800	1600	132%	<10000	<10000	<10000	1800	<100	100
DEET	ng/L	690	690	680	111%	510	480	510	640	<1.0	5.0
TCEP	ng/L	410	410	410	102%	<1000	<1000	<1000	420	<10	<10
Gemfibrozil	ng/L	3200	3300	3100	97%	3500	3000	3400	2900	1.1	0.981
Bisphenol A	ng/L	420	510	540	135%	680	540	610	490	<5.0	<5.0
Naproxen	ng/L	13000	3800	3300	101%	2700	2500	3100	5500	1.9	1.8
Triclosan	ng/L	1400	580	590	102%	870	660	940	640	<1.0	<1.0
BHA	ng/L	370	310	340	130%	240	290	290	320	<1.0	<1.0
Musk Ketone	ng/L	<250	<250	<250	98%	<2500	<2500	<2500	26	<25	<25
Ibuprofen	ng/L	16000	1900	2000	98%	1100	980	950	700	<1.0	4.4
Diphenhydramine	ng/L	1500	1600	1600	95%	1400	1400	1500	1300	<1.0	<1.0
Cimetidine	ng/L	630	860	800	100%	710	570	710	<2.0	<2.0	<2.0
Triclocarban	ng/L	180	170	180	114%	200	200	230	130	<2.0	<2.0
Acetaminophen	ng/L	200000	2500	3400	112%	<500	<500	<500	290	<5.0	<5.0
Sucralose	ng/L	28000	33000	26000	120%	34000	24000	32000	15000	<25	<25

Table E-11. Facility C, Winter (Solid Phase) Raw TOrC Results.

Date Collected		3/15/2010 9:17	3/15/2010 9:17	3/15/2010 9:17
C - Winter Sub Location		RAS Solid	RAS Solid Duplicate	RAS Solid Triplicate
Sulfamethoxazole	ng/g	55	42	44
Atenolol	ng/g	44	44	50
Trimethoprim	ng/g	<110	<110	<110
Iopromide	ng/g	<180	<180	<180
Caffeine	ng/g	110	90	150
Fluoxetine	ng/g	59	<55	61
Meprobamate	ng/g	<5.5	<5.5	<5.5
Carbamazepine	ng/g	17	11	<11
Benzophenone	ng/g	680	<550	<550
Primidone	ng/g	<5.5	<5.5	<5.5
TCPP	ng/g	<1100	<1100	<1100
TCEP	ng/g	<110	<110	<110
Diphenhydramine	ng/g	220	230	260
Gemfibrozil	ng/g	86	89	97
Bisphenol A	ng/g	<5500	<5500	<5500
Naproxen	ng/g	66	71	85
Triclosan	ng/g	4100	4400	4500
BHA	ng/g	63	65	62
Musk Ketone	ng/g	<3800	<3800	<3800
Ibuprofen	ng/g	52	45	45
Cimetidine	ng/g	27	24	22
Triclocarban	ng/g	5700	6200	6000
Acetaminophen	ng/g	<37	<37	<37
Sucralose	ng/g	<1800	<1800	<1800

E.2.6 Facility C, Summer

Table E-12. Facility C, Summer (Aqueous Phase) Raw TOrC Results.

Date Collected		9/23/2010	9/23/2010	9/23/2010	9/23/2010	9/23/2010	9/23/2010	9/23/2010	9/23/2010	9/23/2010	9/23/2010
C - Summer Sub Location		Secondary Influent	Secondary Influent Duplicate	Secondary Influent Matrix Spike	Mixed Liquor	RAS Aqueous Phase	RAS Aqueous Phase Analytical Duplicate	RAS Aqueous Phase Analytical Triplicate	Final Effluent	Field Blank	Rinse blank
Sulfamethoxazole	ng/L	1900	1700	111%	1300	1100	1200	1200	1200	< 0.25	< 0.25
Atenolol	ng/L	2700	2600	121%	2200	1900	2100	2000	2500	< 1.0	< 1.0
Trimethoprim	ng/L	780	780	86%	830	600	680	640	730	< 0.25	< 0.25
Iopromide	ng/L	650	570	50%	530	< 1000	< 1000	< 1000	480	< 10	< 10
Caffeine	ng/L	91000	95000	110%	5700	2100	2200	2100	9000	< 5.0	< 5.0
Fluoxetine	ng/L	61	63	97%	56	< 50	< 50	< 50	58	< 0.50	< 0.50
Meprobamate	ng/L	320	320	77%	330	290	330	300	330	< 0.25	< 0.25
Carbamazepine	ng/L	290	300	110%	350	290	320	290	290	< 0.50	< 0.50
Benzophenone	ng/L	1900	1900	94%	< 500	< 5000	< 5000	< 5000	310	< 50	130
Primidone	ng/L	150	170	146%	170	130	140	140	140	< 0.50	< 0.50
TCPP	ng/L	2000	2000	110%	2000	< 10000	< 10000	< 10000	2100	< 100	< 100
DEET	ng/L	2300	2100	116%	840	560	600	570	720	< 1.0	< 1.0
TCEP	ng/L	570	530	114%	570	< 1000	< 1000	< 1000	550	< 10	< 10
Gemfibrozil	ng/L	3200	3000	97%	3200	2900	3200	3000	2900	0.98	< 0.25
Bisphenol A	ng/L	370	430	86%	430	< 500	< 500	< 500	400	< 5.0	< 5.0
Naproxen	ng/L	17000	17000	113%	2000	710	780	780	1000	< 0.50	< 0.50
Triclosan	ng/L	2500	2000	104%	870	410	430	430	760	< 1.0	< 1.0
BHA	ng/L	400	440	108%	230	140	190	200	280	< 1.0	< 1.0
Musk Ketone	ng/L	< 250	< 250	108%	< 250	< 2500	< 2500	< 2500	41	< 25	< 25
Ibuprofen	ng/L	18000	17000	99%	1200	200	230	210	230	< 1.0	< 1.0
Diphenhydramine	ng/L	1700	1800	92%	1600	1100	1100	1100	1400	< 0.50	< 0.50
Cimetidine	ng/L	560	560	104%	670	480	550	500	< 0.50	< 0.50	< 0.50
Triclocarban	ng/L	490	490	100%	330	270	230	270	320	< 1.0	< 1.0
Acetaminophen	ng/L	140000	160000	116%	< 500	< 500	< 500	< 500	< 500	< 5.0	< 5.0
Sucralose	ng/L	27000	25000	119%	28000	26000	29000	27000	25000	< 5.0	< 5.0

Table E-13. Facility C, Summer (Solid Phase) Raw TOrC Results.

Date Collected		9/23/2010	9/23/2010	9/23/2010	9/23/2010
C - Summer Sub Location		Secondary Influent Solid	RAS Solid	RAS Solid Duplicate	RAS Solid Triplicate
Sulfamethoxazole	ng/g	<31	19	22	20
Atenolol	ng/g	<120	<42	<42	<42
Trimethoprim	ng/g	<1200	<420	<420	<420
Iopromide	ng/g	<2000	<670	<670	<670
Caffeine	ng/g	<610	<210	<210	<210
Fluoxetine	ng/g	<610	<210	<210	<210
Meprobamate	ng/g	<61	<21	<21	<21
Carbamazepine	ng/g	<120	<42	<42	<42
Benzophenone	ng/g	<6100	<2100	<2100	<2100
Primidone	ng/g	<61	<21	<21	<21
TCPP	ng/g	<12000	<4200	<4200	<4200
TCEP	ng/g	<1200	<420	<420	<420
Diphenhydramine	ng/g	720	190	190	200
Gemfibrozil	ng/g	<110	93	78	83
Bisphenol A	ng/g	<32000	<40000	<40000	<40000
Naproxen	ng/g	<140	<50	<50	<50
Triclosan	ng/g	15000	4300	4400	4800
BHA	ng/g	<360	<120	<120	<120
Musk Ketone	ng/g	<43000	<15000	<15000	<15000
Ibuprofen	ng/g	<240	<82	<82	<82
Cimetidine	ng/g	<220	<74	<74	<74
Triclocarban	ng/g	13000	4100	4500	4400
Acetaminophen	ng/g	<420	<140	<140	<140
Sucralose	ng/g	<20000	<6700	<6700	<6700

E.2.7 Facility D, Winter

Table E-14. Facility D, Winter (Aqueous Phase) Raw TOrC Results.

Date Collected		3/8/2010	3/8/2010	3/10/2010	3/10/2010	3/10/2010	3/10/2010	3/11/2010	3/12/2010	3/8/2010	3/8/2010	3/11/2010	3/8/2010
D - Winter Sub Location		Secondary Influent	Secondary Effluent	RAS Aqueous Phase	RAS Aqueous Phase Analytical Duplicate	RAS Aqueous Phase Analytical Triplicate	Centrate	Centrate Sample Duplicate	Centrate Matrix Spike	Post-Centrate Reaeration Basins	Final Effluent	Field blank	Rinse blank
Sulfamethoxazole	ng/L	1300	2000	960	1000	930	190	170	116%	1800	840	<0.25	<0.25
Atenolol	ng/L	2700	4100	600	620	590	1600	1600	88%	1500	2200	<1.0	<1.0
Trimethoprim	ng/L	710	1400	730	780	680	170	160	118%	690	670	<0.25	<0.25
Iopromide	ng/L	1900	3600	<1000	<1000	<1000	880	980	89%	1500	140	<10	<10
Caffeine	ng/L	500000	110	<500	<500	<500	220	200	92%	130000	140	<5.0	68
Fluoxetine	ng/L	32	110	<50	<50	<50	69	60	95%	19	59	<0.50	1.3
Meprobamate	ng/L	160	370	230	240	210	310	330	69%	170	200	<0.25	<0.25
Carbamazepine	ng/L	370	780	330	350	320	3400	3300	106%	380	340	<0.50	<0.50
Benzophenone	ng/L	1400	770	<5000	<5000	<5000	2600	2600	124%	610	400	<50	480
Primidone	ng/L	140	350	140	120	130	150	140	117%	150	140	<0.50	<0.50
TCPP	ng/L	2600	4200	<10000	<10000	<10000	2100	1800	93%	2000	3000	<100	<100
DEET	ng/L	780	140	180	130	110	640	630	167%	480	110	<1.0	6.5
TCEP	ng/L	380	740	<1000	<1000	<1000	350	330	115%	350	390	<10	17
Gemfibrozil	ng/L	3600	5000	2600	2900	2300	10000	9400	86%	2800	2500	<0.25	<0.25
Bisphenol A	ng/L	510	570	<500	<500	<500	6200	6300	127%	160	30	<5.0	<5.0
Naproxen	ng/L	13000	800	1300	1200	940	2200	1900	125%	5800	770	<0.50	1.6
Triclosan	ng/L	460	570	<100	<100	<100	1300	1100	126%	340	330	<1.0	80
BHA	ng/L	280	460	<100	<100	<100	<100	<100	111%	120	58	<1.0	<1.0
Musk Ketone	ng/L	<250	<250	<2500	<2500	<2500	<2500	<2500	94%	<250	46	<25	<25
Ibuprofen	ng/L	17000	260	1800	1400	1200	20000	20000	96%	9700	260	<1.0	8.1
Diphenhydramine	ng/L	1500	430	270	260	230	920	930	137%	480	270	<1.0	34
Cimetidine	ng/L	620	1400	610	880	900	2400	2200	106%	950	<2.0	<2.0	<2.0
Triclocarban	ng/L	220	210	<200	<200	<200	180	200	111%	160	160	<2.0	140
Acetaminophen	ng/L	170000	<500	<500	<500	<500	<500	<500	136%	4200	<500	<5.0	<5.0
Sucralose	ng/L	19000	49000	19000	20000	17000	26000	31000	97%	18000	38000	<25	<25

Table E-15. Facility D, Winter (Solid Phase) Raw TOrC Results.

Date Collected		3/10/2010 14:06	3/10/2010 14:06	3/10/2010 14:06
D - Winter Sub Location		RAS Solid	RAS Solid Duplicate	RAS Solid Triplicate
Sulfamethoxazole	ng/g	220	200	190
Atenolol	ng/g	31	33	31
Trimethoprim	ng/g	220	230	220
Iopromide	ng/g	<260	<260	<260
Caffeine	ng/g	1200	470	670
Fluoxetine	ng/g	190	170	140
Meprobamate	ng/g	<8.0	<8.0	<8.0
Carbamazepine	ng/g	34	34	32
Benzophenone	ng/g	<800	<800	<800
Primidone	ng/g	<8.0	<8.0	<8.0
TCPP	ng/g	<1600	<1600	<1600
TCEP	ng/g	<160	<160	<160
Diphenhydramine	ng/g	260	230	230
Gemfibrozil	ng/g	260	240	210
Bisphenol A	ng/g	<8400	<8400	<8400
Naproxen	ng/g	160	170	130
Triclosan	ng/g	4200	4200	3600
BHA	ng/g	<46	<46	<46
Musk Ketone	ng/g	<5600	<5600	<5600
Ibuprofen	ng/g	140	160	180
Cimetidine	ng/g	190	200	170
Triclocarban	ng/g	10000	10000	8600
Acetaminophen	ng/g	<550	<550	<550
Sucralose	ng/g	<2600	<2600	<2600

E.2.8 Facility D, Summer

Table E-16. Facility D, Summer (Aqueous Phase) Raw TOrC Results.

Date Collected		9/16/2010	9/16/2010	9/16/2010	9/16/2010	9/16/2010	9/16/2010	9/16/2010	9/16/2010	9/16/2010	9/16/2010	9/16/2010	9/16/2010
D - Summer Sub Location		Secondary Influent	Secondary Effluent	RAS Aqueous Phase	RAS Aqueous Phase Analytical Duplicate	RAS Aqueous Phase Analytical Triplicate	Centrate	Post-Centrate Reaeration Basins	Post-Centrate Reaeration Basins Duplicate	Post-Centrate Reaeration Basins Matrix Spike	Final Effluent	Field blank	Rinse blank
Sulfamethoxazole	ng/L	1500	1200	890	1000	1000	800	2300	2100	108%	1300	< 0.25	< 0.25
Atenolol	ng/L	2300	1600	610	720	700	1200	1900	2000	117%	1900	< 1.0	< 1.0
Trimethoprim	ng/L	710	680	590	670	660	350	840	820	113%	670	< 0.25	< 0.25
Iopromide	ng/L	1300	1200	1000	1200	1300	910	1100	1200	119%	1100	< 10	< 10
Caffeine	ng/L	110000	160	< 500	< 500	< 500	96	56000	55000	105%	340	< 5.0	< 5.0
Fluoxetine	ng/L	56	51	< 50	< 50	< 50	< 5.0	55	55	97%	55	< 0.50	< 0.50
Meprobamate	ng/L	320	340	300	280	280	480	300	330	116%	340	< 0.25	< 0.25
Carbamazepine	ng/L	300	320	300	350	330	1700	380	410	119%	350	< 0.50	< 0.50
Benzophenone	ng/L	1000	< 500	< 5000	< 5000	< 5000	2800	< 500	< 500	117%	310	< 50	110
Primidone	ng/L	150	140	110	120	100	130	160	160	108%	160	< 0.50	< 0.50
TCPP	ng/L	2000	1900	< 10000	< 10000	< 10000	3600	1900	1900	121%	1800	< 100	< 100
DEET	ng/L	3100	280	< 100	< 100	< 100	1500	1900	1800	118%	290	< 1.0	< 1.0
TCEP	ng/L	500	550	< 1000	< 1000	< 1000	450	570	520	118%	510	< 10	< 10
Gemfibrozil	ng/L	3200	1700	810	920	910	6000	2800	2700	106%	170	< 0.25	< 0.25
Bisphenol A	ng/L	440	230	< 500	< 500	< 500	1800	240	240	104%	< 5.0	< 5.0	< 5.0
Naproxen	ng/L	17000	2100	1100	1100	1200	1800	9700	9500	130%	2600	< 0.50	1.1
Triclosan	ng/L	3100	270	< 100	100	< 100	1200	510	480	124%	310	< 1.0	< 1.0
BHA	ng/L	340	340	< 100	< 100	< 100	140	400	400	155%	210	< 1.0	< 1.0
Musk Ketone	ng/L	< 250	< 250	< 2500	< 2500	< 2500	< 250	< 250	< 250	93%	< 250	< 25	< 25
Ibuprofen	ng/L	20000	230	380	400	410	15000	13000	12000	96%	240	< 1.0	2.2
Diphenhydramine	ng/L	1600	640	840	940	930	70	1600	1700	140%	620	< 0.50	< 0.50
Cimetidine	ng/L	630	660	730	770	760	1300	700	700	99%	< 5.0	< 0.50	< 0.50
Triclocarban	ng/L	800	260	210	210	210	100	270	270	117%	260	< 1.0	< 1.0
Acetaminophen	ng/L	160000	< 50	< 500	< 500	< 500	< 50	29000	31000	111%	< 50	< 5.0	< 5.0
Sucralose	ng/L	29000	31000	28000	27000	27000	31000	31000	34000	94%	23000	< 5.0	< 5.0

Table E-17. Facility D, Summer (Solid Phase) Raw TOrC Results.

Date Collected		9/16/2010	9/16/2010	9/16/2010	9/16/2010
D - Summer Sub Location		Secondary Influent Solid	RAS Solid	RAS Solid Duplicate	RAS Solid Triplicate
Sulfamethoxazole	ng/g	<52	61	58	47
Atenolol	ng/g	<210	<16	<16	<16
Trimethoprim	ng/g	<2100	<160	<160	<160
Iopromide	ng/g	<3300	<250	<250	<250
Caffeine	ng/g	<1000	170	240	170
Fluoxetine	ng/g	<1000	120	180	<79
Meprobamate	ng/g	<100	<8.0	<8.0	<8.0
Carbamazepine	ng/g	<210	16	22	18
Benzophenone	ng/g	<10000	<800	<800	<800
Primidone	ng/g	<100	<8.0	<8.0	<8.0
TCPP	ng/g	<21000	<1600	<1600	<600
TCEP	ng/g	<2100	<160	<160	<160
Diphenhydramine	ng/g	980	450	580	300
Gemfibrozil	ng/g	<180	64	61	52
Bisphenol A	ng/g	<54000	<4100	<4100	<4100
Naproxen	ng/g	<250	62	57	59
Triclosan	ng/g	17000	1800	1900	1500
BHA	ng/g	<610	<47	<47	<47
Musk Ketone	ng/g	<73000	<5600	<5600	<5600
Ibuprofen	ng/g	<410	51	54	50
Cimetidine	ng/g	<370	120	120	110
Triclocarban	ng/g	13000	3600	4700	2900
Acetaminophen	ng/g	<720	<55	<55	<55
Sucralose	ng/g	<33000	<2500	<2500	<2500

E.2.9 Facility E, Winter

Table E-18. Facility E, Winter (Aqueous Phase) Raw TOrC Results.

Date Collected		4/12/2010	4/13/2010	4/14/2010	4/12/2010	4/13/2010	4/14/2010	4/15/2010	4/15/2010	4/15/2010	4/12/2010	4/13/2010	4/14/2010	4/15/2010	4/12/2010
E - Winter Sub Location		Aeration Basin Influent	Aeration Basin Influent Sample Duplicate	Aeration Basin Influent Sample Triplicate	Membrane Effluent	Membrane Effluent Sample Duplicate	Membrane Effluent Sample Triplicate	RAS Aqueous Phase	RAS Aqueous Phase Analytical Duplicate	RAS Aqueous Phase Analytical Triplicate	Final Plant Effluent (after UV)	Final Plant Effluent Sample Duplicate	Final Plant Effluent Sample Triplicate	Field Blank	Rinse Blank
Sulfamethoxazole	ng/L	650	710	680	480	510	510	630	670	580	370	410	380	<0.25	<0.25
Atenolol	ng/L	2600	2700	2800	430	440	440	<100	<100	<100	560	600	560	<1.0	220
Trimethoprim	ng/L	440	470	480	26	27	26	41	38	46	24	25	25	<0.25	<0.25
Iopromide	ng/L	32000	27000	38000	7700	8400	9100	<1000	<1000	<1000	2000	2300	2600	<10	<10
Caffeine	ng/L	120000	120000	130000	<5.0	<5.0	<5.0	<500	<500	<500	30	30	29	<5.0	<5.0
Fluoxetine	ng/L	25	21	20	24	26	29	<50	<50	<50	10	11	12	<0.50	<0.50
Meprobamate	ng/L	280	310	300	62	62	64	56	55	51	61	61	61	<0.25	<0.25
Carbamazepine	ng/L	260	260	260	340	350	360	330	310	310	310	310	300	<0.50	<0.50
Benzophenone	ng/L	1000	940	940	250	220	210	<5000	<5000	<5000	440	380	410	<50	110
Primidone	ng/L	<5.0	<5.0	<5.0	<0.50	<0.50	<0.50	<50	<50	<50	<0.50	<0.50	<0.50	<0.50	<0.50
TCPP	ng/L	1900	2000	2000	1000	950	1000	<10000	<10000	<10000	900	940	1000	<100	<100
DEET	ng/L	420	440	440	17	16	16	<100	<100	<100	17	18	17	<1.0	<1.0
TCEP	ng/L	360	370	370	440	440	440	<1000	<1000	<1000	420	420	420	<10	<10
Gemfibrozil	ng/L	290	300	320	3.6	3.8	3.9	<25	<25	<25	3.6	3.5	3.2	<0.25	<0.25
Bisphenol A	ng/L	430	420	400	<5.0	<5.0	<5.0	<500	<500	<500	<5.0	<5.0	<5.0	<5.0	<5.0
Naproxen	ng/L	12000	12000	14000	13	19	13	83	69	79	27	25	26	<0.50	11
Triclosan	ng/L	1100	1300	1000	12	11	11	<100	<100	<100	3.7	3.0	3.4	<1.0	<1.0
BHA	ng/L	250	240	190	16	14	14	<100	<100	<100	12	13	13	<1.0	<1.0
Musk Ketone	ng/L	<250	<250	<250	<25	<25	<25	<2500	<2500	<2500	<25	<25	<25	<25	<25
Ibuprofen	ng/L	30000	27000	30000	<10	<10	<10	<100	<100	<100	<10	<10	<10	<1.0	<1.0
Diphenhydramine	ng/L	1200	1200	1200	61	58	62	74	69	66	47	48	47	<1.0	<1.0
Cimetidine	ng/L	350	380	310	120	110	110	290	310	350	86	74	65	<2.0	<2.0
Triclocarban	ng/L	550	490	480	200	230	230	270	280	240	67	67	74	<2.0	<2.0
Acetaminophen	ng/L	170000	160000	150000	<500	<500	<500	<500	<500	<500	<500	<500	<500	<5.0	<5.0
Sucralose	ng/L	28000	33000	23000	51000	41000	43000	81000	91000	74000	77000	77000	76000	<25	<25

Table E-19. Facility E, Winter (Solid Phase) Raw TOrC Results.

Date Collected		4/15/2010	4/15/2010	4/15/2010
E - Winter Sub Location		RAS Solid	RAS Solid Duplicate	RAS Solid Triplicate
Sulfamethoxazole	ng/g	180	220	N/A
Atenolol	ng/g	15	22	N/A
Trimethoprim	ng/g	<63	<63	N/A
Iopromide	ng/g	<100	<100	N/A
Caffeine	ng/g	200	260	N/A
Fluoxetine	ng/g	69	110	N/A
Meprobamate	ng/g	<3.2	<3.2	N/A
Carbamazepine	ng/g	31	25	N/A
Benzophenone	ng/g	750	<320	N/A
Primidone	ng/g	<3.2	<3.2	N/A
TCPP	ng/g	<630	2100	N/A
TCEP	ng/g	72	<63	N/A
Diphenhydramine	ng/g	73	97	N/A
Gemfibrozil	ng/g	<5.5	<5.5	N/A
Bisphenol A	ng/g	<1600	<1600	N/A
Naproxen	ng/g	20	17	N/A
Triclosan	ng/g	600	640	N/A
BHA	ng/g	<18	<18	N/A
Musk Ketone	ng/g	<2200	<2200	N/A
Ibuprofen	ng/g	28	26	N/A
Cimetidine	ng/g	100	120	N/A
Triclocarban	ng/g	8600	13000	N/A
Acetaminophen	ng/g	<21	<21	N/A
Sucralose	ng/g	<1000	<1000	N/A

N/A - Instrument failed during extraction and sample was lost

E.2.10 Facility E, Summer

Table E-20. Facility E, Summer (Aqueous Phase) Raw TOrC Results.

Date Collected		8/26/2010	8/26/2010	8/26/2010	8/26/2010	8/26/2010	8/26/2010	8/26/2010	8/26/2010	8/26/2010	8/26/2010
E - Summer Sub Location		Aeration Basin Influent	Aeration Basin Influent Duplicate	Aeration Basin Influent Matrix Spike	Membrane Effluent	RAS Aqueous Phase	RAS Aqueous Phase Analytical Duplicate	RAS Aqueous Phase Analytical Triplicate	Final Plant Effluent (after UV)	Field Blank	Rinse Blank
Sulfamethoxazole	ng/L	2100	2000	102%	940	1100	1100	1100	860	< 0.25	< 0.25
Atenolol	ng/L	2300	2000	114%	160	< 100	< 100	< 100	150	< 1.0	< 1.0
Trimethoprim	ng/L	990	960	103%	66	30	33	31	51	< 0.25	< 0.25
Iopromide	ng/L	< 100	< 100	110%	< 10	< 1000	< 1000	< 1000	< 10	< 10	< 10
Caffeine	ng/L	120000	110000	92%	10	< 500	< 500	< 500	30	< 5.0	< 5.0
Fluoxetine	ng/L	35	32	92%	23	< 50	< 50	< 50	13	< 0.50	< 0.50
Meprobamate	ng/L	290	280	108%	130	220	220	230	140	< 0.25	< 0.25
Carbamazepine	ng/L	500	500	94%	380	350	380	360	350	< 0.50	< 0.50
Benzophenone	ng/L	900	870	122%	84	< 5000	< 5000	< 5000	160	< 50	56
Primidone	ng/L	21	18	107%	16	< 50	< 50	< 50	15	< 0.50	< 0.50
TCPP	ng/L	2300	2000	97%	1400	< 10000	< 10000	< 10000	1300	< 100	< 100
DEET	ng/L	15000	15000	118%	24	< 100	< 100	< 100	23	< 1.0	1.7
TCEP	ng/L	790	750	108%	950	< 1000	< 1000	< 1000	960	< 10	< 10
Gemfibrozil	ng/L	3500	3300	92%	6.5	39	42	44	6.2	< 0.25	< 0.25
Bisphenol A	ng/L	550	500	88%	< 5.0	< 500	< 500	< 500	< 5.0	< 5.0	< 5.0
Naproxen	ng/L	11000	12000	104%	23	120	130	150	19	< 0.50	< 0.50
Triclosan	ng/L	2500	1400	102%	33	< 100	< 100	< 100	13	< 1.0	< 1.0
BHA	ng/L	240	240	126%	27	< 100	< 100	< 100	22	< 1.0	< 1.0
Musk Ketone	ng/L	< 250	< 250	114%	< 25	< 2500	< 2500	< 2500	< 25	< 25	< 25
Ibuprofen	ng/L	15000	18000	104%	< 10	< 100	< 100	< 100	< 1.0	1.1	1.3
Diphenhydramine	ng/L	1200	1100	98%	82	100	110	110	74	< 0.50	< 0.50
Cimetidine	ng/L	< 50	< 50	103%	22	< 50	< 50	< 50	18	< 0.50	< 0.50
Triclocarban	ng/L	1100	510	87%	260	< 100	< 100	< 100	140	< 1.0	< 1.0
Acetaminophen	ng/L	160000	130000	90%	< 5.0	< 500	< 500	< 500	< 5.0	< 5.0	< 5.0
Sucralose	ng/L	34000	34000	87%	28000	44000	50000	56000	39000	< 5.0	< 5.0

Table E-21. Facility E, Summer (Solid Phase) Raw TOrC Results.

Date Collected		8/26/2010	8/26/2010	8/26/2010	8/26/2010
E - Summer Sub Location		Aeration Basin Influent Solid	RAS Solid	RAS Solid Duplicate	RAS Solid Triplicate
Sulfamethoxazole	ng/g	<19	160	160	160
Atenolol	ng/g	<78	<11	<11	<11
Trimethoprim	ng/g	<780	<110	<110	<110
Iopromide	ng/g	<1200	<170	<170	<170
Caffeine	ng/g	500	150	19000	160
Fluoxetine	ng/g	<390	<53	<53	<53
Meprobamate	ng/g	<39	<5.3	<5.3	<5.3
Carbamazepine	ng/g	<78	27	20	21
Benzophenone	ng/g	<3900	<530	<530	<530
Primidone	ng/g	<39	<5.3	<5.3	<5.3
TCPP	ng/g	<7800	1300	1100	1100
TCEP	ng/g	<780	<110	<110	<110
Diphenhydramine	ng/g	270	85	75	75
Gemfibrozil	ng/g	<68	<9.3	<9.3	<9.3
Bisphenol A	ng/g	<20000	<2800	<2800	<2800
Naproxen	ng/g	<92	<13	<13	<13
Triclosan	ng/g	7100	370	340	370
BHA	ng/g	<230	<31	<31	<31
Musk Ketone	ng/g	<27000	<3700	<3700	<3700
Ibuprofen	ng/g	<150	<21	<21	<21
Cimetidine	ng/g	<140	25	26	25
Triclocarban	ng/g	13000	4800	3700	4800
Acetaminophen	ng/g	<270	<37	<37	<37
Sucralose	ng/g	<12000	<1700	<1700	<1700

E.2.11 Facility F, Winter

Table E-22. Facility F, Winter (Aqueous Phase) Raw TOrC Results.

Date Collected		4/29/2010	4/29/2010	4/29/2010	4/29/2010	4/29/2010	4/29/2010	4/29/2010	4/29/2010	4/29/2010	4/29/2010	4/29/2010
F - Winter Sub Location		Primary Clarifier Influent	Primary Clarifier Influent Sample Duplicate	Primary Clarifier Influent Sample Triplicate	Primary Clarifier Influent Matrix Spike	Primary Clarifier Influent Matrix Spike Duplicate	Aeration Basin Influent	Secondary Effluent	RAS Aqueous Phase	RAS Aqueous Phase Analytical Duplicate	RAS Aqueous Phase Analytical Triplicate	Field Blank
Sulfamethoxazole	ng/L	1500	1600	1700	114%	104%	1500	2800	1700	1800	1900	<0.25
Atenolol	ng/L	2300	2400	2400	91%	98%	2900	1900	750	800	810	<1.0
Trimethoprim	ng/L	580	600	600	110%	102%	570	510	370	380	400	<0.25
Iopromide	ng/L	230	220	200	77%	74%	140	<100	<1000	<1000	<1000	<10
Caffeine	ng/L	81000	84000	82000	106%	110%	75000	59	<500	<500	<500	<5.0
Fluoxetine	ng/L	13	10	12	94%	90%	7.5	16	<50	<50	<50	<0.50
Meprobamate	ng/L	340	350	360	93%	92%	330	420	420	440	430	<0.25
Carbamazepine	ng/L	230	240	230	100%	103%	250	260	200	200	200	<0.50
Benzophenone	ng/L	3000	3200	3100	115%	119%	3000	710	<5000	<5000	<5000	99
Primidone	ng/L	140	150	140	105%	106%	130	120	100	100	120	<0.50
TCPP	ng/L	1700	1700	1500	118%	117%	1400	1700	<10000	<10000	<10000	<100
DEET	ng/L	460	450	450	142%	136%	500	350	200	210	200	<1.0
TCEP	ng/L	400	390	390	110%	109%	410	410	<1000	<1000	<1000	<10
Gemfibrozil	ng/L	4100	4500	4600	106%	127%	4700	810	1700	1400	1500	<0.25
Bisphenol A	ng/L	640	660	680	127%	125%	1000	170	<500	<500	<500	<5.0
Naproxen	ng/L	12000	12000	11000	112%	140%	13000	150	400	410	420	<0.50
Triclosan	ng/L	750	520	640	123%	105%	870	110	<100	<100	<100	<1.0
BHA	ng/L	120	120	110	109%	114%	<100	110	<100	<100	<100	<1.0
Musk Ketone	ng/L	<250	<250	<250	126%	101%	<250	<250	<2500	<2500	<2500	<25
Ibuprofen	ng/L	16000	16000	18000	96%	123%	13000	<10	310	340	360	<1.0
Diphenhydramine	ng/L	1100	1100	1100	104%	112%	860	520	880	820	880	<1.0
Cimetidine	ng/L	640	570	600	82%	143%	420	260	280	300	340	<2.0
Triclocarban	ng/L	100	78	92	97%	122%	69	110	<100	<100	<100	<2.0
Acetaminophen	ng/L	130000	140000	150000	115%	108%	120000	<50	<500	<500	<500	<5.0
Sucralose	ng/L	44000	48000	51000	103%	111%	29000	22000	19000	21000	28000	<25

Table E-23. Facility F, Winter (Solid Phase) Raw TOrC Results.

Date Collected		4/29/2010	4/29/2010	4/29/2010
F - Winter Sub Location		RAS Solid	RAS Solid Duplicate	RAS Solid Triplicate
Sulfamethoxazole	ng/g	190	190	150
Atenolol	ng/g	27	28	22
Trimethoprim	ng/g	95	100	67
Iopromide	ng/g	<91	<91	<180
Caffeine	ng/g	230	230	130
Fluoxetine	ng/g	63	72	39
Meprobamate	ng/g	13	13	11
Carbamazepine	ng/g	11	10	11
Benzophenone	ng/g	<290	<290	<290
Primidone	ng/g	<2.9	<2.9	<2.9
TCPP	ng/g	<570	<570	<570
TCEP	ng/g	<57	<57	<57
Diphenhydramine	ng/g	390	390	230
Gemfibrozil	ng/g	290	320	240
Bisphenol A	ng/g	<1500	<1500	<1500
Naproxen	ng/g	49	45	35
Triclosan	ng/g	1400	1300	770
BHA	ng/g	<16	<16	<16
Musk Ketone	ng/g	<2000	<2000	<2000
Ibuprofen	ng/g	44	53	44
Cimetidine	ng/g	27	33	27
Triclocarban	ng/g	2300	3100	1400
Acetaminophen	ng/g	<190	<190	<190
Sucralose	ng/g	<910	<910	<910

E.2.12 Facility G, Low, Medium, and High SRT

Table E-24. Facility G – Low, Medium, and High SRT (Aqueous Phase) Raw TOrC Results.

Date Collected		1/17/1011	1/17/1011	1/17/1011	1/17/1011	1/17/1011	1/19/2011	1/19/2011	1/19/2011	1/17/2011	1/19/2011	1/19/2011	1/19/2011	1/17/2011	1/19/2011	1/19/2011	1/19/2011	1/17/2011	1/19/2011
G High, Low, Medium SRT Sub Location		Primary Influent Aqueous Phase	Secondary Influent High SRT	Secondary Influent High SRT Duplicate	Secondary Influent High SRT Matrix Spike	Secondary Effluent High SRT	RAS Aqueous Phase High SRT	RAS Aqueous Phase High SRT Analytical Duplicate	RAS Aqueous Phase High SRT Analytical Triplicate	Secondary Effluent Low SRT	RAS Aqueous Phase Low SRT	RAS Aqueous Phase Low SRT Analytical Duplicate	RAS Aqueous Phase Low SRT Analytical Triplicate	Secondary Effluent Medium SRT	RAS Aqueous Phase Medium SRT	RAS Aqueous Phase Medium SRT Analytical Duplicate	RAS Aqueous Phase Medium SRT Analytical Triplicate	Rinse blank	Field Blank
Sulfamethoxazole	ng/L	1600	1200	1200	110%	1700	1400	1400	1300	2500	1700	1700	1700	2300	1500	1600	1600	<0.25	<0.25
Atenolol	ng/L	2000	1800	1700	105%	20	<100	<100	<100	980	590	580	550	36	<100	<100	<100	270	<1.0
Trimethoprim	ng/L	830	770	830	112%	14	<25	<25	<25	620	530	540	510	24	<25	<25	<25	<0.25	<0.25
Iopromide	ng/L	<100	<100	<100	103%	<10	<1000	<1000	<1000	<10	<1000	<1000	<1000	<10	<1000	<1000	<1000	<10	<10
Caffeine	ng/L	120000	110000	110000	104%	8.6	<500	<500	<500	15	<500	<500	<500	35	<500	<500	<500	<5.0	<5.0
Fluoxetine	ng/L	45	43	35	87%	24	<50	110	<50	27	<50	<50	<50	26	<50	<50	<50	<0.50	<0.50
Meprobamate	ng/L	1200	1300	1400	106%	130	39	50	42	1200	1000	1100	970	140	110	110	110	<0.25	<0.25
Carbamazepine	ng/L	93	120	120	94%	140	170	200	200	130	210	200	180	140	190	210	180	<0.50	<0.50
Benzophenone	ng/L	810	700	830	80%	<50	<5000	<5000	<5000	170	<5000	<5000	<5000	54	<5000	<5000	<5000	<50	<50
Primidone	ng/L	140	130	120	100%	130	130	140	130	130	110	130	130	130	120	130	130	<0.50	<0.50
TCPP	ng/L	2100	1500	1400	127%	1500	<10000	<10000	<10000	1500	<10000	<10000	<10000	1700	<10000	<10000	<10000	<100	<100
DEET	ng/L	200	190	190	120%	40	<100	<100	<100	180	170	180	170	71	<100	<100	<100	<1.0	<1.0
TCEP	ng/L	450	360	320	106%	290	<1000	<1000	<1000	300	<1000	<1000	<1000	300	<1000	<1000	<1000	<10	<10
Gemfibrozil	ng/L	2900	2800	2900	96%	14	110	110	95	470	320	320	340	55	200	220	220	<0.25	<0.25
Bisphenol A	ng/L	440	440	450	115%	<5.0	<500	<500	<500	<5.0	<500	<500	<500	<5.0	<500	<500	<500	<5.0	<5.0
Naproxen	ng/L	21000	17000	20000	116%	5.0	110	120	94	300	100	110	110	7.8	160	110	120	2.1	<0.50
Triclosan	ng/L	1400	1200	1100	103%	30	<100	<100	<100	150	<100	210	<100	86	<100	<100	<100	<1.0	<1.0
BHA	ng/L	240	260	260	103%	2.0	<100	<100	<100	130	<100	<100	<100	2.8	<100	<100	<100	<1.0	<1.0
Musk Ketone	ng/L	<250	<250	<250	115%	<50	<2500	<2500	<2500	<50	<2500	<2500	<2500	<50	<2500	<2500	<2500	<25	<25
Ibuprofen	ng/L	23000	21000	22000	118%	12	160	170	190	53	<100	110	<100	<10	200	240	190	<1.0	<1.0
Diphenhydramine	ng/L	1600	1500	1500	104%	55	86	150	82	880	1100	1100	1100	53	89	84	91	<0.50	<0.50
Cimetidine	ng/L	550	410	400	95%	350	2800	2500	2600	470	840	890	800	300	1300	1300	1400	<0.50	<0.50
Triclocarban	ng/L	160	140	130	106%	28	<100	<100	<100	43	<100	<100	<100	36	<100	<100	<100	<1.0	<1.0
Acetaminophen	ng/L	250000	250000	240000	119%	<5.0	<500	<500	<500	<5.0	<500	<500	<500	<5.0	<500	<500	<500	<5.0	<5.0
Sucralose	ng/L	32000	30000	29000	117%	29000	38000	39000	40000	36000	32000	33000	32000	37000	38000	37000	35000	<5.0	<5.0

Table E-25. Facility G – Low, Medium, and High SRT (Solid Phase) Raw TOrC Results.

Date Collected		1/19/2011	1/19/2011	1/19/2011	1/19/2011	1/19/2011	1/19/2011	1/19/2011	1/19/2011	1/19/2011	1/19/2011
G High, Low, Medium SRT Sub Location		Primary Influent Solids	RAS Solid Phase High SRT	RAS Solid Phase High SRT Analytical Duplicate	RAS Solid Phase High SRT Analytical Triplicate	RAS Solid Phase Low SRT	RAS Solid Phase Low SRT Analytical Duplicate	RAS Solid Phase Low SRT Analytical Triplicate	RAS Solid Phase Medium SRT	RAS Solid Phase Medium SRT Analytical Duplicate	RAS Solid Phase Medium SRT Analytical Triplicate
Sulfamethoxazole	ng/g	17	180	180	220	93	97	110	200	200	190
Atenolol	ng/g	<29	<3.5	<3.5	<3.5	7.1	8.3	16	<3.7	<3.7	<3.7
Trimethoprim	ng/g	<290	<35	<35	<35	<68	<68	<68	<37	<37	<37
Iopromide	ng/g	<460	<56	<56	<56	<110	<110	<110	<59	<59	<59
Caffeine	ng/g	860	61	35	38	63	200	1300	42	130	130
Fluoxetine	ng/g	99	28	24	25	54	60	71	29	28	34
Meprobamate	ng/g	<14	4.3	3.6	4.1	20	18	21	6.7	8.3	6.7
Carbamazepine	ng/g	<29	7.3	8.1	8.9	10	6.9	9.8	7.6	10	10
Benzophenone	ng/g	1600	290	230	270	<340	<340	<340	230	290	280
Primidone	ng/g	<14	<1.8	<1.8	<1.8	<3.4	<3.4	<3.4	<1.8	<1.8	<1.8
TCPP	ng/g	<2900	<350	<350	<350	<680	<680	<680	<370	<370	<370
TCEP	ng/g	<290	<35	<35	<35	<68	<68	<68	<37	<37	<37
Diphenhydramine	ng/g	390	37	33	34	310	330	380	34	37	37
Gemfibrozil	ng/g	<25	34	31	31	97	97	110	59	55	56
Bisphenol A	ng/g	<2200	<260	<260	<260	<510	<510	<510	<280	<280	<280
Naproxen	ng/g	50	<4.2	<4.2	<4.2	<8.2	<8.2	<8.2	<4.4	<4.4	<4.4
Triclosan	ng/g	50	390	410	420	1400	1100	1300	560	530	590
BHA	ng/g	<84	<10	<10	<10	<20	<20	<20	<11	<11	<11
Musk Ketone	ng/g	<10000	<1200	<1200	<1200	<2400	<2400	<2400	<1300	<1300	<1300
Ibuprofen	ng/g	<58	37	43	24	46	54	59	55	53	56
Cimetidine	ng/g	<52	670	610	600	180	160	190	350	360	370
Triclocarban	ng/g	14000	1200	1200	1400	2000	2000	2500	1400	1400	1500
Acetaminophen	ng/g	<99	<12	<12	<12	<23	<23	<23	<13	<13	<13
Sucralose	ng/g	<4600	850	1100	1100	470	340	430	880	830	1000

E.3 Summary of Coefficient of Variances

E.3.1 Liquid Analysis

Table E-26. Coefficient of Variances for Return Activated Sludge Samples (Liquid Analysis) (Sample Triplicates).

Site	A	A	B	B	C	C	D	D	E	E	F	G	G	G			
Event	Winter	Summer	Summer	Winter	Summer	Winter	Summer	Winter	Winter	Summer	Winter	Low SRT	Medium SRT	High SRT	Average	Min.	Max.
Sulfamethoxazole	0	3.0	6.7	3.0	4.9	10.8	6.6	3.6	7.2	0	5.6	0	3.7	4.2	4.2	0	11
Atenolol	3.2	6.0	6.3		5.0	12.9	8.7	2.5			4.1	3.6			5.8	3	13
Trimethoprim	2.8	4.9		1.1	6.3	4.3	6.8	6.8	9.7	4.9	4.0	2.9			4.9	1	10
Iopromide							13.1								13.1	13	13
Caffeine															NA	NA	NA
Fluoxetine															NA	NA	NA
Meprobamate	6.9	5.6	3.7	3.7	6.8	9.8	4.0	6.7	4.9	2.6	2.3	6.7	0	13.0	5.5	0	13
Carbamazepine	9.1	87.6	5.3	4.2	5.8	5.7	7.7	4.6	3.6	4.2	0	7.8	7.9	9.1	11.6	0	88
Benzophenone															NA	NA	NA
Primidone	6.2			3.6	4.2	14.5	9.1	7.7			10.8	9.4	4.6	4.3	7.4	4	15
TCPP															NA	NA	NA
DEET	3.8				3.6	3.5		25.8			2.8	3.3			7.1	3	26
TCEP															NA	NA	NA
Gemfibrozil	5.3	5.1		2.5	5.0	8.0	6.9	11.5		6.0	10.0	3.5	5.4	8.2	6.5	3	12
Bisphenol A															NA	NA	NA
Naproxen	11.1	9.1		7.4	5.3	11.0	5.1	16.2	9.4	11.5	2.4	5.4	20.4	12.1	9.7	2	20
Triclosan	9.1	10.4			2.7	17.7									10.0	3	18
BHA					18.2										18.2	18	18
Musk Ketone															NA	NA	NA
Ibuprofen	12.1	7.5	4.5		7.2	7.9	3.9	20.8			7.5		12.6	8.8	9.3	4	21
Diphenhydramine	6.0	9.9	9.1	3.3	0	4.0	6.1	8.2	5.8	5.4	4.0	0	4.1	36.0	7.3	0	36
Cimetidine	3.2			6.7	7.1	12.2	2.8	20.3	9.6		10.0	5.3	4.3	5.8	7.9	3	20
Triclocarban					9.0		0		7.9						5.6	0	9
Acetaminophen															NA	NA	NA
Sucralose	6.7	4.2	2.6	6.3	5.6	17.6	2.1	8.2	10.4	12.0	20.8	1.8	4.2	2.6	7.5	2	21

Table E-27. Coefficient of Variances for Process Samples (Liquid Analysis) (Sample Triplicates).

