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MODELING AND EVALUATION OF CONSTITUENTS OF EMERGING CONCERN THROUGH WASTEWATER TREATMENT PROCESSES

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JASON LAUBACHER
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MODELING AND EVALUATION OF CONSTITUENTS OF EMERGING CONCERN THROUGH WASTEWATER TREATMENT PROCESSES

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BY

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Dr. Keith Strevett, Chair

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Dr. David Sabatini

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Dr. Ellen McDonald

To my family and friends who made this possible…

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Abstract

Constituents of emerging concern (CECs) have accumulated in drinking water source supply over the past decades. Although there are currently no established treatment standards, CECs should be of concern to the public and the environment. The goal of this study was to better understand the fate of CECs in a conventional activated sludge (CAS) wastewater treatment plant. To achieve this goal, two objectives were identified: (i) evaluate unit operational changes that increase removal efficiency of CECs and (ii) evaluate the efficacy of advanced treatment options. This research measured 98 CECs throughout a CAS facility. Subsequent to these analyses, a stochastic fate model was developed to quantitatively understand CECs' fate through CAS processes. Results of the model indicate that primary clarifiers and secondary plug flow reactors (PFRs) significantly reduced CEC concentrations. CEC removal percentages in the primary clarifiers range from 9.1% (triclosan) to 79.8% (atenolol). PFR removal percentages range from <0% (meprobamate, gemfibrozil, and sucralose) to >98.6% (caffeine) and overall plant removal percentages range from 6.7% (gemfibrozil) to >98.9% (caffeine). Even with relatively low removal percentages, some influent and effluent CEC concentrations are well below monitoring trigger thresholds, which indicate safe drinking-water concentrations. Furthermore, because wastage rate controls the mean cell residence time, wastage rate is the most influential operational control on the effect on CEC removal. In conclusion, by providing operational and advanced treatment analysis, this modeling approach can help determine key factors in CEC removal from CAS facilities.

Chapter 1: Introduction

Constituents of emerging concern (CECs) are chemicals that are being detected in water that were not previously detected or that are being detected at different levels than anticipated (EPA, 2014). CECs can include household chemicals (detergents, deodorizers), pharmaceuticals (hormones, beta blockers, antibiotics), and personal care products (antacids, caffeine). Because wastewater treatment plant (WWTP) process units are not optimized to remove CECs, these compounds may be discharged into the environment. Accumulation of CECs is a concern for ecosystems, as well as for human consumption via indirect or direct water reuse (Githinji et al., 2010). Several researchers (Bernhard et al., 2006; Clara et al., 2004; Clara at al., 2005; Kimura et al., 2004; Kimura et al., 2007; Radjenović et al., 2007; Wang et al., 2013) have studied the fate of CECs in WWTPs and examined various treatment processes. These treatment processes can include conventional activated sludge (CAS), membrane bioreactors (MBR), reverse osmosis (RO), nanofiltration (NF), aerobic and anaerobic digestion, and advanced oxidation processes (AOPs), including ultraviolet irradiation (UV), hydrogen peroxide (H_2O_2), and ozone disinfection. Of these treatment processes, CAS is one of the most commonly used. CAS removes CECs using two key removal mechanisms: biological degradation and adsorption to biosolids (Lee et al., 2009). Because removal efficiencies are a function of hydraulic retention time (HRT), solids retention time (SRT), and the physical, chemical and biological characteristics of the wastewater (Johnson et al., 2005; Monteith et al., 2008), CEC concentration levels in wastewater vary greatly and can be difficult to predict. However, various researchers (Lee et al., 2009; Luo et al., 2014; and Miège et al., 2008) have compiled CEC removal efficiency data (Table 2-1)

from 153 studies of conventional WWTPs (WWTPs utilizing CAS). As stated above, the primary conclusion among these studies is that CEC removal efficiencies depend upon several factors. However, some common characteristics or commonalities can be observed. For instance, CEC removal percentage increases with increased HRT and SRT (Clara et al., 2005a; Johnson et al., 2005; Monteith et al., 2008). Furthermore, based on the Arrhenius theorem, as temperature increases, CEC removal rates increase (Clara at al., 2004; Monteith et al., 2008). Modeling CECs in a specific WWTP would allow for the evaluation of operational changes to increase CEC removal efficiencies. These changes could include modifications to sludge recycling rates, HRTs, SRTs, biomass makeup and recycling, disinfection processes, and temperature. Finally, because modeling allows for a detailed analysis of the process performance, it provides an indication of what unit processes can be optimized or expanded.

This research will determine key CECs in the City of Norman Water Reclamation Facility (NWRF) and will monitor these CECs in the influent and effluent of major processes within the NWRF. Furthermore, it will develop a stochastic fate model of the NWRF, integrating CECs into the model. More generally, it will help to quantitatively understand CECs through WWTPs and will be a template for further modeling of other WWTPs.

Chapter 2: Literature Review and Background

2.1 Removal Efficiencies of CECs in Conventional WWTPs

There is extensive research on CEC removal efficiencies (Table 2-1) in CAS WWTPs (Lee et al., 2009; Luo et al., 2014; Miège et al., 2008). Although some compounds show similar removal efficiencies from the three studies, other compounds show a wide range due to varying HRT, SRT, and wastewater and biomass makeup. From these studies, it is clear that removal efficiencies are specific to WWTP characteristics and results are quite variable. For instance, removals of acetaminophen, estrone, and ibuprofen do not vary greatly across the three studies. Meanwhile, compounds like bezafibrate, diethyltoluamide (DEET), gemfibrozil, sulfamethoxazole, and tonalide all differ from study to study. Furthermore, Luo et al. (2014) found a large range of removal percentages for some compounds. As mentioned, these ranges in removal percentages are attributed to variability of HRT, SRT, and wastewater and biomass makeup.

Table 2-1: Typical Removal Percentages of CECs in Conventional WWTPs

	Removal Percentage				Removal Percentage		
Compound	**Luo et al., 2014**	**Lee et al., 2009**	**Miège et al., 2008**	**Compound**	**Luo et al., 2014**	**Lee et al., 2009**	**Miège et al., 2008**
17α-Ethynylestradiol	43.8–100		~79	**Estrone**	74.8–90.6		~76
Acetaminophen	98.7–100	98.4		**Galaxolide**	87.8	~60-95	~61
Alkylphenol		~30-95		**Gemfibrozil**	<0–92.3	38.8	~61
Alkylphenol ethoxylate		~75-95		**Glibenclamide**		44.5	
Atenolol	<0–85.1	0	0	**Hydrochlorothiazide**		76.3	
Atrazine	<0–25			**Ibuprofen**	72–100	82.5-~98	~78
Bayrepel acid				**Indomethacin**		23.4	
Bentazone				**Ketoprofen**	10.8–100	51.5-~55	~52
Benzophenone-3	63.8–98.2			**MCPP**		13	
Bezafibrate	9.10–70.5	~40-98	~70	**Mefenamic acid**	<0–70.2	29.4-~70	~25
Bisphenol-A	62.5–99.6	91		**Metoprolol**	3–56.4	0	~30
Caffeine	49.9–99.6			**Naproxen**	43.3–98.6	~65-85.1	~74
Carbamazepine	<0–62.3	0-7	~8	**Nonylphenol**	21.7–99		
Clofibric acid	<0–93.6	27.7-~50	~25	**Octylphenol**	<0–96.7		
Clotrimazole	84.5–93.6			**Ofloxacin**		23.8	
DBP	73.6–75.5			**Paroxetine**		90.6	
DEET	65.6–79.5	17		**Pravastatin**		61.8	
DEHP	25–97			**Propyphenazone**		42.7	0
Diazinon	<0			**Rantidine**		42.2	
Diclofenac	<0–81.4	~24-50.1	~35	**Salicylic acid**	89.6–100		~99
Diuron	26.7–71.9			**Sulfamethoxazole**	4–88.9	55.6	~60
DMP	84.8–93.5			**TCEP**	<0	30	
EDTA		1		**TCPP**	<0	13	
Enrofloxacin				**Tebuconazole**	<0–58.7		
Erythromycin	<0–82.5	23.8		**Tonalide**	84.7	~50-97	~64
Estradiol	92.6–100			**Triclosan**	71.3–99.2		~84
Estriol	100			**Trimethoprim**	<0–81.6		~43

Osachoff et al. (2014), using synthetic wastewater containing pharmaceutical and personal care products, studied removal efficiencies (Table 2-2) in a bench-scale CAS process. The synthetic wastewater contained: caffeine, di(2-ethylhexyl)phthalate, estrone, 17α-ethinylestradiol, ibuprofen, naproxen, 4-nonlyphenol, tonalide, triclocarbon, and triclosan.

Table 2-2: Laboratory Tested Conventional Activated Sludge Removal of Pharmaceuticals (Osachoff et al., 2014)

Pharmaceutical	Influent Concentration (ng/L)	Effluent Concentration (ng/L)	Percent Removed
Caffeine	45,579	250	99.5
Di(2-ethylhexyl)phthalate	40,609	15,565	61.7
Estrone	70	20	71.6
17α-Ethinylestradiol	6.0	1.5	75.1
Ibuprofen	27,600	8667	68.6
Naproxen	15,000	9000	40.0
4-Nonylphenol	31,000	125	99.6
Tonalide	1017	25	97.5
Triclocarbon	3000	73	97.6
Triclosan	3000	250	91.7

Di(2-ethylhexyl)phthalate, estrone, 17α-Ethinylestradiol, and ibuprofen were only moderately removed while naproxen was moderately conserved in the treatment process. Because of their lower removal efficiencies, di(2-ethylhexyl)phthalate, estrone, 17α-Ethinylestradiol, ibuprofen, and naproxen should be noted as potential key CECs for modeling.

2.2 Removal Efficiencies of CECs in MBRs and Advanced Treatment Processes

In addition to compiling data for CAS, Lee et al. (2009) accumulated and analyzed CEC removal efficiencies from MBR, NF, RO, granular activated carbon (GAC), and powdered activated carbon (PAC). MBRs use CAS but replace the secondary clarifier with membrane filtration. NF, RO, GAC, and PAC are considered

advanced treatment (AT) processes and are typically used after WWTP processes like CAS or MBRs. NF and RO use membranes to filter contaminants from the passing wastewater. GAC uses adsorption in a fixed-bed process. In contrast, PAC is a suspended media in the water. All of these advanced treatment (AT) processes performed better than CAS in removing CECs (Lee et al., 2009). Table 2-3 shows removal efficiency characteristics of several AT processes.

Table 2-3: CEC Removal Efficiencies of Various Treatment Processes (Lee et al., 2009)

Process	Compounds Studied	Percent of Compounds with No Removal	Percent of Compounds with Removal Below 50%	Percent of Compounds with Removal Above 90% or Below Detection Limit
MBR	49	14	33	39
CAS	33	9	64	27
NF	57	n.d.	17	82
RO	60	n.d.	12	82
GAC	29	0	0	97
PAC	71	6	31	41

n.d. not determined

Although GAC does have high removal efficiencies, according to Lee et al. (2009), several studies found that competitive adsorption can decrease removal efficiency and the operating life of the filter, especially when organic matter is present (Lee et al., 2009). Competitive adsorption is a process in which compounds compete for adsorption sites on cells. It is controlled by the maximum heat and energy required for adsorption (Gun'ko, 2007). Because of this phenomenon, hydrophilic and large-molecular weight compounds may not be removed as well because they do not have accessibility to the inner pores of carbon in the filter (Lee et al., 2009).