Sample	Primary Influent	Aeration Basin Influent (after screening)	Secondary Effluent	Final Effluent
Site	F	E	E	E
Event	Winter	winter	winter	Winter
Sulfamethoxazole	6.3	4.4	3.5	5.4
Atenolol	2.4	3.7	1.3	4.0
Trimethoprim	1.9	4.5	2.2	2.3
Iopromide	7.1	17.0	8.3	13.0
Caffeine	1.9	4.7		1.9
Fluoxetine	13.1	12.0	9.6	9.1
Meprobamate	2.9	5.1	1.8	0.0
Carbamazepine	2.5	0.0	2.9	1.9
Benzophenone	3.2	3.6	9.2	7.3
Primidone	4.0			
TCPP	7.1	2.9	2.9	5.3
DEET	1.3	2.7	3.5	3.3
TCEP	1.5	1.6	0.0	0.0
Gemfibrozil	6.0	5.0	4.1	6.1
Bisphenol A	3.0	3.7		
Naproxen	4.9	9.1	23.1	3.8
Triclosan	18.1	13.5	5.1	10.4
BHA	4.9	14.2	7.9	4.6
Musk Ketone				
Ibuprofen	6.9	6.0		
Diphenhydramine	0.0	0.0	3.5	1.2
Cimetidine	5.8	10.1	5.1	14.0
Triclocarban	12.4	7.5	7.9	5.8
Acetaminophen	7.1	6.3		
Sucralose	7.4	17.9	11.8	0.8

E.3.2 Solid Analysis

Table E-28. Coefficient of Variances for Return Activated Sludge Samples (Solid Analysis) (Sample Triplicates).

Site	A	A	B	B	C	C	D	D	E	E	F	G	G	G			
Event	Winter	Summer	Summer	Winter	Winter	Summer	winter	Summer	winter	Summer	Winter	Low SRT	Medium SRT	High SRT	Average	Min.	Max.
Sulfamethoxazole	5.1	3.9	7.8	4.6	14.9	7.5	7.5	13.3	NA	0.0	13.1	8.9	2.9	11.9	7.8	0	15
Atenolol	6.8				7.5		3.6				12.5	46.1			15.3	4	46
Trimethoprim	3.1			4.9			2.6				20.4				7.7	3	20
Iopromide															NA	NA	NA
Caffeine	32.4	59.9	18.4	3.7	26.2		48.4	20.9		4.6	29.4	130.2	50.5	31.8	38.0	4	130
Fluoxetine	11.2	16.1		6.4			15.1				29.4	14.0	10.6	8.1	13.9	6	29
Meprobamate											9.4	7.8	12.8	9.0	9.7	8	13
Carbamazepine				9.9			3.5	16.4		16.7	5.4	19.5	15.1	9.9	12.0	3	19
Benzophenone				10.7									12.1	11.6	11.4	11	12
Primidone															NA	0	0
TCPP										9.9					9.9	NA	NA
TCEP															NA	0	0
Diphenhydramine	8.8	23.0	17.3	5.6	8.8	3.0	7.2	31.6		7.4	27.4	10.6	4.8	6.0	12.4	3	32
Gemfibrozil	11.6		8.2	4.5	6.3	9.0	10.6	10.6			14.3	7.4	3.7	5.4	8.3	4	14
Bisphenol A															NA	NA	NA
Naproxen	10.7	3.2		10.1	13.3		13.6	4.2			16.8				10.3	3	17
Triclosan	11.6	26.7	11.2	4.4	4.8	5.9	8.7	12.0		4.8	29.3	12.1	5.4	3.8	10.8	4	29
BHA					2.4										2.4	2	2
Musk Ketone															NA	NA	NA
Ibuprofen	8.9	1.8			8.5		12.5	4.0			11.1	12.4	2.8	28.0	10.0	2	28
Cimetidine	15.7		1.7	17.1	10.3		8.2	4.9		2.3	11.9	8.6	2.8	6.0	8.2	2	17
Triclocarban	19.0	17.3	20.6	0.0	4.2	4.8	8.5	24.3		14.3	37.5	13.3	4.0	9.1	13.6	0	38
Acetaminophen															NA	NA	NA
Sucralose												16.1	9.7	14.2	13.3	10	16

E.4 Background Corrected TOrC Results

The following procedure was used for correcting raw TOrC sample results (Section E.3) for contamination identified in rinse, field, or equipment blanks. The combined contamination from rinse, field, or equipment blanks was subtracted from the liquid TOrC concentrations measured in the field samples for each constituent, respectively, if

a) the combined contamination for a given sample and compound was greater than the standard deviation of the TOrC concentrations measured. This indicated that the sample contamination exceeded the estimated accuracy of the TOrC analysis; or
b) the combined contamination for a given sample and compound exceeded 15 percent of the average TOrC concentration measured in a given sample. This indicated that the contamination contributed significantly to the raw TOrC concentration measured.

Background correction of TOrC results based on the site-specific contamination identified in the rinse, field, and equipment blanks was performed based on the types of samples collected:

Table E-29. Blank Samples Used for TOrC Result Correction.

Type of Sample Collected	Type of Blank Used for Data Correction
Grab samples for aqueous phase analysis	Field Blank
Composite sample for aqueous phase analysis (permanent sampler)	Rinse Blank + Field Blank
Composite sample for aqueous phase analysis (temporary sampler)	Rinse Blank + Field Blank + Equipment Blank
Samples for solid phase analysis:	- (No background correction performed)

Depending on the type of sample Liquid samples collected as grabTables E.29 to E.4.40 summarize the background corrected TOrC results for all field sites based on the above procedure.

Antweiler and Taylor (2008) identified the Kaplan-Meier Method as the most reliable method for treating below detection limit environmental data. This method suggests replacing measurements below the detection limit (here below the reporting limit) with one half of the detection limit (reporting limit). This method was only applied for TOrC concentration measured in process samples or blank samples with reporting limits below 100 ng/L. TOrC data with reporting limits over 100 ng/L was reported as not quantifiable (n.q.).

For the case that standard deviations were not available for a specific sample collected (as sample replicates were only analyzed for selected samples from each field site), the standard deviation for a specific compound and sample was estimated based on the (average) coefficient of variance determined for the same sample matrix (e.g. secondary effluent) at a different field site as summarized in Section E.2.

E.4.1 Facility A, Winter

Table E-30. Facility A, Winter (Aqueous Phase), Background Corrected TOrC Results.

Date Collected		3/31/2011	3/31/2011	3/31/2011	3/31/2011	3/31/2011
A - Winter Sub Location		Aeration Basin Influent	Secondary Effluent	RAS Aqueous Phase (Average)	Centrate (Average)	Final Effluent
Sulfamethoxazole	ng/L	1,200	1,300	1,300	145	190
Atenolol	ng/L	1,100	760	717	560	670
Trimethoprim	ng/L	740	650	733	91	120
Iopromide	ng/L	40	n.d.	n.q.	50	**n.d.**
Caffeine	ng/L	86,000	n.d.	n.q.	25	**n.d.**
Fluoxetine	ng/L	50	43	25	29	48
Meprobamate	ng/L	160	180	167	170	180
Carbamazepine	ng/L	220	200	220	1,400	180
Benzophenone	ng/L	490	70	n.q.	620	**130**
Primidone	ng/L	86	82	70	76	72
TCPP	ng/L	1,900	2,100	n.q.	3,300	**1,700**
DEET	ng/L	890	360	260	290	350
TCEP	ng/L	295	295	n.q.	220	**285**
Gemfibrozil	ng/L	1,500	390	577	1,050	230
Bisphenol A	ng/L	960	215	n.q.	1,400	**20**
Naproxen	ng/L	9,000	510	550	120	160
Triclosan	ng/L	2,000	100	110	870	29
BHA	ng/L	50	38	50	5	**4**
Musk Ketone	ng/L	n.q.	n.d.	n.q.	n.q.	**n.d.**
Ibuprofen	ng/L	15,000	4	457	3,150	**4**
Diphenhydramine	ng/L	950	380	500	150	190
Cimetidine	ng/L	420	300	473	585	**n.d.**
Triclocarban	ng/L	370	120	50	100	130
Acetaminophen	ng/L	150,000	n.d.	n.q.	n.q.	**n.d.**
Sucralose	ng/L	22,000	20,000	22,667	22,000	23,000

n.d.: Not detected (measured concentration at or below blank concentration.
n.q.: Not quantifiable (measured concentration below reporting limit, reporting limit > 100 ng/L).
Bold values: Concentrations for which background concentrations were relevant / Blank corrected concentrations.

E.4.2 Facility A, Summer

Table E-31. Facility A, Summer (Aqueous Phase), Background Corrected TOrC Results.

Date Collected		7/14/2011	7/14/2011	7/14/2011	7/14/2011	7/14/2011
A - Summer Sub Location		Aeration Basin Influent (Average)	Secondary Effluent	RAS Aqueous Phase (Average)	Centrate	Final Effluent
Sulfamethoxazole	ng/L	715	740	697	120	220
Atenolol	ng/L	740	500	257	290	510
Trimethoprim	ng/L	435	380	313	15	130
Iopromide	ng/L	40	n.d.	n.q.	50	**n.d.**
Caffeine	ng/L	58,500	41	n.q.	25	**n.d.**
Fluoxetine	ng/L	38	30	25	13	38
Meprobamate	ng/L	105	120	103	120	120
Carbamazepine	ng/L	165	140	293	3,700	140
Benzophenone	ng/L	440	120	n.q.	1,900	**130**
Primidone	ng/L	56	50	25	56	52
TCPP	ng/L	1,450	1,600	n.q.	4,400	**1,400**
DEET	ng/L	5,850	260	50	440	270
TCEP	ng/L	255	330	n.q.	160	310
Gemfibrozil	ng/L	900	120	79	1,600	100
Bisphenol A	ng/L	280	2,200	n.q.	3,000	**20**
Naproxen	ng/L	6,250	78	277	25	36
Triclosan	ng/L	1,250	57	147	690	12
BHA	ng/L	88	28	50	5	**2**
Musk Ketone	ng/L	n.q.	n.d.	n.q.	290	**n.d.**
Ibuprofen	ng/L	11,000	14	503	17,000	**4**
Diphenhydramine	ng/L	565	200	353	170	100
Cimetidine	ng/L	195	2	25	720	**n.d.**
Triclocarban	ng/L	280	76	50	55	79
Acetaminophen	ng/L	41,000	n.q.	n.q.	n.q.	**n.d.**
Sucralose	ng/L	14,500	14,000	13,667	18,000	8,900

n.d.: Not detected (measured concentration at or below blank concentration.
n.q.: Not quantifiable (measured concentration below reporting limit, reporting limit > 100 ng/L).
Bold values: Concentrations for which background concentrations were relevant / Blank corrected concentrations.

E.4.3 Facility B, Winter

Table E-32. Facility B, Winter (Aqueous Phase), Background Corrected TOrC Results.

Date Collected		2/7/2011	2/7/2011	2/7/2011	2/7/2011	2/10/2011	2/10/2011	2/7/2011	2/7/2011	2/7/2011	2/10/2011
B - Winter Sub Location		Primary Influent	Aeration Basin Influent	Anoxic Zone (Average)	Secondary Effluent	RAS Aqueous Phase (Average)	Centrate	Filter Influent	Filter Effluent	Final Effluent	Creek Above Discharge
Sulfamethoxazole	ng/L	860	790	1,100	590	967	620	230	230	5	1
Atenolol	ng/L	1,800	1,500	254	270	50	5	29	29	30	n.d.
Trimethoprim	ng/L	550	510	650	360	547	10	9	9	n.d.	n.d.
Iopromide	ng/L	40	50	40	**n.d.**	n.q.	50	n.d.	n.d.	n.d.	n.d.
Caffeine	ng/L	66,000	57,000	115	**18**	n.q.	150	21	19	14	34
Fluoxetine	ng/L	41	40	25	35	25	42	1	0	1	n.d.
Meprobamate	ng/L	120	120	140	140	157	210	150	150	140	n.d.
Carbamazepine	ng/L	110	110	140	130	137	1,600	69	69	61	n.d.
Benzophenone	ng/L	480	**650**	n.q.	**n.d.**	n.q.	630	n.d.	n.d.	n.d.	n.d.
Primidone	ng/L	67	**64**	70	**71**	69	84	45	44	41	n.d.
TCPP	ng/L	1,600	**1,045**	1,300	**1,145**	n.q.	3,000	595	545	775	410
DEET	ng/L	600	410	133	79	50	220	48	41	46	62
TCEP	ng/L	230	**245**	190	**235**	n.q.	97	225	220	225	18
Gemfibrozil	ng/L	1,500	1,300	500	74	227	2,000	9	9	6	n.d.
Bisphenol A	ng/L	260	270	25	**n.d.**	n.q.	n.q.	n.d.	n.d.	n.d.	n.d.
Naproxen	ng/L	11,000	9,000	1,950	13	207	330	n.d.	n.d.	n.d.	n.d.
Triclosan	ng/L	2,800	2,400	92	32	50	550	8	n.d.	n.d.	n.d.
BHA	ng/L	50	100	65	**4**	50	50	n.d.	n.d.	n.d.	n.d.
Musk Ketone	ng/L	n.q.	**n.q.**	n.q.	**n.d.**	n.q.	n.q.	13	n.d.	n.d.	n.q.
Ibuprofen	ng/L	11,000	9,000	2,148	**2**	50	20,000	5	n.d.	1	1
Diphenhydramine	ng/L	849	790	320	150	173	450	4	4	3	n.d.
Cimetidine	ng/L	170	180	345	76	300	1,200	n.d.	n.d.	n.d.	n.d.
Triclocarban	ng/L	520	390	87	43	50	52	n.d.	n.d.	n.d.	n.d.
Acetaminophen	ng/L	140,000	130,000	n.q.	**n.d.**	n.q.	25	n.d.	n.d.	n.d.	n.d.
Sucralose	ng/L	25,000	23,000	33,995	18,000	45,667	56,000	16,000	16,000	25,000	120

n.d.: Not detected (measured concentration at or below blank concentration.
n.q.: Not quantifiable (measured concentration below reporting limit, reporting limit > 100 ng/L).
Bold values: Concentrations for which background concentrations were relevant / Blank corrected concentrations.

E.4.4 Facility B, Summer

Table E-33. Facility B, Summer (Aqueous Phase), Background Corrected TOrC Results.

Date Collected		8/19/2010	8/19/2010	8/19/2010	8/19/2010	8/19/2010	8/19/2010	8/19/2010	8/19/2010	8/19/2010	8/23/2010
B - Summer Sub Location		Primary Influent	Landfill Leachate	Aeration Basin Influent	Secondary Effluent (Average)	RAS Aqueous Phase (Average)	Filter Influent	Filter Effluent	Final Effluent	Centrate	Creek Above Discharge
Sulfamethoxazole	ng/L	1,200	670	1,100	580	527	670	98	3	210	1
Atenolol	ng/L	1,800	5	1,800	280	160	110	2	1	5	n.d.
Trimethoprim	ng/L	640	1	580	10	26	3	n.d.	n.d.	10	n.d.
Iopromide	ng/L	40	50	50	n.d.	n.q	n.d.	n.d.	n.d.	50	n.d.
Caffeine	ng/L	66,000	25	64,000	9	n.q	26	14	16	250	34
Fluoxetine	ng/L	20	3	24	28	25	27	n.d.	0	12	n.d.
Meprobamate	ng/L	150	3	160	210	157	200	190	180	190	n.d.
Carbamazepine	ng/L	230	95	190	180	217	200	54	56	1,600	n.d.
Benzophenone	ng/L	1,020	250	1,200	80	n.q	38	n.d.	66	1,100	n.d.
Primidone	ng/L	68	3	76	63	25	78	37	43	76	n.d.
TCPP	ng/L	2,700	n.q.	2,000	2,300	n.q	1,600	1,195	1,400	4,200	410
DEET	ng/L	8,600	12	9,100	9	50	1	2	8	3,200	62
TCEP	ng/L	510	50	480	535	n.q	485	330	325	230	18
Gemfibrozil	ng/L	1,800	39	1,900	3	13	1	1	1	2,600	n.d.
Bisphenol A	ng/L	480	760	470	n.d.	n.q	n.d.	n.d.	n.d.	1,600	n.d.
Naproxen	ng/L	13,000	74	14,000	n.d.	25	n.d.	n.d.	n.d.	170	n.d.
Triclosan	ng/L	1,500	5	1,600	20	50	8	n.d.	0	670	n.d.
BHA	ng/L	140	5	140	n.d.	50	n.d.	n.d.	n.d.	5	n.d.
Musk Ketone	ng/L	n.q.	n.q.	n.q.	n.d.	n.q	n.d.	n.d.	n.d.	n.q.	n.q.
Ibuprofen	ng/L	12,000	5	14,000	4	257	n.d.	n.d.	2	16,000	1
Diphenhydramine	ng/L	1,100	3	1,000	99	127	73	1	1	190	n.d.
Cimetidine	ng/L	290	3	300	2	25	n.d.	n.d.	n.d.	640	n.d.
Triclocarban	ng/L	250	5	240	180	50	160	1	n.d.	200	n.d.
Acetaminophen	ng/L	91,000	25	98,000	n.d.	n.q	n.d.	n.d.	n.d.	25	n.d.
Sucralose	ng/L	25,000	260	25,000	27,000	22,333	23,000	24,000	25,000	36,000	120

n.d.: Not detected (measured concentration at or below blank concentration.
n.q.: Not quantifiable (measured concentration below reporting limit, reporting limit > 100 ng/L).
Bold values: Concentrations for which background concentrations were relevant / Blank corrected concentrations.

E.4.5 Facility C, Winter

Table E-34. Facility C, Winter (Aqueous Phase), Background Corrected TOrC Results.

Date Collected		3/15/2010 9:40	3/15/2010 8:45	3/15/2010 9:17	3/15/2010 8:20
C - Winter Sub Location		Secondary Influent	Mixed Liquor (Average)	RAS Aqueous Phase (Average)	Final Effluent
Sulfamethoxazole	ng/L	1,400	1,100	1,600	640
Atenolol	ng/L	2,400	2,700	2,800	3,400
Trimethoprim	ng/L	710	660	810	710
Iopromide	ng/L	40	820	n.q.	930
Caffeine	ng/L	370,000	140	n.q.	1,200
Fluoxetine	ng/L	34	15	25	48
Meprobamate	ng/L	180	180	213	180
Carbamazepine	ng/L	360	340	363	350
Benzophenone	ng/L	2,175	335	n.q.	**525**
Primidone	ng/L	170	150	143	140
TCPP	ng/L	2,050	1,800	n.q.	**1,650**
DEET	ng/L	690	690	500	640
TCEP	ng/L	400	410	n.q.	**410**
Gemfibrozil	ng/L	3,200	3,300	3,300	2,900
Bisphenol A	ng/L	420	510	n.q.	490
Naproxen	ng/L	13,000	3,800	2,767	5,500
Triclosan	ng/L	1,400	580	823	640
BHA	ng/L	370	310	50	320
Musk Ketone	ng/L	n.q.	n.q.	n.q.	**1**
Ibuprofen	ng/L	16,000	1,900	1,010	**695**
Diphenhydramine	ng/L	1,500	1,600	1,433	1,300
Cimetidine	ng/L	630	860	663	**n.d.**
Triclocarban	ng/L	180	170	50	130
Acetaminophen	ng/L	200,000	2,500	n.q.	290
Sucralose	ng/L	28,000	33,000	30,000	15,000

n.d.: Not detected (measured concentration at or below blank concentration.
n.q.: Not quantifiable (measured concentration below reporting limit, reporting limit > 100 ng/L).
Bold values: Concentrations for which background concentrations were relevant / Blank corrected concentrations.

E.4.6 Facility C, Summer

Table E-35. Facility C, Summer (Aqueous Phase), Background Corrected TOrC Results.

Date Collected		9/23/2010	9/23/2010	9/23/2010	9/23/2010
C - Summer Sub Location		Secondary Influent (Average)	Mixed Liquor	RAS Aqueous Phase (Average)	Final Effluent
Sulfamethoxazole	ng/L	1,900	1,300	1,167	1,200
Atenolol	ng/L	2,700	2,200	2,000	2,500
Trimethoprim	ng/L	780	830	640	730
Iopromide	ng/L	650	530	n.q.	480
Caffeine	ng/L	91,000	5,700	2,133	9,000
Fluoxetine	ng/L	61	56	25	58
Meprobamate	ng/L	320	330	307	330
Carbamazepine	ng/L	290	350	300	290
Benzophenone	ng/L	1,745	n.q.	n.q.	**155**
Primidone	ng/L	150	170	137	140
TCPP	ng/L	1,900	2,000	n.q.	2,100
DEET	ng/L	2,300	840	577	720
TCEP	ng/L	560	570	n.q.	550
Gemfibrozil	ng/L	3,200	3,200	3,033	2,900
Bisphenol A	ng/L	370	430	n.q.	400
Naproxen	ng/L	17,000	2,000	757	1,000
Triclosan	ng/L	2,500	870	423	760
BHA	ng/L	400	230	177	280
Musk Ketone	ng/L	n.q.	n.q.	n.q.	**16**
Ibuprofen	ng/L	18,000	1,200	213	230
Diphenhydramine	ng/L	1,700	1,600	1,100	1,400
Cimetidine	ng/L	560	670	510	**n.d.**
Triclocarban	ng/L	490	330	257	320
Acetaminophen	ng/L	140,000	n.q.	n.q.	**n.q.**
Sucralose	ng/L	27,000	28,000	27,333	25,000

n.d.: Not detected (measured concentration at or below blank concentration.
n.q.: Not quantifiable (measured concentration below reporting limit, reporting limit > 100 ng/L).
Bold values: Concentrations for which background concentrations were relevant / Blank corrected concentrations.

E.4.7 Facility D, Summer

Table E-36. Facility D, Summer (Aqueous Phase), Background Corrected TOrC Results.

Date Collected		9/16/2010	9/16/2010	9/16/2010	9/16/2010	9/16/2010	9/16/2010
D - Summer Sub Location		Secondary Influent	Secondary Effluent	RAS Aqueous Phase (Average)	Centrate	Post-Centrate Reaeration Basins (Average)	Final Effluent
Sulfamethoxazole	ng/L	1,500	1,200	963	800	2,300	1,300
Atenolol	ng/L	2,300	1,600	677	1,200	1,900	1,900
Trimethoprim	ng/L	710	680	640	350	840	670
Iopromide	ng/L	1,300	1,200	1,167	50	1,100	1,100
Caffeine	ng/L	110,000	160	n.q.	25	56,000	340
Fluoxetine	ng/L	56	51	25	3	55	55
Meprobamate	ng/L	320	340	287	480	300	340
Carbamazepine	ng/L	300	320	327	1,700	380	350
Benzophenone	ng/L	950	n.q.	n.q.	2,800	n.q.	**260**
Primidone	ng/L	150	140	110	130	160	160
TCPP	ng/L	1,900	1,800	n.q.	3,600	1,900	**1,700**
DEET	ng/L	3,100	280	50	1,500	1,900	290
TCEP	ng/L	485	535	n.q.	450	570	510
Gemfibrozil	ng/L	3,200	1,700	880	6,000	2,800	170
Bisphenol A	ng/L	440	230	n.q.	1,800	240	**n.d.**
Naproxen	ng/L	17,000	2,100	1,133	1,800	9,700	2,600
Triclosan	ng/L	3,100	270	100	1,200	510	310
BHA	ng/L	340	340	50	140	400	210
Musk Ketone	ng/L	n.q.	n.q.	n.q.	n.q.	n.q.	**n.q.**
Ibuprofen	ng/L	20,000	230	397	15,000	13,000	**239**
Diphenhydramine	ng/L	1,600	640	903	70	1,600	620
Cimetidine	ng/L	630	660	753	1,300	700	**2**
Triclocarban	ng/L	800	260	210	100	270	260
Acetaminophen	ng/L	160,000	n.q.	n.q.	25	29,000	**20**
Sucralose	ng/L	29,000	31,000	27,333	31,000	31,000	23,000

n.d.: Not detected (measured concentration at or below blank concentration.
n.q.: Not quantifiable (measured concentration below reporting limit, reporting limit > 100 ng/L).
Bold values: Concentrations for which background concentrations were relevant / Blank corrected concentrations.

E.4.8 Facility E, Winter

Table E-37. Facility E, Winter (Aqueous Phase), Background Corrected TOrC Results.

Date Collected		4/12/2010 0:00	4/12/2010 0:00	4/15/2010 0:00	4/12/2010 0:00
E - Winter Sub Location		Aeration Basin Influent (Average)	Membrane Effluent (Average)	RAS Aqueous Phase (Average)	Final Plant Effluent (after UV) (Average)
Sulfamethoxazole	ng/L	680	500	627	387
Atenolol	ng/L	2,480	216	n.d.	353
Trimethoprim	ng/L	463	26	42	25
Iopromide	ng/L	32,333	8,400	n.q.	2,300
Caffeine	ng/L	123,333	n.d.	n.q.	25
Fluoxetine	ng/L	22	26	25	11
Meprobamate	ng/L	297	63	54	61
Carbamazepine	ng/L	260	350	317	307
Benzophenone	ng/L	825	92	n.q.	**275**
Primidone	ng/L	3	n.d.	25	n.d.
TCPP	ng/L	1,867	883	n.q.	**847**
DEET	ng/L	433	15	50	16
TCEP	ng/L	357	430	n.q.	420
Gemfibrozil	ng/L	303	4	13	3
Bisphenol A	ng/L	417	n.d.	n.q.	**n.d.**
Naproxen	ng/L	12,667	4	66	15
Triclosan	ng/L	1,133	10	50	2
BHA	ng/L	227	15	50	**12**
Musk Ketone	ng/L	n.q.	n.d.	n.q.	**n.d.**
Ibuprofen	ng/L	29,000	4	50	**4**
Diphenhydramine	ng/L	1,200	60	70	46
Cimetidine	ng/L	347	113	317	75
Triclocarban	ng/L	507	220	263	69
Acetaminophen	ng/L	160,000	n.q.	n.q.	**n.q.**
Sucralose	ng/L	28,000	45,000	82,000	76,667

n.d.: Not detected (measured concentration at or below blank concentration.
n.q.: Not quantifiable (measured concentration below reporting limit, reporting limit > 100 ng/L).
Bold values: Concentrations for which background concentrations were relevant / Blank corrected concentrations.

E.4.9 Facility E, Summer

Table E-38. Facility E, Summer (Aqueous Phase), Background Corrected TOrC Results.

Date Collected		8/26/2010	8/26/2010	8/26/2010	8/26/2010
E - Summer Sub Location		Aeration Basin Influent (Average)	Membrane Effluent	RAS Aqueous Phase (Average)	Final Plant Effluent (after UV)
Sulfamethoxazole	ng/L	2,100	940	1,100	860
Atenolol	ng/L	2,300	160	50	150
Trimethoprim	ng/L	990	66	31	51
Iopromide	ng/L	40	n.d.	n.q.	**n.d.**
Caffeine	ng/L	120,000	5	n.q.	25
Fluoxetine	ng/L	35	23	25	13
Meprobamate	ng/L	290	130	223	140
Carbamazepine	ng/L	500	380	363	350
Benzophenone	ng/L	819	3	n.q.	**79**
Primidone	ng/L	21	n.d.	25	**15**
TCPP	ng/L	2,200	1,300	n.q.	**1,200**
DEET	ng/L	15,000	22	50	21
TCEP	ng/L	790	940	n.q.	960
Gemfibrozil	ng/L	3,500	7	42	6
Bisphenol A	ng/L	550	n.d.	n.q.	**n.d.**
Naproxen	ng/L	11,000	23	133	19
Triclosan	ng/L	2,500	33	50	13
BHA	ng/L	240	27	50	22
Musk Ketone	ng/L	n.q.	n.d.	n.q.	**n.d.**
Ibuprofen	ng/L	15,000	3	50	**n.d.**
Diphenhydramine	ng/L	1,200	82	107	74
Cimetidine	ng/L	25	22	25	18
Triclocarban	ng/L	1,100	260	50	140
Acetaminophen	ng/L	160,000	n.d.	n.q.	**n.d.**
Sucralose	ng/L	34,000	28,000	50,000	39,000

n.d.: Not detected (measured concentration at or below blank concentration.
n.q.: Not quantifiable (measured concentration below reporting limit, reporting limit > 100 ng/L).
Bold values: Concentrations for which background concentrations were relevant / Blank corrected concentrations.

E.4.10 Facility F, Winter

Table E-39. Facility F, Winter (Aqueous Phase), Background Corrected TOrC Results.

Date Collected		4/29/2010 0:00	4/29/2010 0:00	4/29/2010 0:00	4/29/2010 0:00
F - Winter Sub Location*		Primary Clarifier Influent (Average)	Aeration Basin Influent	Secondary Effluent	RAS Aqueous Phase (Average)
Sulfamethoxazole	ng/L	1,600	1,500	2,800	1,800
Atenolol	ng/L	2,367	2,900	1,900	787
Trimethoprim	ng/L	593	570	510	383
Iopromide	ng/L	217	140	50	n.q.
Caffeine	ng/L	82,333	75,000	59	n.q.
Fluoxetine	ng/L	12	8	16	25
Meprobamate	ng/L	350	330	420	430
Carbamazepine	ng/L	233	250	260	200
Benzophenone	ng/L	3,100	3,000	710	n.q.
Primidone	ng/L	143	130	120	107
TCPP	ng/L	1,633	1,400	1,700	n.q.
DEET	ng/L	453	500	350	203
TCEP	ng/L	393	410	410	n.q.
Gemfibrozil	ng/L	4,400	4,700	810	1,533
Bisphenol A	ng/L	660	1,000	170	n.q.
Naproxen	ng/L	11,667	13,000	150	410
Triclosan	ng/L	637	870	110	50
BHA	ng/L	117	50	110	50
Musk Ketone	ng/L	n.q.	n.q.	n.q.	n.q.
Ibuprofen	ng/L	16,667	13,000	5	337
Diphenhydramine	ng/L	1,100	860	520	860
Cimetidine	ng/L	603	420	260	307
Triclocarban	ng/L	90	69	110	50
Acetaminophen	ng/L	140,000	120,000	25	n.q.
Sucralose	ng/L	47,667	29,000	22,000	22,667

n.d.: Not detected (measured concentration at or below blank concentration.
n.q.: Not quantifiable (measured concentration below reporting limit, reporting limit > 100 ng/L).
Bold values: Concentrations for which background concentrations were relevant / Blank corrected concentrations.
*No Rinse blank sample collected at this sampling event. Therefore, correction for blank concentrations was not performed.

E.4.11 Facility G, Low, Medium, and High SRT

Table E-40. Facility G – Low, Medium, and High SRT (Aqueous Phase), Background Corrected TOrC Results.

Date Collected		1/17/1011	1/17/1011	1/17/1011	1/19/2011	1/17/2011	1/19/2011	1/17/2011	1/19/2011
G High, Low, Medium SRT Sub Location		Primary Influent Aqueous Phase	Secondary Influent High SRT (Average)	Secondary Effluent High SRT	RAS Aqueous Phase High SRT (Average)	Secondary Effluent Low SRT	RAS Aqueous Phase Low SRT (Average)	Secondary Effluent Medium SRT (Average)	RAS Aqueous Phase Medium SRT (Average)
Sulfamethoxazole	ng/L	1,600	1,200	1,700	1,367	2,500	1,700	2,300	1,567
Atenolol	ng/L	1,730	1,480	n.d.	50	**710**	573	**n.d.**	50
Trimethoprim	ng/L	830	800	14	13	620	527	24	13
Iopromide	ng/L	40	40	n.d.	n.q.	**n.d.**	n.q.	**n.d.**	n.q.
Caffeine	ng/L	120,000	110,000	4	250	**6**	n.q.	**30**	n.q.
Fluoxetine	ng/L	45	39	24	110	27	25	26	25
Meprobamate	ng/L	1,200	1,350	130	44	1,200	1,023	140	110
Carbamazepine	ng/L	93	120	140	190	130	197	140	193
Benzophenone	ng/L	760	715	n.d.	n.q.	**120**	n.q.	**4**	n.q.
Primidone	ng/L	140	125	130	133	130	123	130	127
TCPP	ng/L	2,100	1,350	1,400	n.q.	**1,400**	n.q.	**1,600**	n.q.
DEET	ng/L	200	190	40	50	180	173	71	50
TCEP	ng/L	440	330	280	n.q.	**290**	n.q.	**290**	n.q.
Gemfibrozil	ng/L	2,900	2,850	14	105	470	327	55	213
Bisphenol A	ng/L	440	445	n.d.	n.q.	**n.d.**	n.q.	**n.d.**	n.q.
Naproxen	ng/L	21,000	18,500	3	108	300	107	**5**	130
Triclosan	ng/L	1,400	1,150	30	50	150	210	86	50
BHA	ng/L	240	260	1	50	130	50	**2**	50
Musk Ketone	ng/L	100	n.q.	n.d.	n.q.	**n.d.**	n.q.	**n.d.**	n.q.
Ibuprofen	ng/L	23,000	21,500	12	173	**52**	110	**4**	210
Diphenhydramine	ng/L	1,600	1,500	55	106	880	1,100	53	88
Cimetidine	ng/L	550	405	350	2,633	470	843	300	1,333
Triclocarban	ng/L	160	135	28	50	43	50	36	50
Acetaminophen	ng/L	250,000	245,000	n.d.	n.q.	**n.d.**	n.q.	**n.d.**	n.q.
Sucralose	ng/L	32,000	29,500	29,000	39,000	36,000	32,333	37,000	36,667

n.d.: Not detected (measured concentration at or below blank concentration.
n.q.: Not quantifiable (measured concentration below reporting limit, reporting limit > 100 ng/L).
Bold values: Concentrations for which background concentrations were relevant / Blank corrected concentrations.

E.5 TOrC Mass Balances for Secondary Treatment

E.5.1 Facility A, Winter

Table E-41. Facility A, Winter, TOrC Mass Balance, Secondary Treatment.

	Total IN (ABI)	Total OUT (SE+WAS)		Overall Removal		Removal by Degradation		Removal by	MB
	Liquid	Liquid	Solids	Sec Inf-Sec Eff.[1)]		in Secondary Treatment[2)]		Sorption[3)]	Error
A - Winter	gram per day	gram per day	gram per day	%	gram per day	%	gram per day	%	%
Sulfamethoxazole	68	73	0.5	-4%	-3	-9%	-6	0.7%	-104%
Atenolol	62	43	0.1	34%	21	31%	19	0.2%	8%
Trimethoprim	42	37	0.8	15%	6	10%	4	1.9%	24%
Iopromide	2	n.q	n.q	n.q	n.q	n.q	n.q	n.q	n.q
Caffeine	4,848	n.q	1.9	n.q	n.q	n.q	n.q	0.0%	n.q
Fluoxetine	3	2	0.4	15%	0	0%	0	15.7%	-3%
Meprobamate	9	10	0.0	-8%	-1	-12%	-1	0.2%	-52%
Carbamazepine	12	11	0.0	13%	2	8%	1	0.3%	31%
Benzophenone	28	n.q	n.q	n.q	n.q	n.q	n.q	n.q	n.q
Primidone	5	5	0.0	9%	0	5%	0	0.4%	36%
TCPP	107	n.q	n.q	n.q	n.q	n.q	n.q	n.q	n.q
DEET	50	20	0.0	61%	31	60%	30	0.0%	2%
TCEP	17	n.q	n.q	n.q	n.q	n.q	n.q	n.q	n.q
Gemfibrozil	85	22	0.2	75%	63	73%	62	0.2%	2%
Bisphenol A	54	n.q	n.q	n.q	n.q	n.q	n.q	n.q	n.q
Naproxen	507	29	0.4	95%	480	94%	478	0.1%	0%
Triclosan	113	6	9.3	94%	106	87%	98	8.2%	-1%
BHA	3	2	0.1	26%	1	19%	1	4.2%	13%
Musk Ketone	n.q	n.q	n.q	n.q	n.q	n.q	n.q	n.q	n.q
Ibuprofen	846	1	0.3	100%	845	100%	844	0.0%	0%
Diphenhydramine	54	22	1.0	61%	33	58%	31	1.9%	3%
Cimetidine	24	17	0.4	31%	7	25%	6	1.9%	14%
Triclocarban	21	7	31.6	45%	9	-83%	-17	151.4%	-52%
Acetaminophen	8,455	n.q	0.1	100%	8,428	n.q	n.q	0.0%	n.q
Sucralose	1,240	1133	n.q	n.q	n.q	n.q	n.q	n.q	n.q

Notes:

n.q.: not quantifiable as measured concentration below the reporting limit and reporting limit larger than 100 ng/L for aqueous phase analysis or 100 ng/g for solid phase analysis in RAS.

1) Negative values indicate that the calculated TOrC mass in the secondary effluent was higher compared to the TOrC mass in the secondary influent.

2) Negative values indicate an overall calculated gain of the TOrC during secondary treatment during the sampling period.

3) Percentages significantly higher than 100 percent resulting in high overall MB errors indicate an accumulation of TOrC on solids in RAS beyond the solid / liquid phase equilibrium during the sampling phase.

E.5.2 Facility A, Summer

Table E-42. Facility A, Summer, TOrC Mass Balance, Secondary Treatment.

	Total IN (ABI)	Total OUT (SE+WAS)		Overall Removal		Removal by Biotransformation in Secondary Treatment2)		Removal by Sorption3)	MB Error
	Liquid	Liquid	Solids	Sec Inf-Sec Eff.1)					
A - Summer	gram per day	gram per day	gram per day	%	gram per day	%	gram per day	%	%
Sulfamethoxazole	54	49	0.2	12%	6	9%	5	0.4%	16%
Atenolol	56	33	0.0	42%	24	42%	23	0.0%	2%
Trimethoprim	33	25	n.q	n.q	n.q	n.q	n.q	n.q	n.q
Iopromide	3	n.q	n.q	n.q	n.q	n.q	n.q	n.q	n.q
Caffeine	4,404	n.q	0.4	100%	4,401	n.q	n.q	0.0%	n.q
Fluoxetine	3	2	0.0	33%	1	31%	1	0.3%	4%
Meprobamate	8	8	0.0	2%	0	0%	0	0.2%	83%
Carbamazepine	12	9	0.0	27%	3	24%	3	0.3%	13%
Benzophenone	33	n.q	n.q	n.q	n.q	n.q	n.q	n.q	n.q
Primidone	4	3	0.0	23%	1	22%	1	0.2%	4%
TCPP	109	n.q	n.q	n.q	n.q	n.q	n.q	n.q	n.q
DEET	440	17	0.0	96%	424	96%	424	0.0%	0%
TCEP	19	n.q	n.q	n.q	n.q	n.q	n.q	n.q	n.q
Gemfibrozil	68	8	0.1	89%	60	88%	60	0.1%	0%
Bisphenol A	21	n.q	n.q	n.q	n.q	n.q	n.q	n.q	n.q
Naproxen	471	5	0.0	99%	465	99%	465	0.0%	0%
Triclosan	94	4	1.9	96%	90	94%	88	2.0%	0%
BHA	7	2	0.1	73%	5	71%	5	0.9%	1%
Musk Ketone	n.q	n.q	n.q	n.q	n.q	n.q	n.q	n.q	n.q
Ibuprofen	828	2	0.1	100%	827	100%	826	0.0%	0%
Diphenhydramine	43	13	0.2	70%	30	68%	29	0.5%	2%
Cimetidine	15	0	0.1	99%	15	98%	14	0.7%	0%
Triclocarban	21	5	18.5	63%	13	-11%	-2	87.6%	-21%
Acetaminophen	3,087	n.q	0.1	99%	3,054	n.q	n.q	0.0%	n.q
Sucralose	1,092	921	n.q	n.q	n.q	n.q	n.q	n.q	n.q

Notes:
n.q.: not quantifiable as measured concentration below the reporting limit and reporting limit larger than 100 ng/L for aqueous phase analysis or 100 ng/g for solid phase analysis in RAS.
1) Negative values indicate that the calculated TOrC mass in the secondary effluent was higher compared to the TOrC mass in the secondary influent.
2) Negative values indicate an overall calculated gain of the TOrC during secondary treatment during the sampling period.
3) Percentages significantly higher than 100 percent resulting in high overall MB errors indicate an accumulation of TOrC on solids in RAS beyond the solid / liquid phase equilibrium during the sampling phase.

E.5.3 Facility B, Winter

Table E-43. Facility B, Winter, TOrC Mass Balance, Secondary Treatment.

	Total IN (ABI)		Total OUT (SE+WAS)		Overall Removal		Removal by Biotransformation		Removal by	MB
	Liquid	Solids	Liquid	Solids	Sec Inf-Sec Eff.[1)]		in Secondary Treatment[2)]		Sorption[3)]	Error
B - Winter	gram per day	gram per day	gram per day	gram per day	%	gram per day	%	gram per day	%	%
Sulfamethoxazole	119	0.0	91	2.9	25%	29	21%	25	2.5%	6%
Atenolol	226	0.0	41	0.1	82%	185	82%	185	0.0%	0%
Trimethoprim	77	0.0	56	2.7	29%	22	24%	18	3.5%	5%
Iopromide	8	0.0	n.q	0.9	99%	7	88%	7	12.3%	-1%
Caffeine	8,582	204.8	n.q	16.7	100%	8,578	100%	8,770	0.2%	0%
Fluoxetine	6	0.0	5	1.5	10%	1	-13%	-1	24.1%	-6%
Meprobamate	18	0.0	22	0.0	-17%	-3	-19%	-3	0.2%	-11%
Carbamazepine	17	0.0	20	0.2	-19%	-3	-22%	-4	1.3%	-9%
Benzophenone	98	0.0	n.q	6.7	22%	22	93%	91	6.8%	-350%
Primidone	10	0.0	11	0.0	-12%	-1	-13%	-1	0.3%	-13%
TCPP	157	0.0	n.q	5.8	-10%	-16	96%	152	3.7%	1065%
DEET	62	0.0	12	NA	81%	50	80%	50	n.q	n.q
TCEP	37	0.0	n.q	0.6	4%	1	98%	36	1.6%	-2753%
Gemfibrozil	196	0.0	11.7	0.8	94%	184	94%	183	0.4%	0%
Bisphenol A	41	0.0	n.q	4.3	99%	40	89%	36	10.7%	-1%
Naproxen	1,355	0.0	2.4	1.6	100%	1,353	100%	1,351	0.1%	0%
Triclosan	361	281.6	5	17.0	99%	355	97%	621	4.7%	-2%
BHA	15	0.0	0.8	0.2	95%	14	94%	14	1.1%	1%
Musk Ketone	n.q	0.0	n.q	20.9	n.q	n.q	n.q	n.q	n.q	n.q
Ibuprofen	1,355	0.0	0	0.1	100%	1,355	100%	1,355	0.0%	0%
Diphenhydramine	119	5.6	23	2.4	82%	96	80%	99	2.0%	0%
Cimetidine	27	0.0	12	1.0	57%	16	51%	14	3.8%	4%
Triclocarban	59	217.6	7	67.3	96%	48	73%	202	114.6%	-96%
Acetaminophen	19,573	0.0	n.q	0.2	100%	19,498	n.q	19,573	0.0%	n.q
Sucralose	3,463	0.0	2822	9.3	21%	739	18%	631	0.3%	13%

Notes:
n.q.: not quantifiable as measured concentration below the reporting limit and reporting limit larger than 100 ng/L for aqueous phase analysis or 100 ng/g for solid phase analysis in RAS.
1) Negative values indicate that the calculated TOrC mass in the secondary effluent was higher compared to the TOrC mass in the secondary influent.
2) Negative values indicate an overall calculated gain of the TOrC during secondary treatment during the sampling period.
3) Percentages significantly higher than 100 percent resulting in high overall MB errors indicate an accumulation of TOrC on solids in RAS during the sampling phase.
RAS solid phase concentrations below the reporting limit were assumed as one half of the reporting limit for mass balance calculations.

E.5.4 Facility B, Summer

Table E-44. Facility B, Summer, TOrC Mass Balance, Secondary Treatment.

	Total IN (ABI)		Total OUT (SE+WAS)		Overall Removal		Removal by Biotransformation		Removal by	MB
	Liquid	Solids	Liquid	Solids	Sec Inf-Sec Eff.[1)]		in Secondary Treatment[2)]		Sorption[3)]	Error
B - Summer	gram per day	gram per day	gram per day	gram per day	%	gram per day	%	gram per day	%	%
Sulfamethoxazole	151	0.0	83	0.7	45%	69	45%	67	0.5%	1%
Atenolol	248	0.0	40	0.1	84%	208	84%	208	0.0%	0%
Trimethoprim	80	0.0	1	0.7	98%	78	97%	78	0.8%	0%
Iopromide	7	0.0	n.q	1.1	99%	7	n.q	n.q	15.9%	n.q
Caffeine	8,813	8.3	n.q	1.5	100%	8,812	n.q	n.q	0.0%	n.q
Fluoxetine	3	0.0	4	0.3	-22%	-1	-32%	-1	10.1%	-1%
Meprobamate	22	0.0	30	0.0	-36%	-8	-37%	-8	0.2%	-2%
Carbamazepine	26	0.0	26	0.1	2%	0	0%	0	0.5%	47%
Benzophenone	165	0.0	n.q	3.3	57%	94	n.q	n.q	2.0%	n.q
Primidone	10	0.0	9	0.0	14%	1	14%	1	0.3%	2%
TCPP	275	0.0	n.q	6.6	-19%	-53	n.q	n.q	2.4%	n.q
DEET	1,253	0.0	1	NA	100%	1,252	100%	1,252	n.q	n.q
TCEP	66	0.0	n.q	0.7	-15%	-10	n.q	n.q	1.0%	n.q
Gemfibrozil	262	1.2	0.4	0.2	100%	261	100%	262	0.1%	0%
Bisphenol A	65	0.0	n.q	17.5	98%	64	n.q	n.q	27.1%	n.q
Naproxen	1,928	0.0	0.0	0.1	100%	1,928	100%	1,928	0.0%	0%
Triclosan	220	286.4	3	6.5	99%	217	98%	497	3.0%	-2%
BHA	19	0.0	0.1	0.2	100%	19	99%	19	1.0%	0%
Musk Ketone	n.q	0.0	n.q	23.6	n.q	n.q	n.q	n.q	n.q	n.q
Ibuprofen	1,928	0.0	1	0.3	100%	1,927	100%	1,927	0.0%	0%
Diphenhydramine	138	8.7	14	0.8	90%	123	90%	131	0.6%	0%
Cimetidine	41	0.0	0	0.4	99%	41	98%	41	0.9%	0%
Triclocarban	33	300.2	26	64.7	91%	3	73%	243	195.8%	-195%
Acetaminophen	13,495	0.0	n.q	0.2	99%	13,423	n.q	n.q	0.0%	n.q
Sucralose	3,443	0.0	3875	1.1	-12%	-408	-13%	-434	0.0%	-6%

Notes:
n.q.: not quantifiable as measured concentration below the reporting limit and reporting limit larger than 100 ng/L for aqueous phase analysis or 100 ng/g for solid phase analysis in RAS.
1) Negative values indicate that the calculated TOrC mass in the secondary effluent was higher compared to the TOrC mass in the secondary influent.
2) Negative values indicate an overall calculated gain of the TOrC during secondary treatment during the sampling period.
3) Percentages significantly higher than 100 percent resulting in high overall MB errors indicate an accumulation of TOrC on solids in RAS during the sampling phase.
RAS solid phase concentrations below the reporting limit were assumed as one half of the reporting limit for mass balance calculations.

E.5.5 Facility C, Winter

Table E-45. Facility C, Winter , TOrC Mass Balance, Secondary Treatment.

	Total IN	Total OUT		Overall Removal		Removal by Biotransformation in Secondary Treatment[2)]		Removal by Sorption[3)]	MB Error
	Liquid	Liquid	Solids	Sec Inf-Sec Eff.[1)]					
C - Winter	gram per day	gram per day	gram per day	%	gram per day	%	gram per day	%	%
Sulfamethoxazole	354	281	1.3	23%	82	20%	72	0.4%	10%
Atenolol	607	684	1.2	-10%	-62	-13%	-78	0.2%	-24%
Trimethoprim	180	168	1.8	9%	16	6%	10	1.0%	26%
Iopromide	10	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q
Caffeine	93,641	n.q.	3.2	100%	93,606	n.q.	n.q.	0.0%	n.q
Fluoxetine	9	4	1.6	55%	5	36%	3	18.8%	-1%
Meprobamate	46	46	0.1	2%	1	-1%	0	0.1%	119%
Carbamazepine	91	86	0.4	7%	7	5%	5	0.4%	28%
Benzophenone	550	n.q.	18.3	85%	465	n.q.	n.q.	3.3%	n.q
Primidone	43	38	0.1	14%	6	12%	5	0.1%	13%
TCPP	519	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q
DEET	175	174	n.q.	2%	4	n.q.	n.q.	n.q.	n.q
TCEP	101	n.q.	1.5	-1%	-1	n.q.	n.q.	1.5%	n.q
Gemfibrozil	810	835	2.5	-1%	-8	-3%	-28	0.3%	-213%
Bisphenol A	106	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q
Naproxen	3,290	956	2.0	71%	2,348	71%	2,332	0.1%	1%
Triclosan	354	148	116.9	56%	198	25%	89	33.0%	-4%
BHA	94	77	1.7	18%	17	16%	15	1.8%	0%
Musk Ketone	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q
Ibuprofen	4,049	476	1.3	88%	3,578	88%	3,572	0.0%	0%
Diphenhydramine	380	404	6.4	-5%	-18	-8%	-31	1.7%	-39%
Cimetidine	159	217	0.6	-34%	-54	-36%	-58	0.4%	-6%
Triclocarban	46	42	161.0	-31%	-14	-346%	-158	353.4%	123%
Acetaminophen	50,617	n.q.	0.5	99%	49,997	n.q.	n.q.	0.0%	n.q
Sucralose	7,086	8336	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q

Notes:

n.q.: not quantifiable as measured concentration below the reporting limit and reporting limit larger than 100 ng/L for aqueous phase analysis or 100 ng/g for solid phase analysis in RAS.

1) Negative values indicate that the calculated TOrC mass in the secondary effluent was higher compared to the TOrC mass in the secondary influent.

2) Negative values indicate an overall calculated gain of the TOrC during secondary treatment during the sampling period.

3) Percentages significantly higher than 100 percent resulting in high overall MB errors indicate an accumulation of TOrC on solids in RAS during the sampling phase.

RAS solid phase concentrations below the reporting limit were assumed as one half of the reporting limit for mass balance calculations.

E.5.6 Facility C, Summer

Table E-46. Facility C, Summer, TOrC Mass Balance, Secondary Treatment.

	Total IN		Total OUT		Overall Removal		Removal by Biotransformation		Removal by	MB
	Liquid	Solids	Liquid	Solids	Sec Inf-Sec Eff.[1)]		in Secondary Treatment[2)]		Sorption[3)]	Error
C - Summer	gram per day	gram per day	gram per day	gram per day	%	gram per day	%	gram per day	%	%
Sulfamethoxazole	393	0.0	262	0.7	36%	141	33%	130	0.2%	7%
Atenolol	559	0.0	444	0.7	24%	133	20%	114	0.1%	14%
Trimethoprim	161	0.0	167	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Iopromide	135	0.0	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Caffeine	18,831	0.0	1123	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Fluoxetine	13	0.0	11	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Meprobamate	66	0.0	67	0.4	3%	2	-1%	-1	0.6%	121%
Carbamazepine	60	0.0	71	0.7	-13%	-8	-19%	-11	1.2%	-34%
Benzophenone	361	0.0	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Primidone	31	0.0	34	0.4	-6%	-2	-11%	-4	1.2%	-64%
TCPP	393	0.0	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
DEET	476	0.0	168	0.0	66%	313	65%	308	0.0%	n.q.
TCEP	116	0.0	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Gemfibrozil	662	0.0	647	3.0	6%	42	2%	12	0.5%	65%
Bisphenol A	77	0.0	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Naproxen	3,518	0.0	394	0.9	89%	3,130	89%	3,123	0.0%	0%
Triclosan	517	505.9	172	159.3	83%	848	68%	692	30.8%	-19%
BHA	83	0.0	46	2.1	46%	38	42%	34	2.6%	4%
Musk Ketone	52	0.0	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Ibuprofen	3,725	0.0	234	1.5	94%	3,492	94%	3,489	0.0%	0%
Diphenhydramine	352	24.3	320	6.8	18%	66	13%	49	1.9%	14%
Cimetidine	116	0.0	134	1.3	-12%	-14	-17%	-20	1.1%	-33%
Triclocarban	101	438.5	66	153.4	87%	469	59%	320	151.3%	-142%
Acetaminophen	28,970	0.0	n.q.	2.5	100%	28,873	100%	28,968	0.0%	0%
Sucralose	5,587	0.0	5672	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.

Notes:
n.q.: not quantifiable as measured concentration below the reporting limit and reporting limit larger than 100 ng/L for aqueous phase analysis or 100 ng/g for solid phase analysis in RAS.
1) Negative values indicate that the calculated TOrC mass in the secondary effluent was higher compared to the TOrC mass in the secondary influent.
2) Negative values indicate an overall calculated gain of the TOrC during secondary treatment during the sampling period.
3) Percentages significantly higher than 100 percent resulting in high overall MB errors indicate an accumulation of TOrC on solids in RAS during the sampling phase.
RAS solid phase concentrations below the reporting limit were assumed as one half of the reporting limit for mass balance calculations.

E.5.7 Facility D, W

Table E-47. Facility D, Summer, TOrC Mass Balance, Secondary Treatment.

	Total IN		Total OUT		Overall Removal		Removal by Biotransformation		Removal by	MB
	Liquid	Solids	Liquid	Solids	Sec Inf-Sec Eff.[1]		in Secondary Treatment[2]		Sorption[3]	Error
D - Summer	gram per day	gram per day	gram per day	gram per day	%	gram per day	%	gram per day	%	%
Sulfamethoxazole	476	0.0	381	1.7	21%	99	20%	93	0.4%	4%
Atenolol	730	0.0	505	0.2	31%	228	31%	225	0.0%	1%
Trimethoprim	225	0.0	216	4.9	5%	10	2%	4	2.2%	14%
Iopromide	409	0.0	382	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Caffeine	34,622	0.0	53	5.9	100%	34,570	100%	34,564	0.0%	0%
Fluoxetine	18	0.0	16	4.6	2%	0	-18%	-3	26.2%	-356%
Meprobamate	103	0.0	108	0.1	-3%	-4	-5%	-5	0.1%	-36%
Carbamazepine	103	0.0	102	0.6	3%	3	1%	1	0.6%	47%
Benzophenone	314	0.0	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Primidone	48	0.0	44	0.1	8%	4	7%	3	0.3%	12%
TCPP	617	0.0	611	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
DEET	984	0.0	88	0.0	91%	896	91%	896	0.0%	0%
TCEP	155	0.0	173	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Gemfibrozil	1,039	0.0	538	1.8	49%	505	48%	499	0.2%	1%
Bisphenol A	148	0.0	74	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Naproxen	5,360	0.0	665	1.8	88%	4,700	88%	4,694	0.0%	0%
Triclosan	982	513.7	85	53.3	93%	1,396	91%	1,357	5.4%	-3%
BHA	108	0.0	107	0.7	1%	1	0%	0	0.7%	3%
Musk Ketone	n.q.	0.0	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Ibuprofen	6,374	0.0	74	1.6	99%	6,302	99%	6,299	0.0%	0%
Diphenhydramine	504	29.6	205	13.6	62%	329	59%	315	2.7%	0%
Cimetidine	205	0.0	211	3.6	-2%	-3	-4%	-9	1.7%	-78%
Triclocarban	252	392.8	83	114.8	82%	531	69%	448	45.5%	-40%
Acetaminophen	50,360	0.0	n.q.	0.8	n.q.	n.q.	100%	50,359	0.0%	n.q.
Sucralose	9,292	0.0	9858	n.q.	n.q.	n.q.	-6%	-566	n.q.	n.q.

Notes:

n.q.: not quantifiable as measured concentration below the reporting limit and reporting limit larger than 100 ng/L for aqueous phase analysis or 100 ng/g for solid phase analysis in RAS.

1) Negative values indicate that the calculated TOrC mass in the secondary effluent was higher compared to the TOrC mass in the secondary influent.

2) Negative values indicate an overall calculated gain of the TOrC during secondary treatment during the sampling period.

3) Percentages significantly higher than 100 percent resulting in high overall MB errors indicate an accumulation of TOrC on solids in RAS during the sampling phase.

RAS solid phase concentrations below the reporting limit were assumed as one half of the reporting limit for mass balance calculations.

E.5.8 Facility E, Winter

Table E-48. Facility E, Winter, TOrC Mass Balance, Secondary Treatment.

	Total IN		Total OUT		Overall Removal		Removal by Biotransformation		Removal by Sorption[3)]	MB Error
	Liquid	Solids	Liquid	Solids	Sec Inf-Sec Eff.[1)]		in Secondary Treatment[2)]			
E - Winter	gram per day	gram per day	gram per day	gram per day	%	gram per day	%	gram per day	%	%
Sulfamethoxazole	0.83	0.000	0.341	0.123	61.2%	0.506	43.9%	0.36	14.9%	4%
Atenolol	0.90	0.000	0.056	0.004	94.0%	0.850	93.3%	0.84	0.4%	0%
Trimethoprim	0.39	0.000	0.023	0.041	94.2%	0.367	83.6%	0.33	10.5%	0%
Iopromide	0.04	0.000	0.022	0.066	91.1%	0.036	-124.3%	-0.05	167.6%	52%
Caffeine	47.21	0.051	0.011	0.119	100.0%	47.210	99.7%	47.13	0.3%	0%
Fluoxetine	0.01	0.000	0.009	0.035	42.7%	0.006	-217.2%	-0.03	253.5%	15%
Meprobamate	0.11	0.000	0.048	0.003	61.2%	0.070	55.3%	0.06	2.2%	6%
Carbamazepine	0.20	0.000	0.136	0.018	34.2%	0.067	21.8%	0.04	8.9%	10%
Benzophenone	0.32	0.000	0.096	0.330	99.5%	0.321	-32.0%	-0.10	102.3%	29%
Primidone	0.01	0.000	n.q.	0.002	n.q.	n.q.	74.2%	0.01	25.8%	n.q.
TCPP	0.87	0.000	0.632	0.898	48.7%	0.421	-76.8%	-0.66	103.8%	45%
DEET	5.90	0.000	0.009	NA	99.9%	5.894	99.8%	5.89	NA	n.q.
TCEP	0.31	0.000	0.339	0.061	-3.0%	-0.009	-28.6%	-0.09	19.5%	-201%
Gemfibrozil	1.38	0.000	0.003	0.004	99.8%	1.375	99.5%	1.37	0.3%	0%
Bisphenol A	0.22	0.000	0.011	0.310	99.0%	0.214	-48.5%	-0.11	143.4%	4%
Naproxen	4.33	0.000	0.010	0.005	99.8%	4.320	99.6%	4.31	0.1%	0%
Triclosan	0.98	0.721	0.013	0.284	98.8%	0.972	69.8%	1.41	28.9%	0%
BHA	0.09	0.000	0.011	0.012	90.2%	0.085	75.5%	0.07	12.7%	2%
Musk Ketone	0.10	0.000	0.056	1.454	88.8%	0.087	-1435.2%	-1.41	1478.5%	51%
Ibuprofen	5.90	0.000	0.005	0.010	99.9%	5.898	99.7%	5.89	0.2%	0%
Diphenhydramine	0.47	0.027	0.030	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Cimetidine	0.02	0.000	0.008	0.019	61.8%	0.012	-41.1%	-0.01	98.2%	8%
Triclocarban	0.43	1.320	0.090	3.420	79.4%	0.344	-711.2%	-1.76	790.3%	0%
Acetaminophen	62.95	0.000	0.011	0.014	100.0%	62.948	100.0%	62.92	0.0%	0%
Sucralose	13.38	0.000	10.479	0.679	28.7%	3.842	16.6%	2.22	5.1%	25%

Notes:
n.q.: not quantifiable as measured concentration below the reporting limit and reporting limit larger than 100 ng/L for aqueous phase analysis or 100 ng/g for solid phase analysis in RAS.
1) Negative values indicate that the calculated TOrC mass in the secondary effluent was higher compared to the TOrC mass in the secondary influent.
2) Negative values indicate an overall calculated gain of the TOrC during secondary treatment during the sampling period.
3) Percentages significantly higher than 100 percent resulting in high overall MB errors indicate an accumulation of TOrC on solids in RAS during the sampling phase.
RAS solid phase concentrations below the reporting limit were assumed as one half of the reporting limit for mass balance calculations.

E.5.9 Facility E, Summer

Table E-49. Facility E, Summer, TOrC Mass Balance, Secondary Treatment.

	Total IN	Total OUT		Overall Removal		Removal by Biotransformation		Removal by	MB
	Liquid	Liquid	Solids	Sec Inf-Sec Eff.[1)]		in Secondary Treatment[2)]		Sorption[3)]	Error
E - Summer	gram per day	gram per day	gram per day	%	gram per day	%	gram per day	%	%
Sulfamethoxazole	0.28	0.169	0.033	42.9%	0.118	26.6%	0.07	12.0%	10%
Atenolol	1.00	n.q.	0.003	93.2%	0.936	n.q.	n.q.	0.3%	n.q.
Trimethoprim	0.19	0.009	0.005	95.6%	0.179	92.4%	0.17	2.8%	0%
Iopromide	13.09	n.q.	0.008	79.8%	10.450	n.q.	n.q.	0.1%	n.q.
Caffeine	49.92	n.q.	0.038	n.q.	n.q.	n.q.	n.q.	0.1%	n.q.
Fluoxetine	0.01	0.009	0.015	6.5%	0.001	-164.6%	-0.01	166.4%	72%
Meprobamate	0.12	0.021	0.000	83.6%	0.100	82.5%	0.10	0.2%	1%
Carbamazepine	0.11	0.116	0.005	-4.4%	-0.005	-14.5%	-0.02	4.4%	-128%
Benzophenone	0.33	n.q.	0.124	91.2%	0.305	62.8%	n.q.	37.2%	-10%
Primidone	0.00	n.q.	0.000	n.q.	n.q.	73.8%	n.q.	26.2%	n.q.
TCPP	0.76	n.q.	0.348	63.1%	0.477	54.0%	n.q.	46.0%	-58%
DEET	0.18	0.006	NA	97.3%	0.171	96.7%	0.17	n.q.	n.q.
TCEP	0.14	n.q.	0.014	6.4%	0.009	n.q.	n.q.	9.8%	n.q.
Gemfibrozil	0.12	0.001	0.000	99.1%	0.122	98.5%	0.12	0.4%	0%
Bisphenol A	0.17	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Naproxen	5.13	0.002	0.003	100.0%	5.126	99.9%	5.12	0.1%	0%
Triclosan	0.46	0.004	0.103	99.2%	0.455	76.7%	0.35	22.4%	0%
BHA	0.09	0.006	0.001	95.0%	0.087	92.3%	0.08	1.6%	1%
Musk Ketone	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Ibuprofen	11.74	0.002	0.004	100.0%	11.737	99.9%	11.73	0.0%	0%
Diphenhydramine	0.49	0.020	0.014	96.1%	0.467	92.9%	0.45	2.9%	0%
Cimetidine	0.14	0.042	0.018	74.6%	0.105	57.4%	0.08	13.0%	6%
Triclocarban	0.21	0.074	1.789	63.0%	0.129	-808.2%	-1.66	872.1%	-1%
Acetaminophen	64.77	n.q.	0.002	n.q.	n.q.	n.q.	n.q.	0.0%	n.q.
Sucralose	11.33	15.681	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.

Notes:
n.q.: not quantifiable as measured concentration below the reporting limit and reporting limit larger than 100 ng/L for aqueous phase analysis or 100 ng/g for solid phase analysis in RAS.
1) Negative values indicate that the calculated TOrC mass in the secondary effluent was higher compared to the TOrC mass in the secondary influent.
2) Negative values indicate an overall calculated gain of the TOrC during secondary treatment during the sampling period.
3) Percentages significantly higher than 100 percent resulting in high overall MB errors indicate an accumulation of TOrC on solids in RAS during the sampling phase.
RAS solid phase concentrations below the reporting limit were assumed as one half of the reporting limit for mass balance calculations.

E.5.10 Facility F, Winter

Table E-50. Facility F, Winter, TOrC Mass Balance, Secondary Treatment.

	Total IN	Total OUT		Overall Removal		Removal by Biotransformation		Removal by	MB
	Liquid	Liquid	Solids	Sec Inf-Sec Eff.[1)]		in Secondary Treatment[2)]		Sorption[3)]	Error
F - Winter	gram per day	gram per day	gram per day	%	gram per day	%	gram per day	%	%
Sulfamethoxazole	516	962.7	3.0	-85.9%	-444	-87.0%	-449	0.6%	-1%
Atenolol	998	652.5	0.4	34.8%	347	34.6%	345	0.0%	0%
Trimethoprim	196	175.5	1.5	10.8%	21	9.8%	19	0.8%	2%
Iopromide	48	18.8	0.8	64.2%	31	59.3%	29	1.6%	5%
Caffeine	25,819	21.1	3.4	99.9%	25,798	99.9%	25,795	0.0%	0%
Fluoxetine	3	5.6	1.0	-117.8%	-3	-154.0%	-4	38.3%	2%
Meprobamate	114	144.7	0.2	-26.7%	-30	-27.5%	-31	0.2%	-2%
Carbamazepine	86	89.5	0.2	-3.6%	-3	-4.1%	-4	0.2%	-10%
Benzophenone	1,033	251.9	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Primidone	45	41.3	0.0	8.1%	4	7.6%	3	0.1%	5%
TCPP	482	599.7	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
DEET	172	120.3	NA	30.3%	52	30.1%	52	n.q.	n.q.
TCEP	141	142.2	0.5	0.4%	1	-1.1%	-2	0.3%	296%
Gemfibrozil	1,618	280.2	4.8	82.8%	1,340	82.4%	1,333	0.3%	0%
Bisphenol A	344	59.1	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Naproxen	4,475	52.1	0.7	98.8%	4,424	98.8%	4,422	0.0%	0%
Triclosan	300	37.9	19.7	86.5%	259	80.8%	242	6.6%	-1%
BHA	17	37.9	0.1	-119.1%	-21	-120.8%	-21	0.8%	-1%
Musk Ketone	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Ibuprofen	4,475	2.3	0.8	100.0%	4,473	99.9%	4,472	0.0%	0%
Diphenhydramine	296	179.7	5.7	39.5%	117	37.4%	111	1.9%	1%
Cimetidine	145	89.6	0.5	38.3%	55	37.7%	54	0.3%	1%
Triclocarban	24	37.9	38.7	-81.6%	-19	-222.3%	-53	162.8%	27%
Acetaminophen	41,311	9.4	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Sucralose	9,983	7578.9	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.

Notes:
n.q.: not quantifiable as measured concentration below the reporting limit and reporting limit larger than 100 ng/L for aqueous phase analysis or 100 ng/g for solid phase analysis in RAS.
1) Negative values indicate that the calculated TOrC mass in the secondary effluent was higher compared to the TOrC mass in the secondary influent.
2) Negative values indicate an overall calculated gain of the TOrC during secondary treatment during the sampling period.
3) Percentages significantly higher than 100 percent resulting in high overall MB errors indicate an accumulation of TOrC on solids in RAS during the sampling phase.
RAS solid phase concentrations below the reporting limit were assumed as one half of the reporting limit for mass balance calculations.

E.5.11 Facility G, Low, Medium, and High SRT

Table E-51. Facility G –High SRT, TOrC Mass Balance, Secondary Treatment.

	Total IN	Total OUT		Overall Removal		Removal by Biotransformation		Removal by	MB
	Liquid	Liquid	Solids	Sec Inf-Sec Eff.[1)]		in Secondary Treatment[2)]		Sorption[3)]	Error
G -High SRT	gram per day	gram per day	gram per day	%	gram per day	%	gram per day	%	%
Sulfamethoxazole	23	32.3	0.3	-41.7%	-9	-43.8%	-10	1.5%	-1%
Atenolol	28	0.0	0.0	n.q.	n.q.	n.q.	n.q.	0.0%	n.q.
Trimethoprim	15	0.3	0.0	98.2%	15	98.0%	15	0.2%	0%
Iopromide	1	0.1	0.0	n.q.	n.q.	n.q.	n.q.	6.3%	n.q.
Caffeine	2,081	0.1	0.1	100.0%	2,081	100.0%	2,080	0.0%	0%
Fluoxetine	1	0.5	0.0	38.1%	0	31.7%	0	6.0%	1%
Meprobamate	26	2.5	0.0	90.4%	23	90.3%	23	0.0%	0%
Carbamazepine	2	2.7	0.0	-17.2%	0	-18.7%	0	0.6%	-5%
Benzophenone	14	0.6	0.5	n.q.	n.q.	n.q.	n.q.	3.3%	n.q.
Primidone	2	2.5	0.0	-4.0%	0	-4.7%	0	0.1%	-16%
TCPP	26	27.6	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
DEET	4	0.8	n.q.	78.9%	3	n.q.	n.q.	n.q.	n.q.
TCEP	6	5.4	0.0	15.1%	1	12.9%	1	0.5%	12%
Gemfibrozil	54	0.3	0.1	99.5%	54	99.4%	54	0.1%	0%
Bisphenol A	8	0.1	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Naproxen	350	0.1	0.0	100.0%	350	100.0%	350	0.0%	0%
Triclosan	22	0.6	0.7	97.2%	21	94.1%	20	3.2%	0%
BHA	5	0.0	0.0	99.6%	5	99.2%	5	0.2%	0%
Musk Ketone	n.q.	0.3	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Ibuprofen	407	0.2	0.1	99.9%	406	99.9%	406	0.0%	0%
Diphenhydramine	28	1.1	0.1	96.3%	27	96.1%	27	0.2%	0%
Cimetidine	8	6.9	1.1	12.8%	1	-4.3%	0	14.0%	24%
Triclocarban	3	0.5	2.2	74.6%	2	-6.1%	0	84.9%	-6%
Acetaminophen	4,634	0.1	0.0	n.q.	n.q.	n.q.	n.q.	0.0%	n.q.
Sucralose	558	553.0	1.7	1.7%	9	0.6%	3	0.3%	46%

Notes:
n.q.: not quantifiable as measured concentration below the reporting limit and reporting limit larger than 100 ng/L for aqueous phase analysis or 100 ng/g for solid phase analysis in RAS.
1) Negative values indicate that the calculated TOrC mass in the secondary effluent was higher compared to the TOrC mass in the secondary influent.
2) Negative values indicate an overall calculated gain of the TOrC during secondary treatment during the sampling period.
3) Percentages significantly higher than 100 percent resulting in high overall MB errors indicate an accumulation of TOrC on solids in RAS during the sampling phase.
RAS solid phase concentrations below the reporting limit were assumed as one half of the reporting limit for mass balance calculations.

Table E-52. Facility G –Medium SRT, TOrC Mass Balance, Secondary Treatment.

	Total IN	Total OUT		Overall Removal		Removal by Biotransformation		Removal by	MB
	Liquid	Liquid	Solids	Sec Inf-Sec Eff.[1]		in Secondary Treatment[2]		Sorption[3]	Error
G -Medium SRT	gram per day	gram per day	gram per day	%	gram per day	%	gram per day	%	%
Sulfamethoxazole	30	56.9	0.5	-91.7%	-27	-94.4%	-28	1.8%	-1%
Atenolol	36	0.0	0.0	100.0%	36	100.0%	36	0.0%	n.q.
Trimethoprim	20	0.6	0.0	97.0%	19	96.7%	19	0.2%	0%
Iopromide	1	0.2	0.1	99.6%	1	72.8%	1	8.0%	n.q.
Caffeine	2,705	0.8	0.3	100.0%	2,704	100.0%	2,704	0.0%	0%
Fluoxetine	1	0.6	0.1	32.9%	0	23.9%	0	8.4%	2%
Meprobamate	33	3.5	0.0	89.6%	30	89.5%	30	0.1%	0%
Carbamazepine	3	3.5	0.0	-17.2%	-1	-19.2%	-1	0.8%	-7%
Benzophenone	18	1.0	0.7	99.3%	17	90.0%	16	4.0%	5%
Primidone	3	3.2	0.0	-4.0%	0	-4.9%	0	0.1%	-19%
TCPP	33	41.2	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
DEET	5	1.8	n.q.	62.6%	3	n.q.	n.q.	n.q.	n.q.
TCEP	8	7.3	0.0	12.1%	1	9.2%	1	0.6%	19%
Gemfibrozil	70	1.4	0.2	98.1%	69	97.8%	69	0.2%	0%
Bisphenol A	11	0.1	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Naproxen	455	0.2	0.0	100.0%	455	100.0%	455	0.0%	0%
Triclosan	28	2.1	1.5	92.3%	26	87.2%	25	5.3%	0%
BHA	6	0.1	0.0	99.3%	6	98.6%	6	0.4%	0%
Musk Ketone	n.q.	0.5	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Ibuprofen	529	0.1	0.1	100.0%	529	99.9%	528	0.0%	0%
Diphenhydramine	37	1.3	0.0	96.5%	36	96.3%	36	0.1%	0%
Cimetidine	10	7.6	1.0	25.5%	3	13.8%	1	9.6%	8%
Triclocarban	3	0.9	3.8	68.0%	2	-41.9%	-1	114.6%	-7%
Acetaminophen	6,024	0.1	0.0	100.0%	6,024	100.0%	6,024	0.0%	n.q.
Sucralose	725	916.8	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.

Notes:
n.q.: not quantifiable as measured concentration below the reporting limit and reporting limit larger than 100 ng/L for aqueous phase analysis or 100 ng/g for solid phase analysis in RAS.
1) Negative values indicate that the calculated TOrC mass in the secondary effluent was higher compared to the TOrC mass in the secondary influent.
2) Negative values indicate an overall calculated gain of the TOrC during secondary treatment during the sampling period.
3) Percentages significantly higher than 100 percent resulting in high overall MB errors indicate an accumulation of TOrC on solids in RAS during the sampling phase.
RAS solid phase concentrations below the reporting limit were assumed as one half of the reporting limit for mass balance calculations.

Table E-53. Facility G – Low SRT, TOrC Mass Balance, Secondary Treatment.

	Total IN	Total OUT		Overall Removal		Removal by Biotransformation		Removal by	MB
	Liquid	Liquid	Solids	Sec Inf-Sec Eff.[1)]		in Secondary Treatment[2)]		Sorption[3)]	Error
G - Low SRT	gram per day	gram per day	gram per day	%	gram per day	%	gram per day	%	%
Sulfamethoxazole	44	92.5	0.4	-108.4%	-48	-110.9%	-49	0.8%	-2%
Atenolol	54	26.3	0.0	52.0%	28	51.5%	28	0.1%	1%
Trimethoprim	29	23.0	0.1	22.5%	7	21.3%	6	0.4%	3%
Iopromide	1	0.5	0.2	98.5%	1	55.1%	1	14.0%	30%
Caffeine	4,036	0.5	1.9	100.0%	4,036	99.9%	4,034	0.0%	0%
Fluoxetine	1	1.0	0.2	29.0%	0	13.1%	0	16.1%	-1%
Meprobamate	50	44.5	0.1	11.1%	5	10.0%	5	0.1%	8%
Carbamazepine	4	4.9	0.0	-8.9%	0	-11.6%	-1	0.8%	-22%
Benzophenone	26	6.7	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Primidone	5	4.8	0.0	-4.0%	0	-5.4%	0	0.1%	-30%
TCPP	50	55.9	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
DEET	7	6.7	n.q.	5.3%	0	n.q.	n.q.	n.q.	n.q.
TCEP	12	11.1	0.1	12.0%	1	7.3%	1	1.0%	30%
Gemfibrozil	105	17.4	0.4	83.5%	87	83.0%	87	0.4%	0%
Bisphenol A	16	0.2	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Naproxen	679	11.1	0.0	98.4%	668	98.4%	668	0.0%	0%
Triclosan	42	5.5	4.7	85.7%	36	75.6%	32	11.2%	-1%
BHA	10	4.8	0.0	50.0%	5	49.1%	5	0.4%	1%
Musk Ketone	n.q.	1.1	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.	n.q.
Ibuprofen	789	2.0	0.2	99.8%	787	99.7%	787	0.0%	0%
Diphenhydramine	55	32.8	1.3	41.1%	23	38.1%	21	2.3%	2%
Cimetidine	15	17.6	0.7	-16.5%	-2	-23.1%	-3	4.4%	-13%
Triclocarban	5	1.6	8.1	50.5%	3	-96.3%	-5	163.5%	-33%
Acetaminophen	8,990	0.2	0.0	100.0%	8,990	100.0%	8,990	0.0%	0%
Sucralose	1,083	1335.7	1.5	-22.0%	-239	-23.5%	-255	0.1%	-6%

Notes:
n.q.: not quantifiable as measured concentration below the reporting limit and reporting limit larger than 100 ng/L for aqueous phase analysis or 100 ng/g for solid phase analysis in RAS.
1) Negative values indicate that the calculated TOrC mass in the secondary effluent was higher compared to the TOrC mass in the secondary influent.
2) Negative values indicate an overall calculated gain of the TOrC during secondary treatment during the sampling period.
3) Percentages significantly higher than 100 percent resulting in high overall MB errors indicate an accumulation of TOrC on solids in RAS during the sampling phase.
RAS solid phase concentrations below the reporting limit were assumed as one half of the reporting limit for mass balance calculations.

E.6 TOrC Result Summary for Chlorination / Dechlorination Treatment

Table E-54. TOrC Result Summary for Chlorination / Dechlorination Treatment.

	A - Winter			A - Summer			B - Winter			B - Summer			D - Summer		
	Secondary Effluent	Final Effluent	Removal During Chlorination / Dechlorination	Secondary Effluent	Final Effluent	Removal During Chlorination / Dechlorination	Filter Effluent	Final Effluent	Removal During Chlorination / Dechlorination	Filter Effluent	Final Effluent	Removal During Chlorination / Dechlorination	Secondary Effluent	Final Effluent	Removal During Chlorination / Dechlorination
Sulfamethoxazole	1,300	190	85%	740	220	70%	230	5	98%	98	3	97%	1,200	1,300	-8%
Atenolol	760	670	12%	500	510	-2%	29	30	-3%	**2**	**1**	6%	1,600	1,900	-19%
Trimethoprim	650	120	82%	380	130	66%	**9**	**n.d.**	100%	**n.d.**	**n.d.**		680	670	1%
Iopromide	**n.d.**	**n.d.**		**n.d.**	**n.d.**		**n.d.**	**n.d.**		**n.d.**	**n.d.**		1,200	1,100	8%
Caffeine	**n.d.**	**n.d.**		**41**	**n.d.**	100%	**19**	**14**	24%	**14**	**16**	-18%	160	340	-113%
Fluoxetine	43	48	-12%	30	38	-27%	**0**	**1**	-65%	**n.d.**	**0**		51	55	-8%
Meprobamate	180	180	0%	120	120	0%	**150**	**140**	7%	**190**	**180**	5%	340	340	0%
Carbamazepine	200	180	10%	140	140	0%	69	61	12%	54	56	-4%	320	350	-9%
Benzophenone	**70**	**130**		**120**	**130**	-8%	**n.d.**	**n.d.**		**n.d.**	**66**		**n.q.**	**260**	
Primidone	**82**	72	12%	50	52	-4%	**44**	**41**	8%	**37**	**43**	-14%	140	160	-14%
TCPP	**2,100**	**1,700**	19%	**1,600**	**1,400**	13%	**545**	**775**	-42%	**1,195**	1,400	-17%	**1,800**	**1,700**	6%
DEET	360	350	3%	260	270	-4%	**41**	46	-12%	**2**	**8**		280	290	-4%
TCEP	**295**	**285**	3%	**330**	310	6%	**220**	**225**	-2%	**330**	**325**	2%	**535**	510	5%
Gemfibrozil	390	230	41%	120	100	17%	9	6	34%	**1**	**1**	26%	1,700	170	90%
Bisphenol A	**215**	**20**	91%	2,200	**20**	99%	**n.d.**	**n.d.**		**n.d.**	**n.d.**		230	**n.d.**	100%
Naproxen	510	160	69%	78	36	54%	**n.d.**	**n.d.**		**n.d.**	**n.d.**		2,100	2,600	-24%
Triclosan	100	29	71%	57	12	79%	**n.d.**	**n.d.**		**n.d.**	**0**		270	310	-15%
BHA	38	**4**	89%	28	**2**	95%	**n.d.**	**n.d.**		**n.d.**	**n.d.**		340	210	38%
Musk Ketone	**n.d.**	**n.d.**		**n.d.**	**n.d.**		**n.d.**	**n.d.**		**n.d.**	**n.d.**		**n.q.**	**n.q.**	
Ibuprofen	**4**	**4**	0%	**14**	**4**	71%	**n.d.**	**1**		**n.d.**	**2**		230	**239**	-4%
Diphenhydramine	380	190	50%	200	100	50%	**4**	**3**	19%	**1**	**1**	39%	640	620	3%
Cimetidine	300	**n.d.**	100%	**2**	**n.d.**	100%	**n.d.**	**n.d.**		**n.d.**	**n.d.**		660	**2**	100%
Triclocarban	120	130	-8%	76	79	-4%	**n.d.**	**n.d.**		**1**	**n.d.**		260	260	0%
Acetaminophen	**n.d.**	**n.d.**		**n.q.**	**n.d.**		**n.d.**	**n.d.**		**n.d.**	**n.d.**		**n.q.**	**20**	
Sucralose	20,000	23,000	-15%	14,000	8,900	36%	16,000	25,000	-56%	24,000	25,000	-4%	31,000	23,000	26%

E.7 Centrate TOrC Mass Loads

Table E-55. Centrate TOrC Mass Loads.

	A - Winter			A - Summer			B - Winter			B - Summer			D - Summer		
	ABI	Centrate (Average)	Centrate Mass Load Fraction of	ABI (Average)	Centrate	Centrate Mass Load Fraction of ABI	ABI	Centrate	Centrate Mass Load	ABI	Centrate	Centrate Mass Load	ABI	Centrate	Centrate Mass Load
Carbamazepine	220	1,400	19%	165	3,700	67%	110	1,600	7%	**190**	1,600	25%	300	1,700	11%
TCPP	**1,900**	3,300	5%	**1,450**	4,400	9%	**1,045**	3,000		2,000	4,200	6%	**1,900**	3,600	4%
Gemfibrozil	1,500	1,050		900	1,600	5%	1,300	2,000	1%	1,900	2,600	4%	3,200	6,000	4%
Bisphenol A	960	1,400	4%	280	3,000	32%	270	**n.q.**		470	1,600	10%	440	1,800	8%
Ibuprofen	15,000	3,150		11,000	17,000	5%	9,000	20,000	1%	14,000	16,000	3%	20,000	15,000	
Note:															
Centrate flows assumed to be 3 % of ABI flow for Facility A. Actual centrate and ABI flows used for Facilities B and D.															
ABI: Aeration basin influent															

E.8 TOrC Load on Solids in Secondary Effluents and Waste Sludge

Table E-56. Relative Fraction of TOrC on Secondary Effluent TSS and WAS TSS of Secondary Influent Load.

	A-Summer		A-Winter		B - Winter		B - Summer		C - Winter		C - Summer	
	TOrC on SE TSS	TOrC on WAS TSS	TOrC on SE TSS	TOrC on WAS TSS	TOrC on SE TSS	TOrC on WAS	TOrC on SE TSS	TOrC on WAS	TOrC on SE TSS	TOrC on WAS	TOrC on SE TSS	TOrC on WAS
	%	%	%	%	%	%	%	%	%	%	%	%
Sulfamethoxazole	0%	0%	0%	1%	0%	2%	0%	0%	0%	0%	0%	0%
Atenolol	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Trimethoprim	NA	NA	0%	2%	0%	3%	6%	2%	0%	1%	NA	NA
Iopromide	NA	NA	NA	NA	NA	12%	NA	15%	NA	NA	NA	NA
Caffeine	3%	0%	NA	0%	39%	0%	8%	0%	1%	0%	NA	NA
Fluoxetine	0%	0%	3%	13%	2%	23%	1%	9%	5%	17%	NA	NA
Meprobamate	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	1%
Carbamazepine	0%	0%	0%	0%	0%	1%	0%	1%	0%	0%	0%	1%
Benzophenone	NA	NA	NA	NA	1%	6%	0%	2%	2%	3%	NA	NA
Primidone	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	1%
TCPP	NA	NA	NA	NA	0%	3%	0%	2%	NA	NA	NA	NA
DEET	0%	0%	0%	0%	0%	0%	0%	0%	NA	NA	0%	0%
TCEP	NA	NA	NA	NA	0%	1%	0%	1%	0%	1%	NA	NA
Gemfibrozil	0%	0%	0%	0%	0%	0%	4%	0%	0%	0%	0%	0%
Bisphenol A	NA	NA	NA	NA	#DIV/0!	10%	NA	25%	NA	NA	NA	NA
Naproxen	0%	0%	0%	0%	5%	0%	NA	0%	0%	0%	0%	0%
Triclosan	8%	2%	27%	7%	23%	2%	15%	1%	9%	29%	4%	15%
BHA	0%	1%	1%	4%	2%	1%	NA	1%	0%	2%	0%	2%
Musk Ketone	NA	NA	NA	NA	4%	NA	4%	NA	NA	NA	NA	NA
Ibuprofen	1%	0%	25%	0%	3%	0%	3%	0%	0%	0%	0%	0%
Diphenhydramine	0%	0%	1%	2%	1%	2%	0%	1%	0%	2%	0%	2%
Cimetidine	13%	1%	0%	2%	1%	4%	8%	1%	0%	0%	0%	1%
Triclocarban	60%	74%	77%	127%	67%	23%	17%	18%	41%	315%	11%	27%
Acetaminophen	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Sucralose	NA	NA	NA	NA	0%	0%	0%	0%	NA	NA	NA	NA

Notes:
TOrC on SE TSS expressed as ratio of TOrC associated with secondary effluent TSS and TOrC load in the liquid phase of secondary effluent.
TOrC on WAS TSS expressed as ratio of TOrC associated with waste activated sludge solidsand total TOrC load in secondary influent (liquid and solids).
NA – not available.

Table E-55. Relative Fraction of TOrC on Secondary Effluent TSS and WAS TSS of Secondary Influent Load. (cont.)

	D - Summer		E - Summer		E - Winter		F - Winter		G - High SRT		G - Medium SRT		G - Low SRT	
	TOrC on SE TSS	TOrC on WAS TSS	TOrC on SE TSS	TOrC on WAS TSS	TOrC on SE TSS	TOrC on WAS TSS	TOrC on SE TSS	TOrC on WAS TSS	TOrC on SE TSS	TOrC on WAS TSS	TOrC on SE TSS	TOrC on WAS TSS	TOrC on SE TSS	TOrC on WAS TSS
	%	%	%	%	%	%	%	%	%	%	%	%	%	%
Sulfamethoxazole	0%	0%	0%	15%	0%	12%	0%	1%	0%	1%	0%	2%	0%	1%
Atenolol	0%	0%	0%	0%	0%	0%	0%	0%	NA	0%	NA	0%	0%	0%
Trimethoprim	NA	NA	0%	10%	0%	3%	0%	1%	1%	0%	0%	0%	0%	1%
Iopromide	NA	NA	3%	167%	0%	0%	1%	1%	NA	6%	NA	8%	NA	12%
Caffeine	3%	0%	12%	0%	NA	0%	2%	0%	6%	0%	2%	0%	90%	0%
Fluoxetine	8%	19%	1%	253%	1%	166%	3%	33%	1%	6%	1%	8%	3%	14%
Meprobamate	0%	0%	0%	2%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Carbamazepine	0%	0%	0%	9%	0%	4%	0%	0%	0%	1%	0%	1%	0%	1%
Benzophenone	NA	NA	57%	102%	2%	37%	NA	NA	NA	3%	33%	4%	NA	NA
Primidone	0%	0%	NA	26%	NA	26%	0%	0%	0%	0%	0%	0%	0%	0%
TCPP	NA	NA	0%	104%	0%	46%	NA	NA	NA	NA	NA	NA	NA	NA
DEET	0%	0%	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
TCEP	NA	NA	0%	20%	0%	10%	0%	0%	0%	0%	0%	1%	0%	1%
Gemfibrozil	0%	0%	0%	0%	0%	0%	0%	0%	1%	0%	1%	0%	0%	0%
Bisphenol A	NA	NA	32%	143%	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Naproxen	0%	0%	0%	0%	1%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Triclosan	18%	3%	4%	17%	12%	22%	7%	6%	7%	3%	3%	5%	9%	10%
BHA	0%	0%	0%	13%	0%	2%	0%	1%	3%	0%	3%	0%	0%	0%
Musk Ketone	NA	NA	30%	1476%	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Ibuprofen	1%	0%	1%	0%	1%	0%	7%	0%	1%	0%	7%	0%	1%	0%
Diphenhydramine	2%	2%	NA	NA	0%	3%	0%	2%	0%	0%	0%	0%	0%	2%
Cimetidine	0%	1%	0%	98%	0%	13%	0%	0%	1%	13%	1%	9%	0%	4%
Triclocarban	40%	13%	1%	195%	10%	869%	14%	140%	23%	80%	20%	109%	55%	146%
Acetaminophen	NA	0%	1%	0%	NA	0%	NA	NA	NA	0%	NA	0%	NA	0%
Sucralose	NA	NA	0%	5%	NA	NA	NA	NA	0%	0%	NA	NA	0%	0%

Notes:
TOrC on SE TSS expressed as ratio of TOrC associated with secondary effluent TSS and TOrC load in the liquid phase of secondary effluent.
TOrC on WAS TSS expressed as ratio of TOrC associated with waste activated sludge solidsand total TOrC load in secondary influent (liquid and solids).
NA – not available.