GAC can be combined with a biologically active layer in what is referred to as biological activated carbon (BAC). Reungoat et al. (2011) found that BAC had removal efficiencies of greater than 90% for 21 pharmaceuticals analyzed. Although adsorption

might have some role in these high removal percentages, biodegradation was found to be the primary removal mechanism (Reungoat et al., 2011).

2.3 Operational Effects on CEC Removal Efficiencies

Several researchers have examined the effects of WWTP operational parameters on CEC removal efficiencies (Johnson et al., 2005; Clara et al., 2005a; Lishman et al., 2006). Johnson et al. (2005) studied the impact that HRT, SRT, biological HRT (HRT in the biological treatment zones), and temperature have on the estrogenic hormone estrone (E1). In analyzing seventeen WWTPs throughout Europe; Johnson et al. (2005) found that E1 removal rates (Figure 2-1) increased as HRT and SRT increased, especially biological HRT. It should be noted that the Pearson product-moment correlation coefficient (R^2), obtained from a linear regression of each parameter, is relatively low. Consequently, there exists a general downward trend (Figure 2-1) from these data but resulting relationships should not be viewed as exact tendencies. It is important to note that the influent concentrations were estimated from excretion rates, population data, and flow, resulting in artificially higher E1 levels at low retention times (Figure 2-1). Temperature did not have a significant effect on E1 removal efficiency.

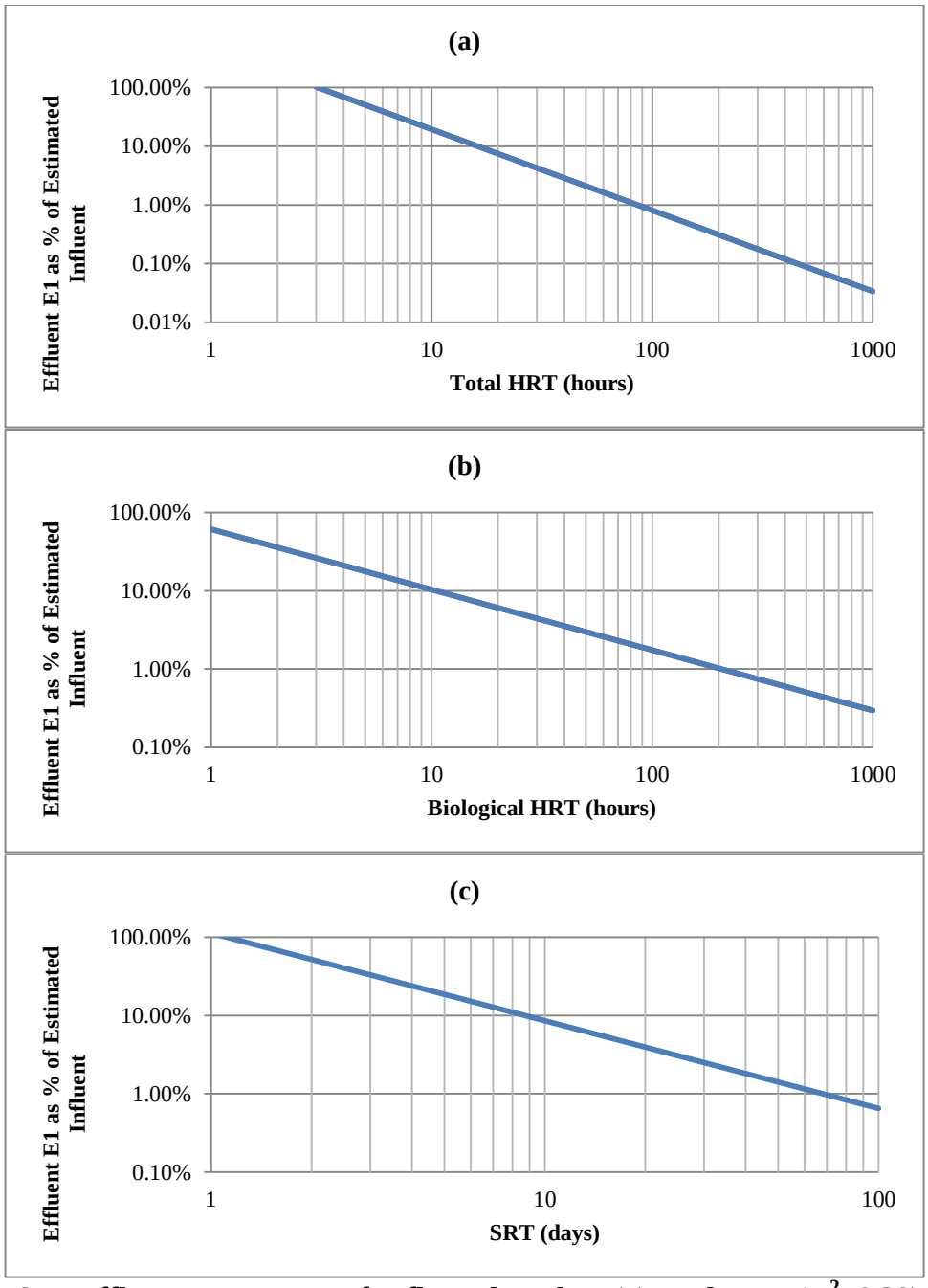

Figure 2-1: Effluent E1 Percent of Influent based on (a) total HRT (R^2=0.39), (b) biological HRT (R^2=0.16), and (c) SRT (R^2=0.28) (Johnson et al., 2005)

Clara et al. (2005a) analyzed E1, 17β-estradiol (E2), 17α-ethinylestradiol (EE2), caffeine, and bezafibrate using bench-scale experiments with varying SRTs along with sampling at five different WWTPs. The study concluded that the critical SRT (the SRT

for which the compound removal is maximized) for E1 and E2 was between 5 and 10 days, with almost complete removal of these two compounds occurring after 10 days. EE2, meanwhile, did not show consistent removal rates. Even for similar SRTs, removal rates varied quite drastically (Clara et al., 2005a). Both E1 and E2 are natural estrogens, while EE2 is a pharmaceutical. This could be the reason for variation in removal through WWTPs. Both caffeine and bezafibrate had removal rates of more than 95%. Furthermore, critical SRTs for caffeine and bezafibrate were found to be 5 and 10 days, respectively (Clara et al., 2005a).

Lishman et al. (2006) analyzed CECs in twelve different WWTPs along the Thames River in Canada. Seven of the twelve WWTPs consisted of only CAS while two of the twelve had CAS and media filtration. The remaining treatment plants used lagoon treatment processes. Among other CECs, Lishman et al. (2006) evaluated concentrations of gemfibrozil, diclofenac, celestolide, phantolide, galaxolide, and tonalide. As expected, gemfibrozil, diclofenac, and celestolide (ADBI) all had increased removal efficiencies as SRT increased. Traseolide (ATII), galaxolide (HHCB), and tonalide (AHTN), meanwhile, did not show these tendencies. For a SRT between 3 and 5 days, no correlation was discovered. However, for SRT over 5 days, ATII removal efficiency increased with increasing SRT. Meanwhile, for HHCB and AHTN, removal efficiency seemed to slightly decrease with increased SRT. This can likely be attributed to the lack of data for larger SRT ranges. In many cases, effluent concentrations of these compounds were below detectable levels (BDL), making it difficult to correlate any patterns in removal efficiency. Other CECs evaluated, including ibuprofen and naproxen, had high (~95%) removal efficiencies but also varied with increased SRT.

For these two compounds, Lishman et al. (2006) noted that removal efficiency tendencies could not be found with treatment configurations or operational parameters.

2.4 Removal Mechanisms

CECs are removed from wastewater by biodegradation and adsorption to biosolids (Lee et al., 2009; Ghalajkhani, 2013). Although volatilization could be considered, it is negligible for most CECs due to their low octanol-water partitioning coefficients (log K_{OW}) and Henry coefficients (K_H) (Clara et al., 2005b). CEC compounds can partition between the neutral (HA) and ionized form (A^-) which impact the rate of sorption or biodegradation (Figure 2-2).

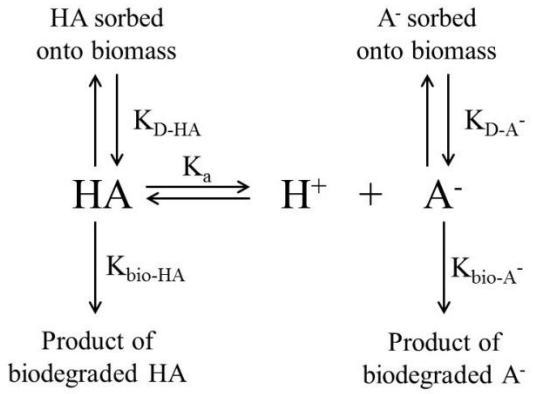

Figure 2-2: Ionized CEC Sorption and Biodegradation Diagram

As presented in Figure 2-2, sorption and biodegradation of ionized CECs must be accounted for in the neutral and ionized forms. In contrast, neutral compounds (not shown) only require sorption and biodegradation rates for the neutral form. However, for this research, it is unknown whether each CEC is in the ionized or neutral form. Therefore, sorption and biodegradation rates are considered to be equal for both forms.

2.4.1 Sorption

Sorption consists of both adsorption from liquid to a solid and desorption, or a solid to liquid phase. The amount of a compound sorbed onto biomass can be modeled by the compound's partitioning coefficient, K_d (Equation 2.1) (Joss et al., 2006). Note: M_s is mass associated with substrate, M_{ss} is mass associated with suspended solids, M_x is mass associated with biomass, L is a unit of length, and T is a unit of time.

$$K_d = \frac{X}{VSS \times S} \qquad \textbf{Equation 2.1}$$

where

K_d is the compound partitioning coefficient (L^3/M_{ss})

X is the sorbed compound concentration (M_s/L^3)

S is the concentration of the compound (M_s/L^3), and

VSS is the volatile suspended solids concentration in the reactor (M_{ss}/L^3)

Rearranged, the amount of sorbed compound is:

$$X = K_d \times VSS \times S \qquad \textbf{Equation 2.2}$$

As shown, sorption is not modeled using a kinetic expression. However, Ternes et al., (2004) found that equilibrium was reached after just 0.5 hours in a batch reactor. Because the clarifiers and the PFR at the NWRF have HRTs greater than 0.5 hours, sorption is assumed to reach equilibrium.

The desorption rate (r_{des} (M_s/L^3)) does not depend on the influent concentration of the compound. Instead, it is dependent on the concentration of the compound on the

biomass. Therefore, r_{des} (Equation 2.3) is equal to K_{des} multiplied by the concentration of the compound sorbed onto the biomass (X) (Ghalajkhani, 2013).

$$r_{des} = K_{des}X \qquad \textbf{Equation 2.3}$$

The rate of desorption is assumed to be slower than adsorption. Therefore, k_{des} is assumed to be 0.1 d^{-1}, meaning that desorption is assumed to happen at 10% of the rate that adsorption takes place (Ghalajkhani, 2013).