E.9 Uncertainty and Error Analysis for TOrC Mass Balances

Table E-57. TOrC Removal by Biotransformation During Secondary Treatment.

Uncertainty Assessment	QA/QC	Quantification
Sample collection in field		
Contamination in field	- Cleaning procedures - Sample container covers - Sampling staff protective wear - Sample replicates for selected samples	- Rinse blanks - Field blanks - Equipment blanks - Variability of sample replicates
Data collection in field		
Incorrect process description	- Close coordination of PFDs with ops staff and management - Field visits where feasible	- Mass balance error assessment for solids (TSS)
System not under steady state	- Close coordination with management and ops staff	- Documentation of daily operation 1-2 months prior to sampling event
Flow measurements	- Solids mass balances	- Mass balance error assessment for solids (TSS)
TSS measurements of RAS, etc.	- Triplicates at facility for RAS / WAS - Independent analysis at CSM	- Variability of triplicate analysis
Inaccurate / variable process and operational parameters	- Analysis of long-term plant data history (1-2 year) to identify suspicious data	- Sensitivity analysis in TOrC fate models
Sample handling		
Loss during shipment / handling / sample processing	- On-site sample preservation - Immediate sample extraction - Preservation study - Isotope Dilution	- Recoveries / Loss estimates from preservation study
Contamination at receiving Lab	- Lab DI water analysis for TOrC - Field blanks	- Results from lab DI water analysis - Results from field blanks - Correction for blank contamination

Uncertainty Assessment	QA/QC	Quantification
Sample analysis at receiving lab		
Analytical Errors, accuracy, precision	- Analytical Replicates for selected samples - Lab internal QA/AC procedures - Calibration and standard testing - Isotope dilution method to overcome matrix affects	- Variability of analytical replicates - Variability of Standard tests - Matrix Spikes - Matrix Replicates
Variability of results	- Sample replicates for selected samples and different matrices - Inter-lab comparison (CSM, SNWA, Milwaukee)	- Variability of sample replicates - Results of interlab comparison
Data analysis		
Errors during data transfer and calculation	- Standardized spreadsheet calculations - Independent calculation check	
Data interpretation		
Unaccounted TOrC fate processes for loss	- TOrC mass balance error estimate	- Calculated TOrC mass balance error

APPENDIX F

MASS BALANCE CALCULATIONS

F.1 TSS Mass Balances for Secondary Treatment

Solids were used as a conservative parameter to assess the mass balances around the secondary clarifiers (or membrane bioreactor) at each facility. The percent recovery of solids in this mass balance was defined as:

TSS recovery = MLSS, mg/L * (Q_{RAS} + $Q_{AB\ Inf.}$) / [TSS_{SE} * Q_{SE} + (Q_{WAS}+Q_{RAS})*TSS_{RAS}]

(Equation 1)

Where,

MLSS =	Mixed Liquor Suspended Solid Concentration in Aeration Basins, mg/L
Q_{WAS}=	Waste Activated Sludge Flow, mgd
Q_{SE}=	Secondary Effluent Flow, mgd
Q_{RAS} =	RAS flow, mgd
$Q_{AB\ Inf.}$=	Aeration basin influent flow (including relevant plant internal recycle streams, mgd
TSS_{SE} =	TSS concentration in secondary effluent, mg/L
TSS_{RAS}=	TSS concentration in RAS, mg/L

F.2 TOrC Mass Balances for Secondary Treatment

Mass balance calculations for the indicator compounds were established based on mass flows in and out of control volumes set around the secondary treatment systems of each field site. TOrC mass flows for liquid streams were calculated as follows:

$$M_{L,TOrC}\left(\frac{g}{d}\right) = Q\left(\frac{10^6 gal}{d}\right)\cdot \times \left(\frac{3.78L}{gal}\right) \times C_{L,TOrC}\left(\frac{ng}{L}\right) \times \left(\frac{g}{10^9 ng}\right)$$

(Equation 2)

Where,

$M_{L,TOrC}$ =	Mass Flow of TOrC in Liquid Phase
Q =	Flow
$C_{L,TOrC}$ =	Concentration of TOrC in Liquid Phase

The mass flow of TOrC associated with (bio)solids were calculated as follows:

$$M_{S,TOrC}\left(\frac{g}{d}\right) = Q_{WAS}\left(\frac{10^6 gal}{d}\right) \times TSS_{WAS}\left(\frac{\dot{mg}}{L}\right) \times \left(\frac{g}{10^3 mg}\right) \times \left(\frac{3.78L}{gal}\right) \times C_{S,TOrC}\left(\frac{ng}{g}\right) \times \left(\frac{g}{10^9 ng}\right)$$

(Equation 3)

Where,

$M_{S,TOrC}$ = Mass Flow of TOrC in Solid Phase
Q_{WAS} = Waste Activated Sludge Flow
TSS_{WAS} = Total Suspended Solids in WAS
$C_{S,TOrC}$ = Concentration of TOrC in Solid Phase

The removal of TOrC during secondary treatment gave an indication of the biotransformation of TOrC. Recall that the target compounds were specifically selected with properties that would minimize losses due to volatilization during wastewater treatment. The removal due to degradation was calculated with the following mass balance around the secondary treatment systems of each field site:

$$\text{TOrC Removal, Biotransform.} = 1 - [\,(M_{L,\text{Secondary Effluent}} + M_{S,\text{Secondary Effluent}} + M_{S,WAS} + M_{L,WAS}) / (M_{L,\text{Secondary Influent}} + M_{S,\text{Secondary Influent}}]$$

(Equation 4)

Where,

$M_{LS,\text{Secondary Influent}}$ = Mass Flow of TOrC in liquid and solid phase of Secondary Influent (including all plant internal recycle flows)
M_L = Mass Flow of TOrC in Liquid phase of designated flow
M_S = Mass Flow of TOrC in Solid Phase of designated flow

The removal of TOrC from the liquid phase of the secondary influent to the solid phase gave indication of sorption during secondary treatment and was calculated as follows:

$$\text{TOrC Removal, Sorption} = (M_{S,\text{Secondary Effluent}} + M_{S,WAS} - M_{S,\text{Secondary Influent}}) / M_{L,\text{Secondary Influent}}$$

(Equation 5)

The overall liquid stream TOrC removal during secondary treatment was calculated as follows:

$$\text{TOrC Removal, Sec. Treat} = 1 - [(M_{L,\text{Secondary Effluent}} + M_{S,\text{Secondary Effluent}})/(M_{L,\text{Secondary Influent}} + M_{S,\text{Secondary Influent}}]$$

(Equation 6)

The TOrC mass balance error was calculated as follows:

$$\text{TORC Mass Balance Error, \%} = 1 - \frac{(\text{TOrC Removal, Sorption} + \text{TOrC Removal, Biotransform.})}{\text{TOrC Removal, Sec. Treat}}$$

(Equation 7)

APPENDIX G

BIOTRANSFORMATION RATE PARAMETERS AND BIOSORPTION PARTITION COEFFICIENTS

G.1 Summary of Literature Values

Table G-1. Literature Summary of Sorption Coefficients for TOrC Indicators.

Compound	CAS	K_d[i] (L/kg) DM-AS	K_d[i] (L/kg) DM-Primary	K_d[i] (L/kg) MP-AS	K_d (L/kg) Lit. data
Acetaminophen	103-90-2	< 30	< 30	< 30	1160[e]
Atenolol	29122-68-7	< 30	46	35	4.37[f], 64[e]
Benzophenone	119-61-9	-	-	-	161[c]
Bisphenol A	80-05-7	431 (±35)	314 (±66)	505 (±83)	217-273[c]
Caffeine	58-08-2	< 30	< 30	< 30	
Carbamazepine	298-46-4	50 (±1)	65 (±5)	36 (±2)	17[b], 66[c], 1.2[d], 135[e]
DEET	134-62-3	42	100 (±19)	< 30	-
Gemfibrozil	25812-30-0	45	45 (±9)	< 30	100[c], 19.3[e]
Ibuprofen	15687-27-1	< 30	< 30	< 30	80[c], 7.1[d], 0[e]
Iopromide	73334-07-3	-	-	-	11[d]
Meprobamate	57-53-4	< 30	42 (±12)	< 30	-
Naproxen	22204-53-1	< 30	< 30	< 30	24[c]
Primidone	125-33-7	< 30	45 (±10)	< 30	7[b]
Sulfamethoxazole	723-46-6	< 30	< 30	< 30	77[e], 256[g]
TCEP	115-96-8	65 (±20)	162 (±72)	<30	-
Trimethoprim	738-70-5	119 (±49)	251 (±99)	193 (±104)	253[e]

DM-AS – Denver Metro activated sludge; DM-Primary – Denver Metro primary sludge ; MP-AS – Mines Park activated sludge
[b]Wick et al. 2009, [c]Urase and Kikuta 2005, [d]Ternes et al. 2004, [e]Radjenovic et al. 2009, [f]Scheurer et al. 2010, [g]Göbel et al. 2005, [i]Dickenson et al. 2010

Table G-2. Literature Summary of Biotransformation Rates for TOrC Indicators.

Compound	K_b (min^{-1})	95% CI ± (min^{-1})	k_b $L/(g_{ss} \cdot d)$	$T_{1/2}$ * (hrs)	Reference
Acetaminophen	1.16E-001	3.67E-002	119	0.14	Dickenson et al., 2010 (Mines Park)
Acetaminophen	2.44E-002	3.90E-003	69	0.24	Joss et al., 2006
Atenolol	2.39E-002	1.72E-003	25	0.68	Dickenson et al., 2010 (Mines Park)
Atenolol	1.35E-002	3.16E-003	8.6	1.93	Dickenson et al., 2010 (Denver Metro)
Atenolol	1.06E-003	1.11E-004	1.4	11.66	Wick et al., 2009
Bisphenol A	1.23E-002	5.44E-003	13	1.31	Dickenson et al., 2010 (Mines Park)
Bisphenol A	4.77E-002	2.60E-002	31	0.54	Dickenson et al., 2010 (Denver Metro)
Caffeine	9.50E-002	1.31E-002	98	0.17	Dickenson et al., 2010 (Mines Park)
Caffeine	3.97E-001	6.85E-002	254	0.07	Dickenson et al., 2010 (Denver Metro)
Carbamazepine			<0.1		Wick et al., 2009
Carbamazepine			<0.1		Dickenson et al., 2010 (Mines Park)
Carbamazepine			<0.1		Dickenson et al., 2010 (Denver Metro)
DEET	5.64E-003	8.24E-004	5.8	2.87	Dickenson et al., 2010 (Mines Park)
DEET	9.82E-003	8.60E-004	6.3	2.65	Dickenson et al., 2010 (Denver Metro)
Gemfibrozil	1.87E-002	3.92E-003	19	0.86	Dickenson et al., 2010 (Mines Park)
Gemfibrozil	2.79E-003	9.94E-004	1.8	9.32	Dickenson et al., 2010 (Denver Metro)
Gemfibrozil	2.83E-003	5.67E-004	8.0	2.08	Joss et al., 2006
Ibuprofen	9.92E-003	2.48E-003	28	0.59	Joss et al., 2006
Ibuprofen	2.36E-002	6.24E-003	24	0.69	Dickenson et al., 2010 (Mines Park)
Ibuprofen	2.00E-002	1.66E-002	13	1.30	Dickenson et al., 2010 (Denver Metro)
Iopromide	7.26E-004	1.59E-004	2.0	8.12	Joss et al., 2006
Meprobamate			<0.1		Dickenson et al., 2010 (Mines Park)
Meprobamate			<0.1		Dickenson et al., 2010 (Denver Metro)
Naproxen	5.14E-004	1.59E-004	1.5	11.46	Joss et al., 2006
Naproxen	9.20E-003	1.74E-003	9.5	1.76	Dickenson et al., 2010 (Mines Park)
Naproxen	1.43E-001	1.05E-001	92	0.18	Dickenson et al., 2010 (Denver Metro)
Primidone			<0.1		Wick et al., 2009
Primidone			<0.1		Dickenson et al., 2010 (Mines Park)
Primidone			<0.1		Dickenson et al., 2010 (Denver Metro)
Sulfamethoxazole	2.97E-004	5.56E-005	0.31	54.46	Dickenson et al., 2010 (Mines Park)
Sulfamethoxazole	7.80E-004	3.45E-004	0.50	33.32	Dickenson et al., 2010 (Denver Metro)
TCEP			<0.1		Dickenson et al., 2010 (Mines Park)
TCEP			<0.1		Dickenson et al., 2010 (Denver Metro)
Triclosan	2.59E-002	9.90E-003	27	0.62	Dickenson et al., 2010 (Mines Park)
Triclosan	2.10E-003	6.17E-004	1.3	12.38	Dickenson et al., 2010 (Denver Metro)
Trimethoprim			<0.1		Dickenson et al., 2010 (Mines Park)
Trimethoprim			<0.1		Dickenson et al., 2010 (Denver Metro)

* half-life in a 1 g_{ss}/L solution; CI: confidence interval

G.2 K_d and K_b Values From Full-Scale Testing

The kinetic disappearance of a TOrC due to biotransformation was described by a pseudo first order model:

$$\frac{dC_T}{dt} = -k_b X_{ss} C_T \qquad \textit{(Equation 1)}$$

where C_T is the total compound concentration (ng/L), t is the time (min), k_b is the reaction rate constant (L/g_{ss}•min), and X_{SS} the suspended solids concentration (g_{ss}/L). The model in Eq. 1 assumes that X_{ss} is constant while the compound is undergoing biotransformation, where the pseudo first-order rate constant, $K_b = k_b X_{ss}$. The model also assumes that the biotransformation rate, k_b, is the same in both aqueous and solid phases. To assess sorption effects, partitioning equilibrium between aqueous and solid phases may be assumed, where the sorption partition coefficient, K_d, is defined as:

$$K_d = \frac{C_s}{C_w} \qquad \textit{(Equation 2)}$$

where K_d is in units of L/g-SS, C_s is the sorbed compound concentration on the solids (ng/g_{ss}) at equilibrium, and C_w is the compound concentration in the aqueous phase (ng/L) at equilibrium. The total substrate concentration is

$$C_T = C_w + C_s X_{SS} = C_w(1 + K_d X_{SS}) \qquad \textit{(Equation 3)}$$

Substituting Eq. 3 into Eq. 1 and solving the differential equation, the observed aqueous compound concentration at any time can be expressed as:

$$C_w = \frac{C_0}{1 + K_d X_{SS}} e^{-k_b X_{SS} t} \qquad \textit{(Equation 4)}$$

where C_0 is the initial total compound concentration.

The model in Eq. 4 assumes instantaneous sorption. However, sorption kinetics maybe important and should be included in overall removal kinetics from the aqueous phase. By considering sorption as a first order reaction where the aqueous concentration asymptotes to its partitioning equilibrium concentration, Eq. 4 can be modified as:

$$C_w = C_0 e^{-k_b X_{SS} t} \frac{1 + K_d X_{SS} e^{-k_{sor} t}}{1 + K_d X_{SS}} \qquad \textit{(Equation 5)}$$

where k_{sor} is the first-order reaction rate of sorption. For preliminary data analysis it was assumed the sorbed concentration for all TOrC reaches 99% of its equilibrium concentration in two hours, then k_{sor} = -ln(0.01)/120 min = 0.038 min^{-1}. This assumption was verified by performing sorption kinetic tests. K_d values were calculated using the Freundlich equation at aqueous TOrC concentrations of C_w = 1000 ng/L.

Kd values on RAS collected from all full-scale facilities were calculated using the following equation:

$$\log K_D = \log(\frac{c_S}{c_L} * 1000) \qquad \textit{(Equation 6)}$$

Where,

K_D: Sorption coefficient (-)
Cs: Solid phase TOrC concentration (ng/g RAS TSS)
C_L: Liquid phase TOrC concentration (ng/L)

Table G-3. Sorption Coefficients K_D for RAS Samples (Field Testing).

K_D (RAS Field Testing)	A - Winter	A - Summer	B - Winter	B - Summer	C - Winter	C - Summer	D - Summer	E - Winter	E - Summer	F - Winter	G - High SRT	G - Medium SRT	G - Low SRT
Sulfamethoxazole	1.94	1.97	2.12	2.10	1.47	1.24	1.76	2.50	2.76	1.99	2.15	2.10	1.77
Atenolol	1.49				1.22					1.51			1.26
Trimethoprim	2.41		2.33					2.88		2.36			
Iopromide													
Caffeine													
Fluoxetine			3.40								2.37		
Meprobamate								1.47	1.76		1.96	1.82	1.28
Carbamazepine		1.65	1.84	1.78			1.76	1.95	2.40	1.73	1.63	1.68	1.66
Benzophenone							-						
Primidone		2.09					1.56			1.13			
TCPP													
DEET													
TCEP													
Gemfibrozil	1.92	2.42	2.17	3.23	1.44	1.45	1.83		2.69	2.27	2.48	2.42	2.49
Bisphenol A													
Naproxen	2.19		2.52		1.43		1.72	2.38		2.02			
Triclosan	4.29	3.61	4.17	4.07	3.72	4.03	4.24						3.78
BHA													
Musk Ketone													
Ibuprofen	2.24	1.68		1.97	1.67		2.11			2.14	2.30	2.42	2.68
Diphenhydramine	2.68	2.32	2.78	2.76	2.22	2.24	2.69	3.09		2.59	2.51		2.49
Cimetidine	2.34	3.12	2.17	3.12	1.56		2.19	2.54	3.60	1.98	2.38	2.43	2.32
Triclocarban		5.07	4.76	5.07	5.08	4.23	4.25	4.61	5.55				
Acetaminophen													
Sucralose									1.85		1.42		1.11

G.3 K_d Values From Bench-Scale Testing

Table G-4. Sorption Coefficients K_d for MLSS Samples.

log Kd	B - Summer	C - Winter	D - Winter	E - Winter	F - Winter	G	Mines Park Low SRT	Mines Park Medium SRT	Mines Park High SRT
Atenolol	-	2.53	2.87	-	2.58	2.35	-	-	-
Benzophenone	2.31	2.59	3.27	2.35	2.97	2.38	-	3.06	3.09
Bisphenol A	-	2.52	2.70	3.18	-	-	-	2.28	-
Carbamazepine	2.01	-	2.37	1.98	-	-	1.67	1.79	
Cimetidine	-	-	2.36	2.72	2.28	2.19	2.53	2.47	2.79
DEET	1.97	-	2.11		2.14		1.89	1.77	1.87
Diphenhydramine	-	2.47	2.60	2.57	2.70		2.34	2.48	2.53
Fluoxetine	3.09	2.89	3.23	3.06	-	2.84	3.03	3.25	3.02
Gemfibrozil	1.86	2.11	2.34	1.65	2.56	2.08	1.68	2.02	2.44
Ibuprofen	1.65	2.62	2.41	1.71	2.62	2.03	2.16	2.21	2.23
Iopromide	-	-	-	-	-	-	-	-	-
Meprobamate	2.36	-	2.23	2.39	2.09		1.86	1.85	1.70
Naproxen	1.41	1.91	2.38	1.79	2.36	2.23	1.94	1.90	2.39
Sulfamethoxazole	2.36	2.28	2.81	2.40		1.94	2.39	2.93	2.12
Triclocarban	-	-	4.23	3.21	3.62	-	-	-	4.41
Triclosan	3.28	-	3.98	3.49	3.09	-	3.47	-	3.74
Trimethoprim	2.33	2.49	2.29	2.60	2.58	2.10	2.28	2.25	2.26

G.4 K_b Values from Bench-Scale Testing

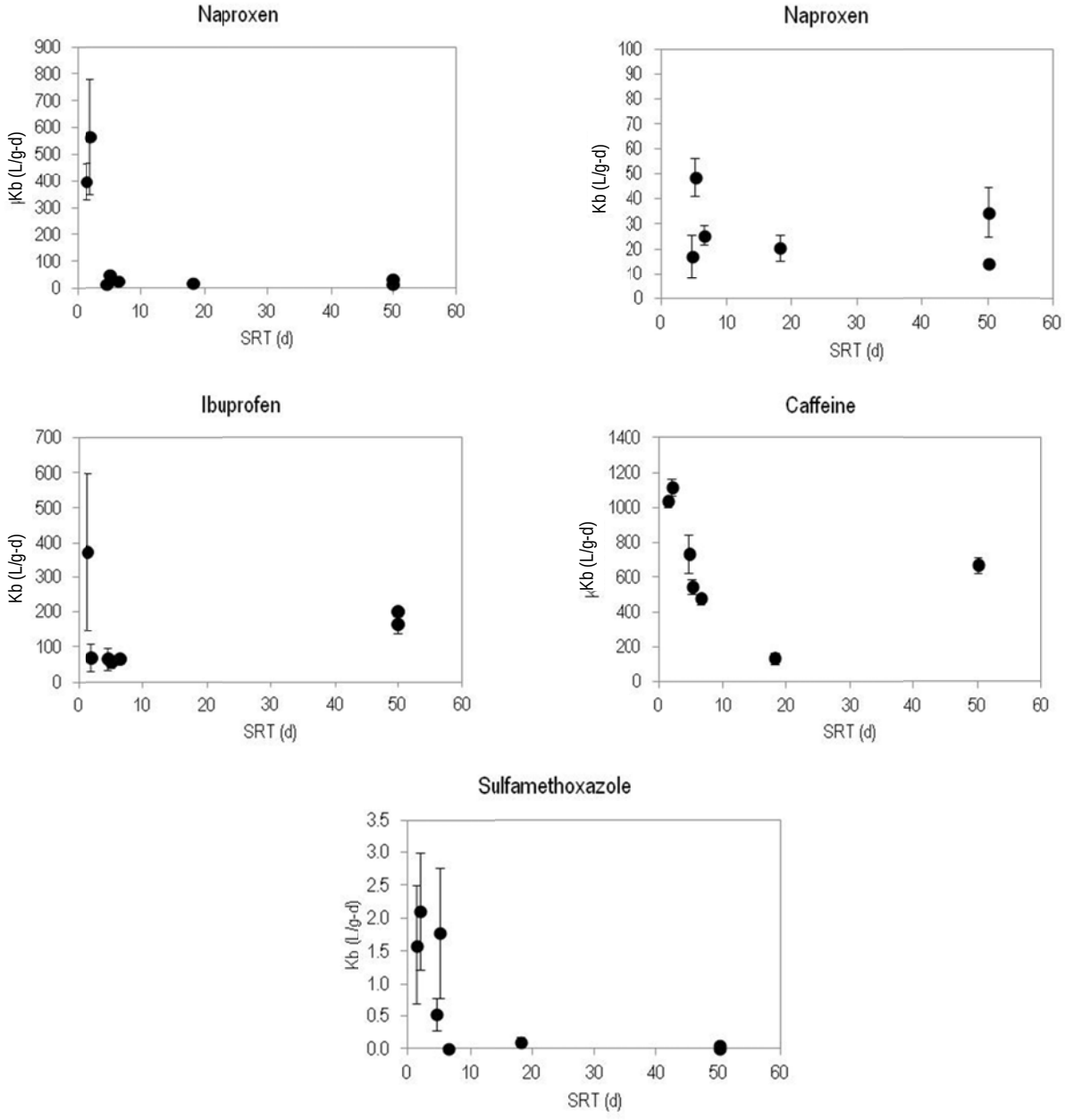
Table G-5. Biotransformation Rate Constants K_b for MLSS Samples.

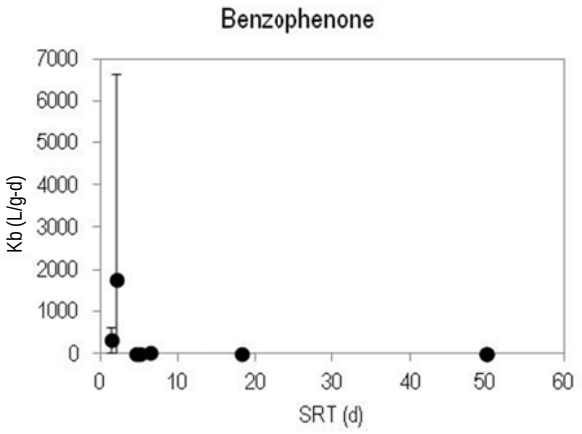
	C Winter		C Summer		F Winter		D Winter		D Summer		B Summer		E Winter		E Summer		Range	
Kb	K_b	CI	K_b	CI	K_b	CI	K_b	CI	K_b	CI	K_b	CI	K_b	CI	K_b	CI	**Min** K_b	**Max** K_b
Compound	(L/g-d)	(L/g-d)	(L/g-d)	(L/g-d)	(L/g-d)	(L/g-d)	(L/g-d)	(L/g-d)	(L/g-d)	(L/g-d)	(L/g-d)	(L/g-d)	(L/g-d)	(L/g-d)	(L/g-d)	(L/g-d)	(L/g-d)	(L/g-d)
Atenolol	0.9	0.2	NA	NA	3.3	1.0	8.3	1.6	11.0	3.7	12.8	2.8	9.0	6.0	17.0	0.7	0.9	17
Benzophenone	NA	NA	NA	NA	24	24	15	12	13.3	6.3	9.9	8.3	1.9	2.2	4	4.4	1.88	24
Bisphenol A	0.11	0.14	NA	NA	NA	NA	3.7	3.3	NA	NA	NA	NA	NA	NA	NA	NA	0.11	4
Caffeine	1116	47	1033	31	473	28	543	41	734	109	130	33	668	48	NA	NA	130.1	1115.8
Carbamazepine	0	NA	0	NA	0	NA	0	NA	0	NA	0	NA	0	NA	0	NA	0	0
Cimetidine	NA	NA	0.07	0.05	0.2	0.2	0.7	0.3	0.4	0.08	5.9	2.9	0.27	0.16	0.5	0.6	0.07	5.9
DEET	0.14	0.09	11	2.4	0.2	0.2	4.4	1.0	11	4.7	3.2	1.2	1.4	0.2	12	2.7	0.14	12
Diphenahydramine	2.0	0.8	11	9.5	29	28	17.5	NA	610	444	245	208	288	135	255	155	2.0	609.5
Fluoxetine	897	532	811	358	980	307	1512	597	1548	461	832	265	617	290	645	267	616.6	1548
Gemfibrozil	0	NA	0	NA	1.1	0.8	0.1	0.11	2.2	0.8	1.20	0.2	10	2.6	14	4.4	0.0	14
Ibuprofen	69	38	374	225	65	13	57	18	65	30	NA	NA	201	13	165	26	56.6	373.9
Meprobamate	NA	NA	NA	NA	NA	NA	0	NA	0	NA	NA	NA	NA	NA	NA	NA	0.0	0.0
Naproxen	565	216	400	67	25	3.9	49	7.6	17	8.5	20	5.2	35	9.9	14	1.1	14.4	565
Primidone	0	NA	0	NA	0	NA	0	NA	0	NA	0	NA	0	NA	0	NA	0	0
Sulfamethoxazole	2.1	0.9	1.6	0.9	0.06	0.04	1.8	1.0	0.5	0.2	0.11	0.07	0	NA	0.05	0.04	0	2.1
TCEP	0	NA	0	NA	0	NA	0	NA	0	NA	0	NA	0	NA	0	NA	0	0
Triclocarban	0	NA	0	NA	0	NA	0	NA	0	NA	0	NA	0	NA	0	NA	0	0
Triclosan	1.2	1.0	0.6	0.7	572	430	NA	NA	923	709	728	494	NA	NA	NA	NA	0.6	923
Trimethoprim	0	NA	0	NA	0.13	0.3	0	NA	0.08	0.03	0.8	0.8	0.7	0.8	0.3	0.8	0	0.8

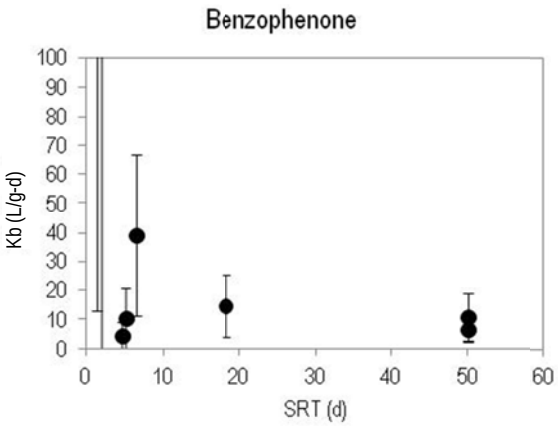
Note:
CI: 95 % Confidence Interval.

G.5 K_b Values Versus SRT

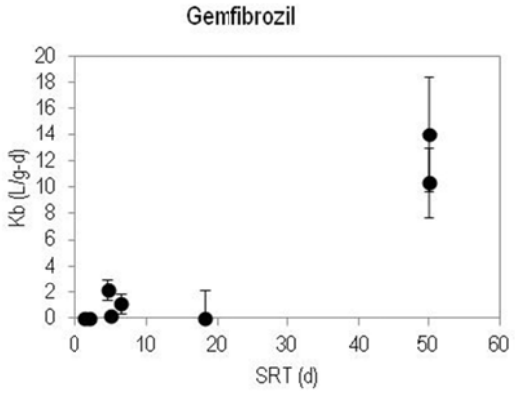
G.5.1 Negative Trend

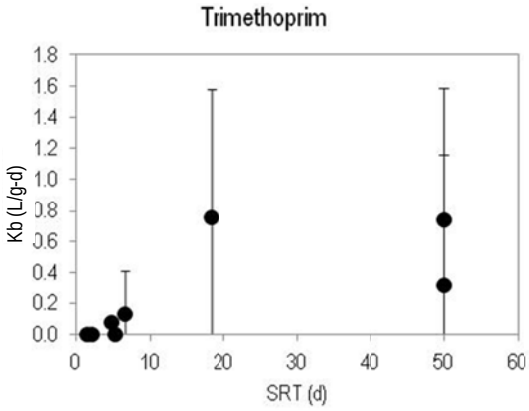




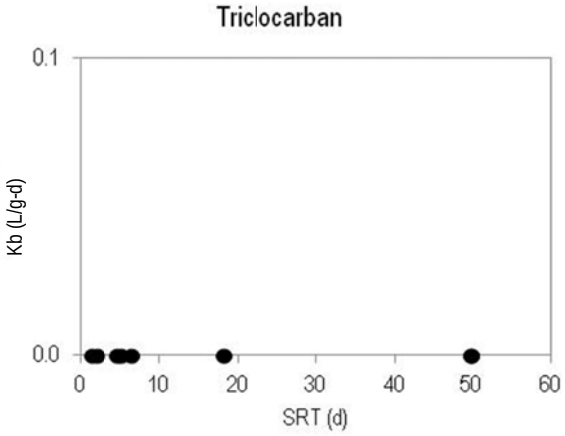


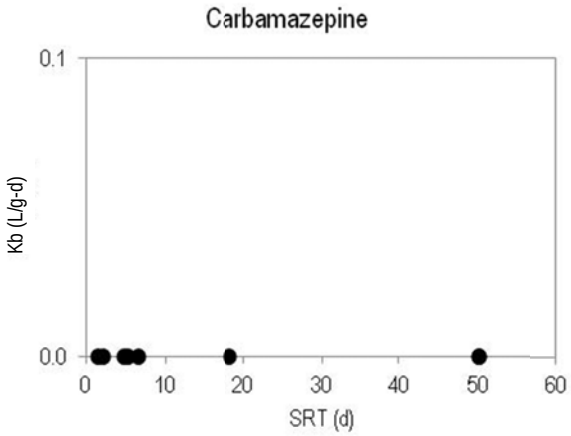
G.5.2 Positive Trend

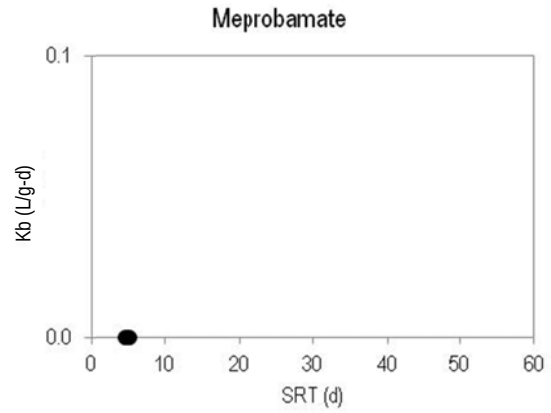


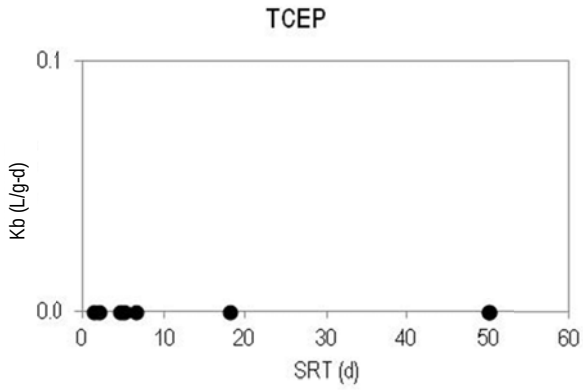


G.5.3 Recalcitrant

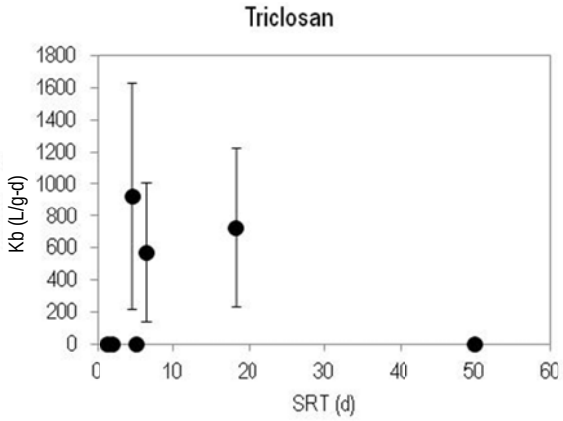


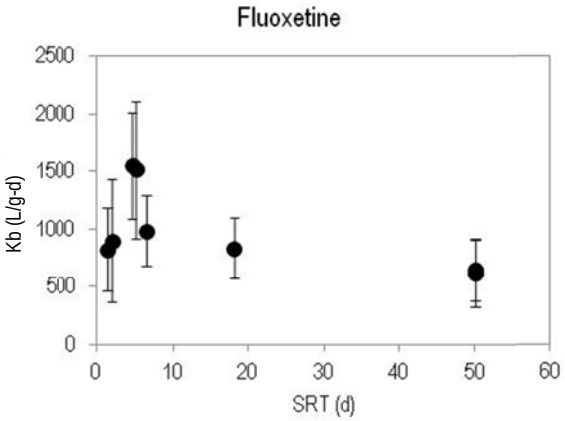


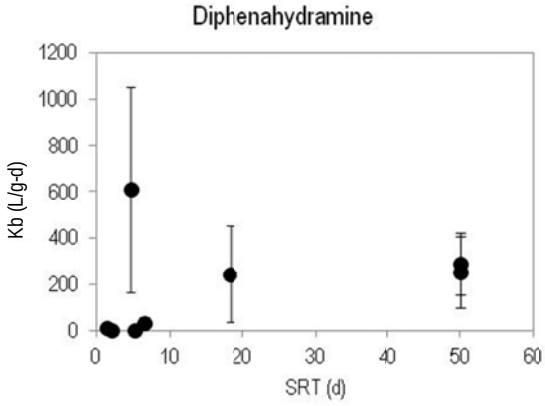


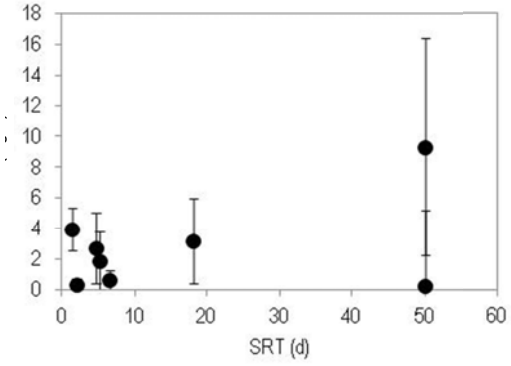


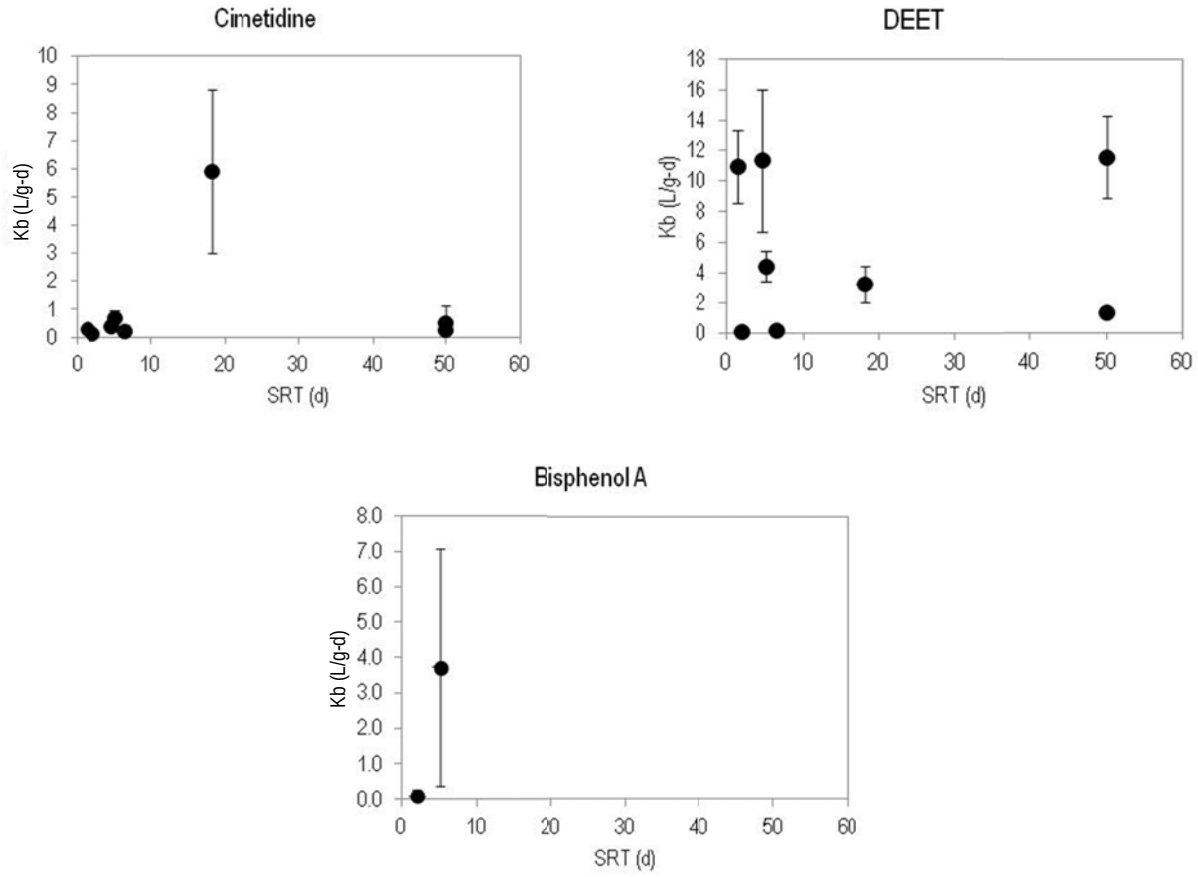
G.5.4 No clear trend



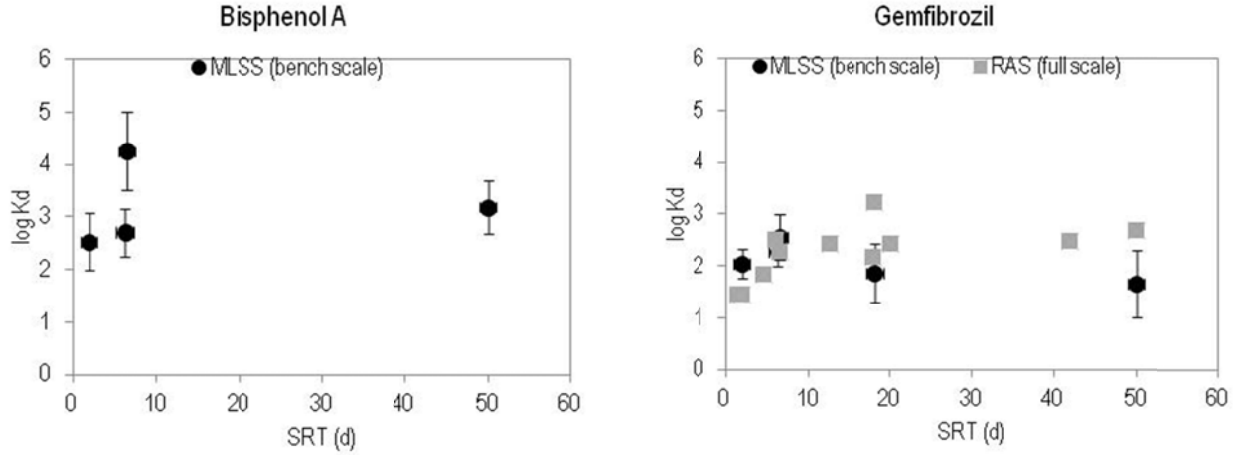


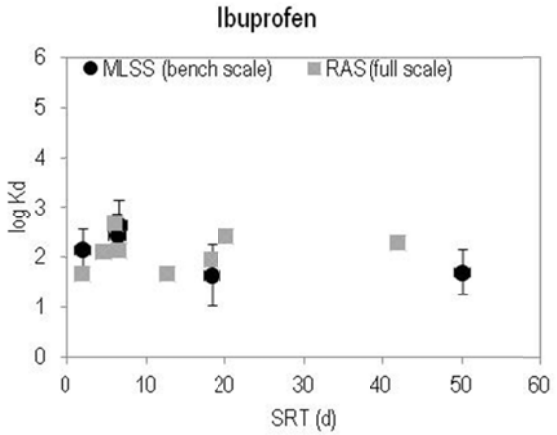


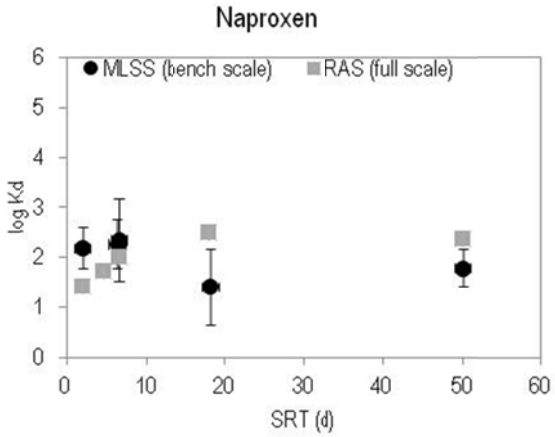


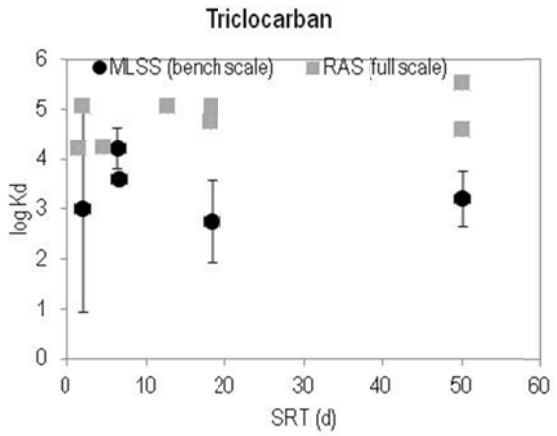


G.6 K_D Values Versus SRT




Ibuprofen
MLSS (bench scale)
RAS (full scale)
log Kd
SRT (d)