Githinji et al. (2010) analyzed ciprofloxacin and amoxicillin, determining sorption rates and biodegradation tendencies. The experimental sorption rates determined are presented in Figure 2-3.

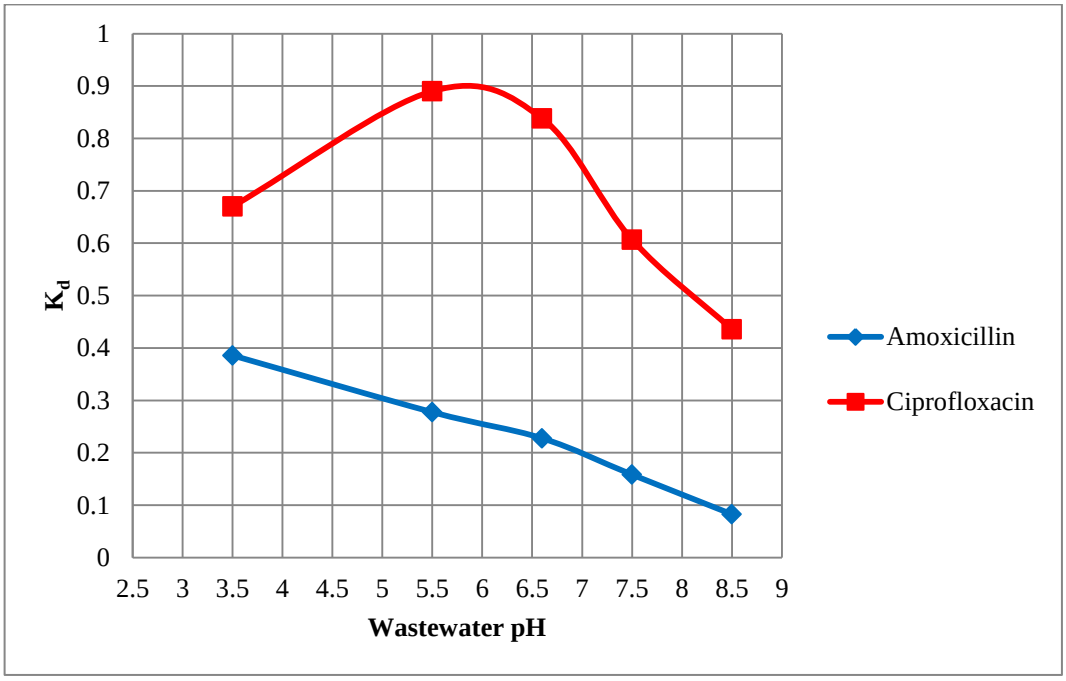

Figure 2-3: Sorption Coefficients of Amoxicillin and Ciprofloxacin under varying pH (Githinji et al., 2010)

The key conclusion developed from this study is that ciprofloxacin had higher adsorption rates than amoxicillin and amoxicillin portioning coefficients decreased with increasing values of pH. Ciprofloxacin partitioning coefficients reached a maximum at a

pH of 5.5 and decreased as pH increased after that point. Because amoxicillin has a higher pKa value than ciprofloxacin, it dissociates in water at a higher rate. Therefore, amoxicillin has less electrostatic attraction and sorbs to solids at a lower rate than ciprofloxacin (Githinji et al., 2010). At higher pH, amoxicillin and ciprofloxacin compounds are more negatively charged, resulting in less electrostatic attraction with solids in the system. Consequently, the sorption potential of these compounds decreases at higher pH values (Githinji et al., 2010). This should be considered when selecting sorption coefficients for CECs. Furthermore, neither antibiotic significantly degraded within 48 hours, indicating the importance of an adsorption removal mechanism (Githinji et al., 2010).

2.4.2 Biodegradation

Lee et al. (2012) used a Monod biokinetic expression to model triclosan degradation in wastewater. The same concept can be used for other CECs with the alteration of half saturation constants (K) and maximum specific rate of substrate utilization ($\hat{q}$). The Monod expression, in terms of substrate utilization (r_{ut}), is presented in Equation 2.4 (Rittmann and McCarty, 2001).

$$r_{ut} = -\hat{q}\frac{S}{K+S}X_a \qquad \textbf{Equation 2.4}$$

where

r_{ut} is the rate of substrate utilization ($M_s/L^3 \cdot T$)

$\hat{q}$ is the maximum specific rate of substrate utilization ($M_s/M_x \cdot T$)

S is the concentration of the rate-limiting substrate (M_s/L^3)

K is the half-saturation coefficient of the substrate (M_s/L^3), and

X_a is the active biomass concentration (M_x/L^3)

It should be noted that this is a pseudo-order utilization rate, resulting in two boundary conditions. At low concentrations of substrate (S<<K, which is the case for CECs), the net specific growth rate (μ) can be modeled as a first-order rate (Figure 2-4).

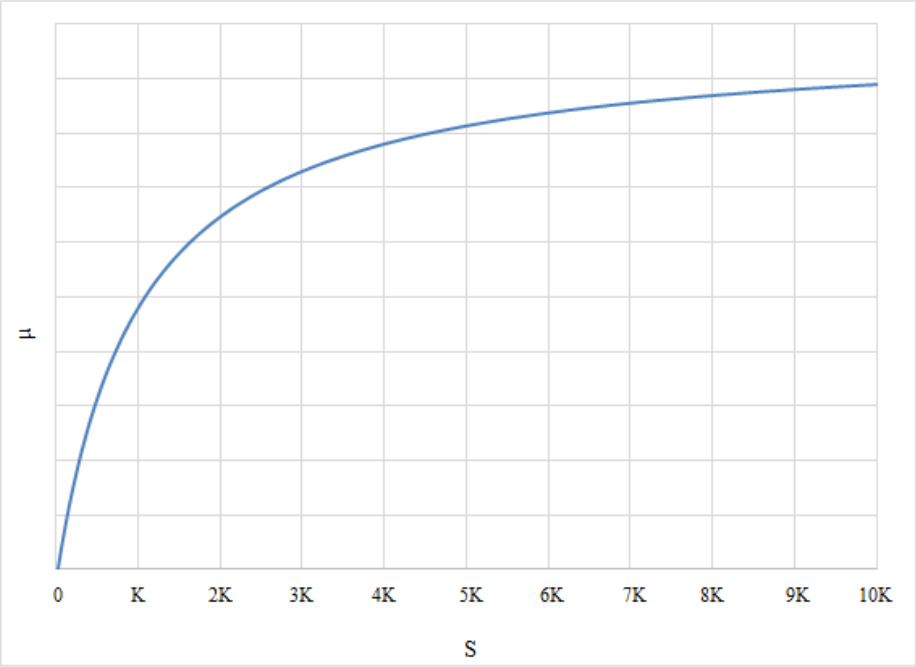

Figure 2-4: Net Specific Growth Rate vs. Substrate Concentration

Based on the observation that the CEC exists at low concentrations in the waste stream, it can be assumed that first-order rates apply to CEC biodegradation. Therefore, the net rate of biomass growth, r_{net}, can be defined by Equation 2.5.

$$r_{net} = Y\hat{q}\frac{S}{K+S}X_a - bX_a \qquad \textbf{Equation 2.5}$$

where

r_{net} is the net rate of active biomass growth ($M_x/L^3 \cdot T$)

Y is the true yield (M_x/M_s), and

b is the endogenous-decay coefficient (1/T)

Because half-saturation coefficients are not well documented, a simpler modeling method for biodegradation is to use biodegradation constants. As noted, because first-order rates apply, Equation 2.6 can be used in determining removal due to biodegradation (Joss et al., 2006; Tran et al., 2015).

$$r_{ut} = -k_{bio} X_a S \qquad \textbf{Equation 2.6}$$

where

k_{bio} is the biodegradation constant ($L^3/M_x \cdot T$)

Similar to Equation 2.5, r_{net} can then be described using Equation 2.7.

$$r_{net} = Y k_{bio} X_a S - b X_a \qquad \textbf{Equation 2.7}$$

However, because CEC concentrations are small compared to biomass concentrations, their effect on biomass can be considered negligible. For this reason and to simplify modeling, the net rate of biomass growth was modeled as the negative rate of CEC utilization (Equation 2.6).

2.5 Modeling CECs in GPS-X

Based on a thorough literature review, much of the CEC research focus has been centered around bench/pilot scale studies; with little attention aimed at treatment process optimization. However, Ghalajkhani (2013); Monteith et al. (2008) and Schraa et al. (2006), have provided a framework for using a standard process model (GPS-X, Hydromantis, Ontario Canada) to study CEC fate in municipal wastewater systems.

CECs were integrated into the models using the Model Developer (MD) tool. MD allows for the creation of new models using a matrix format. New models allow for the addition of rates and kinetic and stoichiometric relationships, as well as other model parameters (Hydromantis, 2014).

Ghalajkhani (2013) used GPS-X to model the fate of xenobiotic organic compounds (XOCs). XOCs stem from personal care products, pharmaceuticals, excreted hormones, and household and industrial chemicals. Using data from existing research for calibration (Collado et al., 2012; Zhao et al., 2007), the following sorption and biotransformation constants were determined for ibuprofen (Table 2-4) and bisphenol-A (Table 2-5). $K_{d\text{-}HA}$ is the solid-liquid partitioning coefficient for the neutral form of an iodized compound; $K_{d\text{-}A\text{-}}$ is the solid-liquid partitioning coefficient for the ionized form of an ionized compound; $K_{d\text{-}N}$ is the solid-liquid partitioning coefficient for a neutral compound; $K_{bio\text{-}HA}$ is the aerobic biodegradation rate constant for the neutral form of an ionized compound; and $K_{bio\text{-}N}$ is the aerobic biodegradation rate constant for a neutral compound (Ghalajkhani, 2013).

Table 2-4: Calibrated Ibuprofen Partitioning and Biotransformation Coefficients (Ghalajkhani, 2013)

Parameter	Lower Bound	Upper Bound	Optimal Value ± Standard Error
$K_{d\text{-}HA}$ (L/mg biomass)	1.59E-05	7.53E-04	3.23E-4±6.02E-5
$K_{bio\text{-}HA}$ (L/mg biomass/d)	0.0681	0.2877	0.1943±0.10
$K_{d\text{-}A\text{-}}$ (L/mg biomass)	1.32E-06	6.26E-05	1.96E-5±5.72E-6

Note: The biodegradation rate for the ionized form of an ionized compound, $K_{bio\text{-}A\text{-}}$, was not provided.

Table 2-5: Calibrated Bisphenol-A Partitioning and Biotransformation Coefficients (Ghalajkhani, 2013)

Parameter	Lower Bound	Upper Bound	Optimal Value ± Standard Error
$K_{d\text{-}N}$ (L/mg biomass)	5.75E-05	7.19E-04	4.935E-4±5.3E-5
$K_{bio\text{-}N}$ (L/mg biomass/d)	0.0047	0.0697	0.0502±7.9E-3

Rate constants similar to those shown in Table 2-4 and Table 2-5 will be needed in order to model other CECs. Once CECs are selected for modeling, biodegradation constants and partitioning coefficients will be estimated from literature values.

Monteith et al. (2008) developed equations for sorption and biotransformation processes (including parent and daughter cells) of the estrogenic hormones E1, E2, and synthetic estrogen EE2. These equations were developed via literature review and the results were compared with actual field data in order to calibrate the model. Table 2-6 presents the initial and calibrated physical and chemical properties that Monteith et al. (2008) used in modeling. The calibrated initial properties were adjusted after comparing the modeled results to literature data (Monteith et al., 2008).

Table 2-6: Initial Physical and Chemical Properties of Three Estrogenic Hormones (Monteith et al., 2008)

Property	E1	E2	EE2
Molecular weight (Daltons)	270.4	272.4	296.4
Density (g/cm^3)	1.23	1.2	1.2
Henry's coefficient (L_{liq}/L_{gas})	1.54E-08	1.47E-10	3.21E-10
Log K_{ow}	3.13	4.01	3.67
Initial Aerobic k_{bio} (m^3/g VSS-d)	0.205	0.429	0.00097
Initial Anoxic k_{bio} (m^3/g VSS-d)		0.125	
Initial Anaerobic k_{bio} (m^3/g VSS-d)		0.222	
Calibrated Aerobic k_{bio} (m^3/g VSS-d)	0.0216	0.024	0.00097
Calibrated Anoxic k_{bio} (m^3/g VSS-d)		0.007	
Calibrated Anaerobic k_{bio} (m^3/g VSS-d)		0.013	

After calibration, the model was analyzed with varying temperature, SRT, HRT, and total suspended solids (TSS) concentrations. Under 9 to 11°C, sorption impacts removal rates more than biotransformation. At these low temperatures, biotransformation kinetics decrease, and the compounds are removed primarily from sorption to biosolids. However, above 9 to 11 °C, it was found that biotransformation plays a larger role on the removal of the hormones (Monteith et al., 2008). Generally, as temperature increases, so does the removal of the estrogenic hormones (Figure 2-5).

This is likely due to the Arrhenius equation, which states that kinetic constants increase as temperature increases.

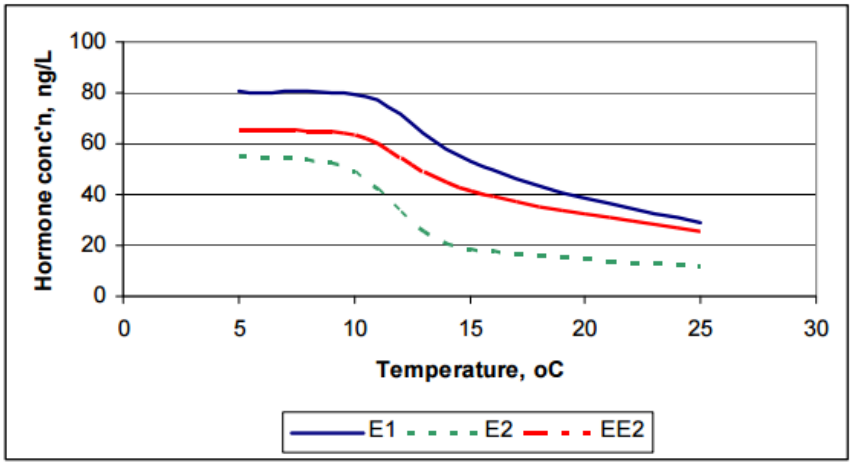

Figure 2-5: Effluent Estrogenic Hormone Concentrations vs. Varying Temperature (Monteith et al., 2008)

Monteith et al. (2008) also studied isothermal SRT impact on hormone concentrations. At 20°C, no significant changes in effluent concentration were observed after an aerobic SRT of 5 days (Figure 2-6). However, at a constant temperature of 10°C, E2 concentrations decreased as aerobic SRT increased (Figure 2-7). E1 and EE2 decreased, but not substantially.

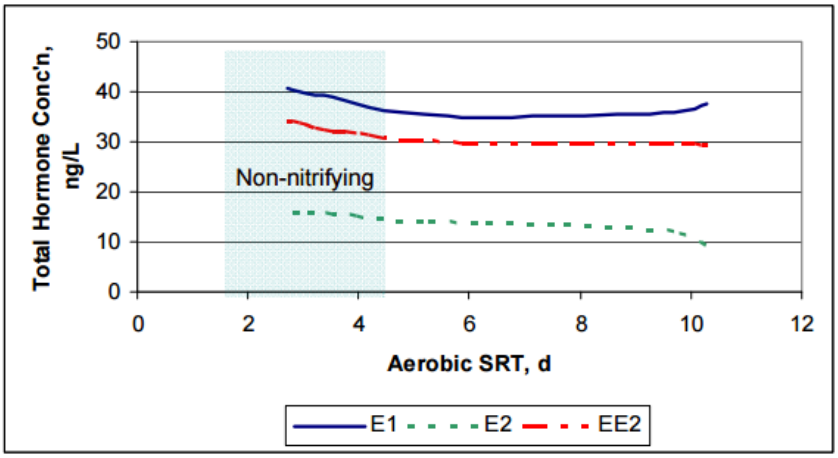

Figure 2-6: Effluent Estrogenic Hormone Concentrations vs. Aerobic SRT, 20°C (Monteith et al., 2008)

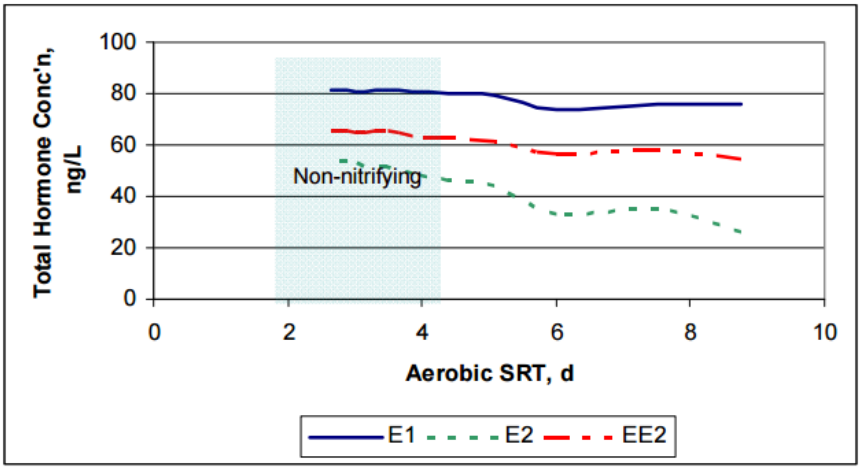

Figure 2-7: Effluent Estrogenic Hormone Concentrations vs. Aerobic SRT, 10°C (Monteith et al., 2008)

The effects of aeration HRT were examined on the estrogenic hormone levels. As expected, increased aeration HRT resulted in decreased levels of total hormone concentrations. In this case, removal efficiency plateaued after a HRT of about five days.

Monteith et al. (2008) also examined the effect that TSS concentrations have on the hormone concentrations. Because the majority of the estrogenic hormones in the primary and final effluents were free and not bound, TSS did not have a large effect on the hormone concentrations (Figure 2-8).

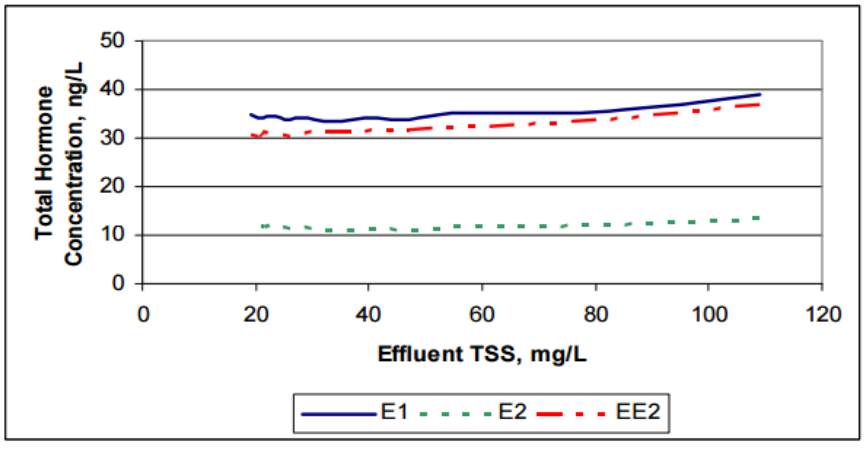

Figure 2-8: Effluent Estrogenic Hormone Concentrations vs. TSS Concentration (Monteith et al., 2008)

Schraa et al. (2006) modeled pharmaceutical wastewater through a WWTP that contained fungal and bacterial integrated fixed-film activated sludge (IFAS). Schraa et al. (2006) used the *mantis* model, a modified activated sludge model (ASM), because of the following modifications from ASM: temperature dependence of kinetic parameters; growth limitation due to low ammonia conditions; simultaneous nitrification and denitrification; and updated kinetic parameters. After calibration, modeling was used to analyze the WWTP with treatment processes offline, varying temperatures, and lower air flowrates in the reactors (Schraa et al., 2006).

2.6 NWRF Characteristics

The NWRF has an average flowrate of about 10 MGD (from 2012 and 2013 data). Utilizing CAS, it consists of primary and secondary clarification, a plug flow reactor (PFR) aeration basin, and anaerobic digesters. The current unit processes and sizes are shown in Table 2-7. Figure 2-9 and Figure 2-10 display a labeled aerial view and a process flow diagram with sampling locations, respectively.