Naproxen
MLSS (bench scale)
RAS (full scale)
log Kd
SRT (d)


Triclocarban
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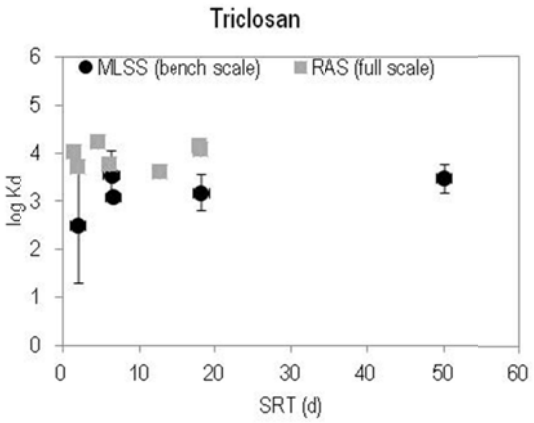
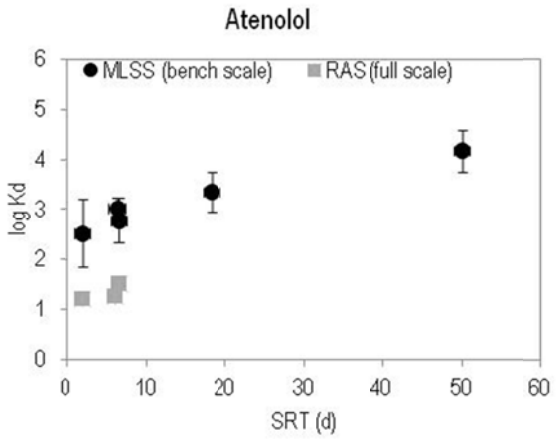
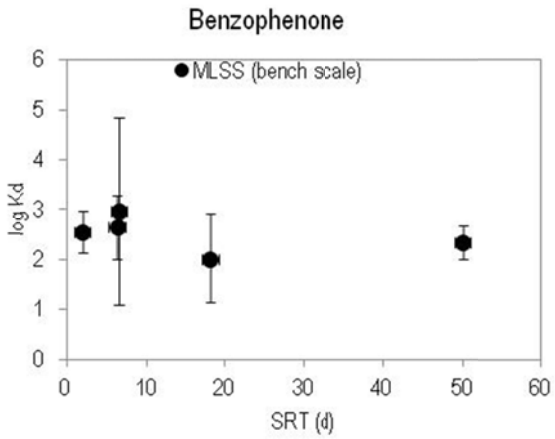
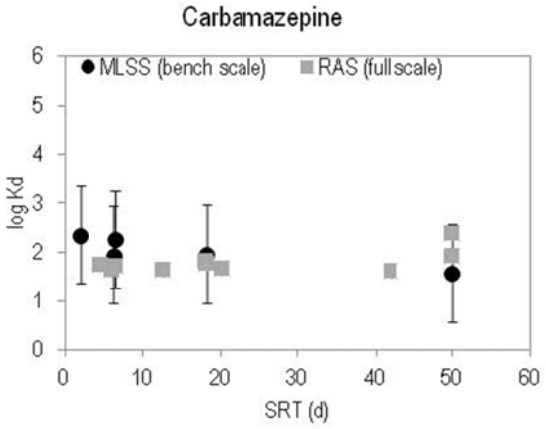
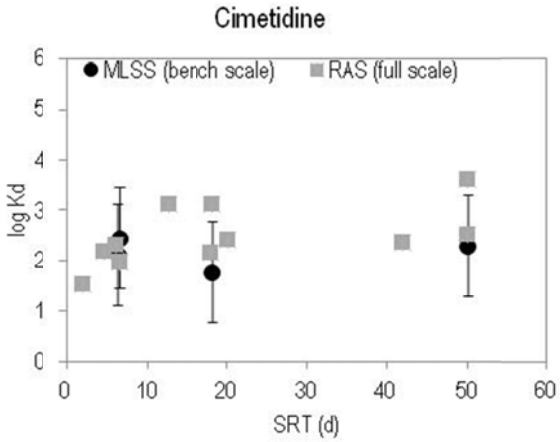
RAS (full scale)
log Kd
SRT (d)

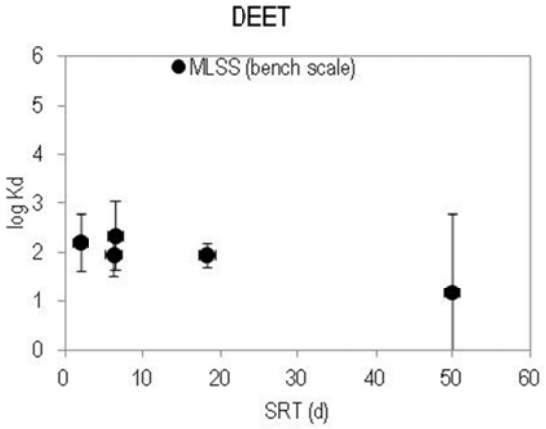

Triclosan
MLSS (bench scale)
RAS (full scale)
log Kd
SRT (d)

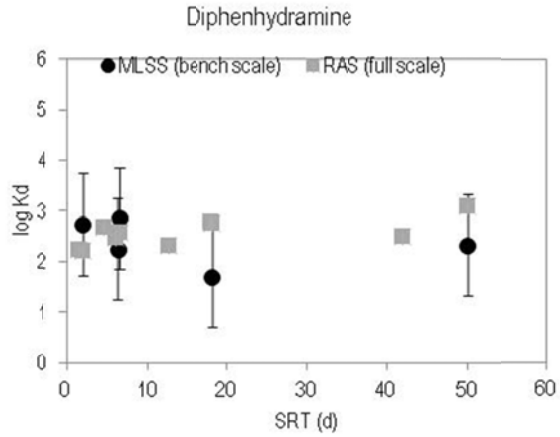

Atenolol
MLSS (bench scale)
RAS (full scale)
log Kd
SRT (d)

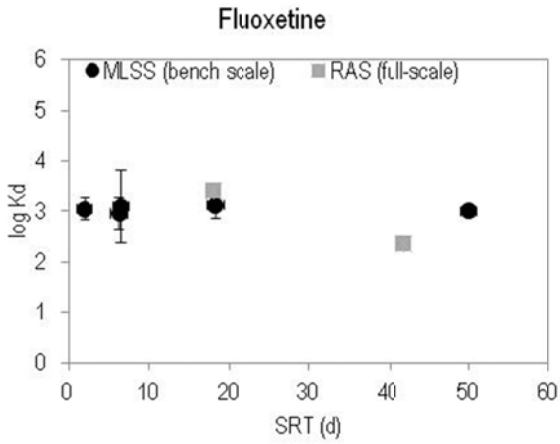

Benzophenone
MLSS (bench scale)
log Kd
SRT (d)

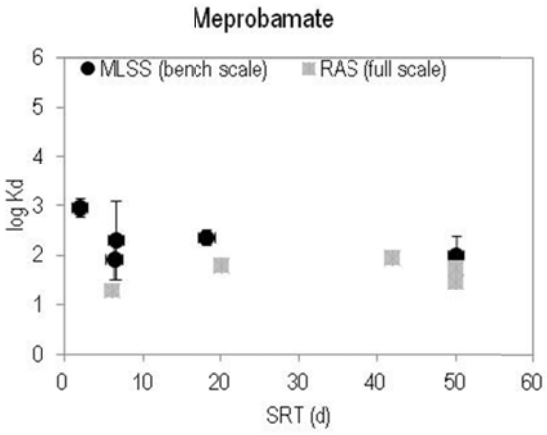

Carbamazepine
MLSS (bench scale)
RAS (full scale)
log Kd
SRT (d)

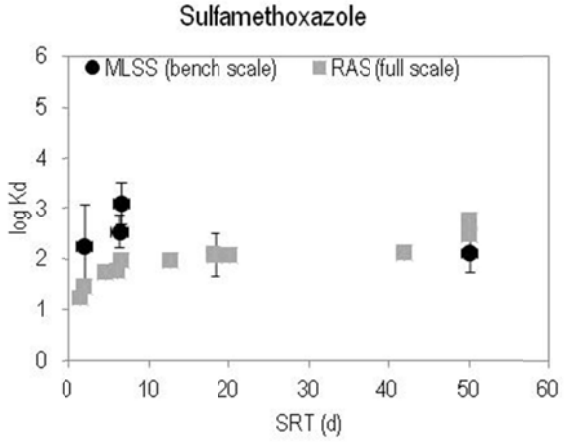

Cimetidine
MLSS (bench scale)
RAS (full scale)
log Kd
SRT (d)

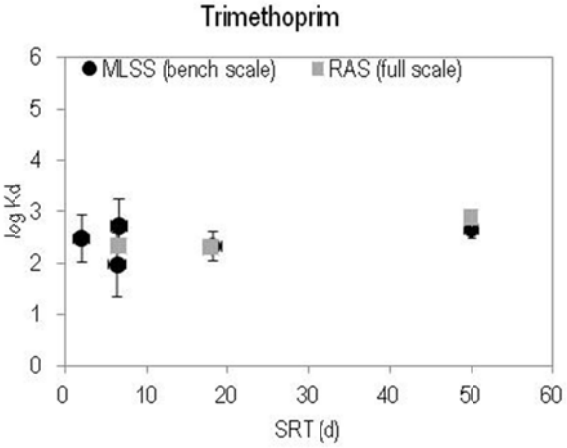

DEET
MLSS (bench scale)
log Kd
SRT (d)


Diphenhydramine
MLSS (bench scale)
RAS (full scale)
log Kd
SRT (d)


Fluoxetine
MLSS (bench scale)
RAS (full-scale)
log Kd
SRT (d)


Meprobamate
MLSS (bench scale)
RAS (full scale)
log Kd
SRT (d)


Sulfamethoxazole
MLSS (bench scale)
RAS (full scale)
log Kd
SRT (d)
0
1
2
3
4
5
6
0
10
20
30
40
50
60


Trimethoprim
MLSS (bench scale)
RAS (full scale)
log Kd
SRT (d)
0
1
2
3
4
5
6
0
10
20
30
40
50
60

APPENDIX H

PROCESS MODEL COMPARISON

H.1 Review of TOrC Fate Models for Conventional Wastewater Treatment

The following is a review of existing steady-state mass balance models that predict the removal of TOrC in a wastewater treatment plant (WWTP). These WWTPs include primary treatment followed by activated-sludge (i.e., suspended growth) secondary treatment processes for BOD removal only or for nutrient removal. Numerous WWTP emission models have been developed. Please note that these models are not intended to simulate conditions in an actual WWTP in detail, but instead provide a screening level of the fate of specific chemicals in a WWTP. This review only focuses on models with the following features:

- Available in the form of a Windows application.
- Widely used for exposure assessment.
- Modeling capability for user-defined substances.
- Can predict quantities of a given chemical 1) present in the aqueous phase, 2) volatilized to air, 3) sorbed by sludge, and 4) biotransformed.

The following models satisfy the above criteria and are reviewed in the following sections:

- WATER9 version 2.0.
- STP Model versions 2.11 and STPWin.
- SimpleTreat versions 4.0 and EUSES.
- ASTreat version 1.0.
- TOXCHEM+ version 3.0.
- EnviroPro Designer 7.5.

Table H-1, Table H-2, and Table H-3 provide comparison summaries of the availability, source, required input parameters, and capability of these TOrC mass balance models. The following sections provide a summary of relevant model features and a comparison of advantages and possible limitations of the existing models.

Table H-1. Description, Availability, and Source of TOrC Mass Balance Models.

Model	Version	Origin/ Country	Computer/ Platform Interface	Availability (Demo/Full)	Source	Website or email
WATER9	2.0	U.S. EPA/U.S.	Windows/ Graphical	-/Free	U.S. EPA	www.epa.gov/ttn/chief/software/water
TOXCHEM+	3.0	Enviromega/ Canada	Windows/ Graphical	Free/ Cost $4,000 per copy	Hydromantis	www.hydromantis.com/TOXCHEM.html
STP Model	2.11	Canadien Modelling Centre at Trent University/ Canada	Windows/ Graphical	-/Free	Canadian Modelling Centre at Trent University	http://www.trentu.ca/academic/aminss/envmodel/models/STP211.html
STPWin (STP embedded in EPI Suite)	4.0	U.S. EPA/U.S.	Windows/ Graphical	-/Free	U.S. EPA	www.epa.gov/oppt/exposure/pubs/episuite.htm
ASTreat	1.0	Procter & Gamble/ U.S.	Windows/ Graphical	-/Free	Procter & Gamble	Drew McAvoy mcavoy.dc@pg.com
SimpleTreat	4.0	Netherlands National Institute for Public Health and the Environment/ Netherlands	Windows/ Spreadsheet	-/Free	Netherlands National Institute for Public Health and the Environment	Jaap Stuijs j.stuijs@rivm.nl
EUSES (SimpleTreat embedded)	2.1	Netherlands National Institute for Public Health and the Environment/ Netherlands	Windows/ Graphical	-/Free	European Commission Joint Research	ecb.jrc.ec.europa.eu/euses/
EUSES (SimpleTreat embedded)	2.1	Netherlands National Institute for Public Health and the Environment/ Netherlands	Windows/ Graphical	-/Free	Centre	ecb.jrc.ec.europa.eu/euses/
EnviroPro Designer	7.5	Intelligen/ U.S.	Windows/ Graphical	Free/Cost $4,995 per copy	Intelligen	www.intelligen.com

Table H-2. Capability Comparison of TOrC Mass Balance Models.

	WATER9	TOXCHEM+	STP Model	STPWin (STP embedded in EPI Suite)	ASTreat	SimpleTreat	EUSES (Simple Treat embedded)	EnviroPro Designer
User-Friendly: Process Input Data	Extensive input data required	Extensive input data required	Minimal input data required	No input data required	Minimal input data required	Minimal input data required	unknown	Extensive input data required
User-Defined Process Configuration	Yes	Yes	No	No	No	No	No	No
Example Treatment Reactor Units	activated sludge treatment, DAF, trickling filter, lagoon, biofilter, oil/water separator, aerated biotreatment	activated sludge treatment, DAF, trickling filter, rotating biological contactor, chlorine disinfection, PAC addition	activated sludge treatment	activated sludge treatment	activated sludge treatment	activated sludge treatment	activated sludge treatment	activated sludge treatment, anoxic reactor, trickling filter, plug flow aerobic reactor
Sludge Treatment Reactor Units	not available	Concentrator, anaerobic/aerobic digesters, sludge dewatering, centrifuge, belt filter, drying bed	not available	not available	digester and sludge dewatering	not available	not available	Anaerobic digester
Compound Database	Yes	Yes	Yes	Yes	No	No	unknown	Yes
# of Compounds	2000	227	15	-	-	-	unknown	1750
User-Defined Compounds	Yes	Yes	Yes	No	Yes	Yes	Yes	Yes
Property Estimation Techniques	Yes (UNIFAC)	No	No	Yes (EPI Suite)	No	No	unknown	No
Biodegrdation Models	Zero and first order	anaerobic/ aerobic (suspended or fixed-film) first order; aerobic	anaerobic / aerobic half lives or	anaerobic/ aerobic half lives	first and second order or Monod	first order and Monod	first order and Monod	first order, Haldane, Grau and Monod

	WATER9	TOXCHEM+	STP Model	STPWin (STP embedded in EPI Suite)	ASTreat	SimpleTreat	EUSES (Simple Treat embedded)	EnviroPro Designer
		Monod	biodegra-dability "ready test" results					
Simulation of Multiple Compounds	Yes (100 Compounds)	Yes	No	No	No	No	No	Yes
# WW Influents	Multipe	1	1	1	1	1	1	1
Output Data	Individual Units & Entire Process	Individual Units & Entire Process	Individual Units & Entire Process	Entire Process Only	Individual Units & Entire Process	Individual Units & Entire Process	Entire Process Only	Individual Units & Entire Process
Validation for nonvolatile compounds (Total Removal)	under estimated within the 75-100% range	Predictive within the 75-100% range	Predictive or over estimate d within the 75-100% range		predictive within the 75-100% range	predictive within the 75-100% range		
Validation Study Reference	Crechen Technologies (2006)	Crechen Technologies (2006)	Wang et al. 2007, Crechen Technol ogies (2006)		Crechen Technologi es (2006)	Crechen Technologies (2006), Artola-Garicano et al. (2003)		

The models originate from the United States, Canada, or the Netherlands. All the models are readily accessible, windows-based, and provide a graphical interface, with the exception of SimpleTreat, which uses a spreadsheet interface. These models are public-domain software except for TOXCHEM+ and EnviroPro Designer, which must be purchased. A comparison of their capabilities and limitations follows:

1) **Model Inputs**: Extensive wastewater and process input parameters are necessary for WATER9, TOXCHEM+, and EnviroPro Designer models. Minimal input data is required for STP, SimpleTreat and ASTreat models and no input data is required for STPWin. For the most part, all input variables are readily available from operations. A model with minimal or no input process parameters is a model that is potentially easier to use, if it has similar predictivity capabilities as models with extensive process input parameters. It is not clear how certain wastewater and process input parameters effect TOrC removal, especially for models that require extensive process input parameters.
2) **Treatment Configurations**: WATER9, TOXCHEM+, and EnviroPro Designer models provide the capability of simulating complex and different treatment configurations. The other models only simulate emissions for a single conventional activated sludge treatment process, which contains primary treatment followed by activated-sludge (suspended growth) secondary treatment. Only WATER9 has the capability of handling multiple influents simultaneously.
3) **Solids Treatment**: Only TOXCHEM+, ASTreat, and EnviroPro Designer models provide modeling of TOrC fate during sludge digester treatment.
4) **User-Defined Compounds and Fate Properties**: User-defined compounds and compound properties can be incorporated in all the models with one exception, being STPWin. This exception is less flexible and relies mostly on estimated compound properties calculated by the EPI Suite program (user-defined biodegradation half-lives can be used).
5) **Breadth of Integrated Compound Databases**: WATER9, TOXCHEM+, STP, STPWin, and EnviroPro Designer programs provide compound databases, which allows a user to simply enter a compound of interest within the database and the program is able to retrieve the appropriate compound property data. These databases comprise 2,000 (Water9), 1,750 (EnviroPro Designer), 227 (TOXCHEM+) and 15 (STP) compounds. ASTreat and SimpleTreat do not contain compound databases.
6) **Integrated Tools for Estimating Unknown Compound Properties**: In case that compound property information is not directly available in the databases, WATER9 and STPWin are able to estimate some compound properties with program-imbedded quantitative structure property relationships (QSPRs). WATER9 is not able to estimate biodegradation parameters, whereas STPWin is able to do this. The utilization of QSPR estimation techniques is an attractive feature as compound property data (e.g., biodegradability) is unavailable for many emerging compounds.

7) **Key Fate Parameters**: The predictions of the fate of nonvolatile compounds (the current project only focuses on nonvolatile compounds) by sorption and biodegradation removal mechanisms are primarily dictated by two parameters: octanol-water partition coefficient (used for estimating the aqueous-solids partitioning coefficient) and biodegradation rate constant. Note, the octanol-water partition coefficient may not be the best parameter for the prediction of aqueous-solids partitioning, especially when specific compound and solid interactions occur, such as charge interactions. Reliable methods in the form of QSPRs need to be established for estimating activated sludge biodegradation rate constants and solids-water partitioning coefficients for certain compounds, such as positively charged compounds.

8) **Biodegradation Kinetics**: Generally, aerobic biodegradation is simulated in the models using zero-order, first-order, second-order, or Monod kinetics. Most of the models are set up to accommodate at least two of these kinetic simulations that the user can choose from; first-order or Monod models being the most common options. None of the models is equipped to provide options for all four types of kinetics mentioned above. In addition to aerobic biodegradation, TOXCHEM+, EnviroPro Designer, STP, and STPWin models allow for modeling of anaerobic biodegradation. TOXCHEM+ also allows for biodegradation of TOrCs by suspended or fixed slim activated-sludge. The biodegradation data for activated sludge is very limited and rate constants measured in accordance to standard test protocols are not readily available in the literature.

9) **Simulating Multiple Compounds in Parallel**: WATER9, EnviroPro Designer and TOXCHEM+ allows for multiple compounds to be modeled simultaneously. This is an attractive user feature when screening of multiple compounds is necessary. Fate information for multiple compounds can be quickly reported in a concise format. These models assume the simulation of the fate of multiple TOrCs simultaneously do not result in any interactions (synergism or antagonism) between compounds that would affect their fate. The other models do not have this capability.

10) **Model Output**: Except for STPWin and EUSES models, all the models report TOrC fate information for both, individual processes and the entire plant. Individual process fate information is necessary for knowing which treatment process is responsible for TOrC removal.

11) **Accuracy of Model Prediction**: Based on limited validations studies, some models under estimated (WATER9), over estimated (STP) or was predictive (TOXCHEM+, ASTreat, SimpleTreat) for nonvolatile compounds that were removed in the 75-100% range. The studies that have been performed primarily focused on polyaromatic hydrocarbons and polybromodiphenyl ethers type of compounds. The models need further validation for a structurally and chemically diverse set of emerging compounds, such as pharmaceuticals and personal care products. No validations studies have been performed for nonvolatile compounds that are moderately removed (<75% removal).

H.2 ASTreat Model Input Summary

Table H-3. ASTreat Model Input Summary.

Treatment Characteristics		B - Winter	C - Winter	C - Summer	D - Summer	E - Winter	E - Summer	F - Winter
Secondary Influent								
Influent Flow Rate	m3/d	34443.5	31652	25880	26243	405	394	34444
HRT	hrs	0	0	0	0	0	0	0
Influent TSS	mg/L	106	108	163	96	210	258	63
Removal of solids	%	0	0	0	0	0	0	0
Solids in Primary Sludge	%	0	0	0	0	0	0	0
Secondary Treatment								
SRT	days	18.2	2	1.4	4.6	>50	40-80	6.5
HRT	hrs	9.6	2.4	2.4	4.5	4.1	4.1	2.6
Tank Depth	m	5	5.36	5.36	5.0	5.18	5.18	5.00
MLSS	mg/L	3619	2563	2227	2590	7857	8053	3700
Secondary Clarifier								
Effluent TSS	mg/L	5.1	11.8	8.3	28	5	<2	7
RAS TSS	mg/L	9333	4543	3722	4838	8722	10233	8625

H.3 Actual TOrC Removal versus ASTreat Predictions

H.3.1 Model Input: Biotransformation Rates K_b

Table H-4. Matrix Selection Table for Selecting the ASTreat K_b Input Parameter.

	K_b values (L/g-d)								
Compound \ SRT (d)	2	5	7	10	15	20	30	40	50
Acetaminophen[b]	69	69	69	69	69	69	69	69	69
Atenolol[c]		K_b = 0.82(SRT)			10	10	10	10	10
Benzophenone	11	11	11	11	11	11	11	11	11
Bisphenol A	0.1	3.7	NA	NA	NA	NA	NA	NA	NA
Caffeine	1074	510	510	510	510	510	510	510	510
Carbamazepine	0	0	0	0	0	0	0	0	0
Cimetidine	0.36	0.36	0.36	0.36	0.36	0.36	0.36	0.36	0.36
DEET[a]					See footnote				
Diphenahydramine	15	15	15	72	167	262	262	262	262
Fluoxetine	980	980	980	980	980	980	980	980	980
Gemfibrozil	0	1.2	1.2	1.2	1.2	1.8	5.3	8.7	12
Ibuprofen	142	142	142	142	142	142	142	142	142
Iopromide[b]	2	2	2	2	2	2	2	2	2
Meprobamate	0	0	0	0	NA	NA	NA	NA	NA
Naproxen	482	27	27	27	27	27	27	27	27
Primidone	0	0	0	0	0	0	0	0	0
Sucralose	0	0	0	0	0	0	0	0	0
Sulfamethoxazole	1.1	1.1	0.05	0.05	0.05	0.05	0.05	0.05	0.05
TCEP	0	0	0	0	0	0	0	0	0
Triclocarban	0	0	0	0	0	0	0	0	0
Triclosan	0.91	741	741	741	741	741	741	741	741
Trimethoprim	0.05	0.05	0.05	0.27	0.36	0.6	0.6	0.6	0.6

a – Based on aeration basin influent (ABI) concentration. Below 3000 ng/L, use K_b (L/g-d) = 0.0039x where x is the ABI concentration. For 3000-15000 ng/L, use K_b = 11.5. The biotransformation rate for DEET in activated sludge was found to be linear function with DEET influent concentrations, up to 3 µg/L.

b – For acetaminophen and iopromide experimental literature K_b values (Joss et al. 2006) are proposed.

Italicized numbers are suggested values based on linear interpolation.

For an SRT value not appearing on the chart, find the upper and lower SRT and choose the lower Kb value.

c - A linear relationship was used for atenolol between SRT 2-10 days.

H.3.2 ASTreat Evaluation Raw Data

Table H-5. Actual TOrC Removal versus ASTreat Model Prediction.

		Actual Measured Total Removal	ASTreat Simulated Bio. Removal	ASTreat Simulated Sorp. Removal	ASTreat Simulated Total Removal	Difference
Atenolol	B - Winter	84%	96%	0%	96%	12%
	C - Winter	0%	17%	0%	17%	17%
	C - Summer	24%	97%	0%	97%	73%
	D - Summer	31%	79%	0%	79%	48%
	E - Winter	94%	91%	0%	91%	-3%
	E - Summer	93%	95%	0%	95%	2%
	F - Winter	35%	52%	0%	52%	17%
Benzophenone	B - Summer	57%	95%	0%	95%	38%
	C - Winter	85%	100%	0%	100%	15%
	C - Summer	n.q.	99%	0%	99%	NA
	D - Summer	n.q.	78%	4%	82%	NA
	E - Winter	100%	67%	1%	68%	-32%
	E - Summer	91%	82%	0%	82%	-9%
	F - Winter	n.q.	89%	0%	89%	NA
Bisphenol A	B - Summer	98%	NA	NA	NA	NA
	C - Winter	n.q.	2%	6%	9%	NA
	C - Summer	n.q.	NA	NA	NA	NA
	D - Summer	n.q.	NA	NA	NA	NA
	E - Winter	99%	NA	NA	NA	NA
	E - Summer	n.q.	NA	NA	NA	NA
	F - Winter	n.q.	NA	NA	NA	NA
Caffeine	B - Summer	100%	100%	0%	100%	0%
	C - Winter	100%	99%	0%	99%	-1%
	C - Summer	n.q.	100%	0%	100%	NA
	D - Summer	100%	100%	0%	100%	0%
	E - Winter	100%	100%	0%	100%	0%
	E - Summer	n.q.	NA	NA	NA	NA
	F - Winter	100%	99%	0%	99%	-1%
Carbamazepine	B - Summer	2%	0%	2%	2%	0%
	C - Winter	7%	0%	2%	2%	-6%
	C - Summer	0%	0%	5%	5%	5%
	D - Summer	3%	0%	2%	2%	-1%
	E - Winter	34%	0%	1%	1%	-34%
	E - Summer	0%	0%	1%	1%	1%
	F - Winter	0%	0%	1%	1%	1%

Table H-5. Actual TOrC Removal versus ASTreat Model Prediction.

		Actual Measured Total Removal	ASTreat Simulated Bio. Removal	ASTreat Simulated Sorp. Removal	ASTreat Simulated Total Removal	Difference
Cimetidine	B - Summer	99%	92%	0%	92%	-7%
	C - Winter	0%	1%	1%	2%	2%
	C - Summer	0%	10%	1%	11%	11%
	D - Summer	0%	12%	2%	14%	14%
	E - Winter	62%	22%	3%	25%	-36%
	E - Summer	75%	NA	NA	NA	NA
	F - Winter	38%	6%	1%	8%	-31%
DEET	B - Summer	100%	86%	0%	86%	-14%
	C - Winter	2%	3%	3%	6%	4%
	C - Summer	66%	80%	1%	81%	15%
	D - Summer	91%	80%	0%	80%	-11%
	E - Winter	100%	61%	0%	61%	-39%
	E - Summer	97%	93%	0%	93%	-4%
	F - Winter	30%	7%	1%	8%	-22%
Diphenhydramine	B - Summer	90%	100%	0%	100%	10%
	C - Winter	0%	30%	3%	33%	33%
	C - Summer	18%	79%	1%	81%	63%
	D - Summer	62%	100%	0%	100%	38%
	E - Winter	n.q.	100%	0%	100%	NA
	E - Summer	96%	100%	0%	100%	4%
	F - Winter	40%	90%	0%	91%	51%
Gemfibrozil	B - Summer	100%	69%	0%	70%	-30%
	C - Winter	0%	0%	1%	1%	1%
	C - Summer	6%	0%	1%	1%	-5%
	D - Summer	49%	42%	1%	44%	-5%
	E - Winter	100%	92%	0%	92%	-8%
	E - Summer	99%	95%	0%	95%	-5%
	F - Winter	83%	27%	1%	28%	-55%
Ibuprofen	B - Summer	100%	NA	NA	NA	NA
	C - Winter	88%	83%	0%	83%	-5%
	C - Summer	94%	99%	0%	99%	6%
	D - Summer	99%	96%	0%	96%	-3%
	E - Winter	100%	100%	0%	100%	0%
	E - Summer	100%	99%	0%	99%	-1%
	F - Winter	100%	96%	0%	96%	-4%

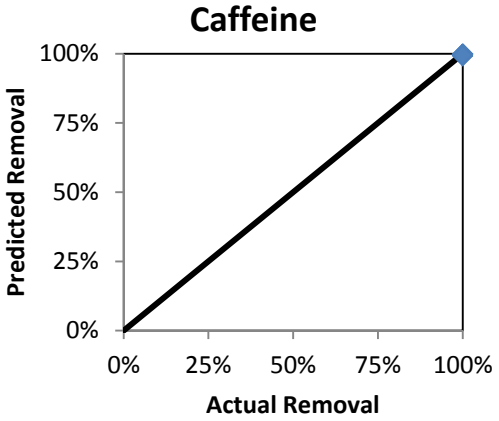
Table H-5. Actual TOrC Removal versus ASTreat Model Prediction.

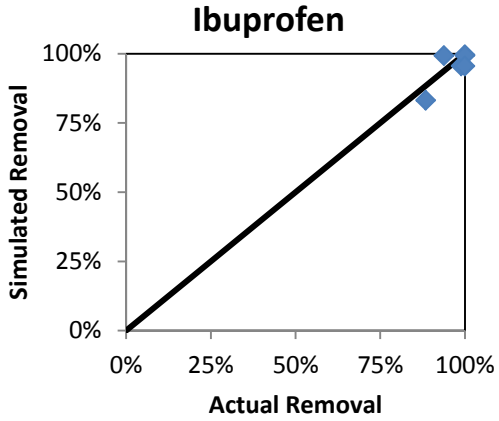
		Actual Measured Total Removal	ASTreat Simulated Bio. Removal	ASTreat Simulated Sorp. Removal	ASTreat Simulated Total Removal	Difference
Meprobamate	B - Summer	-36%	0%	3%	3%	39%
	C - Winter	2%	0%	12%	12%	9%
	C - Summer	3%	0%	14%	14%	11%
	D - Summer	0%	0%	1%	1%	1%
	E - Winter	61%	NA	NA	NA	NA
	E - Summer	84%	NA	NA	NA	NA
	F - Winter	0%	0%	0%	0%	0%
Naproxen	B - Summer	100%	98%	0%	98%	-2%
	C - Winter	71%	99%	0%	99%	28%
	C - Summer	89%	99%	0%	99%	10%
	D - Summer	88%	85%	0%	86%	-2%
	E - Winter	100%	98%	0%	98%	-2%
	E - Summer	100%	95%	0%	95%	-5%
	F - Winter	99%	89%	0%	89%	-9%
Primidone	B - Summer	14%	0%	0%	0%	-14%
	C - Winter	14%	0%	0%	0%	-14%
	C - Summer	0%	0%	0%	0%	0%
	D - Summer	8%	0%	0%	0%	-8%
	E - Winter	n.q.	0%	0%	0%	NA
	E - Summer	n.q.	0%	0%	0%	NA
	F - Winter	8%	0%	0%	0%	-8%
Sucralose	B - Summer	0%	0%	0%	0%	0%
	C - Winter	n.q.	0%	0%	0%	NA
	C - Summer	n.q.	0%	0%	0%	NA
	D - Summer	n.q.	0%	0%	0%	NA
	E - Winter	29%	0%	0%	0%	-29%
	E - Summer	n.q.	0%	0%	0%	NA
	F - Winter	n.q.	0%	0%	0%	NA
Sulfamethoxazole	B - Summer	45%	17%	1%	18%	-27%
	C - Winter	23%	31%	2%	33%	10%
	C - Summer	36%	36%	3%	39%	3%
	D - Summer	21%	15%	3%	18%	-3%
	E - Winter	61%	0%	1%	1%	-60%
	E - Summer	43%	6%	1%	7%	-36%
	F - Winter	0%	2%	3%	5%	5%

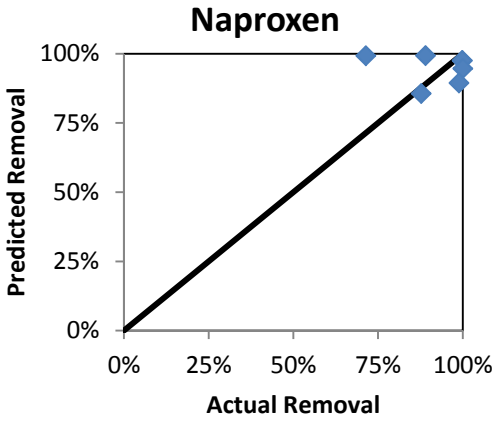
Table H-5. Actual TOrC Removal versus ASTreat Model Prediction.

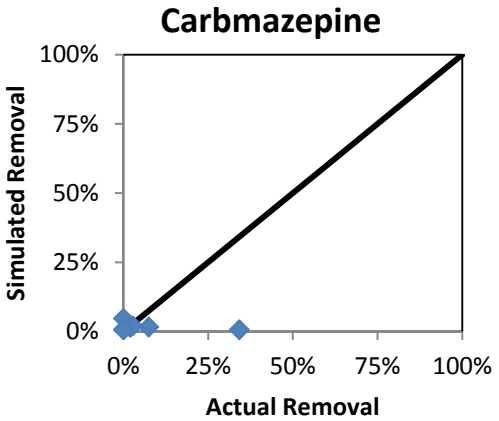
		Actual Measured Total Removal	ASTreat Simulated Bio. Removal	ASTreat Simulated Sorp. Removal	ASTreat Simulated Total Removal	Difference
TCEP	B - Summer	0%	0%	0%	0%	0%
	C - Winter	0%	0%	1%	1%	1%
	C - Summer	n.q.	0%	0%	0%	NA
	D - Summer	n.q.	0%	0%	0%	NA
	E - Winter	0%	2%	1%	2%	2%
	E - Summer	6%	0%	0%	0%	-6%
	F - Winter	0%	0%	0%	0%	0%
Triclocarban	B - Summer	96%	0%	85%	85%	-11%
	C - Winter	-31%	2%	84%	86%	NA
	C - Summer	87%	0%	69%	69%	-17%
	D - Summer	82%	0%	51%	51%	-31%
	E - Winter	79%	0%	63%	63%	-17%
	E - Summer	63%	0%	92%	92%	29%
	F - Winter	-82%	NA	NA	NA	NA
Triclosan	B - Summer	99%	100%	0%	100%	1%
	C - Winter	56%	14%	32%	46%	-10%
	C - Summer	83%	8%	55%	63%	-20%
	D - Summer	93%	99%	0%	100%	6%
	E - Winter	99%	NA	NA	NA	NA
	E - Summer	99%	NA	NA	NA	NA
	F - Winter	86%	99%	0%	99%	13%
Trimethoprim	B - Summer	98%	58%	2%	60%	-38%
	C - Winter	9%	0%	2%	2%	-7%
	C - Summer	n.q.	0%	6%	6%	NA
	D - Summer	5%	3%	2%	5%	0%
	E - Winter	94%	43%	6%	48%	-46%
	E - Summer	96%	26%	6%	32%	-64%
	F - Winter	11%	4%	3%	7%	-4%

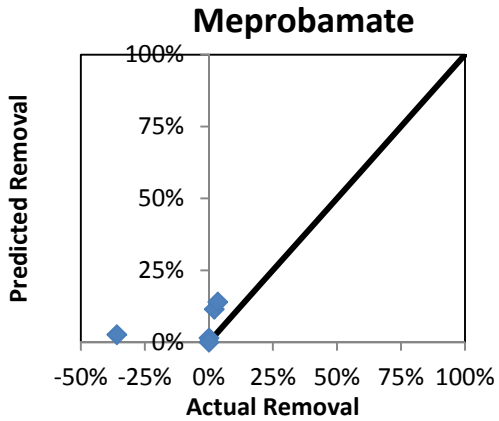
H.3.3 ASTreat Model Evaluation Graphs

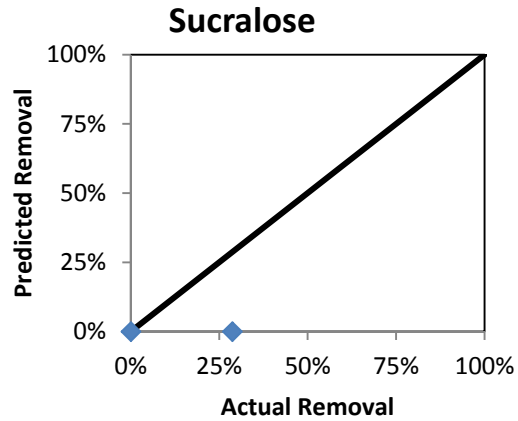


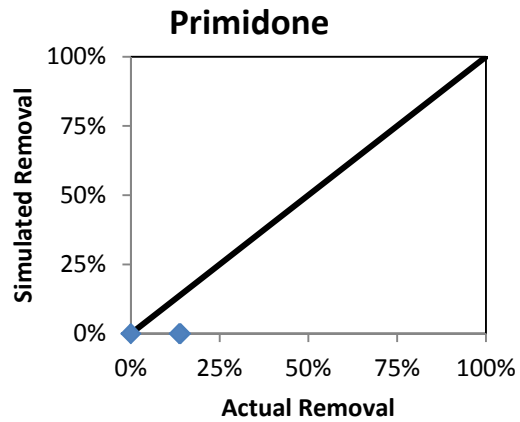


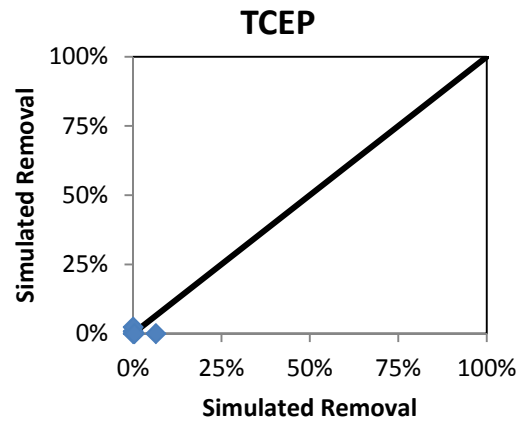


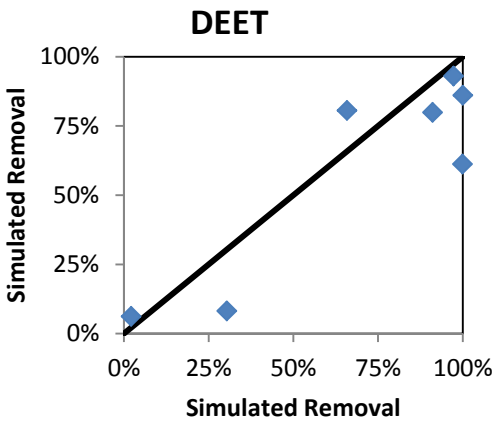


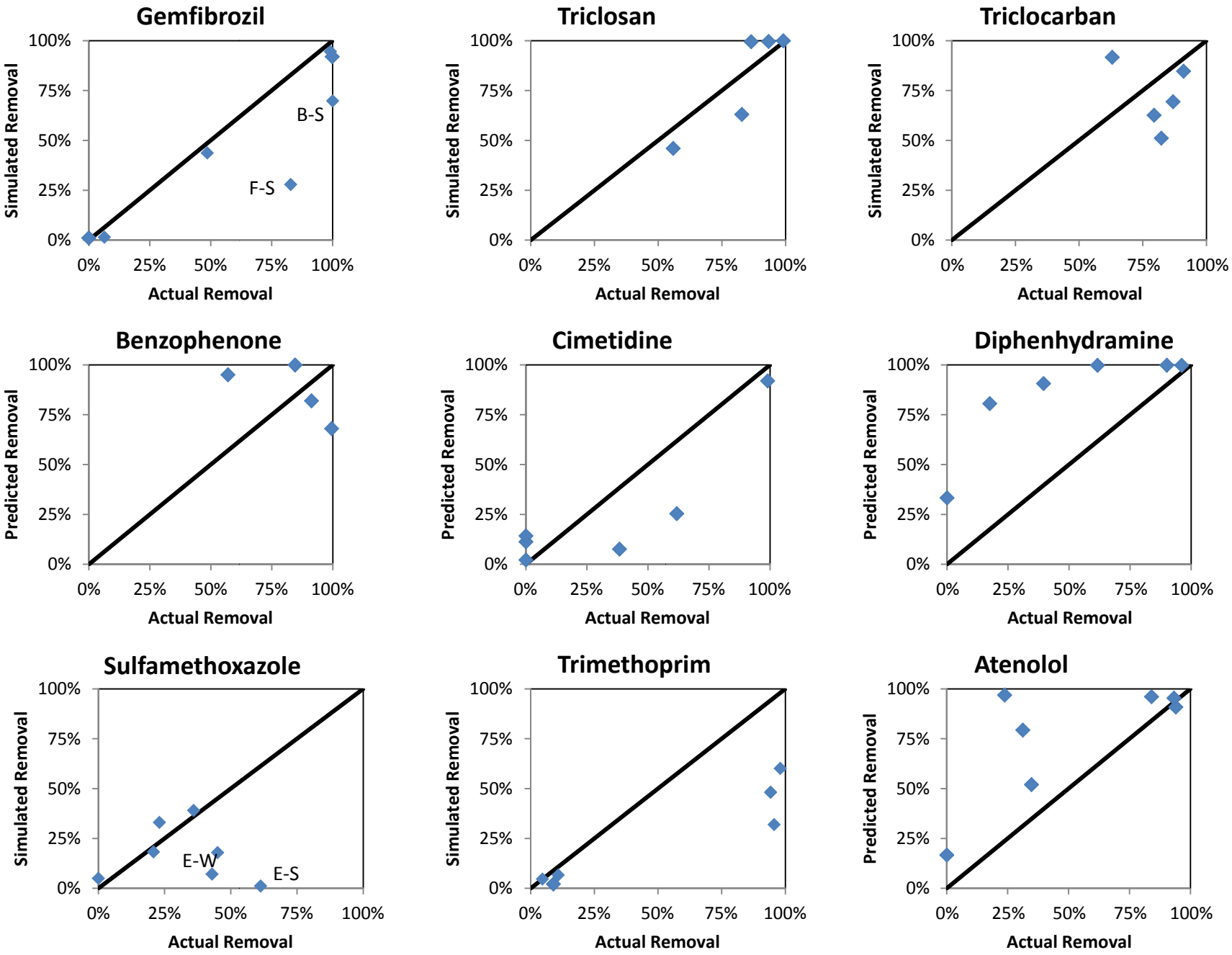










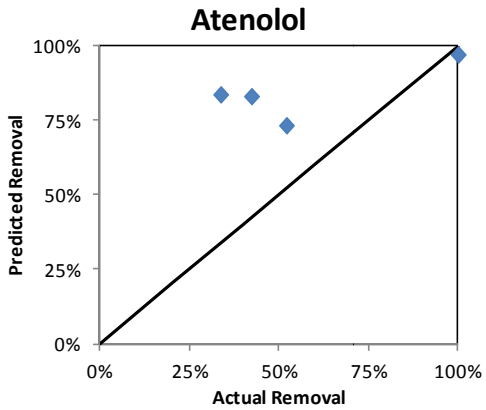

Gemfibrozil
Simulated Removal
Actual Removal
B-S
F-S
Triclosan
Simulated Removal
Actual Removal
Triclocarban
Simulated Removal
Actual Removal
Benzophenone
Predicted Removal
Actual Removal
Cimetidine
Predicted Removal
Actual Removal
Diphenhydramine
Predicted Removal
Actual Removal
Sulfamethoxazole
Simulated Removal
Actual Removal
E-W
E-S
Trimethoprim
Simulated Removal
Actual Removal
Atenolol
Predicted Removal
Actual Removal
0%
25%
50%
75%
100%