Table 2-7: Current NWRF Layout

2015 NWRF Layout
Bar Screen
2 Grit Chambers
2 Primary Clarifiers @ 0.200 MG each 2 Primary Clarifiers @ 0.288 MG each
3 Chamber Aeration Basin @ 0.990 MG per chamber
2 Secondary Clarifiers @ 0.676 MG each 2 Secondary Clarifiers @ 1.33 MG each
4 Gravity Thickeners @ 0.019 MG each
4 Anaerobic Digesters @ 0.633 MG each

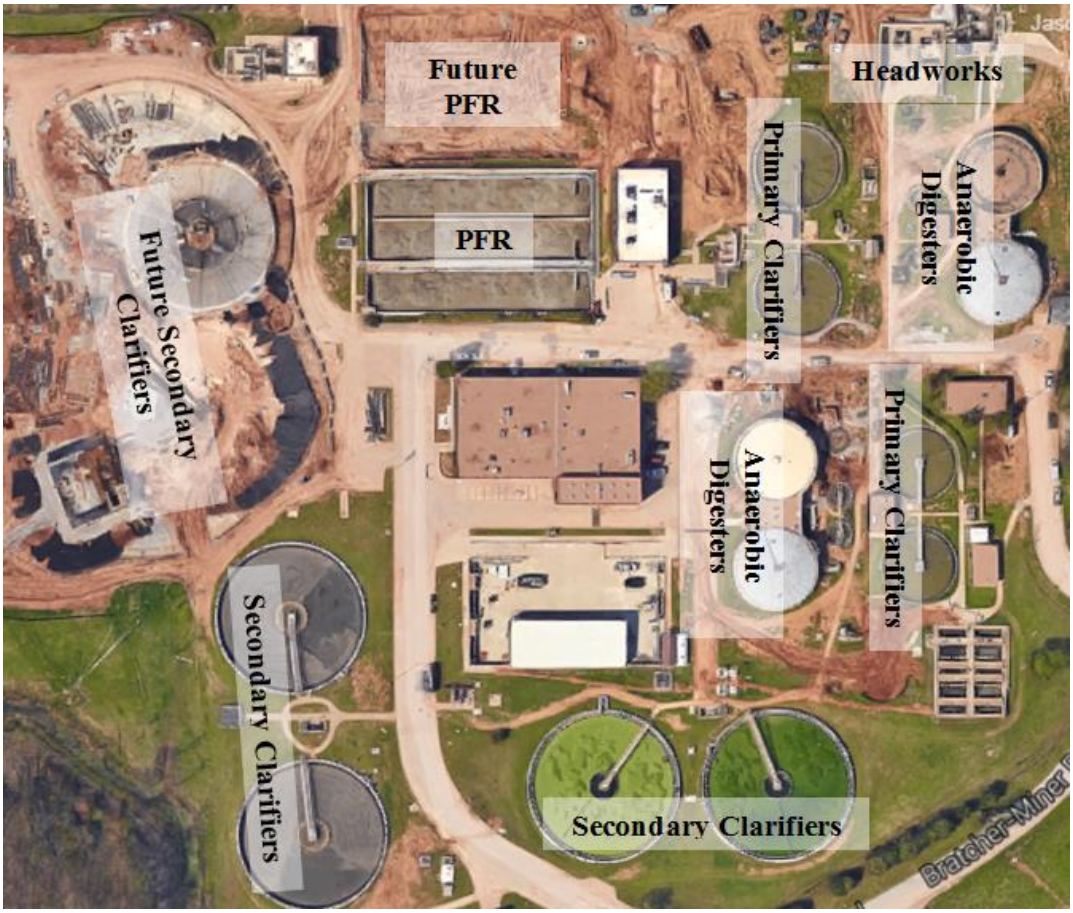

Figure 2-9: Aerial View of the NWRF

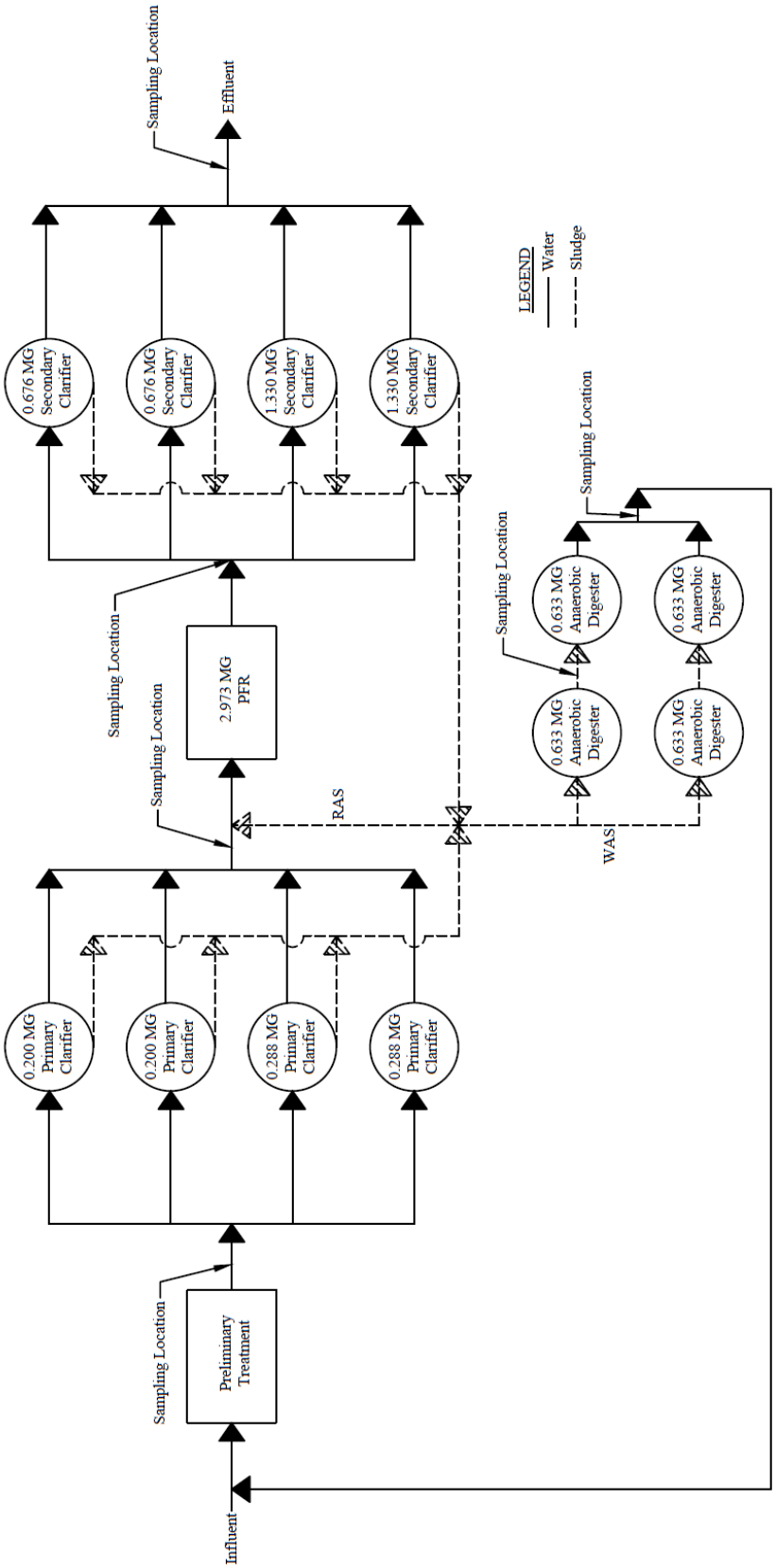

Figure 2-10: NWRF Process Flow Diagram

Chapter 3: Hypothesis and Objectives

It is hypothesized that utilizing MBRs will be more effective than operational changes to the CAS process at removing CECs in the NWRF. From literature, MBRs typically have higher removal efficiencies than CAS (Lee et al., 2009). MBRs are desirable because of their small space requirements, their capability of replacing secondary clarifiers (EPA, 2007), and their ability to be placed inside or outside an existing CAS aeration basin (Lee et al., 2009). Furthermore, because MBRs are able to maintain higher concentrations of biomass, less volume is needed in CAS aeration basins (EPA, 2007). Finally, MBRs provide additional pathogen barriers, providing increased removal that may be desirable for water reuse applications (Alan Plummer Associates, Incorporated, 2015).

3.1 Objective 1

The first objective of this research is to evaluate the impact of operational parameters (HRT, SRT, sludge recycling, disinfection adjustments, etc.) on the removal efficiency of CECs. To achieve this objective the following tasks have been identified: (i) develop a model of the current NWRF layout (base model), (ii) calibrate the base model, (iii) validate the base model, (iv) integrate CECs using MD to develop an enhanced model, (v) calibrate the enhanced model, and (vi) validate the enhanced model.

3.2 Objective 2

The second objective is to evaluate AT options (such as MBR, NF, RO, UV disinfection, GAC, and BAC) that help to increase removal efficiency of CECs. This objective will use the advanced model to further the understanding of the fate through AT processes.

3.3 Goal

The goal of this research is to develop a stochastic model to optimize CEC removal efficiencies and operations at the NWRF.

Chapter 4: Methodology

The scope of this research included: reviewing literature regarding the fate of CECs through WWTPs; analyzing water quality data of the influent and effluent of major treatment processes from the NWRF; determining rate constants and biological and physiochemical properties of CECs to be modeled; developing a base model in GPS-X of the current layout of the NWRF; calibrating and validating the base model; developing an enhanced model that uses MD to integrate CECs into the base model; calibrating and validating the enhanced model; developing an expanded model that expands the enhanced model to include the future layout of the NWRF; and developing an advanced model to evaluate operational changes and AT options to increase removal efficiencies of CECs.

4.1 Outline

The first step of this research was to complete a thorough literature review. Common CECs in wastewater and typical removal efficiencies were determined. Due to the vast numbers of CECs that could be used and due to budget limitations, indicator CECs were modeled. In order to select CECs for modeling, CECs with similar physiochemical and biological characteristics and function were grouped together. After grouping, indicator CECs were used to represent the group. Although validators did not always behave the same as indicators, most validators performed the same as its indicator CEC through at least one treatment process (Table 5-4). Therefore, indicators from a resource document by Alan Plummer Associates, Incorporated (2015) were used for modeling in order to better understand entire groups of CECs. The sampling

locations at the NWRF were the preliminary treatment effluent, primary clarifier effluent, aeration basin effluent, secondary (final) clarifier effluent, primary anaerobic digester effluent, and secondary anaerobic digester effluent. After selection of CECs, literature values were again used to determine biodegradation constants and partitioning coefficients of CEC (Table 4-2).

4.2 Base Model Development, Calibration, and Validation

During CEC literature review and selection, the base NWRF model was developed. Due to limitations of the GPS-X model, only half of the plant was modeled. Because the NWRF has four primary, four secondary clarifiers, four thickeners, and four anaerobic digesters (as of 2015), only two of each of these treatment processes were modeled. The PFR's volume, meanwhile, was divided by two and all three chambers were kept for modeling purposes. Furthermore, because only one-half of the plant was modeled, the influent flowrate was divided by two. Because the flow was halved, one of each size of clarifier (both primary and secondary) was used for modeling. In the model, flow was further split to account for the size of each clarifier. These splits, along with the current NWRF and modeled physical parameters are shown in Table 4-1.

Table 4-1: NWRF and Base Model Physical Parameters

2015 NWRF Layout	Base and Enhanced Model Layout
Bar Screen	Bar Screen
2 Grit Chambers	1 Grit Chamber
2 Primary Clarifiers @ 0.200 MG each 2 Primary Clarifiers @ 0.288 MG each	1 Primary Clarifier @ 0.200 MG (40% of flow) 1 Primary Clarifier @ 0.288 MG (60% of flow)
3 Chamber Aeration Basin @ 0.990 MG per chamber	3 Chamber Aeration Basin @ 0.495 MG per chamber
2 Secondary Clarifiers @ 0.676 MG each 2 Secondary Clarifiers @ 1.33 MG each	1 Secondary Clarifier @ 0.676 MG (34% of flow) 1 Secondary Clarifier @ 1.33 MG (66% of flow)
4 Gravity Thickeners @ 0.019 MG each	2 Gravity Thickeners @ 0.019 MG each
4 Anaerobic Digesters @ 0.633 MG each	2 Anaerobic Digesters @ 0.633 MG each

Splitting the plant allowed for the model to be calibrated using the data provided by the NWRF. The data provided by the NWRF included typical WWTP parameters, including: temperature, carbonaceous biological oxygen demand (cBOD), ammonia, TSS, dissolved oxygen (DO), alkalinity, and pH from 2012 and 2013 (Appendix A: NWRF Typical Wastewater Parameters).

Calibration involved adjustment of model parameters so that modeled effluent concentration levels of cBOD, ammonia, and TSS closely match actual levels found from sampling over the entire year of 2013. The model was then validated by confirming the effluent concentrations of cBOD, ammonia, and TSS from 2012. Validation confirms the calibration of the system, verifying that modeled effluent concentrations match data from the NWRF. With validation, the effluent data should closely match the levels from the model.

4.3 Enhanced Model Development, Calibration, and Validation

The next step was to integrate CECs into the base model using the MD tool. The MD tool allows custom libraries to be created within GPS-X. MD uses a matrix format

and can be used to add new contaminant parameters and alter rate equations and constants, making it possible to precisely model varying wastewater parameters. In this case, CEC parameters were added to the base model, creating the enhanced model. During this process, the five sections of the MD tool were populated. These sections are: GPS-X Libraries, Stoichiometric Matrix, Model Kinetics, Model Parameters, and Composite Variables. The GPS-X Libraries section contains the existing state variables and composite variable stoichiometry parameters. State variables are used by GPS-X to perform mass balance calculations. They include the various forms of COD, nitrogen, phosphorus, and other wastewater parameters. Composite variables are calculated from the state variables and include: TSS, volatile suspended solids (VSS), total $cBOD_5$, total COD, total Kjeldahl nitrogen (TKN), TN, total phosphorus, and total carbon. The Stoichiometric Matrix contains state variables in columns and kinetic processes in rows, showing the stoichiometric relationship between the state variables and the rate processes within the model. It allows the addition of process rates such as the sorption, desorption, and biodegradation of CECs. The Model Kinetics section has the kinetic equations used in the model. It incorporated Equation 2.2 to Equation 2.6 to quantify CEC sorption, desorption, biodegradation, and biomass production from CEC biodegradation, respectively. The Model Parameters tab contains state variables, stoichiometric parameters, and kinetic parameters. This section allows for the entry of new rate constants and is where desorption constants, partitioning coefficients, and biodegradation constants were entered into the model. The Model Parameters section also allows for the application of Arrhenius coefficients, making it possible to analyze

temperature's effect on CEC removal. Finally, the Composite Variables tab shows fixed composite variable stoichiometry (Hydromantis, 2014).

After CECs were integrated, the enhanced model was calibrated and validated in a similar way to the base model. In this case, indicator CECs from certain groups (Alan Plummer Associates, Incorporated, 2015) were selected for calibration (Table 4-2), while other CECs from the same group were used for validation (Table 4-3). Along with compiling a list of indicator CECs, Alan Plummer Associates (2015) also compiled monitoring trigger thresholds (MTTs) for each CEC. These MTTs assume a 150-pound person that consumes 2 liters of water per day to estimate acceptable concentrations of CECs based on tolerable daily intake values (Alan Plummer Associates, Incorporated, 2015).

Table 4-2: Indicator CEC Sorption and Biodegradation Constants

Indicator CEC	Class	MTT (ng/L)	K_d (L/kg)	k_{bio} (L/g – d)	Validation CEC
17β-Estradiol (E2)♦	Hormone	<1	426-2003[a] 461±212[f]	350±42[j] (Aerobic) 460±60[j] (Anoxic) 175±10[j] (Anaerobic)	Estrone (E1)
Atenolol	Beta Blocker	4,000	0.21[d] 64±88[e] 17-97[g]	0.69[g] 1.1±0.1-1.9±0.2[l]	Lopressor
TCEP♦	Flame Retardant	5,000	<30-162±72[k] †	†	TCPP
Caffeine	Stimulant	-	199.5-794.3[i]	39.6-50.9[n]	Theobromine (Caffeine degradate)
Gemfibrozil	Lipid Regulator	800,000	75-1106[a] 19.3±9.3[e] 47.9-275.4[h]	6.4-9.6[c]	Bezafibrate♦
Iopromide	X-Ray Contrast Agent	750,000	11±1[b] 6.9[f]	1.6-2.5[c]	Iohexol
Meprobamate	Anti-Anxiety	200,000	316.2-631.0[i]	-	Diazepam♦
DEET	Repellant	200,000	58.9-128.8[h] 63.1-1258.9[i]	-	N/A*
Primidone	Anti Convulsant	10,000	<30-45±10[k] 7±1[l]	<0.1[l]	N/A*
Sucralose	Sugar Substitute	150,000,000	95.5±28.9-761.1±323.5[m]	0.003-0.009[m]	Acesulfame-K
Triclosan	Antibacterial	2,100,000	1905-9550[h]	1.2-3.6[n]	Triclocarban♦

* Note: Validation CECs that are similar to the indicator CEC do not exist in the sampling suite.
† Note: Several studies have shown zero removal of CEC (Luo et al., 2014; Meyer and Bester, 2004)
♦ Note: Concentrations were below MRL during analysis

Table 4-3: Validation CEC Sorption and Biodegradation Constants

Class	Validation CEC	K_d (L/kg)	k_{bio} (L/g – d)
Hormone	**Estrone (E1)**	170-365[a] 303±59[f]	162±25[j] (Aerobic) 30±10[j] (Anoxic) 10±1[j] (Anaerobic)
Beta Blocker	**Lopressor**	7-19[g]	0.58[g]
Flame Retardant	**TCPP**	┼	┼
Caffeine Degradate	**Theobromine**	^	^
Lipid Regulator	**Bezafibrate**♦	158.5-501.2[i]	2.1-3.0[c]
X-Ray Contrast Agent	**Iohexol**	-	1.8-2.4[c]
Anti-Anxiety	**Diazepam**♦	21±8-44±26[b] 81.3-295.1[h]	0.035[c] <0.016[l]
Sugar Substitute	**Acesulfame-K**	47.5±4.5- 365.9±338.4[m]	0.0448-0.0594[m]
Antibacterial	**Triclocarban**♦	25703[h]	

* Note: Validation CECs that are similar to the indicator CEC do not exist in the sampling suite.
┼ Note: Several studies have shown zero removal of CEC (Luo et al., 2014; Meyer and Bester, 2004)
♦ Note: Concentrations were below MRL
^ Literature data not found. Values are assumed to be similar to caffeine constants.

[a] Urase and Kikuta, 2005
[b] Ternes et al., 2004
[c] Joss et al., 2006
[d] Jones et al., 2002
[e] Radjenović et al., 2009
[f] Carballa et al., 2008
[g] Maurer et al., 2007
[h] Hyland, 2014
[i] Okuda et al., 2009
[j] Joss et al., 2004
[k] Stevens-Garmon et al., 2011
[l] Wick et al., 2009
[m] Tran et al., 2015
[n] Blair et al., 2015

CECs have varying biodegradability based on whether the treatment process is aerobic, anoxic, and anaerobic. At the NWRF, both sets of digesters are currently anaerobic. However, the digester modules in GPS-X are not compatible with the MD tool. The digesters have large variability in removal percentages (Table 5-2). However, a lack of modeling could result in incorrect concentrations in the digester effluents.

Table 4-2 and Table 4-3 served as a preliminary list of expected CECs to model. However, some of the CECs listed were below the method reporting limit (MRL) (as noted in the tables). After removal percentages were determined for each CEC (Table 5-2), each pair of indicator and validation CECs was confirmed to have similar removal

percentages in the primary clarifiers, PFR, or both unit processes. In contrast to base model calibration, instead of adjusting just model parameters, CEC rate constants and coefficients were adjusted as part of the calibration process.

4.4 Expanded and Advanced Models

After the enhanced model was calibrated and validated, the expanded model was developed. The expanded model utilized the enhanced model but was modified with currently proposed (and ongoing) plant expansion treatment processes. This included adjustments to certain treatment processes, as well as a volume expansion of the aeration basin and final clarifiers. The current plant expansion also includes the addition of a UV disinfection process. With the initial expanded model developed, multiple scenarios were analyzed to determine the NWRF performance on CEC removal efficiency with varying conditions. Next, in the advanced model, additional AT processes were integrated and analyzed. These processes were simulated to determine their effects on CEC removal efficiency.

4.5 Model Limitations

A portion of the expansion at the NWRF is the addition of UV disinfection. Although GPS-X has a disinfection treatment process, UV is not an option. Furthermore, in order to use a treatment process to model CECs, the unit must be compatible with the MD tool. Although the MD tool is compatible with primarily suspended and attached growth processes, other treatment processes are available. Below, the options given for model generation are shown (Figure 4-1). Since UV was

not included as an option in GPS-X, it was not included in the expanded or advanced models.

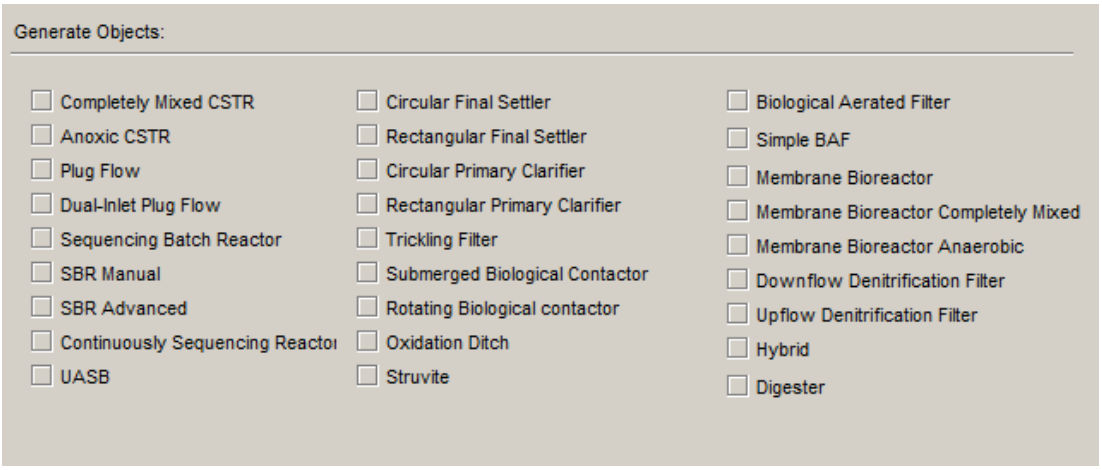

Figure 4-1: GPS-X Model Generation Treatment Processes

Chapter 5: Results and Discussion

5.1 Sampling and Analysis

Sampling was completed on January 27, 2016. In order to monitor the wastewater as it passed through the plant, samples were taken at different times throughout the day based on the units' hydraulic retention time (HRT). It was assumed that the data would be more representative of each treatment processes' removal capability if HRT was taken into consideration. Table 5-1 displays each unit's estimated HRT along with the time of sampling for each. A few items should be addressed regarding the sampling times and locations:

- The first sampling point was the preliminary treatment effluent. It was assumed that there were no changes in CEC concentrations between the plant influent and preliminary treatment effluent. Therefore, the preliminary effluent only had to be sampled at an early enough time to be able to sample the rest of the plant on the same day.
- The primary and secondary digesters have HRTs of multiple days. Because time was of importance, these treatment processes were sampled at 9:30 AM, without taking HRT into consideration.
- The NWRF does not have a sampling location for the PFR effluent. Therefore, the PFR effluent was actually taken towards the bottom of the secondary clarifier. This should not have a significant effect on the CEC concentrations.