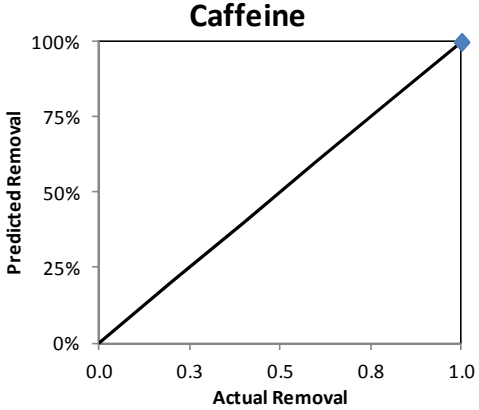
H.3.4 ASTreat Validation Raw Data

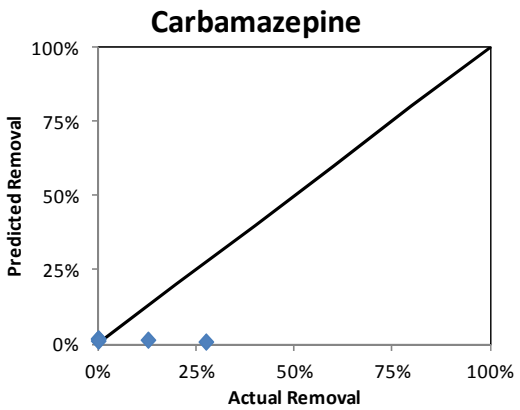
	Actual removal		Actual removal			Predicted removal		Predicted removal		
Location	A - Winter	A - Summer	G - Low SRT	G - Med SRT	G - High SRT	A - Winter	A - Summer	G - Low SRT	G - Med SRT	G - High SRT
Acetaminophen	100%	99%	100.0%	100.0%	n.q.	97.9%	97.1%	97.4%	99.3%	99.4%
Atenolol	34%	42%	52.0%	100.0%	n.q.	83.6%	83.0%	73.2%	97.0%	98.7%
Benzophenone	n.q	n.q	n.q.	99.3%	n.q.	88.2%	84.2%	85.6%	95.7%	96.2%
BHA	26%	73%	50.0%	99.3%	99.6%	n/a	n/a	n/a	n/a	n/a
Bisphenol A	n.q	n.q	n.q.	n.q.	n.q.	n/a	n/a	n/a	n/a	n/a
Caffeine	n.q	100%	100.0%	100.0%	100.0%	99.7%	99.6%	99.6%	99.9%	99.9%
Carbamazepine	13%	27%	-8.9%	-17.2%	-17.2%	1.3%	0.6%	1.6%	1.7%	1.0%
Cimetidine	31%	99%	-16.5%	25.5%	12.8%	20.5%	15.5%	17.6%	42.3%	45.7%
DEET	61%	96%	5.3%	62.6%	78.9%	70.2%	84.9%	29.6%	60.2%	63.9%
Diphenhydramine	61%	70%	41.1%	96.5%	96.3%	91.1%	97.2%	89.1%	99.8%	99.8%
Fluoxetine	15%	33%	29.0%	32.9%	38.1%	99.8%	99.8%	99.8%	99.9%	100.0%
Gemfibrozil	75%	89%	83.5%	98.1%	99.5%	45.2%	37.3%	39.9%	78.5%	89.3%
Ibuprofen	100%	100%	99.8%	100.0%	99.9%	99.0%	98.6%	98.7%	99.7%	99.7%
Iopromide	n.q	n.q	98.5%	99.6%	n.q.	57.9%	49.6%	54.7%	79.7%	82.3%
Meprobamate	-8%	2%	11.1%	89.6%	90.4%	1.9%	1.0%	1.1%	n/a	n/a
Musk Ketone	n.q	n.q	n.q.	n.q.	n.q.	n/a	n/a	n/a	n/a	n/a
Naproxen	95%	99%	98.4%	100.0%	100.0%	94.8%	92.9%	93.6%	98.2%	98.4%
Primidone	9%	23%	-4.0%	-4.0%	-4.0%	0.8%	0.4%	1.0%	1.0%	0.6%
Sucralose	n.q	n.q	-22.0%	n.q.	1.7%	0.8%	0.4%	1.0%	1.0%	0.6%
Sulfamethoxazole	-4%	12%	-108.4%	-91.7%	-41.7%	5.4%	3.6%	5.1%	12.3%	13.5%
TCEP	n.q	n.q	12.0%	12.1%	15.1%	0.8%	0.4%	1.0%	1.0%	0.6%
TCPP	n.q	n.q	n.q.	n.q.	n.q.	n/a	n/a	n/a	n/a	n/a
Triclocarban	45%	63%	50.5%	68.0%	74.6%	69.7%	58.2%	75.4%	82.9%	50.6%
Triclosan	94%	96%	85.7%	92.3%	97.2%	99.8%	99.7%	99.7%	99.9%	99.9%
Trimethoprim	15%	n.q	22.5%	97.0%	98.2%	19.4%	18.7%	5.3%	55.5%	58.3%

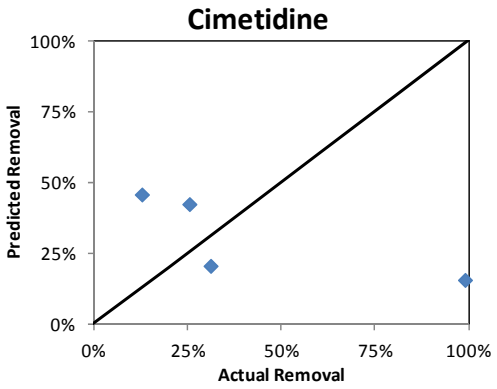
H.3.5 AST

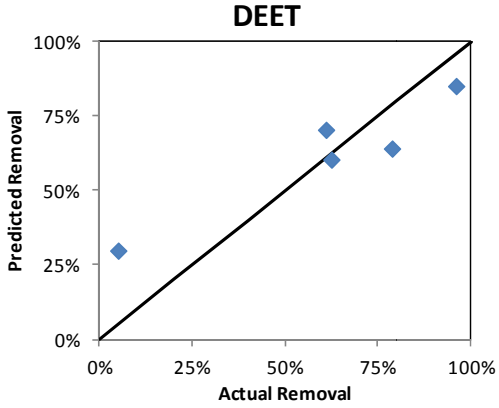
reat Mode l Validation Graphs

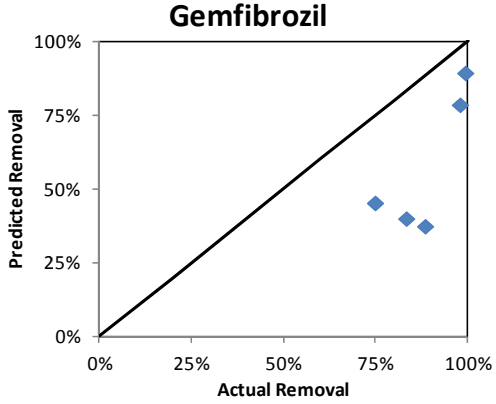


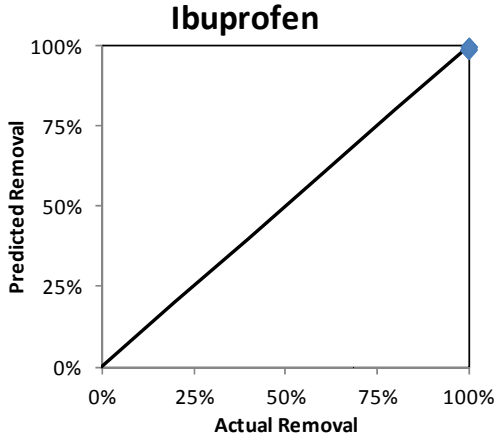


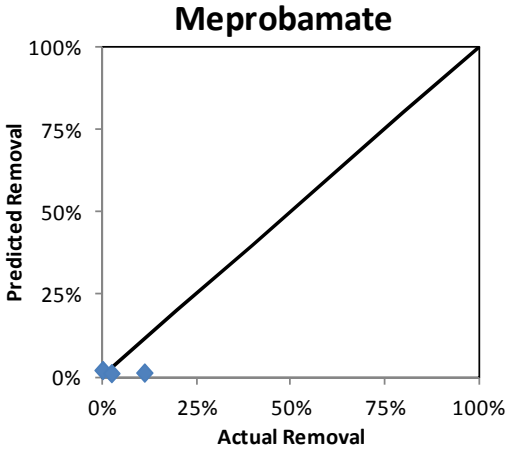


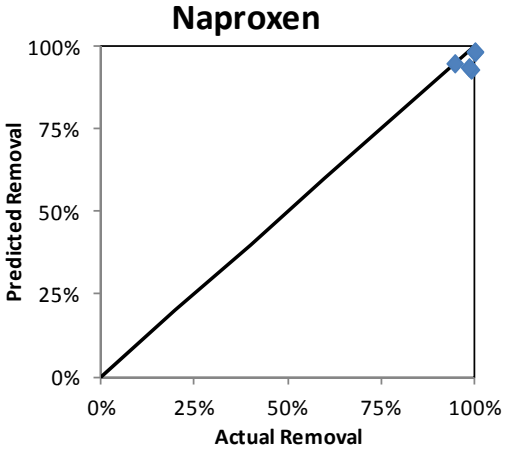


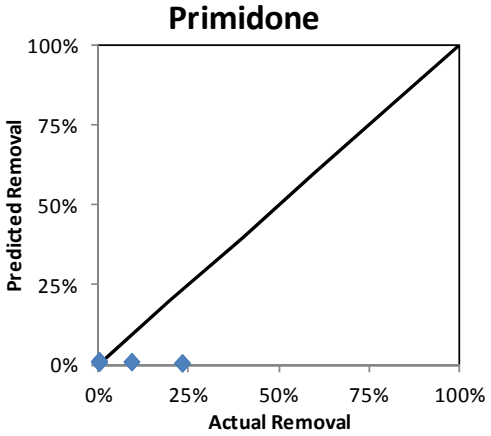


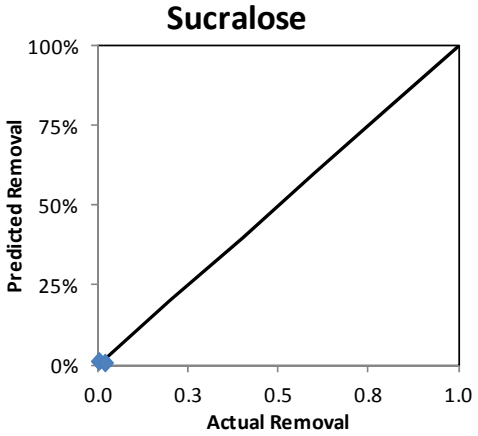


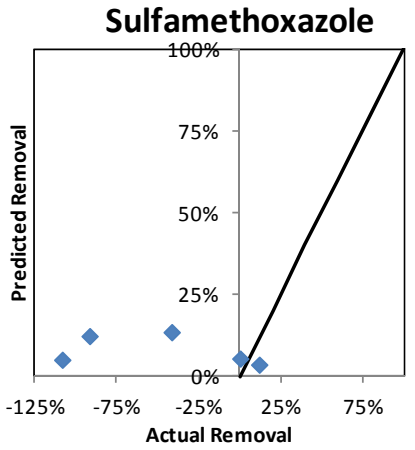


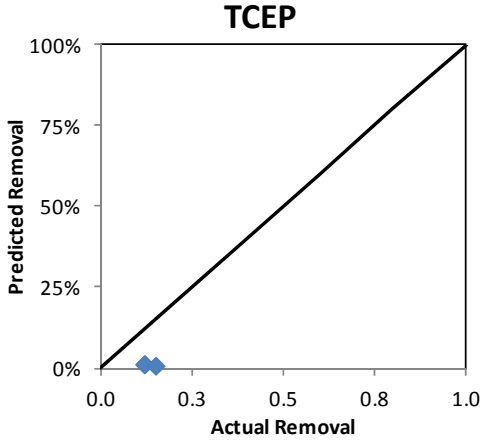


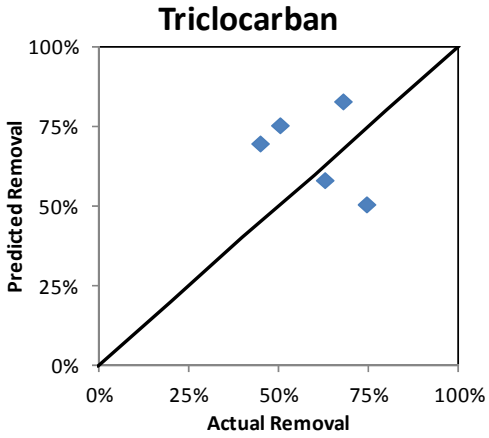



Primidone
Predicted Removal
Actual Removal
0%
25%
50%
75%
100%


Sucralose
Predicted Removal
Actual Removal
0%
25%
50%
75%
100%
0.0
0.3
0.5
0.8
1.0


Sulfamethoxazole
Predicted Removal
Actual Removal
100%
75%
50%
25%
0%
-125%
-75%
-25%
25%
75%


TCEP
Predicted Removal
Actual Removal
100%
75%
50%
25%
0%
0.0
0.3
0.5
0.8
1.0


Triclocarban
Predicted Removal
Actual Removal
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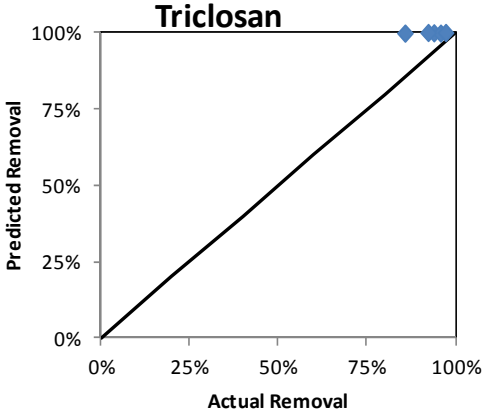
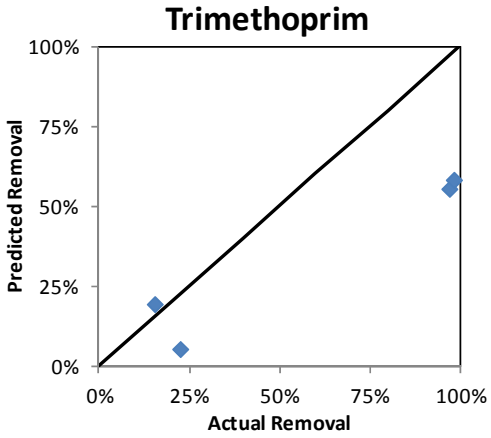
75%
50%
25%
0%
0%
25%
50%
75%
100%


Triclosan
Predicted Removal
Actual Removal
100%
75%
50%
25%
0%
0%
25%
50%
75%
100%


Trimethoprim
Predicted Removal
Actual Removal
100%
75%
50%
25%
0%
0%
25%
50%
75%
100%

H.4 Sensitivity/Uncertainty Analysis

H.4.1 Sensitivity Analysis

The sensitivity of eight parameters within the model ASTREAT was analyzed in order to determine which parameters, when varied, have the greatest impact on the output. A sensitivity parameter was calculated by comparing percent removal values (state variable or SV) from a calibrated model run to values obtained by varying a single parameter (parameter variable or P) by a fixed percentage. Parameter variables included: biotransformation rate, partitioning coefficient, sludge retention time (SRT), hydraulic retention time (HRT), concentration of mixed liquor suspended solids (MLSS), aeration basin (AB) depth, concentration of total suspended solids (TSS) in the return activated sludge (RAS), and influent concentration.

Three compounds, DEET, gemfibrozil, and triclocarban were used to establish different scenarios that are representative of various compounds in this study: 1) significant biotransformation rate, 2) low biotransformation rate with significant sorption, and 3) zero biotransformation rate with high sorption.

The sensitivity parameter (SP) was calculated according to the following equation

$$SP\ \% = 100 * \frac{\left|\frac{\Delta SV}{SV}\right|}{\left|\frac{\Delta P}{P}\right|}$$

where

ΔSV = change in the state variable resulting from the parameter change
SV = state variable value prior to parameter change
ΔP = change in parameter variable
P = parameter value prior to parameter change

Baseline values for the calibrated model are shown in Table H-6. The process treatment conditions at Utility A in the summer (A#2) were employed. The k_b values for the 3 compounds represent experimental data from a single sludge from Utility D sampled in the summer, while the K_d values are experimental values averaged from five different sludges (Utilites B, C, D, E, and F).

A summary is presented in Table H-7. In Scenario 1 (DEET), K_b and HRT are equally sensitive and no other parameters showed sensitivity. This indicates that when there is significant biotransformation , these two parameters have the greatest impact on the percent removal. Scenario 2 (Gemfibrozil) shows the same result as Scenario 1, indicating that even using a lower biotransformation rate results in a higher sensitivity for this parameter compared to sorption. In Scenario 3 (Triclocarban), where biotransformation is not present, four parameters (K_d, HRT, SRT, MLSS) show similar sensitivity. However, SRT shows a reverse trend in percent removal (data not shown) compared to other parameters; a decrease in SRT resulted in an increase in removal. Three parameters (AB depth, RAS TSS, influent) are not sensitive in any scenario. In each scenario, a decrease in the parameter had a stronger effect on sensitivity than an increase in the parameter. Also, sensitivity may not be linear. In a graph of % parameter change (-20% to 20%) versus percent removal, the best-fit line is polynomial (Figure H-1). This trend might be more apparent if the range for % parameter change were increased.

Table H-6. Baseline Model Input Values Used for the Sensitivity Analysis.

Parameter Variable	Unit	Value	Parameter Variable		Unit	Value
SRT[1]	d	12.5	K_b[2]	DEET	1/d	21
				Gemfibrozil		4.0
HRT[1]	h	6.7		Triclocarban		0
			K_d[2]	DEET	L/kg	86
MLSS[1]	mg/L	1740		Gemfibrozil		120
				Triclocarban		2329
AB depth[1]	m	4.27	Influent[1]	DEET	ng/L	5850
				Gemfibrozil		900
RAS TSS[1]	mg/L	4460		Triclocarban		280

1 – Operational and water quality data for Utility A#2; 2 – Measured for sludge from Utility D.

Table H-7. Sensitivity Parameter Results for ±10% Parameter Change.

Scenario 1: DEET			Scenario 2: Gemfibrozil			Scenario 3: Triclocarban		
P	SP (-10%)	SP (+10%)	P	SP (-10%)	SP (+10%)	P	SP (-10%)	SP (+10%)
K_b	16.4	12.9	K_b	49.1	43.4	K_b	n/a	n/a
K_d	0	0	K_d	0	0	K_d	88	84.8
SRT	0	0	HRT	50.9	43.4	HRT	118	114.9
HRT	16.4	12.9				SRT	134	110.6
MLSS	0	0				MLSS	115	112.1
AB depth	0	0				AB depth	0	0
RAS TSS	0	0				RAS TSS	0	1.4
influent	0	0				influent	0	0

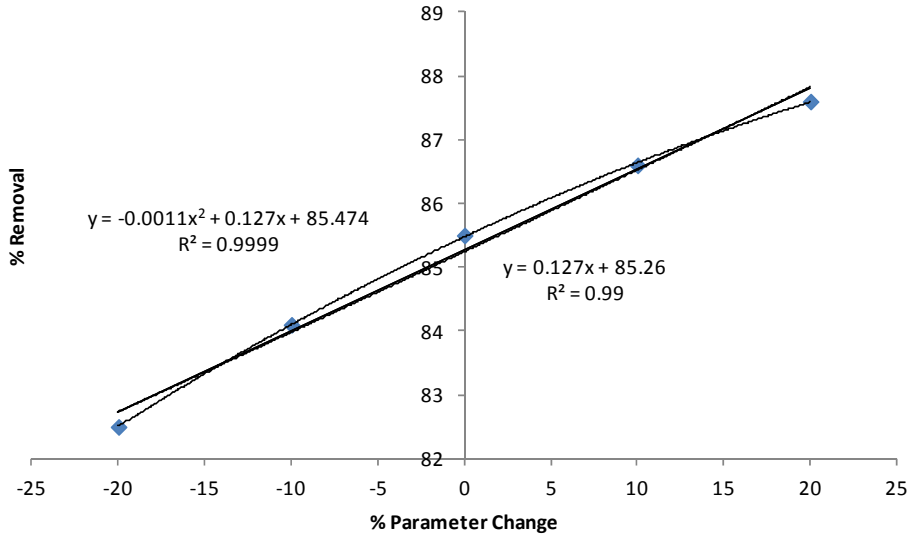


Figure H-1. Effect of K_b or HRT Parameter Change on DEET % Removal for Scenario 1.

H.4.2 Uncertainty Analysis

In conjunction with the sensitivity analysis (Utility A#2 process treatment conditions; K_b values from Utility D, K_d values averaged from Utilites B, C, D, E, and F), eight parameters within the model ASTreat were analyzed in order to determine the magnitude of uncertainty associated with the experimental values. For each compound (n=16), the percent removal was calculated by concurrently changing each parameter by 1 standard deviation and then comparing the result to the baseline model scenario. Only the parameters expected to be sensitive, as determined in the sensitivity analysis, were used for each compound in the uncertainty analysis.

Standard deviations for SRT, HRT, and MLSS were uniform for all compounds and are shown in Table H-8. For K_b and K_d, each compound had a unique, experimentally-determined standard deviation. The coefficient of variation (% CV) for each compound is included in Table H-9 for reference.

Table H-9 shows the results for the uncertainty analysis. Compounds with high baseline percent removal show low uncertainty, as implied by the small range for percent removal. Compounds with low baseline percent removal may appear to have high uncertainty based on the % change in removal; however, the range is still very small, which indicates low uncertainty. In general, compounds at the extremes (i.e., above 95% and below 5%) for percent removal have low uncertainty. Altering the parameters by one standard deviation in either direction in ASTreat shows very little effect on the output, even if the compound has a high K_b % CV such as diphenhydramine. Compounds exhibiting low uncertainty with extreme removal include: caffeine, carbamazepine, diphenhydramine, ibuprofen, sucralose, triclosan, and trimethoprim. Of these compounds, the ASTreat model was a good match to field data for caffeine, carbamazepine, ibuprofen, sucralose, and triclosan.

On the other hand, compounds falling in the range of 5-95% for percent removal have higher uncertainty. Atenolol, benzophenone, cimetidine, DEET, gemfibrozil, naproxen, sulfemthoxazole and triclocarban had higher uncertainty removal ranges, 10-34%. Figure H-2 compares the predicted values including the uncertainty error with observed values. It appears that the percent removal is a stronger indicator for uncertainty compared to K_b % CV. For example, gemfibrozil (53% removal) shows greater uncertainty than ibuprofen (97.1% removal) despite larger K_b % CV for ibuprofen.

Table H-8. Standard Deviations for Uniform Parameters.

Parameter Variable	Baseline	St. dev.
SRT (d)	12.5	2
HRT (h)	6.7	2
MLSS (mg/L)	1740	15%

Table H-9. Percent Change for Removal and Range for Comparing Baseline Model Results to ±1 Standard Deviation Change.

Compound	Baseline % removal	K_b % CV	K_d % CV	% change in removal -1 st. dev.	% change in removal +1 st. dev.	Range for % removal
Atenolol	85.1	34	0.30	-15	7	18.1
Benzophenone	87.3	48	0.70	-18	6	21.2
Caffeine	99.7	15	0.41	0	0	0.2
Carbamazepine	0.6	0	1.95	-59	110	1.0
Cimetidine	16.9	19	1.35	-36	37	12.3
DEET	85.5	41	3.32	-17	7	20.8
Diphenhydramine	99.7	73	1.22	-1	0	1.5
Gemfibrozil	53.0	36	1.89	-38	26	33.7
Ibuprofen	97.1	47	2.07	-5	1	5.9
Naproxen	89.8	50	2.48	-16	5	18.8
Sucralose	0.4	0	n/a	-69	102	0.7
Sulfamethoxazole	22.5	46	0.95	-59	61	27.0
Triclocarban	7.0	0	0.16	-59	85	10.1
Triclosan	99.8	77	0.18	0	0	0.2
Trimethoprim	3.8	41	0.70	-88	131	8.3

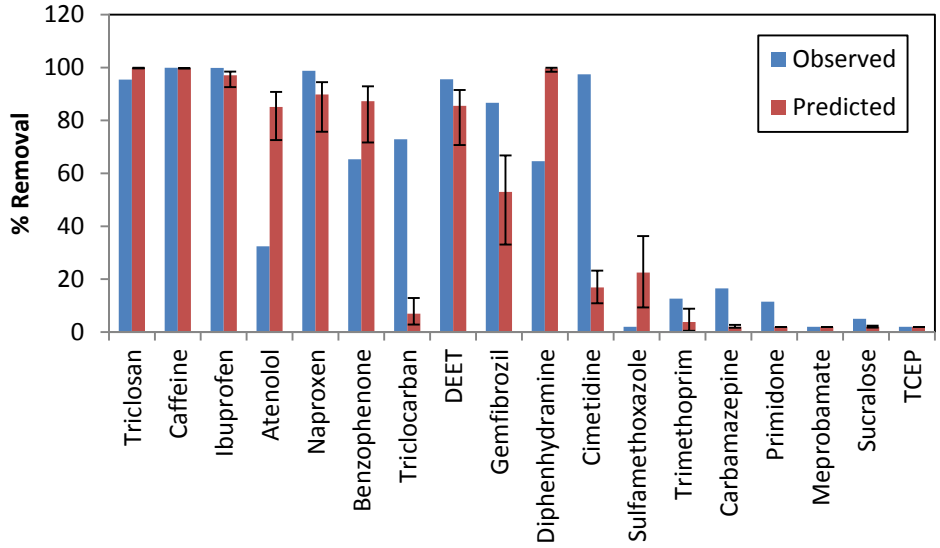
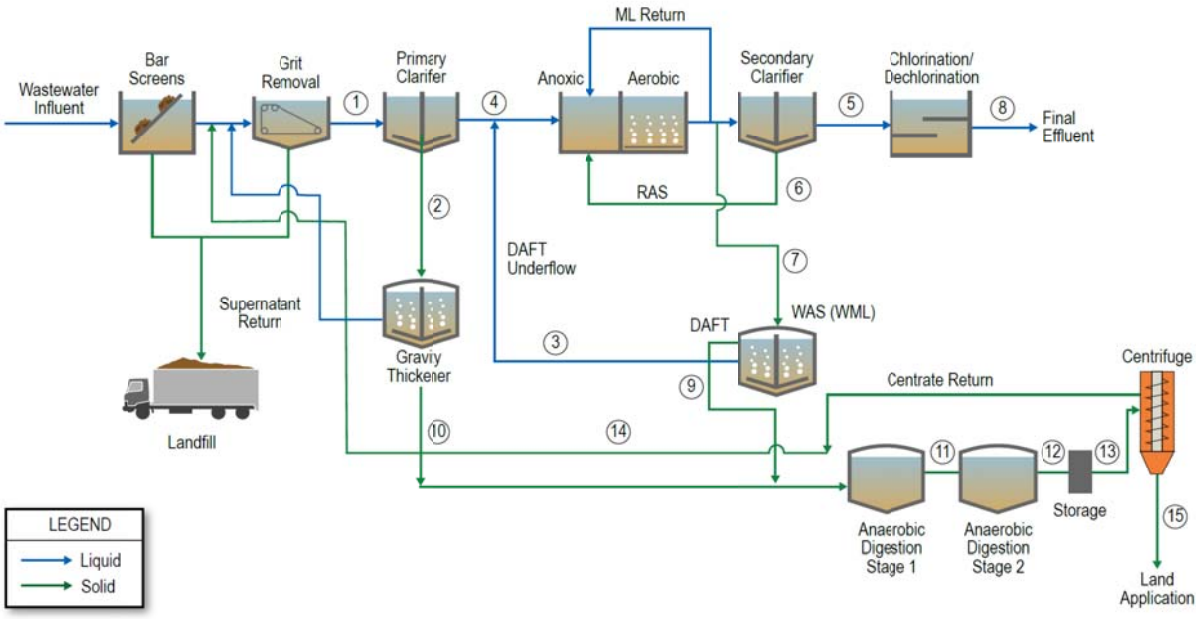


Figure H-2. Comparison of Observed and Predicted Removals with Uncertainty Range.

APPENDIX I

ANAEROBIC DIGESTION STUDY RESULTS

I.1 Process Flow Diagram – Facility A



Sampling Locations: Additional samples for Anaerobic Digestion study in italic.

Primary, Secondary & Disinfection Treatments

1. *Primary influent (composite)*
2. *Primary sludge (grab)*
3. *DAFT underflow (composite)*
4. Aeration Basin Influent (composite)
5. Secondary clarifier effluent (composite)
6. RAS (grab sample)
7. *WAS/ML (grab sample)*
8. Final Plant Effluent after dechlorination (composite)

Sludge Thickening, Anaerobic Digestion, and Biosolids Dewatering

9. DAFT overflow, TWAS (with polymer addition) (manual composite)

10. Gravity thickener underflow, TPS (manual composite)

11. Anaerobic digestion sludge effluent: Stage 1 (manual composite)

12. Anaerobic digestion sludge effluent: Stage 2 (manual composite)

13. Anaerobic digested sludge storage effluent (manual composite)

14. Centrate (grab sample)

15. Dewatered biosolids sample (grab sample)

I.2 Solids Treatment Performance – Facility A

A detailed description of the solids treatment parameters during the field sampling campaign are provided in Table I.2-1.

Table I.2-1. Solids Treatment at Facility A During Digester Sampling Campaign.

Process	Operational Parameter
Gravity Thickening	
Number of GT units in use	1
Tank dimensions (L x W), each (ft x ft)	42' Diameter x 15' Sidewall Depth
Solids loading rate (lbs/hr-ft^2)	562.5lbs/hr/ 1385 ft^2 = 0.406
Hydraulic loading rate (gpm/ft^2)	694.4 gpm/ 1385 ft^2 = 0.501
Solids capture (%)	> 98%
PS solids concentration (% TS)	< 0.5% TS
Thickened PS concentration (% TS)	5 – 6% TS
Dissolved Air Flotation	
Number of DAF units in use	1
Tank dimension (L x W), each (ft x ft)	27' Diameter x 11.75' Depth
Solids loading rate (lbs/hr-ft^2)	284.95 lbs/hr / 573 ft^2 = 0.50
Hydraulic loading rate (gpm/ft^2)	284.7 gpm / 573 ft^2 = 0.50
Polymer Addition (Type, Dosage)	Cationic, ~ 2 pounds/dry ton
Solids capture (%)	> 98%
WAS solids concentration (mg/L TSS)	1,800 – 2,100 mg/l TSS
Thickened WAS concentration (% TS)	4 – 4.5% TS

Process	Operational Parameter
Digester No. 1 (Primary)	
Diameter, ft	90
Side Water Depth, ft	26.75
Volume, gal	1,200,000
Hydraulic Residence Time, days	20
Volatile Solid Loading Rate, lbs VS/cf/day	12,917 lbs VS / 160,430 ft^3 = 0.0805
VS destruction, %	60% per Van Kleek
Temperature, °C	36°C
Digester No. 2 (Secondary)	
Diameter, ft	90
Side Water Depth, ft	21
Volume, gal	1,000,000 (Operated in fill and draw operation)
Hydraulic Residence Time, days	15
Volatile Solid Loading Rate, lbs VS/cf/day	Unknown gas production, not calculated
VS destruction, %	< 10% per Van Kleek
Temperature, °C	36°C
Pre-Dewatering Storage Tank No. 1	
Diameter, ft	70
Side Water Depth, ft	8
Volume, gal	490,000 (includes cone bottom)
Hydraulic Residence Time, days	N/A
Pre-Dewatering Storage Tank No. 2	
Diameter, ft	70
Side Water Depth, ft	8
Volume, gal	490,000 (includes cone bottom)
Hydraulic Residence Time, days	N/A
Centrifugation	
Number of units in use	2
Digested Sludge Solids, % TS	2 – 3%TS
Dewatered Sludge Solids, % TS	20 – 24%TS

I.3 Analytical Methods

I.3.1 Procedure for Total TOrC Concentrations (Aqueous + Solids)

I.3.1.1 Sample Extraction

The samples analyzed for total TOrC concentrations were extracted using a Dionex 200 Accelerated Solvent Extraction (ASE) system. The samples were first frozen at -4°C, and then put in a -80°C freezer for 24 hours. Samples were then lyophilized to remove water using a LabConco 10411E Free Drier at 24°C and 0.006 megabars. Stainless steel extraction cells (22 mL) were fit with a Dionex Glass fiber filter (19.8 mm) before being packed with freeze-dried solids and sand. Isotope surrogate standards, 100 µL of a 4,000 ng/L solution for ESI+ compounds and an 8,000 ng/L solution for ESI- compounds, were spiked directly into the extraction cell. The samples were extracted with 40 mL of methanol. Operational parameters for the ASE method are provided in Table I.3-1.

To clean-up the 40 mL extracts, each extract was diluted with 1,000 mL of ultra pure water and loaded onto a Waters 176 Oasis® HLB Solid Phase Extraction cartridge. Each cartridge was eluted with 5 mL methanol/5 mL 9:1 MTBE:methanol and evaporated under nitrogen gas to a volume of 1 mL. The eluted extract was then diluted with ultra pure water prior to analysis by LC-MS/MS (135 µL of extract diluted up to 1.35 mL with water in an autosampler vial). The samples were analyzed by the same procedure as described in the *Procedure for Aqueous TOrC Concentrations* section below.

Table I.3-1. Operational Parameters for DIONEX 200 ASE.

Cell Preheat	5 min
Heat Up Time	5 min
Static Extraction Time	5 min
Flush Percentage	100%
Purge Time for Nitrogen Gas	60 sec
Number of Cycles	3
Temperature	100^0C
Pressure	10.3 MPa
Solvent A	Methanol
Solvent B	HPLC Water

I.3.2 Procedure for Aqueous TOrC Concentrations

I.3.2.1 Sample Extraction

The target compounds were extracted from aqueous samples onto hydrophilic-lipophilic balance (HLB) solid phase extraction (SPE) cartridges from Waters Corporation. Cartridges were sequentially preconditioned with 5 mL $MeCl_2$, 5 mL MTBE, 5 mL methanol, and 5 mL of reagent water. Sample volumes of 20-30 mL were measured into 50 mL polypropylene conical tubes and spiked with isotopically-labeled standards before being loaded onto the SPE cartridges (see Table I.3-2 for details of isotopic standards). After loading the samples onto the SPE cartridges, they were rinsed with an additional 5 mL of HPLC grade water and dried under nitrogen. The SPE cartridges were then eluted with 5 mL of methanol followed by a 10/90 methanol/MTBE (v/v) mixture. The eluents

were first added to 50 mL centrifuge tubes, capped and shaken, and then poured directly onto the SPE cartridge to maximize analyte recoveries. The resultant extracts were dried under nitrogen in a heated (30˚C) water bath to a final volume of 1 mL. Finally, samples were diluted to 10/90 methanol/water (v/v) ratio for analysis by liquid chromatography tandem mass spectrometry (LC-MS/MS) with isotope dilution.

I.3.2.2 Sample Analysis

Samples were analyzed using LC-MS/MS conditions adapted from Vanderford and Snyder (2006). Briefly, each extract was injected twice and analyzed via electrospray ionization (ESI) in both positive and negative ionization modes. An Agilent 1200 Series Binary Pump and LEAP technologies CTC Analytics HTS PAL autosampler equipped with a 1 mL sample loop was used for all analysis. Compounds were separated using a 150 mm x 4.6 mm Luna C18 column with a 5 μm particle size. Mass spectrometry was performed using an Applied Biosystems 3200 QTrap. Compound and source dependent parameters were optimized for each TOrC and were similar to previously-reported values (Vanderford et al., 2003).

I.3.2.3 Calibration and Quality Assurance

The instrument was calibrated for each analyte at concentrations between 2.5 and 10,000 ng/L with stable isotope addition for positive and negative ionization mode compounds. Correlation coefficients for the calibration curve typically exceeded 0.995. An additional challenge when working with wastewater samples is that TOrCs may be present in concentrations spanning six orders of magnitude. This is problematic, as the typical linear concentration range is only four orders of magnitude (2.5 ng/L to 10,000 ng/L): spanning an additional order of magnitude or more is generally not possible in a single calibration curve. To quantitate across the complete range, samples were reinjected when necessary at an additional ten-fold dilution (i.e., caffeine, ibuprofen), which corresponds to a calibration curve from 250 ng/L to 50,000 ng/L.

Quantification was performed using Applied Biosystems Analyst software. Sample results were not reported if the analyte peak was less than 30 times greater than background noise. The recovery of the stable isotope surrogate was calculated for each sample and those less than 10% were not reported. Reported values reflect correction based on stable isotope recovery. Stable isotope recovery varied by compound (rather than sample). Typical recoveries were between 10-70%, with most being greater than 25%. Field blanks were prepared for each site and analyzed with typical stable isotope additions to ensure samples were not contaminated during the sampling process.

Table I.3-2. Target Compounds and Stable Isotope Standards Employed and Their Corresponding Retention Time, Molecular Weight, Precursor Ion, Production and Various Mass Spectrometry Tuning Parameters.

Native	RT min	Pre m/z	Pro m/z	DP V	CE eV	CXP V	EP	CEP	Isotope	RT min	Pre m/z	Pro m/z	DP V	CE eV	CXP V	EP	CEP
ESI Positive																	
Atenolol	5.4	267.1	145.1	41	35	4	4	16	Atenolol – d_7	5.4	274.1	145.2	41	35	4	5	16
Benzophenone	11.0	183.0	105.0	31	21	4	4	10	Benzophenone – d_{10}	11.0	193.0	110.1	36	23	4	4	14
Caffeine	6.5	195.1	138.0	36	27	4	4	10	Caffeine – d_9	6.5	204.2	144.1	41	29	4	6.5	12
Carbamazepine	9.2	237.1	165.0	31	55	4	4	14	Carbamazepine – d_{10}	9.2	247.2	204.2	41	29	4	7	14
Cimetidine	5.4	253.1	95.1	26	37	4	4	14	Cimetidine – d_3	5.4	256.0	95.1	26	37	4	3.5	14
DEET	9.9	192.1	119.0	36	23	4	6.5	12	DEET – d_4	9.9	199.2	126.2	41	23	4	4	12
Diphenhydramine	7.5	256.1	167.3	26	19	4	2	18	Diphenhydramine – d_5	7.5	261.2	172.0	16	17	4	2.5	14
Fluoxetine	8.9	310.0	44.1	21	27	6	5	20	Fluoxetine – d_{10}	8.9	315.1	44.1	16	33	4	4.5	16
Meprobamate	7.9	219.1	158.2	21	13	4	7.5	12	Meprobamate – d_3	7.9	222.1	161.2	16	13	4	9	12
Sulfamethoxazole	6.6	254.0	156.0	31	21	4	4	14	Sulfamethoxazole – d_4	6.6	258.0	160.2	36	21	4	4.5	12
Trimethoprim	5.7	291.0	261.2	51	35	4	5.5	16	Trimethoprim – d_9	5.7	300.1	234.2	51	35	4	6	16
TCEP	8.9	284.9	223.0	36	17	4	7	14	TCEP- d_{12}	8.9	297.0	232.0	36	17	4	7	16
TCPP	10.8	329.0	99.1	31	35	4	7	12									
ESI Negative																	
Bisphenol A	8.8	227.0	212.0	-40	-26	-2	-4	-14	Bisphenol A – d_{16}	8.8	241.1	142.1	-90	-38	-2	-8	-21
Gemfibrozil	11.3	249.0	121.0	-25	-18	0	-8.5	-14	Gemfibrozil – d_6	11.3	255.0	120.9	-25	-18	0	-5	-12
Ibuprofen	9.3	205.0	161.2	-20	-10	0	-9	-12	Ibuprofen – d_3	9.3	208.0	164.2	-15	-15	0	-7.5	-12
Naproxen	7.2	229.0	169.0	-10	-38	-2	-3	-14	Naproxen – d_3	7.2	231.9	173.2	-5	-24	-2	-4	-36
Triclocarban	12.3	312.9	159.8	-40	-18	-2	-4	-24	Triclocarban – d_4	12.3	316.8	159.9	-30	-20	-2	-4	-22
Triclosan	12.4	285.8	35.1	-25	-32	-4	-4.5	-38	Triclosan – $^{13}C_6$	12.4	292.8	35	-20	-22	-4	-10	-12

RT = Retention Time Pre = Precursor Ion Pro = Product Ion DP = Declustering Potential CE = Collision Energy
CXP = Collision Cell Exit Potential EP = Entrance Potential CEP = Collision Cell Entrance Potential

I.4 Laboratory-Scale Anaerobic Digestion

The laboratory-scale anaerobic bioreactor was fully operational on July 11th, 2011.

I.4.1 Design and Operation of Bioreactor

The bioreactor was inoculated with anaerobic digester sludge from the second stage digester at Facility A. During the length of this study (87 days; July 11th to Oct 6th, 2011) the system had minimal operational problems. A schematic of the complete system setup is provided in Figure I.4-1.

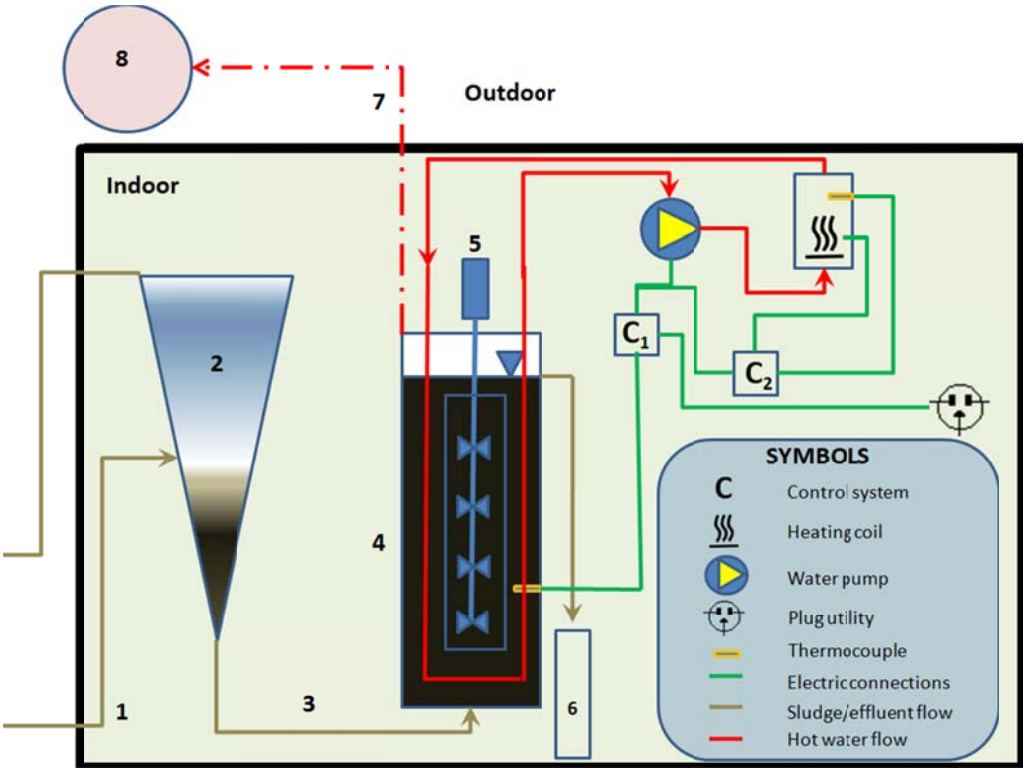


Figure I.4-1. Schematic of Laboratory-Scale Anaerobic Digester.

I.4.2 Bioreactor Feed

Settled solids from a laboratory-scale primary clarifier were used as feed to the anaerobic bioreactor (Figure I.4-2). The primary clarifier was fed with raw wastewater collected from a student housing complex located at the Colorado School of Mines (see Table 7-5 for characteristics of raw wastewater). The clarifier had an effective volume of 96 L with an average HRT of two hours.

Primary sludge from the clarifier was collected for 24 hours before feeding it to the bioreactor. The clarifier was emptied on a daily basis immediately after feeding the bioreactor. Thus, only 24 hour old sludge was used as feed to the anaerobic bioreactor.