Table 5-1: Treatment Process Sampling Times

Treatment Process	HRT (hours)	Sampling Time
Preliminary Treatment Effluent	N/A	6:37 AM
Primary Clarifier Effluent	3	9:35 AM
PFR Effluent	6	3:40 PM
Secondary Clarifier Effluent	3	6:37 PM
Primary Digester Effluent	N/A*	9:30 AM
Secondary Digester Effluent	N/A*	9:30 AM

* HRT is several days and was not considered during sampling due to time constraints.

Eurofins Eaton Analytical performed the analysis of 98 CECs. However, only 38 (Table 5-2) of these were above the MRL in one or more of the treatment processes (Appendix B: CECs (and MRLs) Analyzed). Furthermore, each indicator CEC is significantly lower than its MTT concentration. Several CECs increase in concentration as they move through the plant (Table 5-2). If more samples could have been collected (during other days and even seasons), it is likely that fewer CECs would have negative removal percentages. However, it is worth noting that there would likely still be CECs with negative removal percentages. This is due to the fact that biodegraded products can convert back to the parent compound during treatment processes (Jelić et al., 2012). For instance, theobromine could have converted back to caffeine. Due to the high percent removal of both compounds, though, this was likely not the case for theobromine. Negative removal percentages can also be attributed to the desorbing of CECs in a unit operation. Previously sorbed CECs can desorb, causing an increase in concentration. Furthermore, instrumental errors can result in small negative removal percentages (Verlicchi et al., 2012).

Table 5-2: NWRF CEC Removal Percentages

	Prelim. Treat. Effl.	Prim. Clar. Effl.	PFR Effl.	Sec. Clar. Effl.	Prim. Dig. Effl.	Sec. Dig. Effl.
Compound (MTT in ng/L)	ng/L	ng/L	ng/L	ng/L	ng/L	ng/L
1,7-Dimethylxanthine	4200	3500	14	13	18	18
4-nonylphenol - semi quantitative	1200	<100	460	510	400	570
4-tert-Octylphenol	950	380	330	350	210	390
Acesulfame-K	26000	22000	1400	1400	7400	7200
Acetaminophen	26000	12000	<500	<500	<500	<500
Albuterol	17	<5	<5	<5	<5	<5
Amoxicillin	15000	15000	16000	18000	12000	11000
Atenolol (4,000)	990	200	100	90	96	<5
Atrazine	<5	<5	<5	<5	63	55
Azithromycin	290	270	270	200	140	180
Butalbital	9.4	10	10	11	<5	<5
Caffeine	45000	36000	<500	<500	<500	<500
Carbamazepine	88	110	110	110	140	200
Cotinine	940	710	48	57	240	770
DEET (200,000)	290	220	<100	<100	140	300
Diltiazem	42	34	27	24	<5	<5
Estrone (E1)	12	<5	<5	<5	<5	<5
Ethylparaben	200	<20	<20	<20	<20	<20
Gemfibrozil (800,000)	1500	1200	1500	1400	1100	1800
Iohexol	61000	44000	36000	37000	5500	370
Iopromide (750,000)		410	16	16	28	31
Lidocaine	320	<5	290	290	270	<5
Lopressor	1400	3000	960	1200	1500	1800
Meprobamate (200,000)	51	34	44	45	42	29
Methylparaben	100	<20	<20	<20	<20	<20
Metolachlor	11	11	6.9	10	81	74
Naproxen	140	170	19	<10	32	<10
Primidone		88	100	94	69	52
Propylparaben	670	180	10	<5	24	77
Salicylic Acid	750	430	<100	<100	<100	<100
Simazine	140	150	170	160	7.7	<5
Sucralose (150,000,000)	23000	4900	22000	19000	26000	23000
Sulfamethoxazole	990	1100	900	1000	32	<5
TCPP	160	<100	180	160	410	<100
Theobromine	8200	6800	<100	<100	<100	<100
Theophylline	12000	9200	<200	<200	<200	<200
Triclosan (2,100,000)	11	<10	<10	<10	<10	<10
Trimethoprim	260	310	380	440	<50	<50

In the next step, CECs were arranged and graphed according to overall plant removal percentage (Figure 5-1 to Figure 5-6). CECs that have removal percentages

greater than 90% generally are significantly (95% confidence interval (CI) of 67.2 to 100% for PFR removal percentage) removed in the PFR. CECs that have removal percentages between 50 and 90% are removed more in the primary clarifiers than in the PFR. CECs with percentage removals lower than 50% do not show any general trends. Several of these compounds increase in concentration during the treatment process, which could be due to biodegraded compound converting back to their parent compounds, desorption of previously sorbed compounds, or sampling/instrumental errors.

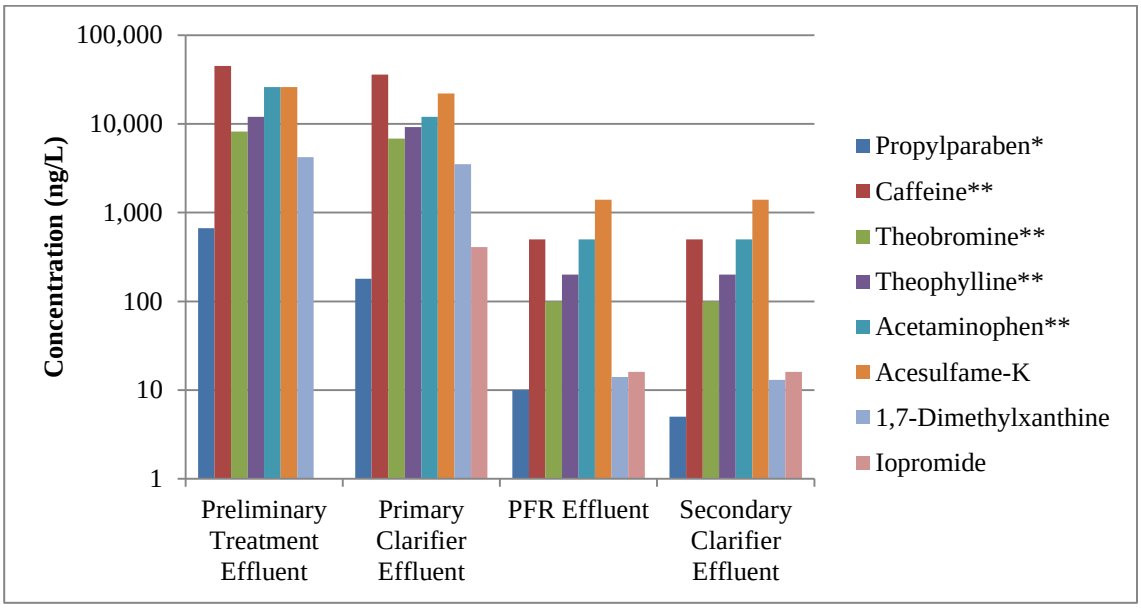

Figure 5-1: NWRF CEC Concentrations with Removal Percentage Greater than 95%

* Concentrations were below the MRL in the plant effluent.
**Concentrations were below the MRL in the PFR and plant effluents.
***Concentrations were below the MRL in the primary clarifiers, PFR, and plant effluents.

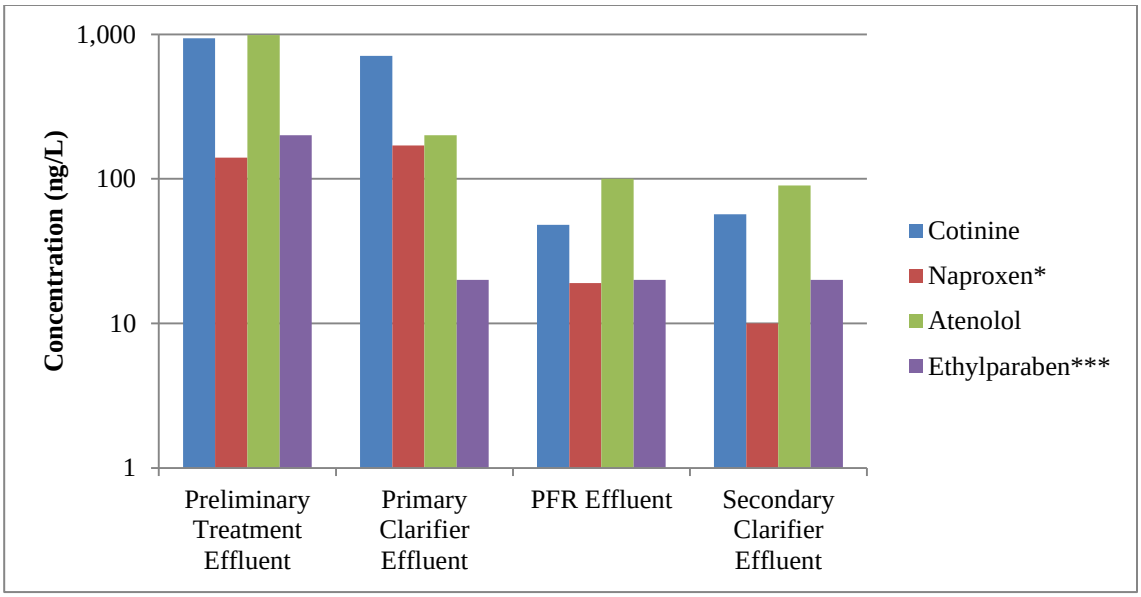

Figure 5-2: NWRF CEC Concentrations with Removal Percentage between 90 and 95%

* Concentrations were below the MRL in the plant effluent.
**Concentrations were below the MRL in the PFR and plant effluents.
***Concentrations were below the MRL in the primary clarifiers, PFR, and plant effluents.

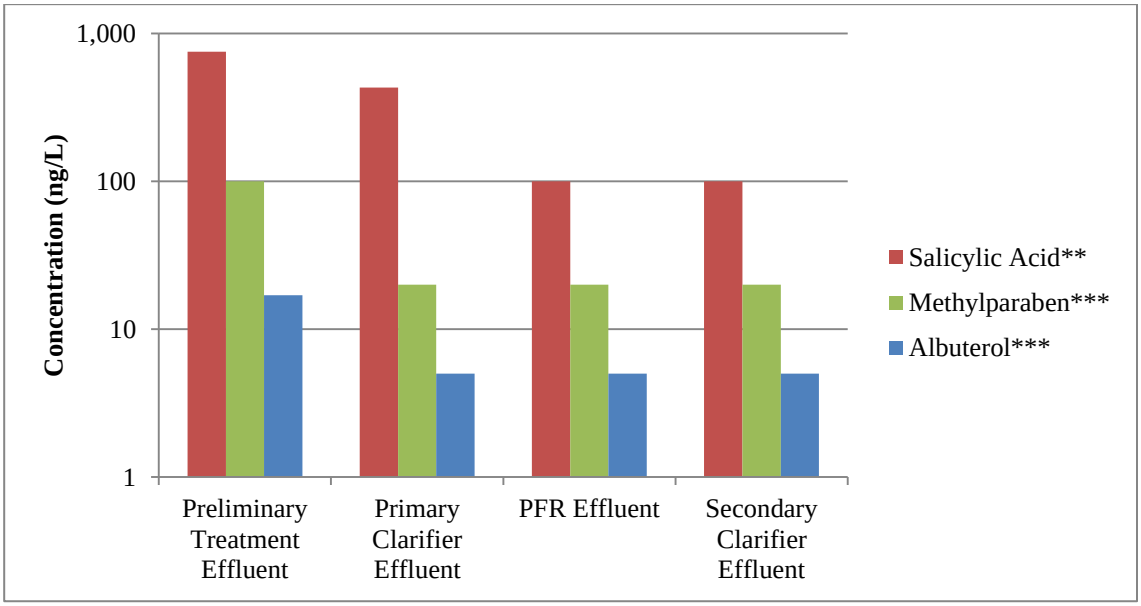

Figure 5-3: NWRF CEC Concentrations with Removal Percentage between 70 and 90%

* Concentrations were below the MRL in the plant effluent.
**Concentrations were below the MRL in the PFR and plant effluents.
***Concentrations were below the MRL in the primary clarifiers, PFR, and plant effluents.