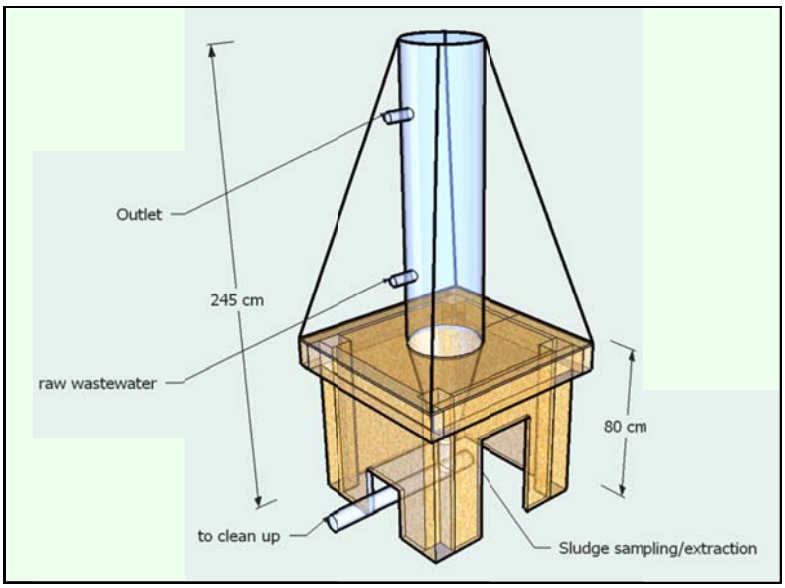


Figure I.4-2. Design of the Primary Clarifier.

I.4.3 Anaerobic Bioreactor

The anaerobic bioreactor was designed as a completely mixed anaerobic reactor. It consisted of a 6-inch diameter clear PVC pipe with flanges. The bottom and top of the reactor were sealed with a rubber gasket between PVC plates screwed tightly to the flanges. The total volume of the bioreactor was 16 L, with an effective liquid volume of 13.3 L. The inlet and outlet fittings were screwed into the top and bottom plates with Teflon tape. The bioreactor was checked for leaks by filling the reactor with water under a positive pressure.

The influent feed enters through the bottom of the reactor (see Figure I.4-1). A bottom feed promotes the settled solids to rise in the reactor. The bioreactor was fed in a batch mode where 665 mL of primary sludge was fed daily. The feed volume was measured by collecting the overflow (effluent) in a 1-L graduated cylinder. An average HRT of 22 days was maintained over the 87-day evaluation period.

Mixing of the bioreactor was accomplished by the draft tube technique. This technique used four propellers connected to a shaft powered by a variable speed motor. The apparatus was housed inside a 2-inch diameter PVC tube. Proper mixing was verified by observing the movement of solids within the bioreactor.

A heat exchanger was used to maintain an operating temperature of 35°C in the bioreactor. The heat exchanger consisted of hot water (50°C) flowing through a stainless steel pipe inside the bioreactor. The recirculating hot water was maintained at temperature by passing it through an electric heating coil located outside of the bioreactor. The temperature of the bioreactor (35°C) and the recirculating water (50°C) were controlled by temperature controllers. If the temperature in the bioreactor decreased by 1°C, then a controller would start the water recirculating pump and the heating coil. A second controller would make sure that the temperature of the hot water did not exceed 50°C. A schematic of the heating system is provided in Figure I.4-1.

Biogas produced during the experiment was vented to a reservoir outside of the testing facility. When approximately 75% of the reservoir volume was filled, the biogas was released and flared.

I.4.4 Sampling and Analytical Methods

Performance of the anaerobic bioreactor was assessed by taking weekly samples of influent and effluent and then analyzing these samples for total solids (TS), volatile solids (VS), total suspended solids (TSS), volatile suspended solids (VSS), chemical oxygen demand (COD), alkalinity (Alk), pH, total nitrogen (TN), nitrate nitrogen (NO_3-N), ammonia nitrogen (NH_3-N), total phosphorus (TP), and orthophosphates (Ortho-P).

I.4.4.1 Sampling Conventional Parameters

Performance samples were collected for 60 days (~3 HRTs) to evaluate steady state conditions and then for an additional 27 days to assess TOrC removals. The samples were collected in 250 mL amber bottles, and then stored at 4°C until being processed for analysis. The system was also checked on a daily basis for pH and temperature.

I.4.4.2 Sampling Trace Organic Compounds

Removal of the indicator TOrCs was evaluated by collecting daily samples, except on weekends, over a 27-day period after the system had reached steady state conditions. The samples were collected in 500-mL amber bottles containing 3-mL of a sodium azide solution (200 g/L) as a preservative. The samples were then storage at -20°C. On a weekly basis, the daily samples were thawed and then mixed to form a 5-d weekly composite sample. The weekly composite samples were then stored at -80°C until processed for analysis.

I.4.4.3 Analytical Methods

Total solids (TS), volatile solids (VS), total suspended solids (TSS), and volatile suspended solids (VSS) were analyzed according to Standard Methods for the Examination of Water and Wastewater (APHA, 2006). Chemical oxygen demand (COD), total nitrogen (TN), nitrate nitrogen (NO_3 - N), ammonia nitrogen (NH_3 -N), total phosphorus (TP), and orthophosphates (Ortho-P) were analyzed using HACH colorimeter methods. The HACH kits are identified as: COD: Dichromate #8000 (High range 20-1500 mg/L); TN: Persulfate digestion #10208 (Range 1-16 mg/L); NO_3-N: Dimethylphenol #10206 (range 0.23-16.5 mg/L NO_3-N); NH_3-N: Salicylate #10205 (range 2-47 mg/L NH_3-N); TP and Ortho-P: ascorbic acid #10209-10210 (range 0.5-5 mg/L PO_3-P).

The pH was measured using an AB15 pH meter from Fisher Scientific. The pH meter was calibrated before use with a pH 4 and 7 buffer. Alkalinity was determined by titration with 1.6 N H_2SO_4 for effluent samples and 0.16 N H_2SO_4 for influent samples. The samples were titrated to a pH of 4.6 using the HACH digital titrator.

TOrC samples were thawed, lyophilized (LabConco 10411E Freeze Drier), and extracted by accelerated solvent extraction (ASE). Individual labeled standards were added to the samples before ASE. The extracted ASE samples were concentrated via SPE followed by LC-MS/MS analysis. Details of the analytical methods maybe found in section *I.3 Analytical Methods*.

I.5 Laboratory Fate Parameter Procedures

The fate paramenter procedures are outlined below.

I.5.1 Batch Sorption Method

The batch sorption experiments followed the method described in Kerr et al. (2000). In these experiments anaerobic digester sludge collected from Facility A was first frozen at -4°C, and then placed in a -80°C freezer for 24 hours. Samples were then freeze dried for 48 hours to remove excess water using a LabConco 10411E Freeze Drier at 24°C and 0.006 megabar. Freeze dried material was weighed into a 50 mL plastic centrifuges tube, and washed 10 times with distilled water to remove any excess dissolved organic carbon (DOC) released during the lyophilization process. In between each washing step, the plastic tubes were centrifuged using an Eppendorf-5810 centrifuge at 4000 rpm (3220 rcf) for 10 minutes.

The sorption experiments were conducted at ambient laboratory temperatures (20°C ± 2°C). In these experiments, the washed freeze-dried solids were resuspended in a synthetic wastewater to a known solids mass content. The experimental solids-to-water ratio (r_{sw}) was achieved by pipetting an appropriate volume of the slurry directly into a 15-mL reactor vessel and then diluted with synthetic wastewater up to 10 mL. For the compounds analyzed by LC-ESI (positive)-MS/MS, two experimental r_{sw} values were employed (800 mg/L and 2500 mg/L) to capture the range of sorption of the suite of analytes. For those compounds analyzed in negative ion mode, only the lower of these r_{sw} values was necessary (800 mg/L). Next, a mixture of TOrCs was spiked into the reactor vessels at concentrations ranging from 0 to 10,000 ng/L. Five separate concentrations were assessed for each TOrC so that an isotherm could be generated. Each concentration was conducted in triplicate to account for variability in the test method. The equilibration time was set at 2 hours to avoid microbial regrowth in the system, as justified by (Kerr et al., 2000). Following the 2-hour equilibration period, the samples were centrifuged (Eppendorf- 5810) at 2000 rpm (805 rcf) for 15 minutes. The supernatants were then analyzed for the TOrCs by the same procedure as described in *I.3 Analytical Methods* under the *Procedure for Aqueous TOrC Concentrations* section.

The isotherms were constructed directly from the supernatant results (i.e., not from background-corrected aqueous concentrations). While this is a less-direct approach than background-correcting the aqueous concentrations, this approach ensured that the highly variable aqueous background levels did not bias the results. As a result, actual measurements of the aqueous concentrations of any of the TOrCs can be used to estimate solid-phase (i.e. sorbed) concentrations without any background offsets. This approach did, however, require calculation of both the additional mass loss from the spiked aqueous phase (i.e., background correction) and an estimation of the background solid-phase concentration to enable an estimation of the actual solid-phase concentration. Mass balance calculations had been performed for previous experiments with fresh activated sludge by extracting the solid phase, and good agreement was shown between the measured sorbed analyte concentrations and those derived from the aqueous loss method (measuring the fraction in water as the aqueous analyte concentration over the spiked concentration). For this reason only the aqueous phase was measured for the experiments with freeze dried anaerobically digested sludge.

A Freundlich isotherm model was developed for each of the TOrCs by performing a linear regression on the log transformed C_w (aqueous phase) and C_s (solid phase) concentrations. The slope and intercept values from these regressions were used to estimate the Freundlich

model parameters (K_f and *n*) for each analyte. The resultant Freundlich isotherm parameters were then used in the interpolation of Log K_d values for each analyte. An aqueous concentration of 1,000 ng/L ($K_{d,int}$) was used to compare the sorption affinity for each TOrC.

I.5.2 Batch Anaerobic Biodegration Test

This test provided the rates of primary biodegradation of TOrCs in the presence of anaerobic digester sludge. Fresh anaerobic digester sludge was collected from the first stage anaerobic digester at Facility A. The collected sample had a pH ~7.4, temperature of ~30°C, and total solids concentration 22.4 g/L. The anaerobic digester sludge was manipulated inside of an anaerobic chamber containing nitrogen and hydrogen gases. A known amount of fresh sludge was spiked with the indicator TOrC compounds (i.e., atenolol, amitriptyline, atrazine, benzophenone, bisphenol A, caffeine, carbamazepine, cimetidine, DEET, diclofenac, dilantin, diphenhydramine, fluoxetine, gemfibrozil, ibuprofen, meprobamate, naproxen, primidone, sulfamethoxazole, TCEP, TCPP, triclocarban, triclosan, and trimethoprim). These TOrCs were spiked at concentrations that ranged from 20-70 µg/L, except for triclosan and triclocarban which were spiked from 1000-2000 µg/L due to expected higher background levels. Norfluoxetine and methylparaben, additional unspiked compounds, were also assessed in collected samples. Afterward 20 mL of spiked sludge was distributed to 50 mL clear glass serum bottles, capped with glass-tight septums, and crimped with aluminum rings (Figure I.5-1). Each serum bottle represented a time point. Triplicate test vessels were prepared. Serum bottles were then removed from the anaerobic chamber and purged with N2 to remove any residual H2. Reactors were stored in a dark incubator at 35 ± 3°C. An unspiked biotic control was used to assess the initial background levels and sludge activity by evaluating gas production. An abiotic control with spiked TOrCs was also performed. The sludge for the abiotic control was inactivated using a combination of heat sterilization (autoclaved for 90 minutes and 120°C) and chemical inactivation (5% sodium azide and 5 mM nickel/barium chloride with 60 minutes of mixing).

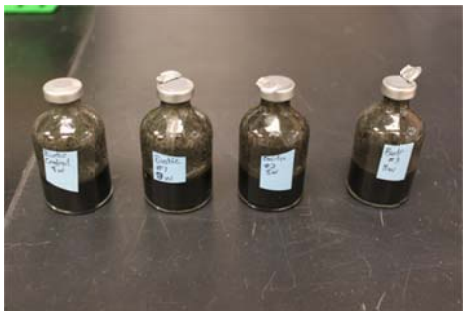


Figure I.5-1. Serum Bottles. Reactors.

Figure I.5-2. Monitoring Pressure Within Reactors.

The pressure within the reactors was monitored over the course of the experiment (up to 56 days) as an indirect measure of anaerobic gas production and biological activity (Figure I.5-2). The kinetic pressure profiles are presented in Figure I.5-3. The pressure in the biotic reactors increased up to 30 psi over the course of the study, indicating significant gas production in the reactor vessels. Gas production was also qualitatively observed via syringe displacement. The biotic control profile was similar to the biotic reactors, suggesting that the activity was similar between the reactors despite the introduction of TOrCs (i.e., no inhibitory effects). As expected, the pressure did not increase in the abiotic reactor, indicating no anaerobic respiration and biological activity.

TOrC samples were collected at the following sampling time points: 0, 2, 8, and 48 hours, and 3 and 7 weeks. At the designated sampling times the serum bottles were frozen at -80°C. Prior to analysis, the samples were thawed, lyophilized (LabConco 10411E Freeze Drier), and extracted by accelerated solvent extraction (ASE). Individual labeled standards were added to the samples before ASE. The extracted ASE samples were concentrated via SPE followed by LC-MS/MS analysis. Details of the analytical methods maybe found in section *I.3 Analytical Methods*.

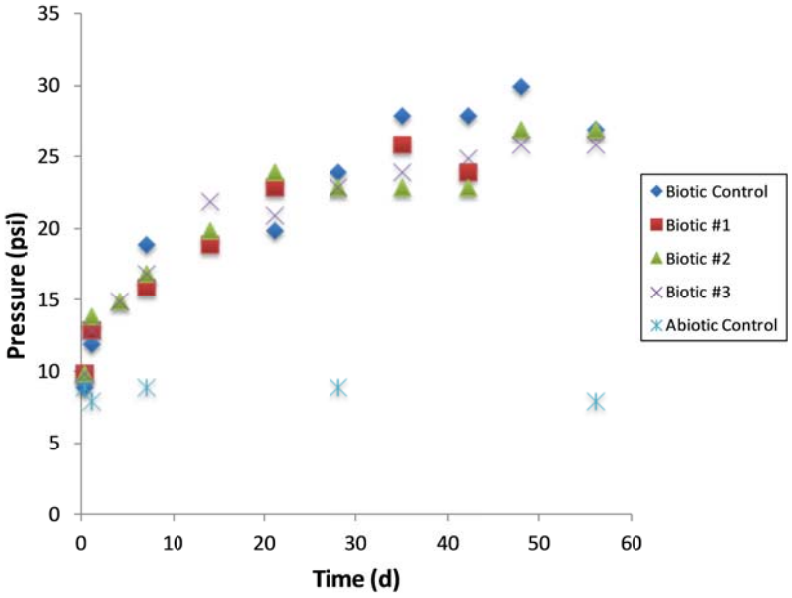


Figure I.5-3. Kinetic pressure profiles.

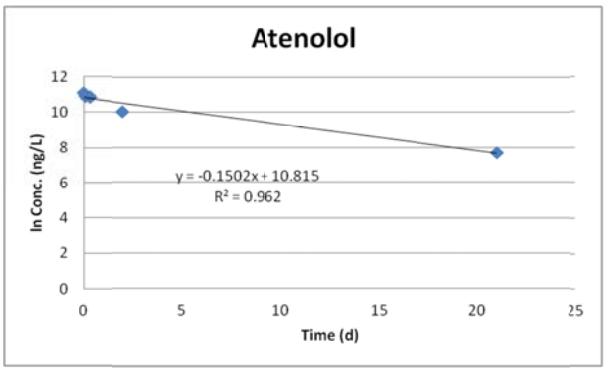
I.6 Calculations

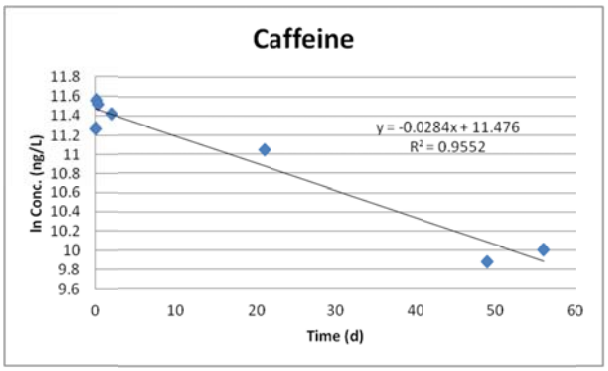
I.6.1 Batch Sorption Experiments – Freundlich Isotherm Model Parameters

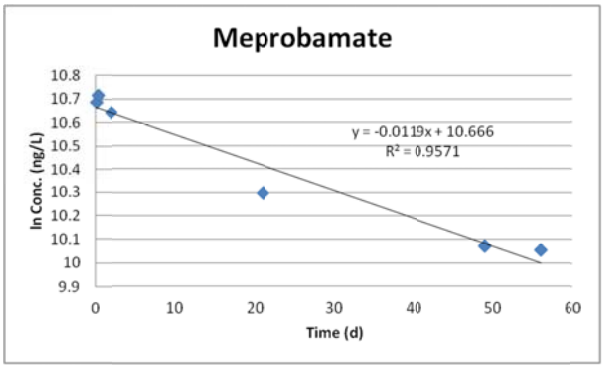
Chemical	LOG K_f	n	R^2	Int. LOG K_d	LOG K_f	n	R^2	Int. LOG K_d
Bisphenol A	2.39	0.86	0.76	1.89	2.24	0.88	0.76	1.89
Ibuprofen					3.05	0.65	0.61	1.98
Triclocarban	4.32	0.88	0.96	3.99	4.93	0.69	0.98	3.99
Triclosan	3.43	0.91	0.95	3.54	4.96	0.53	0.95	3.54
Atenolol	2.68	0.81	0.65	2.10	2.54	0.78	0.60	1.87
Benzophenone	2.30	0.94	0.70	2.12	2.94	0.78	0.67	2.29
Carbamazepine	0.54	1.32	0.74	1.51	-0.16	1.51	0.92	1.36
Cimetidine	2.59	0.86	0.92	2.17	0.27	1.51	0.81	1.79
DEET	-1.28	1.83	0.93	1.21	-0.28	1.46	0.99	1.12
Diphenhydramine	1.37	1.35	0.86	2.43	-0.86	1.99	0.82	2.10
Fluoexetine	1.95	1.51	0.80	3.47	-0.10	2.17	0.80	3.40
Sulfamethoxazole	2.60	0.69	0.88	1.68	2.56	0.59	0.72	1.33
Trimethoprim	1.27	1.09	0.86	1.53	1.61	0.96	0.99	1.48

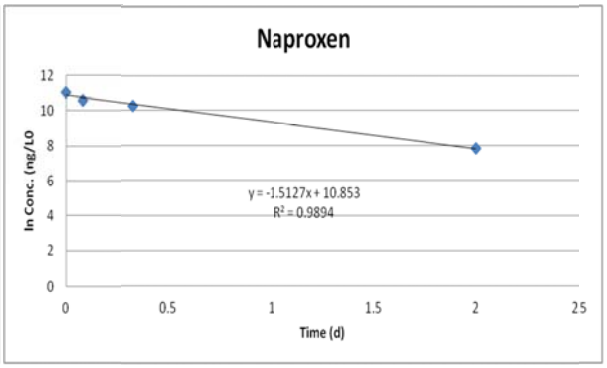
Int. LOG K_d – interpolated log K_d value at aqueous concentration of 1 µg/L

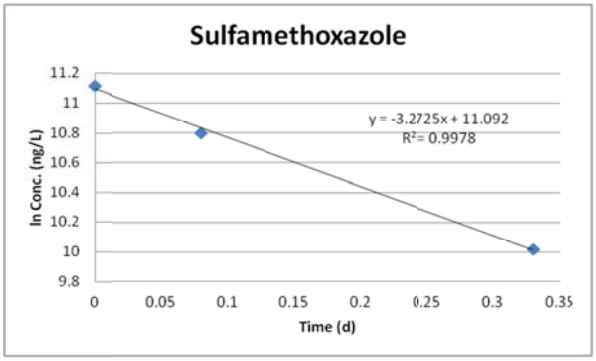
I.6.2 Batch Biotransformation Experiments – First-Order Rate Constants

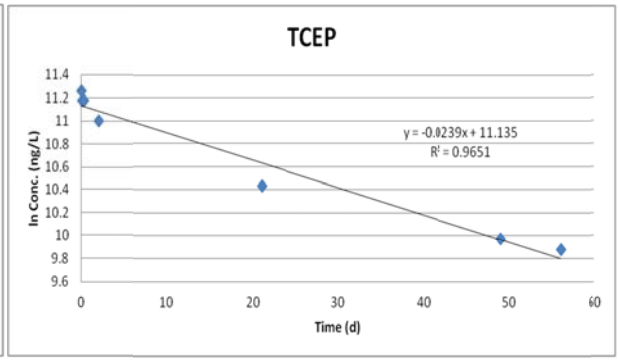


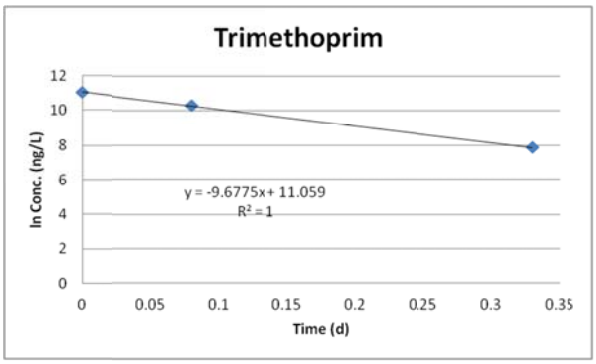












I.6.3 TOrC Mass Balance Calculations – Facility A

TOrC	GT Conc. (ng/g)	DAFT Conc. (ng/g)	AD1 Conc. (ng/g)	AD2 Conc. (ng/g)	GT Flux (mg/h)	DAFT Flux (mg/h)	AD1 Flux (mg/h)	AD2 Flux (mg/h)	GT+DAFT -AD1 Flux (mg/h)	AD1 Removal (%)	AD1-AD2 Flux (mg/h)	AD2 Removal (%)	Total Removal (%)
Atenolol	117.7	22.4	27.5	9.4	18.56	2.52	3.76	1.09	17.32	82.13	2.66	70.82	94.78
Bisphenol A	811.2	508.1	1472.9	1532.1	127.9	57.28	201.73	179.10	-16.51	-8.91	22.62	11.21	3.30
Caffeine	3270.9	390.5	178.7	204.1	515.9	44.02	24.47	23.85	535.41	95.62	0.61	2.51	95.73
Cabamazepine	90.1	25.6	317.4	307.5	14.21	2.88	43.47	35.94	-26.37	-154.27	7.52	17.30	-110.26
DEET	141.3	164.9	180.9	202.7	22.28	18.59	24.77	23.69	16.09	39.38	1.08	4.35	42.02
Fluoexetine	171.0	302.8	515.9	445.9	26.96	34.13	70.65	52.12	-9.55	-15.63	18.53	26.22	14.69
Gemfibrozil	37.9	86.4	193.7	158.3	5.97	9.74	26.52	18.50	-10.81	-68.78	8.02	30.24	-17.73
Meprobamate	4.5	19.0	48	4.9	0.70	2.14	6.57	0.57	-3.72	-130.53	6.00	91.28	79.91
TCEP	133.7	111.2	442.3	370.3	21.08	12.53	60.57	43.28	-26.95	-80.16	17.28	28.53	-28.74
TCPP	157.9	278.5	1245.2	691.2	24.90	31.39	170.54	80.80	-114.24	-202.91	89.74	52.62	-43.52
Triclocarban	6129.4	8911.5	12193	8318.8	966.7	1004.7	1669.9	972.49	301.46	15.29	697.41	41.76	50.66
Trimethoprim	149.7	296.8	75.4	36.1	23.60	33.46	10.32	4.22	46.74	81.90	6.10	59.13	92.60

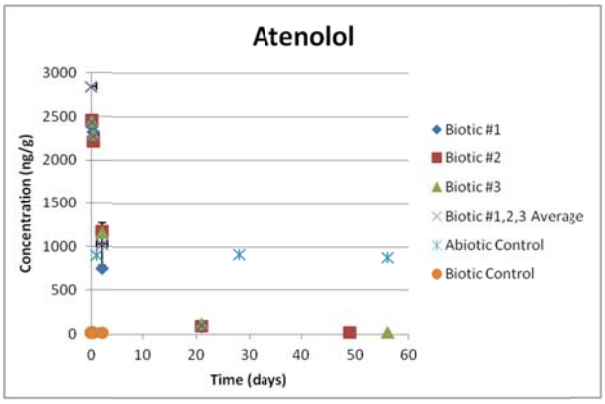
GT = primary sludge gravity thickener; DAFT = secondary sludge dissolved air floatation thickener; AD1 = first stage anaerobic digester; AD2 = second stage anaerobic digester

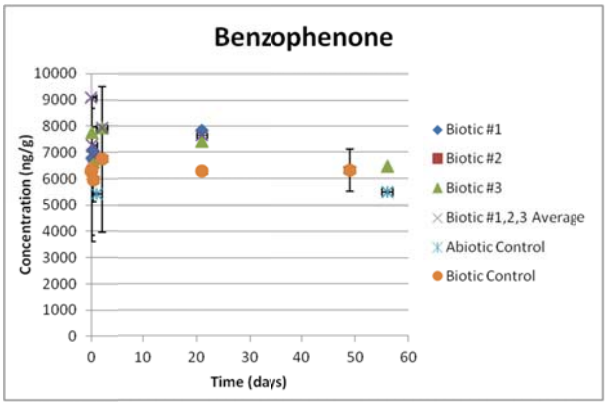
GT TSS = 39125 mg/L; DAFT TSS = 35375 mg/L; AD1 TSS = 18975 mg/L; AD2 TSS = 17017 mg/L

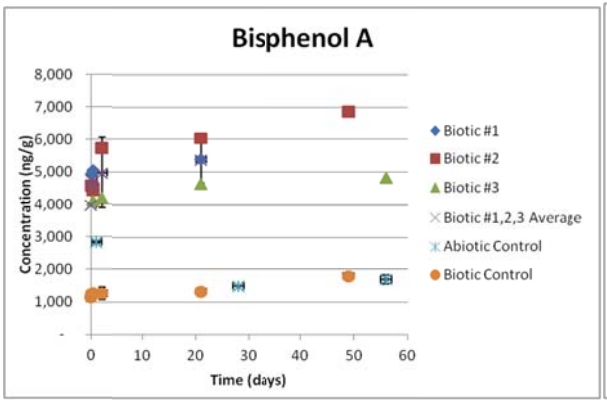
GT Flow = 1065 gph; DAFT Flow = 842 gph; AD1 Flow = 1907 gph; AD2 Flow = 1815 gph

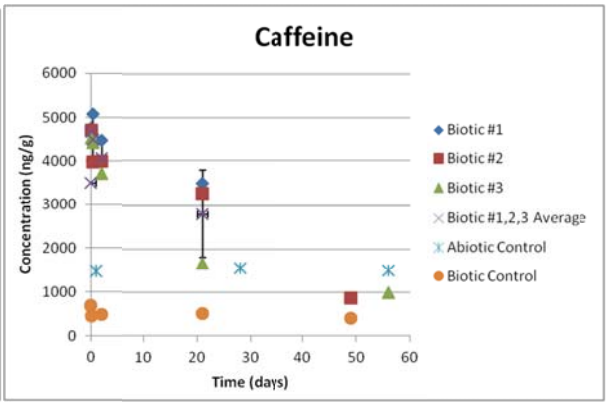
I.7 Raw Data

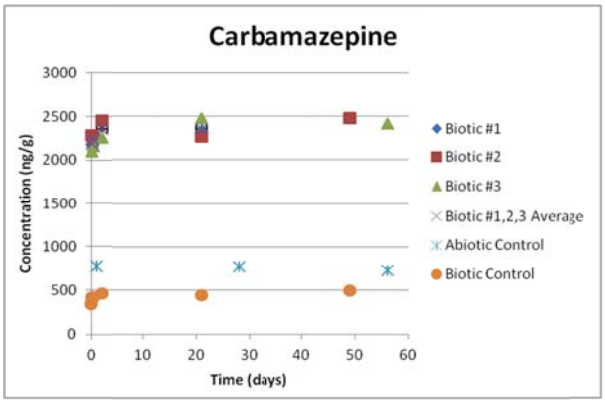
I.7.1 Batch Biotransformation Experiments

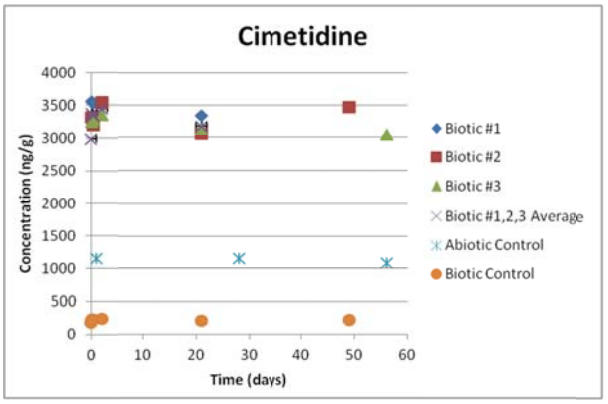


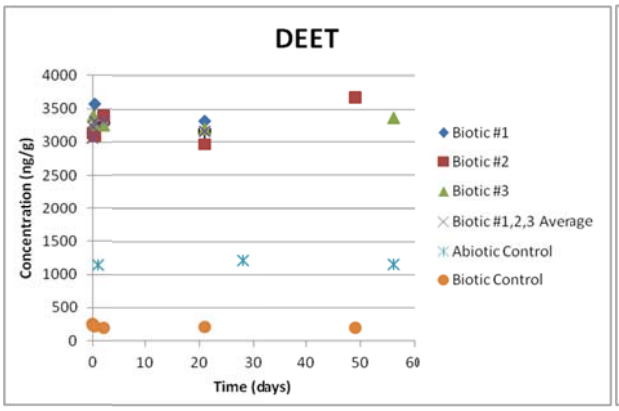


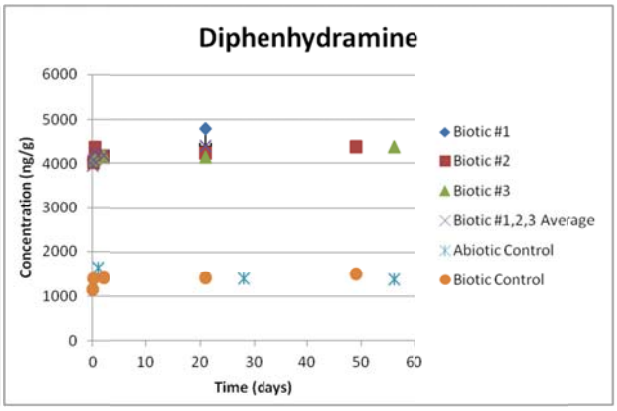









DEET
Concentration (ng/g)
Time (days)
Biotic #1
Biotic #2
Biotic #3
Biotic #1,2,3 Average
Abiotic Control
Biotic Control


Diphenhydramine
Concentration (ng/g)
Time (days)
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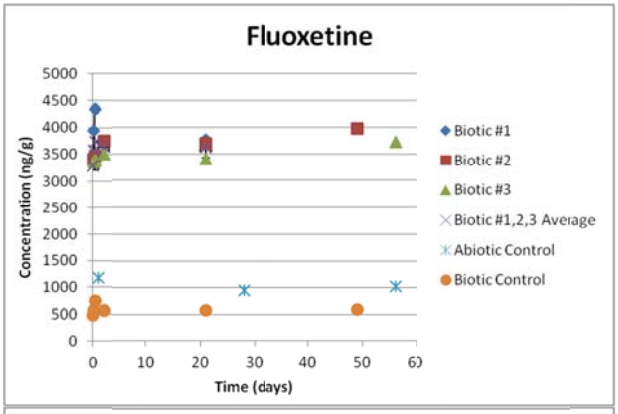
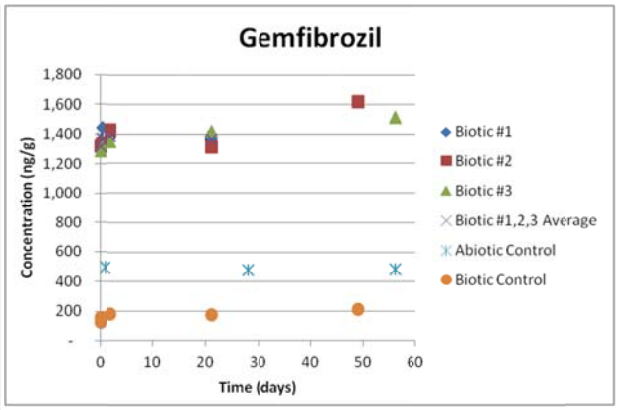
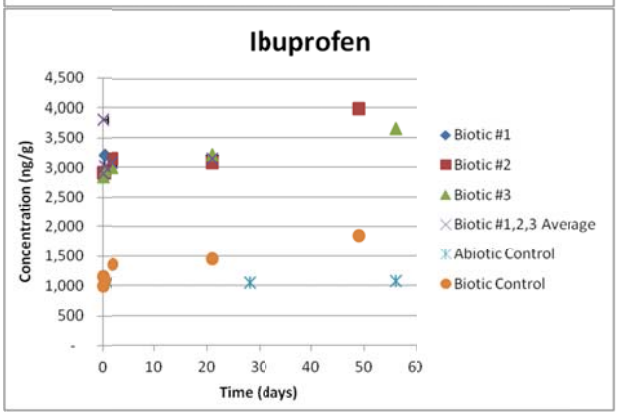
Biotic #2
Biotic #3
Biotic #1,2,3 Average
Abiotic Control
Biotic Control


Fluoxetine
Concentration (ng/g)
Time (days)
Biotic #1
Biotic #2
Biotic #3
Biotic #1,2,3 Average
Abiotic Control
Biotic Control


Gemfibrozil
Concentration (ng/g)
Time (days)
Biotic #1
Biotic #2
Biotic #3
Biotic #1,2,3 Average
Abiotic Control
Biotic Control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Concentration (ng/g)
Time (days)
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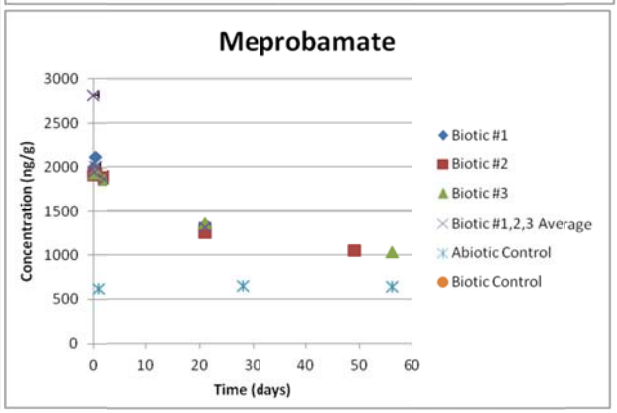
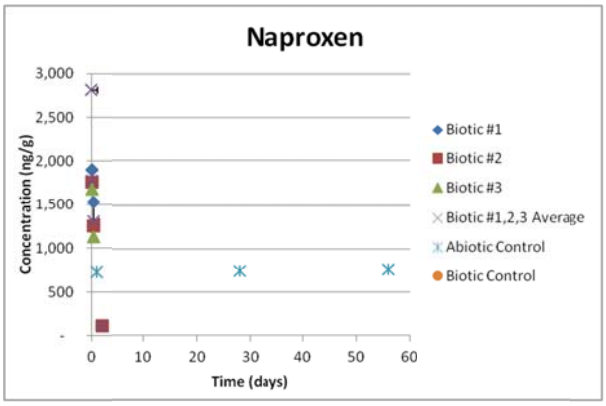
Biotic #2
Biotic #3
Biotic #1,2,3 Average
Abiotic Control
Biotic Control


Meprobamate
Concentration (ng/g)
Time (days)
Biotic #1
Biotic #2
Biotic #3
Biotic #1,2,3 Average
Abiotic Control
Biotic Control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Concentration (ng/g)
Time (days)
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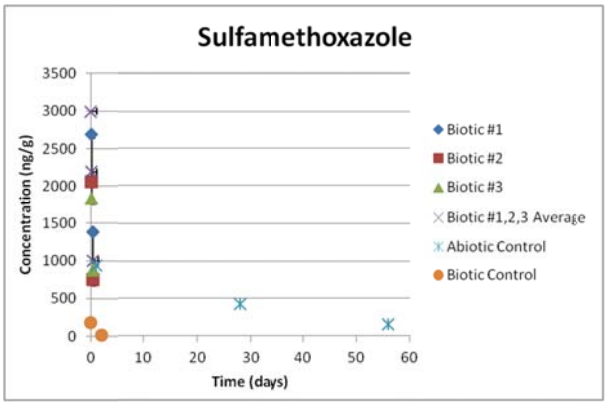
Biotic #2
Biotic #3
Biotic #1,2,3 Average
Abiotic Control
Biotic Control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Time (days)
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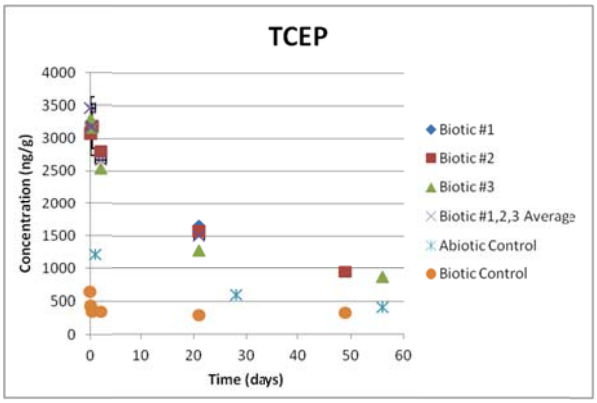
Biotic #2
Biotic #3
Biotic #1,2,3 Average
Abiotic Control
Biotic Control


TCEP
Concentration (ng/g)
Time (days)
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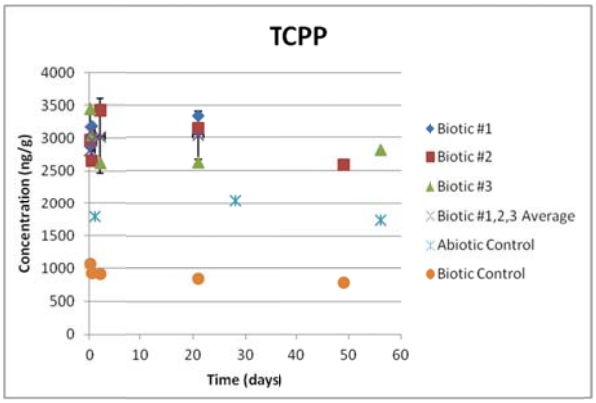
Biotic #2
Biotic #3
Biotic #1,2,3 Average
Abiotic Control
Biotic Control


TCPP
Concentration (ng/g)
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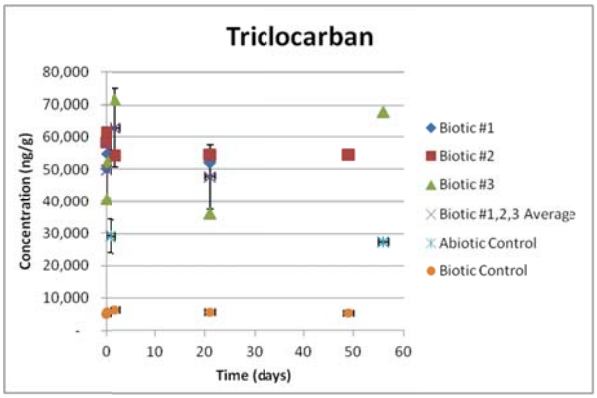
Biotic #1,2,3 Average
Abiotic Control
Biotic Control


Triclocarban
Concentration (ng/g)
Time (days)
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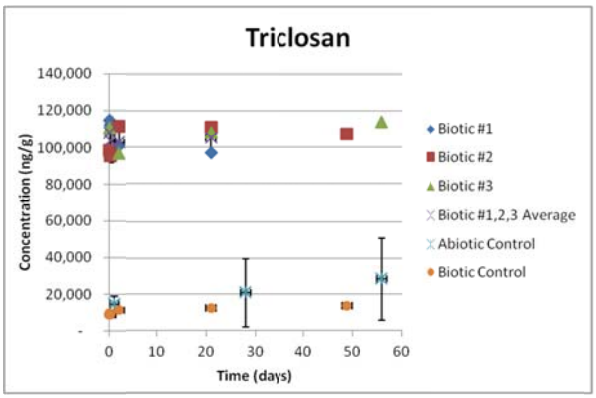
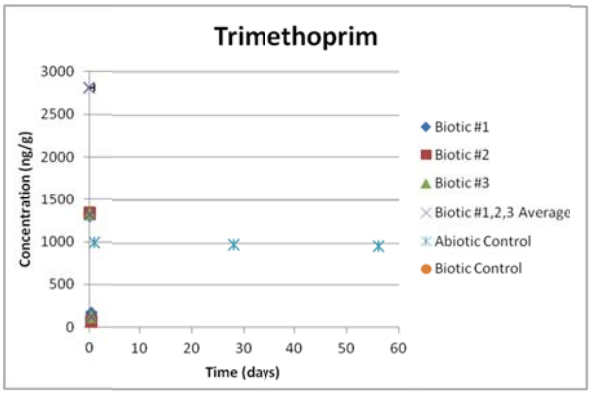
Biotic #2
Biotic #3
Biotic #1,2,3 Average
Abiotic Control
Biotic Control


Triclosan
Concentration (ng/g)
Time (days)
Biotic #1
Biotic #2
Biotic #3
Biotic #1,2,3 Average
Abiotic Control
Biotic Control


Trimethoprim
Concentration (ng/g)
Time (days)
Biotic #1
Biotic #2
Biotic #3
Biotic #1,2,3 Average
Abiotic Control
Biotic Control

I.7.2 Laboratory-Scale Anaerobic Bioreactor

	Week 1		Week 2		Week 3	
Compound	Influent (ng/g)	Effluent (ng/g)	Influent (ng/g)	Effluent (ng/g)	Influent (ng/g)	Effluent (ng/g)
Benzophenone	2876	4733	5222	7136	1616	4755
Bisphenol A	495	1800	749	1854	364	2027
Caffeine	9153	5476	8818	8252	7727	5833
Cimetidine	590	456	512	660	-	417
DEET	174	237	130	461	95	441
Diphenhydramine	140	548	119	212	121	441
Fluoxetine	59	180	57	71	45	147
Ibuprofen	1306	752	1241	1704	881	806
Naproxen	691	336	351	655	452	265
Sulfamethoxazole	303	13	212	-	1034	-
TCEP	609	352	552	583	324	941
TCPP	1599	1257	990	2194	750	2574
Triclocarban	9316	17000	11133	8155	6136	18064
Triclosan	148860	281429	115764	116505	112216	367647
Trimethoprim	498	39	581	33	347	33

APPENDIX J

TORC REMOVAL AS A FUNCTION OF PROCESS OPERATION

J.1 TOrC Removal as a Function of Solid Retention Time

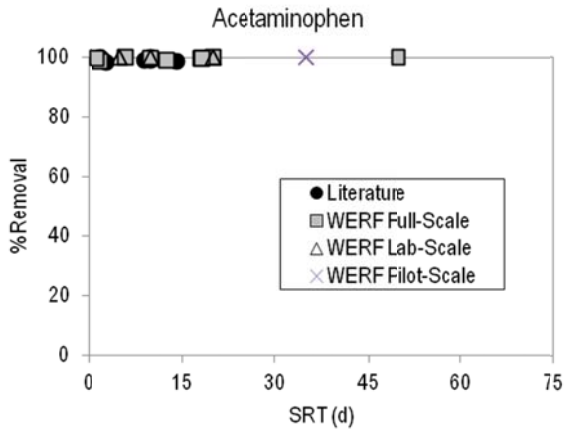


Figure J-1. Acetaminophen Removal versus SRT.

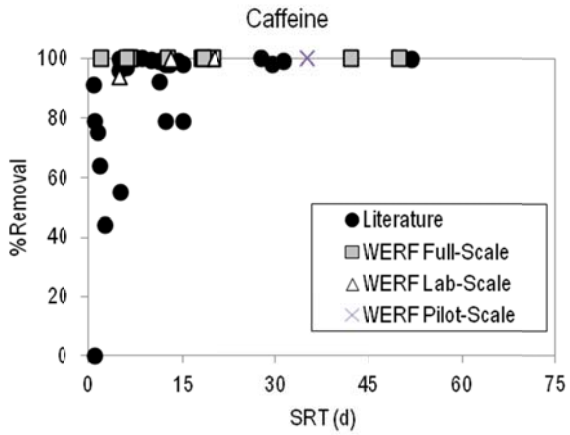


Figure J-2. Caffeine Removal versus SRT.

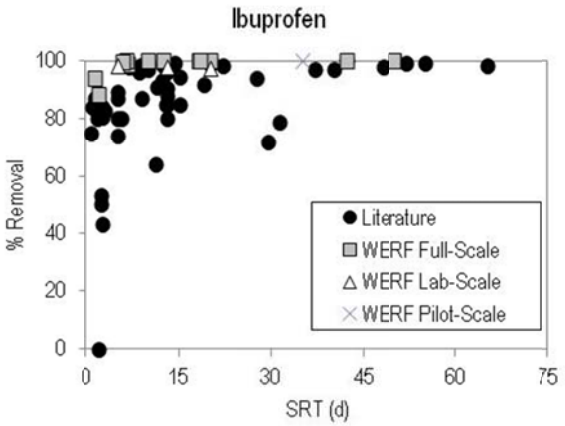


Figure J-3. Ibuprofen Removal versus SRT.

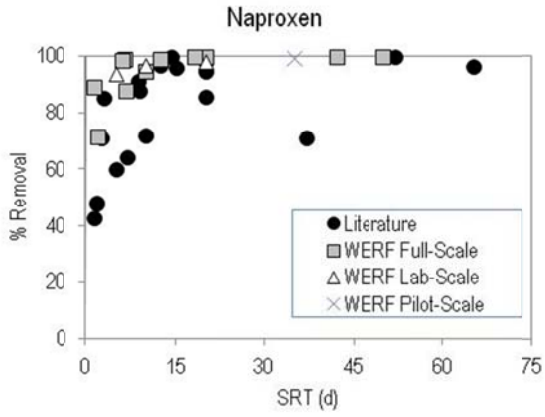


Figure J-4. Naproxen Removal versus SRT.

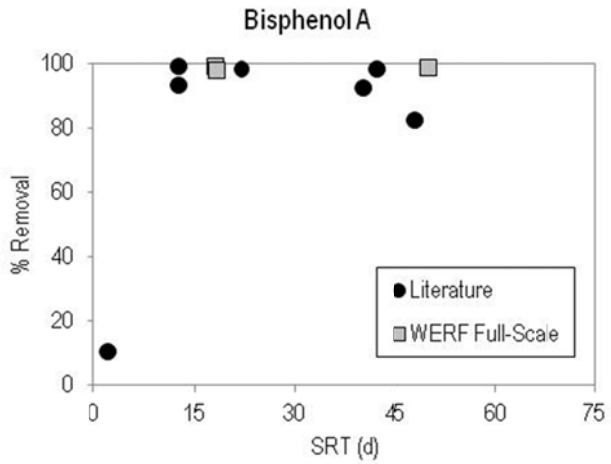


Figure J-5. Bisphenol A Removal versus SRT.

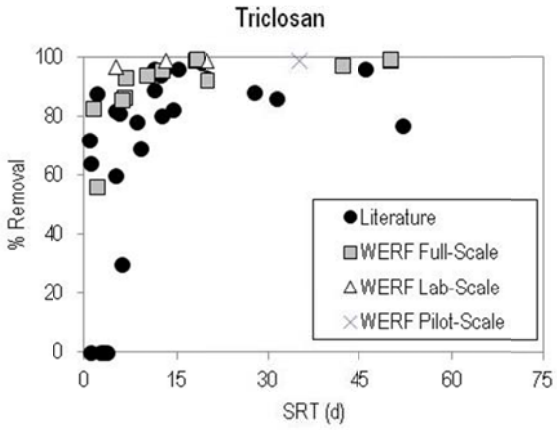


Figure J-6. Triclosan Removal versus SRT.

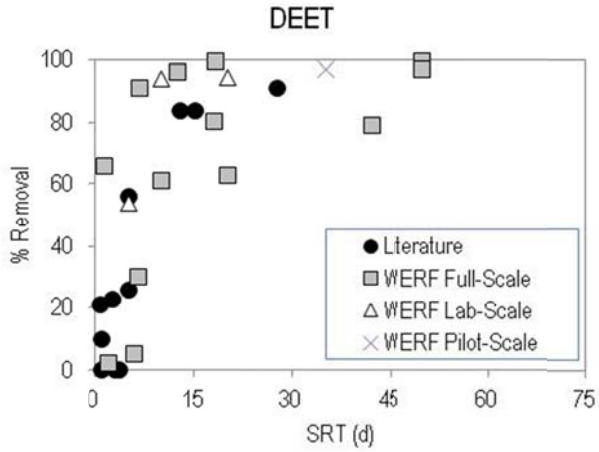


Figure J-7. DEET removal versus SRT.

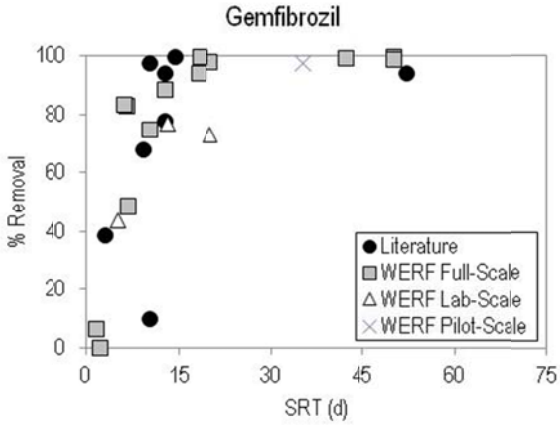


Figure J-8. Gemfibrozil removal versus SRT.

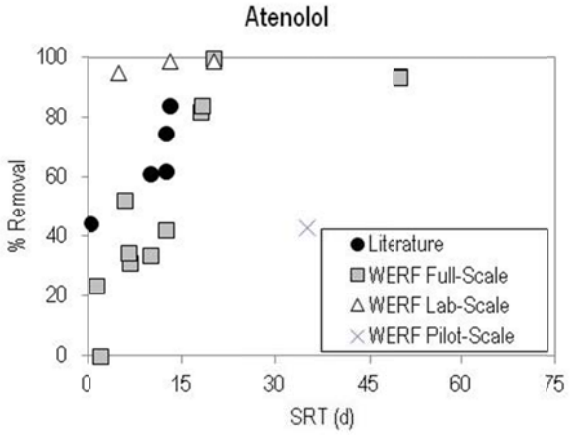


Figure J-9. Atenolol Removal versus SRT.

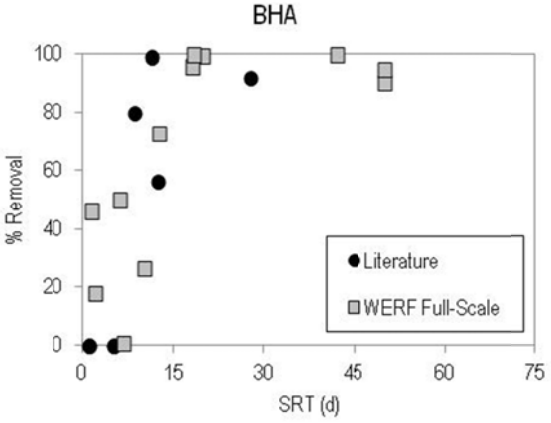


Figure J-10. BHA Removal versus SRT.

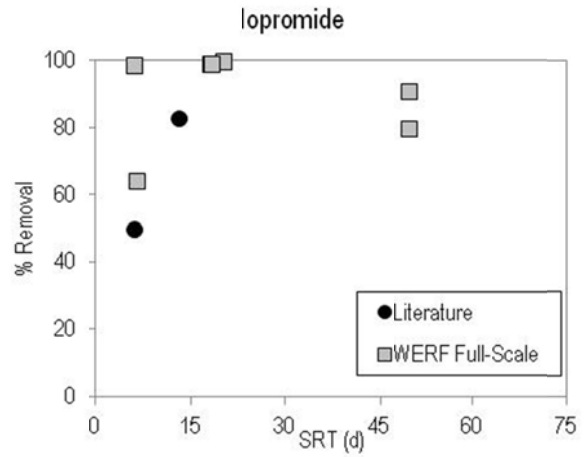


Figure J-11. Iopromide Removal versus SRT.

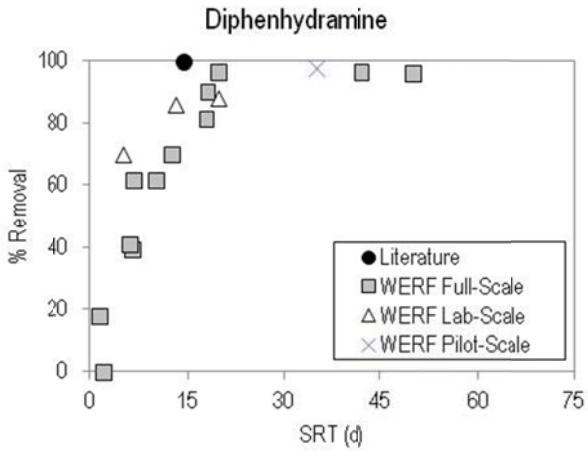


Figure J-12. Diphenhydramine Removal versus SRT.

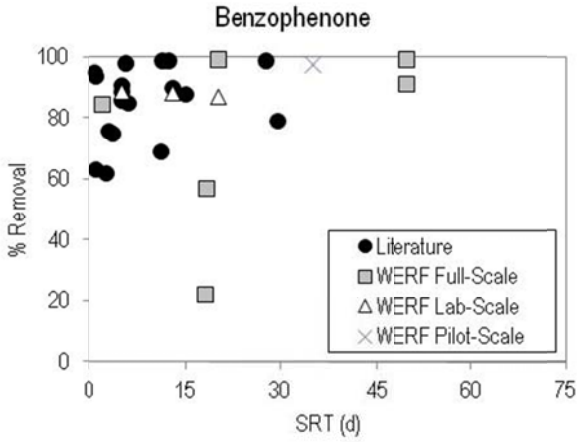


Figure J-13. Benzophenone Removal versus SRT.

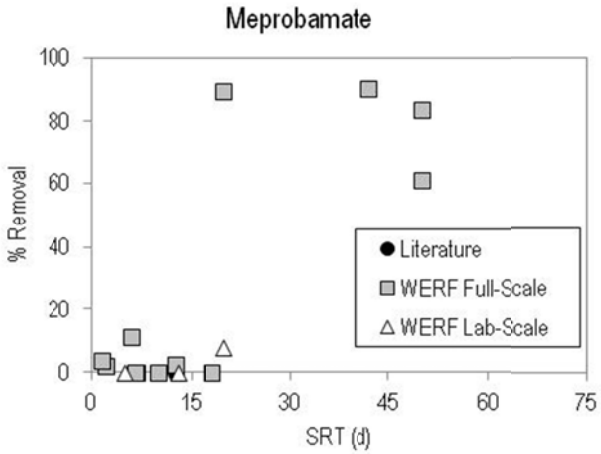


Figure J-14. Meprobamate Removal versus SRT.

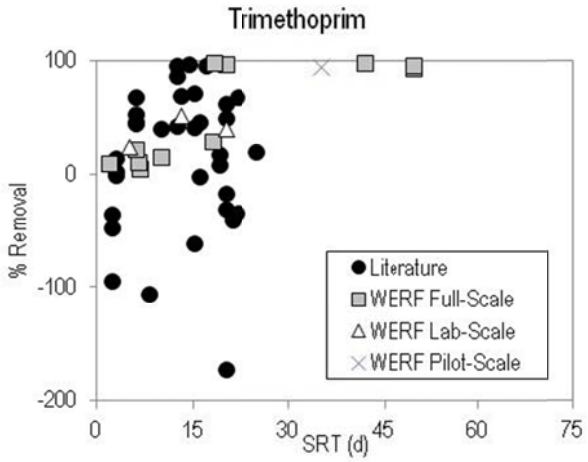


Figure J-15. Trimethoprim Removal versus SRT.

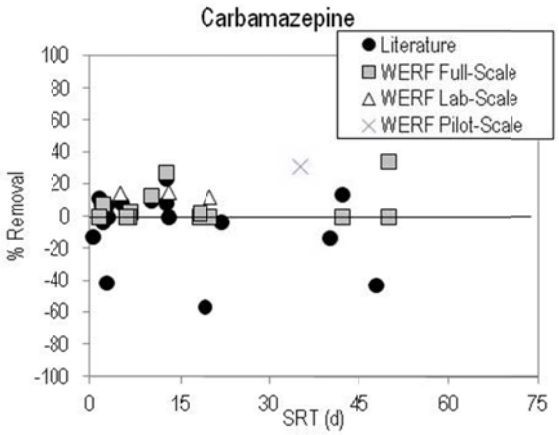


Figure J-16. Carbamazepine Removal versus SRT.

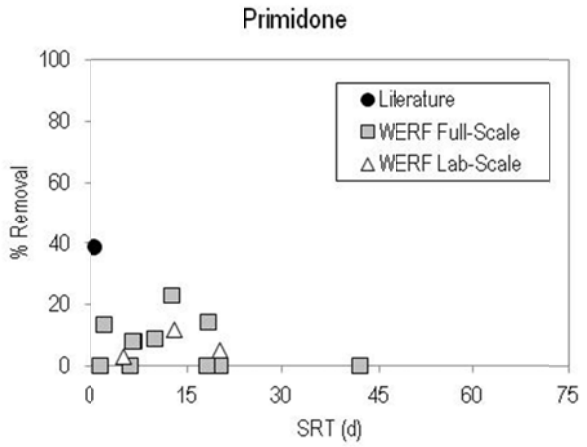


Figure J-17. Primidone Removal versus SRT.

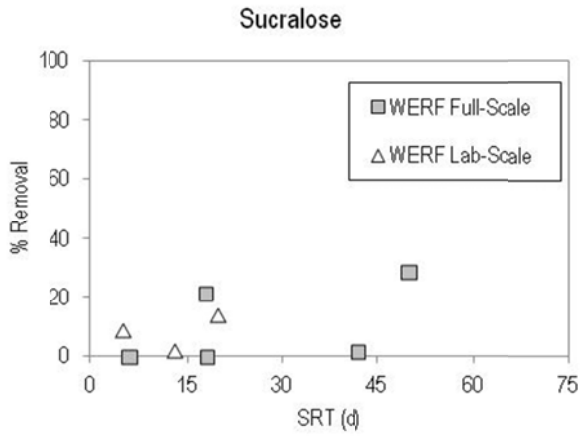


Figure J-18. Sucralose Removal versus SRT.

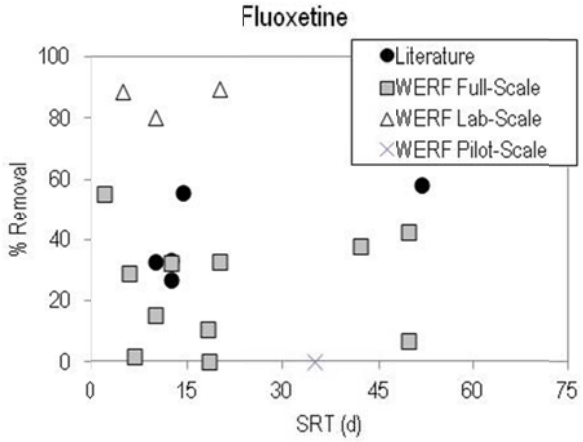


Figure J-19. Fluoxetine Removal versus SRT.

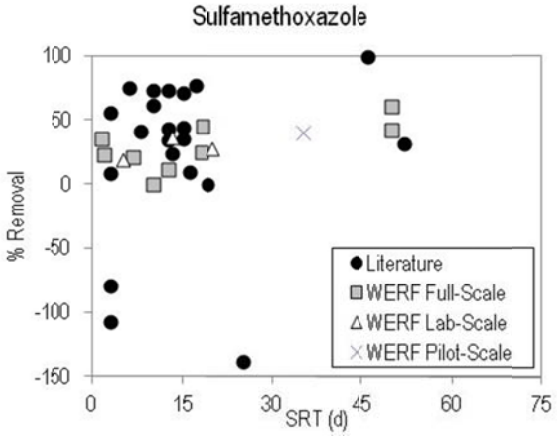


Figure J-20. Sulfamethoxazole Removal versus SRT.

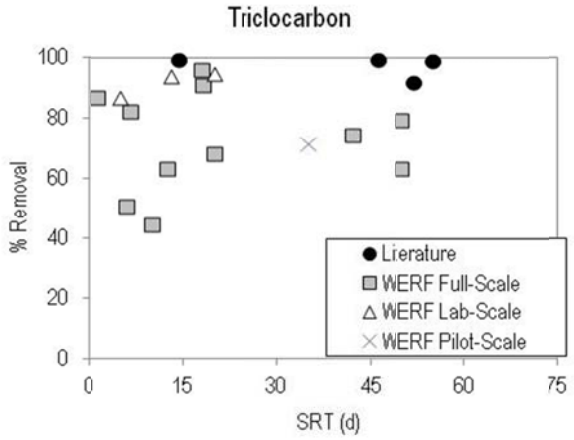


Figure J-21. Triclocarbon Removal versus SRT.

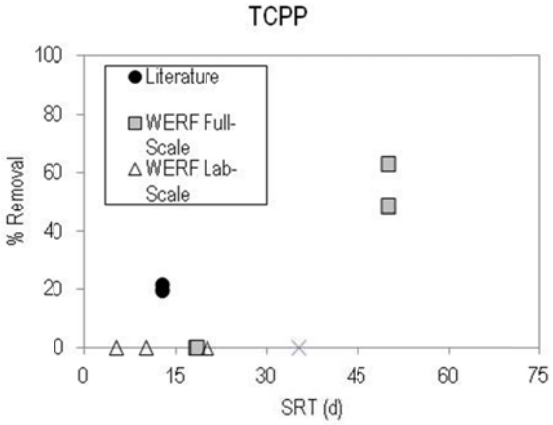


Figure J-22. TCPP Removal versus SRT.

J.2 Solid Retention Time vs. Hydraulic Retention Time

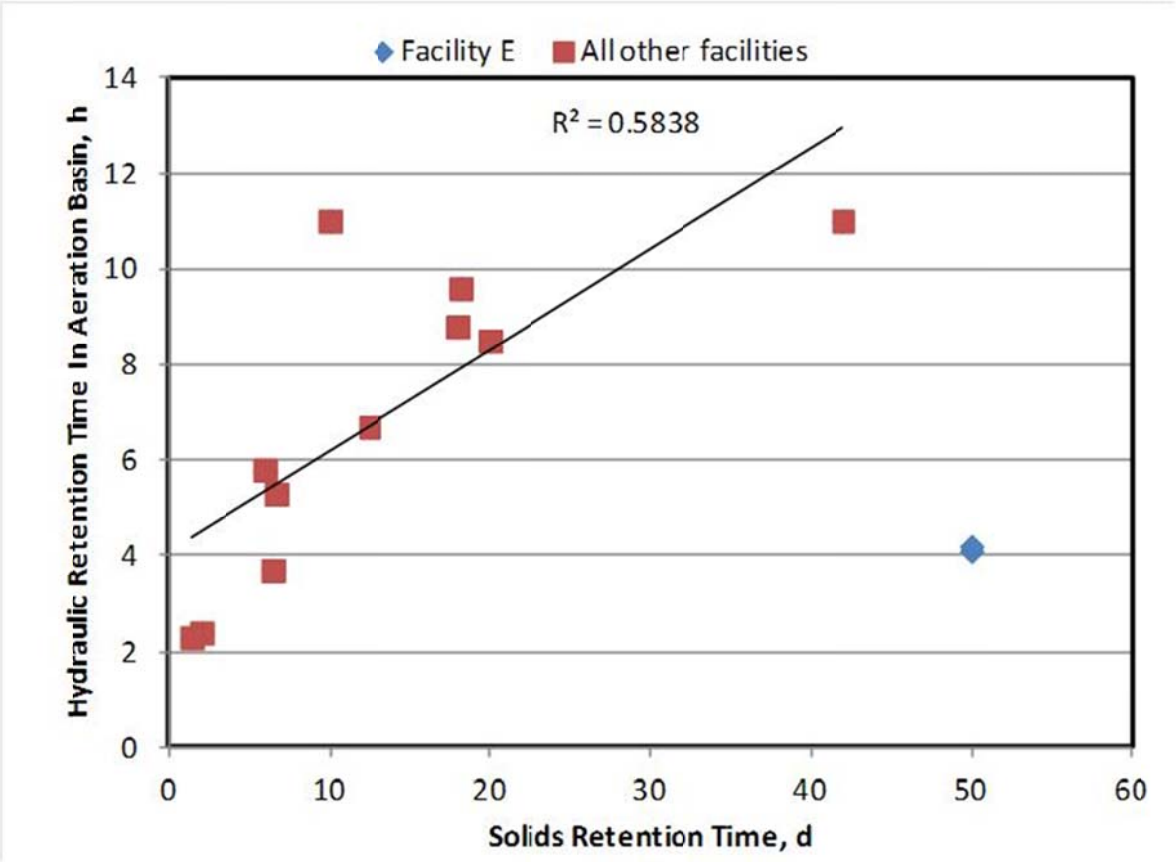


Figure J-23. Hydraulic Retention Time Versus Solid Residence Time for Facilities A to G.

J.3 Laboratory-Scale Experiments

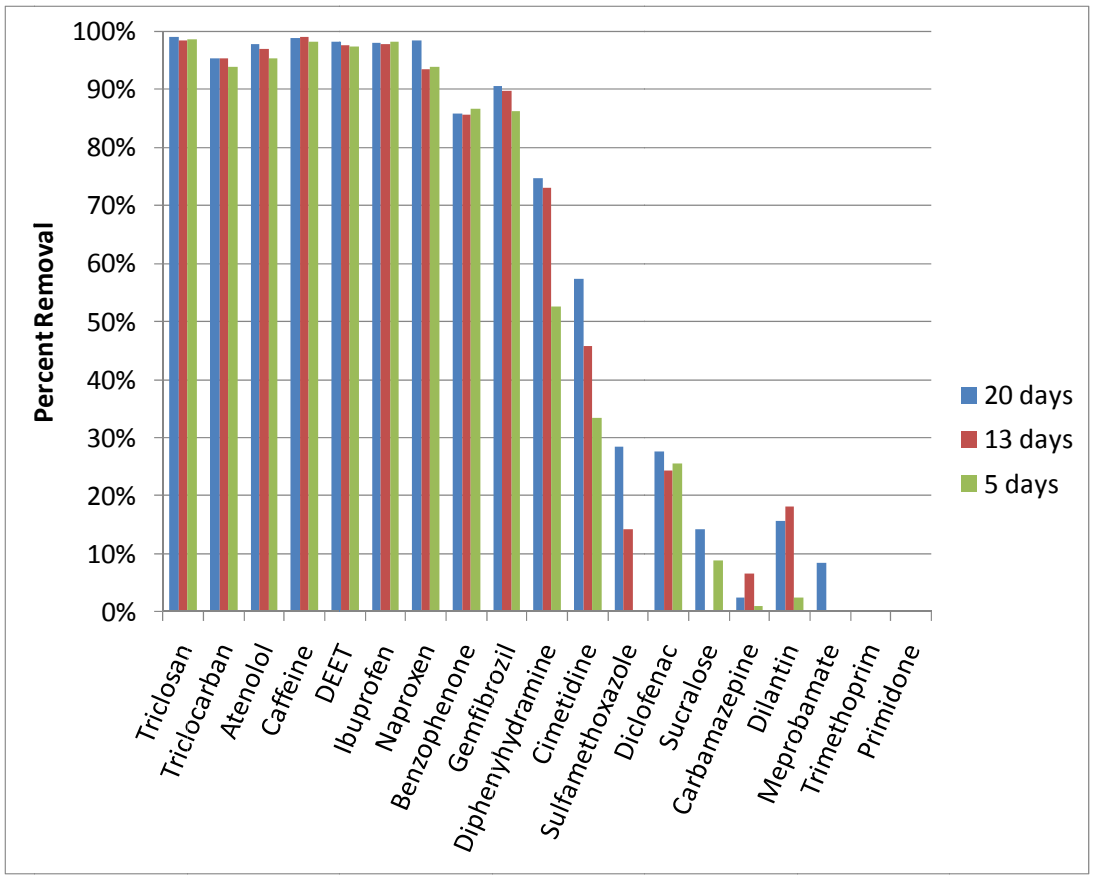


Figure J-24. Effect of SRT on the Removal of TOrCs during Laboratory Tests.

APPENDIX K

COST BENEFIT DATA

K.1 Secondary Treatment Upgrade

Construction costs were developed using a 25% estimating contingency and 10% contractor overhead and profit. Direct costs include excavation, concrete structures, mechanical equipment, and simplified piping. Lump sum percentages were used for electrical and instrumentation. Unit prices for raw materials came from cost estimating databases, as well as representative cost quotes for major equipment such as pumps, aeration blowers, and secondary clarifier mechanisms.

K.1.1 Cost Estimate Design Basis

Table K-1 outlines the process and equipment sizing assumptions for the low SRT, moderate SRT, and high SRT secondary treatment facilities.

Table K-1. Process Design Upgrade (Based on Scenarios Presented in Table 5-2).

	Low SRT (2.6 days)	Moderate SRT (6.5 days)	High SRT (9 days)
Aeration Basins			
Units, -	3	5	6
Volume each, MG	0.83	0.83	0.83
Total volume, MG	2.5	3.8	5.0
Secondary Clarifiers			
Units, -	3	5	5
Diameter each, ft	53	53	53
Side water depth, ft	14	14	14
Surface area each, sf	2,210	2,210	2,210
Total surface area, sf	6,620	11,030	11,030
Solid loading rate, ppd/sf	28	28	28
Blowers			
Oxygen transfer rate, ppd	16,300	29,300	31,200
Blower size each, scfm	2,400	2,400	2,400
Units	3	6	6
Firm capacity, scfm	7,200	14,400	14,400

K.1.2 Cost Estimate Details

Table K-2 outlines the operational costs for secondary treatment upgrades.

Table K-2. Operational Costs for Secondary Treatment Upgrades

	Low SRT	Moderate SRT	High SRT
	Horsepower	Horsepower	Horsepower
Aeration Blowers	450	900	900
MLR Pumps	150	250	300
RAS Pumps	150	250	250
WAS Pumps	10	10	10
Secondary Clarifier Mechanism	3	5	5
Total Horsepower	763	1,415	1,465
Annual Power Use (kwh)	4,986,174	9,246,968	9,573,716
Annual Power Cost ($)[1]	$398,894	$739,757	$765,897
Annual Maintenance Cost ($)[2]	$90,000	$150,000	$170,000
Total Operating Cost	$490,000	$890,000	$940,000

Notes:
1. Assumes power cost of $0.08/kwh.
2. Assumes annual maintenance cost of $10,000 for secondary clarifiers and associated facilities, and $20,000 for aeration basins and associated facilities.

K.2 Ozone

The cost estimate for ozone is based upon the use of liquid oxygen (LOX).

K.2.1 Cost Estimate Design Basis

Based on an ozone transfer dose range of 2.0 to 5.0 mg/L and treatment plant flow range of 8 mgd to 16 mgd, and assuming an 11% concentration of the production gas, the LOX tanks are designed for about 10 days of storage and total capacity of LOX tank would be 3,000 gallons. The LOX storage facility and the ozone dissipation chamber would be an outdoor installation. Nitrogen gas addition is included in the cost analysis. The ozone requirements for this project require a single 300 pounds per day generator. The ozone generators are generally recommended with redundancy (1 duty + 1 standby). During any plant flow and dose requirement, one duty ozone generator will be able to comfortably produce the amount of ozone needed at the plant. The ozone generation facility would be located in a building with an electrical room.

Ozone gas produced from ozone generators can be fed into the process water in a number of ways. The primary purpose is to dissolve the ozone gas efficiently to maximize the effectiveness of the generated ozone. The addition of ozone using side stream injection involves taking a portion (typically 10-15% of the total flow for an ozone dose in the 2-5 mg/L range) of the main flow and boosting it to a higher pressure to operate a high-efficiency venturi injector system. One pipeline flash reactor with three stainless steel injectors and three degas separators with relief valves is proposed for this project. The ozone side stream pump station would be located outside with canopy.

Any ozone contacting process will transfer at most 98% of the ozone in the feed gas. The un-transferred ozone must be destroyed prior to release to the atmosphere. The un-transferred ozone, or off-gas, is collected at the top of a basin or from the degasification unit and conveyed

to an ozone destruction system. The system typically uses a catalyst that readily converts ozone into oxygen (manganese dioxide, for example) so that essentially no ozone will be emitted to the atmosphere from the transfer process. The destruct system also has a preheater to prevent moisture from condensing on the catalyst and a blower to pull the off-gas through the catalyst bed. The two ozone destruct unit is provided by ozone generators suppliers.

K.2.2 Cost Estimate Details

Tables K-3 through K-5outline the estimates and cost of the ozone system.

Table K-3. Equipment Cost Estimate of Ozone System.

Description	Number of units	Equipment cost, $
Liquid oxygen (LOX) feed system		$175,000
• Storage Tank	1	Inclusive
• Vaporizers	2	Inclusive
• GOX Filter	1	Inclusive
• LOX/GOX Instruments & Valves, PRV station	1	Inclusive
Ozone Generator & Power Supply Unit (skid mounted ozone generator including: instruments, valves, piping and wiring)	2	$927,000
Controls - PLC based Master Ozone Control Panel	1	Inclusive
Ozone Injection System	1	$216,000
Instrumentation and Monitors		Inclusive
Field Valves	1	Inclusive
Closed Loop Cooling Water System (skid mounted)	2	Inclusive
Destruct Units	2	Inclusive
Nitrogen System	1	Inclusive
Miscellaneous Items		Inclusive
• Engineering, Freight, Warranty, Project Mgt.,	---	Inclusive
• Testing, Commissioning, etc	---	Inclusive
Total Equipment Cost		$1,318,000

Table K-4. Project Cost Estimate for the Ozone System.

Description	Percentage	Project Cost
Ozone Dissipation Chamber		$217,000
Liquid Oxygen System		$225,000
Ozone Generation Facility		$1,461,000
Ozone side stream pump station		$471,000
Electrical & Instrumentation		$755,000
Mechanical		$782,000
TOTAL DIRECT CONSTRUCTION COSTS		$3,912,000
Contingency	25.0%	$978,000
Subtotal		$4,891,000
General Contractor Overhead, Profit & Risk	10.0%	$489,000
TOTAL ESTIMATED CONSTRUCTION COST		$5,380,000
Engineering, Legal & Administration Fees	25.0%	$1,345,000
Owner's Reserve for Change Orders	10.0%	$538,000
TOTAL ESTIMATED PROJECT COST		$7,263,000

Table K-5. Operation and Maintenance Cost Estimate of Ozone System.

Description	Cost
LOX[1]	$57,000
Energy Cost[2]	$74,000
Labor Cost[3]	$20,000
Annual Repair and Replacement Cost[4]	$13,000
Total Annual O&M Cost	$164,000

Notes:
1. LOX Rate = $110/ton.
2. Power cost = $0.08/kW-hr.
3. Labor rate = $50.00/hr.
4. Annual parts replacement cost is based upon the 1% of the equipment cost.

K.3 Actiflo™ – CARB

K.3.1 Actiflo™-CARB Pilot Test Criteria

Table K-6. Actiflo™-CARB Pilot Testing Criteria at MMSD.

Operational parameters	Value
Influent flowrate	75 – 95 gpm
System HRT	27 – 34 min
Rise rate	13 – 14 gpm/sf
Waste rate (Residuals)	1,300 – 2,020 ml/min
Residuals concentration	8.8 – 12.0 g/L
PAC type	PICAHYDROSOL AFP23
PAC dosage	10 – 20 mg/L
Coagulant type	Ferric Chloride
Coagulant dosage (as Fe)	1.5 – 6.0 mg/L
Polymer type	Hydrex 6161
Polymer dosage	1.5 – 3.2
Microsand effective size	82 µm
Microsand concentration	14 – 16 g/L

K.3.2 Cost Estimate Details

Table K-7. Project Cost Estimate for the Actiflo™-CARB System.

Description	Percentage	Project cost
Equipment Cost		$2,000,000
Electrical & Instrumentation		$300,000
Mechanical		$300,000
TOTAL DIRECT CONSTRUCTION COSTS		$2,600,000
Contingency	25	$650,000
Subtotal		$3,250,000
General Conditions, General Contractor Overhead, Profit & Risk	10	$325,000
Subtotal		$3,575,000
TOTAL ESTIMATED CONSTRUCTION COST		$3,575,000
Engineering, Legal & Administration Fees	25	$893,750
Owner's Reserve For Change Orders	10	$357,500
TOTAL ESTIMATED PROJECT COST		$4,826,250

Table K-8. Operation and Maintenance Cost Estimate of Actiflo System.

Description	Cost
Polymer[1]	$146,000
Sand Consumption[2]	$5,000
Coagulant (As $FeCl_3$)[3]	$41,000
Fresh PAC[4]	$402,000
Energy Cost[5]	$62,000
Labor [6]	$20,000
Annual Repair and Replacement Cost[7]	$20,000
Total Annual O&M Cost	$696,000

Notes:
1. Polymer cost = $4,000/ton.
2. Sand consumption cost = $200/ton.
3. Coagulant cost = $340/ton.
4. Fresh PAC cost = $2,200/ton.
5. Power cost = $0.08/kW-hr.
6. Labor rate = $50.00/hr.
7. Annual parts replacement cost is based upon the 1% of the equipment cost.

K.3.3 Actiflo™ – CARB Results from MMSD

Date	Carbon dosage (mg/L)	Flow rate (gpm)	Contact time (min)	Waste rates (residuals) (mL/min)	Coagulant dosage as Fe (mg/L)	Polymer dosage (mg/L)	Residuals concentration (g/L)	Fluoxitine (ng/L)			Carbamazepine (ng/L)			Trimethoprim (ng/L)			Sulfamethoxazole (ng/L)		
								Inf.	Eff.	% removv.	Inf.	Eff.	% removv.	Inf.	Eff.	% removv.	Inf.	Eff.	% removv.
4/18/2011	10	95	27	1650	1.5	1.5	9.9-10.4	20	15	22%	86	28	68%	220	26	88%	585	256	56%
4/19/2011	10	75	34	1300	2.1	1.5	7.7-8.2	31	29	6%	95	44	53%	219	54	75%	669	346	48%
4/20/2011	10	75	34	1300	2.1	1.5	8.2-8.6	321	13	96%	262	71	73%	408	32	92%	567	344	39%
4/21/2011	10	95	27	1650	2.1	3.2	10.5-11.3	481	9	98%	274	73	73%	362	41	89%	523	275	47%
4/25/2011	20	95	27	2020	2.1	3.2	11.0-11.5	23	5	77%	50	17	67%	141	4	97%	244	137	44%
4/27/2011	20	75	34	1600	2.1	3.2	8.8-9.5	223	5	98%	220	18	92%	296	3	99%	293	73	75%
4/28/2011	20	95	27	2020	2.1	3.2	11.4-12.0	254	53	79%	141	21	85%	258	2	99%	406	69	83%
7/26/2011	10	75	34	1300	5.4	3.0	9.2-9.8	1786	119	93%	646	31	95%	980	14	99%	2357	473	80%
7/27/2011	10	95	27	1650	5.4	3.2	10.1-10.6	444	290	35%	439	207	53%	802	121	85%	1870	862	54%
7/28/2011	10	75	34	1300	6.0	3.3	11.0-11.4	305	254	17%	181	70	61%	320	50	84%	1061	469	56%
8/1/2011	20	95	27	2020	5.6	3.2	9.7-9.9	733	147	80%	2922	13	100%	367	11	97%	1202	110	91%
8/2/2011	20	75	34	1600	5.6	3.2	8.9-9.2	3038	1096	64%	662	70	89%	983	35	96%	1558	181	88%
8/3/2011	20	95	27	2020	5.6	3.0	10.0-10.4	2222	1026	54%	825	84	90%	1135	70	94%	1537	366	76%
8/4/2011	20	75	34	1600	5.6	3.1	9.5-9.9	689	59	91%	277	26	91%	652	24	96%	1248	365	71%

Date	Carbon dosage (mg/L)	Flow rate (gpm)	Contact time (min)	Waste rates (residuals) (mL/min)	Coagulant dosage as Fe (mg/L)	Polymer dosage (mg/L)	Residuals concentration (g/L)	Diltiazem (ng/L)			Diphenhydramine (ng/L)			Caffeine (ng/L)			Triclosan (ng/L)		
								Inf.	Eff.	% removv.	Inf.	Eff.	% removv.	Inf.	Eff.	% removv.	Inf.	Eff.	% removv.
4/18/2011	10	95	27	1650	1.5	1.5	9.9-10.4	45	0	100%	69	21	70%	64	25	60%	231	0	100%
4/19/2011	10	75	34	1300	2.1	1.5	7.7-8.2	111	18	84%	117	23	80%	103	103	0%	228	25	89%
4/20/2011	10	75	34	1300	2.1	1.5	8.2-8.6	229	16	93%	149	21	86%	1962	363	81%	388	8	98%
4/21/2011	10	95	27	1650	2.1	3.2	10.5-11.3	183	12	94%	128	18	86%	2057	340	83%	436	6	99%
4/25/2011	20	95	27	2020	2.1	3.2	11.0-11.5	87	0	100%	72	10	86%	92	20	79%	177	3	98%
4/27/2011	20	75	34	1600	2.1	3.2	8.8-9.5	209	0	100%	168	2	99%	1523	53	97%	266	2	99%
4/28/2011	20	95	27	2020	2.1	3.2	11.4-12.0	198	0	100%	91	4	96%	1862	213	89%	223	29	87%
7/26/2011	10	75	34	1300	5.4	3.0	9.2-9.8	407	23	94%	600	23	96%	1746	1244	29%	196	24	88%
7/27/2011	10	95	27	1650	5.4	3.2	10.1-10.6	406	64	84%	554	142	74%	2130	1613	24%	250	79	68%
7/28/2011	10	75	34	1300	6.0	3.3	11.0-11.4	175	40	77%	253	67	74%	329	241	27%	1002	92	91%
8/1/2011	20	95	27	2020	5.6	3.2	9.7-9.9	239	17	93%	269	13	95%	675	574	15%	490	30	94%
8/2/2011	20	75	34	1600	5.6	3.2	8.9-9.2	392	32	92%	506	45	91%	2135	794	63%	900	100	89%
8/3/2011	20	95	27	2020	5.6	3.0	10.0-10.4	557	78	86%	637	92	86%	3333	740	78%	1998	593	70%
8/4/2011	20	75	34	1600	5.6	3.1	9.5-9.9	261	22	92%	443	28	94%	3482	40	99%	452	93	79%

K.4 Ultrafiltration and Reverse Osmosis

K.4.1 Basis of Cost Estimate

Typically, MF or UF is provided upstream of RO to serve as pretreatment for removing particulate matter from the WWTP secondary effluent. The MF membranes have a nominal pore size of 0.1 microns and are typically of hollow fiber construction. The membrane material in recent past has typically been polypropylene, although newer polyvinylidene fluoride (PVDF) membranes provide the added benefit of oxidant resistance. The MF/UF system can be one of two different configurations: pressurized membrane cartridges mounted on skids or vacuum driven membranes in submerged tanks. Both types are available from several manufacturers. Since these systems are proprietary, the MF/UF units will vary by manufacturer, not just in the MF/UF unit/tank itself, but also in the ancillary equipment and infrastructure/piping to be considered during the design of the new facility. MF/UF ancillary equipment includes automatic (self-cleaning) strainers, backwash supply and waste equipment and tankage, chemical CIP equipment and tankage, compressed air systems, piping systems, and electrical and control systems. The automatic strainers are located upstream of the MF system and help to remove remaining large particulate matter.

The RO membranes have a nominal "pore" size of 0.001-0.0001 microns and are typically of spiral wound construction (flat membrane sheet with feed spacer wrapped together in a spiral). Typically, composite polyamide is the membrane material of choice for recycled water applications. The RO system is typically constructed of commodity components and is comprised of skids with pressure vessels, manifold piping, and RO membrane elements. The skids may also contain dedicated RO feed pumps and cartridge filters, or this equipment can be manifolded separately. The RO system also contains chemical CIP tankage and equipment. The cartridge filters, typically located upstream of the RO feed pumps, help to remove any remaining particulate matter before entering the RO pressure vessels. RO systems are typically designed and furnished by an original equipment manufacturer (OEM).

The MF/RO design criteria assumed for this cost estimate are as follows:

- All buildings were designed at grade.
- There are a total of 8 MF tanks (n+1, 14% of capacity each).
- The MF tanks are constructed out of coated steel.
- The MF nominal design flux is 24 gallons per square foot per day (gfd).
- The MF recovery is 90%.
- The average MF chemical clean-in-place (CIP) frequency is 30 days.
- The average MF membrane life is five years.
- The RO system is a low pressure, two-stage system.
- There are a total of 8 RO skids (25% of capacity each, no redundancy).
- The RO nominal design flux is 10 gfd.
- The RO recovery is 75%.
- The average RO CIP frequency is 90 days.
- The average RO membrane life is four years.
- The MF/RO system will be located inside a single-story, concrete-masonry building with a metal roof.
- All stainless steel piping is not electropolished.

Another key consideration of MF/RO systems is disposal of backwash/CIP wastes and RO reject. The available means of reject disposal can significantly impact the feasibility and application of RO. For this preliminary evaluation, it is assumed that the MF backwash waste, neutralized MF maintenance wash waste, and neutralized MF and RO CIP waste will not require special disposal, but can be discharged back to the WWTP headworks. Likewise, it is assumed that RO reject is disposed of by blending into the wastewater treatment plant effluent (prior to chlorination) without impacting plant operations or ability to meet discharge permits. It should be noted that for this preliminary evaluation, it was assumed there would be no additional impact to wastewater treatment plant (WWTP) capacity, or to WWTP operations, maintenance, or disposal costs, for treating the recycle/waste flows (and solids) from the MF/RO system. No user or connection fees were included for these recycle/waste flow streams.

Water quality parameters, such as silica, total dissolved solids (TDS), and many others, as well as upstream treatment processes and chemical additions (e.g. coagulants and chlorine/chloramines) can have a significant impact on RO system operation/maintenance and performance. Several of these parameters, such as high silica concentration, can also significantly impact the feasibility of RO. For this cost estimate, the following water quality conditions are assumed:

- The silica concentrations in the RO feed are not a concern (i.e., less than 30 mg/L). If silica concentrations are significantly higher, it is likely that RO is not a feasible treatment process (due to possible irreversible scaling).
- The TDS concentrations in the RO feed are less than 1000 mg/L.
- No coagulants (e.g., alum, ferric chloride, permanganate, and/or polymer) are added prior to RO as they have the potential to cause or contribute to fouling.
- Additionally, this estimate includes the costs of the following systems for pre-treatment of the RO feed and post-treatment of the RO permeate.
- Anti-scalant and acid dosing systems for the RO feed.
- A pH adjustment system using calcium hydroxide for RO permeate.
- A decarbonation tower for the RO permeate.

K.4.2 Cost Estimate Details

Table K-9. Project Cost Estimate for the UF System.

Description	Percentage	Project Cost
Equipment Cost		$9,633,000
Electrical & Instrumentation		$1,444,000
Mechanical		$1,444,000
TOTAL DIRECT CONSTRUCTION COSTS		$12,522,000
Contingency	25	$3,130,000
Subtotal		$15,653,000
General Conditions, General Contractor Overhead, Profit & Risk	10	$1,565,000
Subtotal		$17,218, 000
TOTAL ESTIMATED CONSTRUCTION COST		$17,218, 000
Engineering, Legal & Administration Fees	25	$4,304, 000
Owner's Reserve For Change Orders	10	$1,721, 000
TOTAL ESTIMATED PROJECT COST		$23,245, 000

Table K-10. Project Cost Estimate for the RO System.

Description	Percentage	Project cost
Equipment Cost		$14,449, 000
Electrical & Instrumentation		$2,167, 000
Mechanical		$2,167, 000
TOTAL DIRECT CONSTRUCTION COSTS		$18,784, 000
Contingency	25	$4,696, 000
Subtotal		$23,480, 000
General Conditions, General Contractor Overhead, Profit & Risk	10	$2,348, 000
Subtotal		$25,828, 000
TOTAL ESTIMATED CONSTRUCTION COST		$25,828, 000
Engineering, Legal & Administration Fees	25	$6,457, 000
Owner's Reserve For Change Orders	10	$2,582, 000
TOTAL ESTIMATED PROJECT COST		$34,868, 000

Table K-11. Operation and Maintenance Cost Estimate of UF and RO System.

Description	UF cost	RO cost
Membrane Replacement and Chemical Cost	$806,000	$1,208,000
Energy Cost[1]	$664,000	$966,000
Labor [2]	$40,000	$40,000
Other Replacement Cost[3]	$78,000	$116,000
Total Annual O&M Cost	$1,588,000	$2,330,000

Notes:

1. Power cost = $0.08/kW-hr.
2. Labor rate = $50.00/hr.
3. Annual parts replacement cost is based upon the 1% of the equipment cost.

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