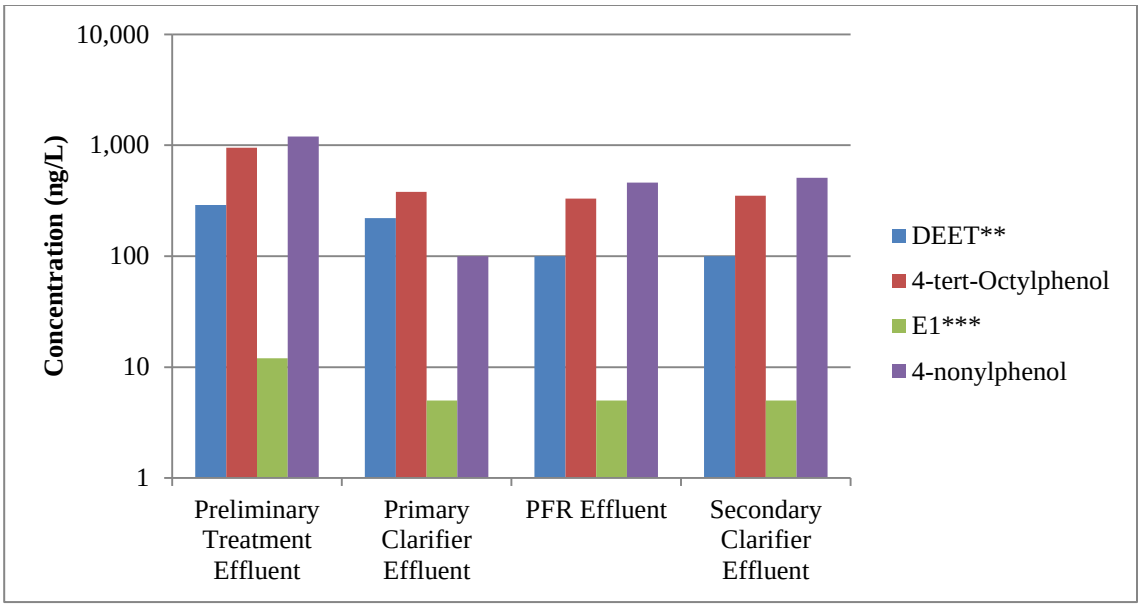

Figure 5-4: NWRF CEC Concentrations with Removal Percentage between 50 and 70%

* Concentrations were below the MRL in the plant effluent.
**Concentrations were below the MRL in the PFR and plant effluents.
***Concentrations were below the MRL in the primary clarifiers, PFR, and plant effluents.

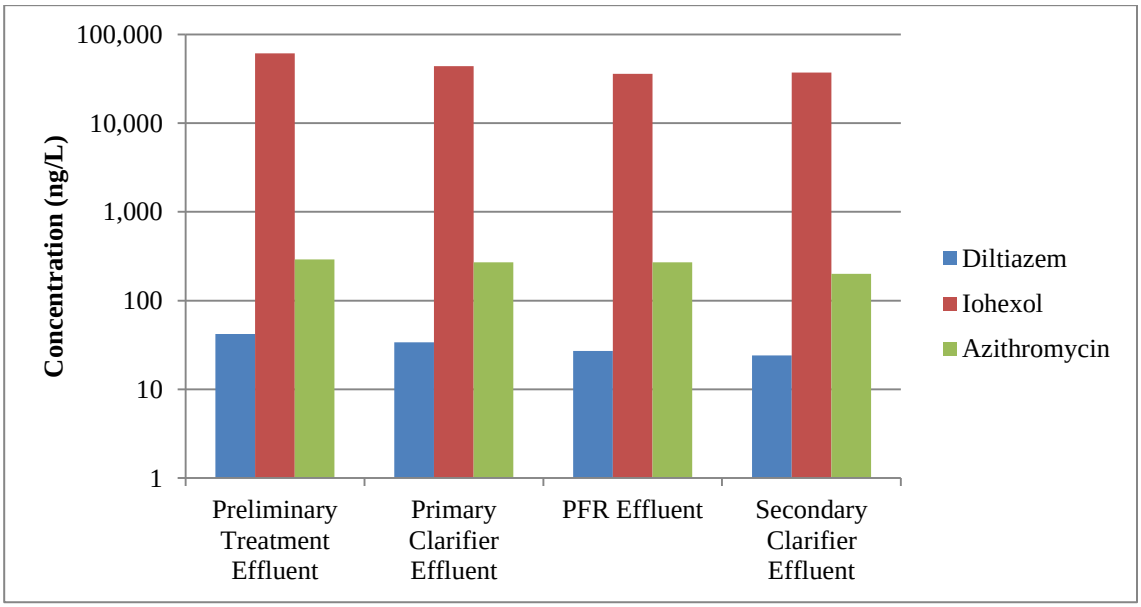

Figure 5-5: NWRF CEC Concentrations with Removal Percentage between 30 and 50%

* Concentrations were below the MRL in the plant effluent.
**Concentrations were below the MRL in the PFR and plant effluents.
***Concentrations were below the MRL in the primary clarifiers, PFR, and plant effluents.

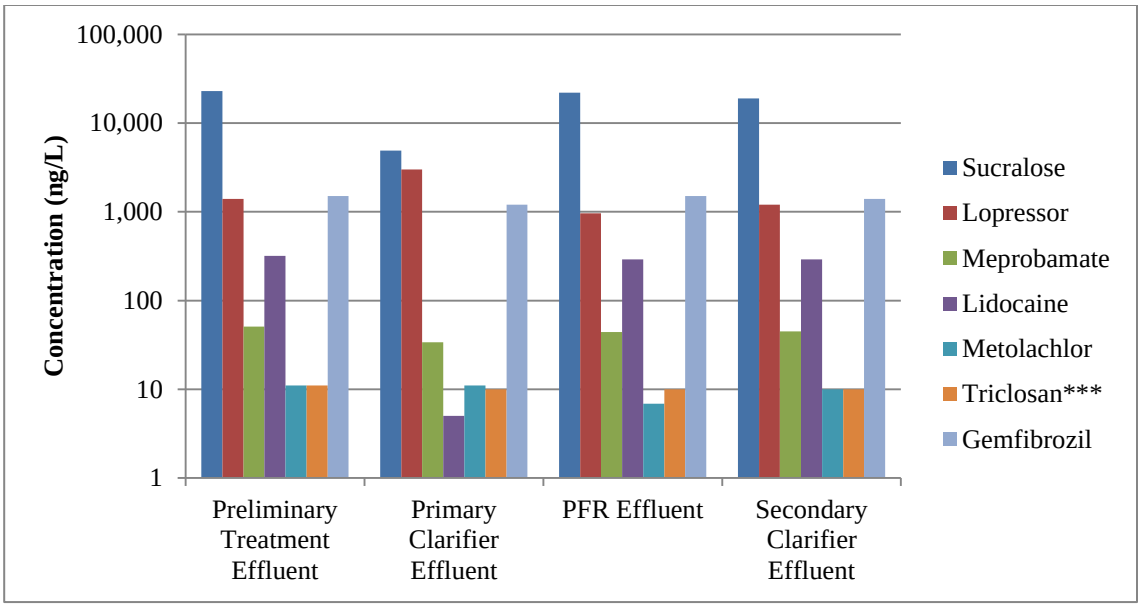

Figure 5-6: NWRF CEC Concentrations with Removal Percentage between 0 and 30%

* Concentrations were below the MRL in the plant effluent.
**Concentrations were below the MRL in the PFR and plant effluents.
***Concentrations were below the MRL in the primary clarifiers, PFR, and plant effluents.

Averages, standard deviations, and 95% CIs were calculated for each range of CECs (Table 5-3). Several removal percentage groups have only one or two CECs in the group. Because of this, some averages, standard deviations, and 95% CIs have large ranges. For CECs with concentrations below the MRL, the MRL concentrations were used in calculating the removal percentage.

Table 5-3: Statistical Analysis of NWRF CEC Removal Percentages

		Plant			Primary Clarifiers			PFR		
Plant Rem. %	**No. of CECs**	**Avg. Rem. %**	**Std. Dev.**	**95% CI**	**Avg. Rem. %**	**Std. Dev.**	**95% CI**	**Avg. Rem. %**	**Std. Dev.**	**95% CI**
90 to 100	12	95.9	3.6	93.9 - 97.9	41.4	29.7	24.6 - 58.2	83.9	29.6	67.2 - 100
80 to 90	2	83.3	4.7	76.8 - 89.8	61.3	26.4	26.4 - 97.9	38.4	54.3	-
70 to 80	1	70.6	-	-	70.6	-	-	0.0	-	-
60 to 70	2	64.3	1.7	61.9 - 66.7	42.1	25.4	6.9 - 77.3	33.9	29.3	0 - 74.5
50 to 60	2	57.9	0.6	57.1 - 58.7	75.0	23.6	42.3 - 100	-	-	-
40 to 50	1	42.9	-	-	19.0	-	-	20.6	-	-
30 to 40	2	35.2	5.9	27.0 - 43.4	17.4	14.8	0 - 37.9	9.1	12.9	-
20 to 30	0	-	-	-	-	-	-	-	-	-
10 to 20	3	14.5	2.8	10.6 - 18.4	-	-	-	-	-	-
>0 to 10	4	8.6	1.3	7.3 - 9.9	31.9	45.1	-	-	-	-

Note: Negative removal percentages are not included in average, standard deviation, or 95% CI calculations.

To narrow the scope of the research, indicator and validator CECs (Table 4-2) were isolated from other CECs and plotted in the same manner as above (Figure 5-7 to Figure 5-9). The total plant removal percentages for each CEC are shown in parentheses in the legend. Almost every CEC that is removed greater than 30% in the overall plant shows moderate removal percentage in the primary and secondary clarifiers and CECs with removal percentages greater than 90% are considerably removed in the PFR. This is expected as VSS and X_a levels are about six and twenty times larger in the PFR than in the clarifiers, respectively (Figure 5-17).

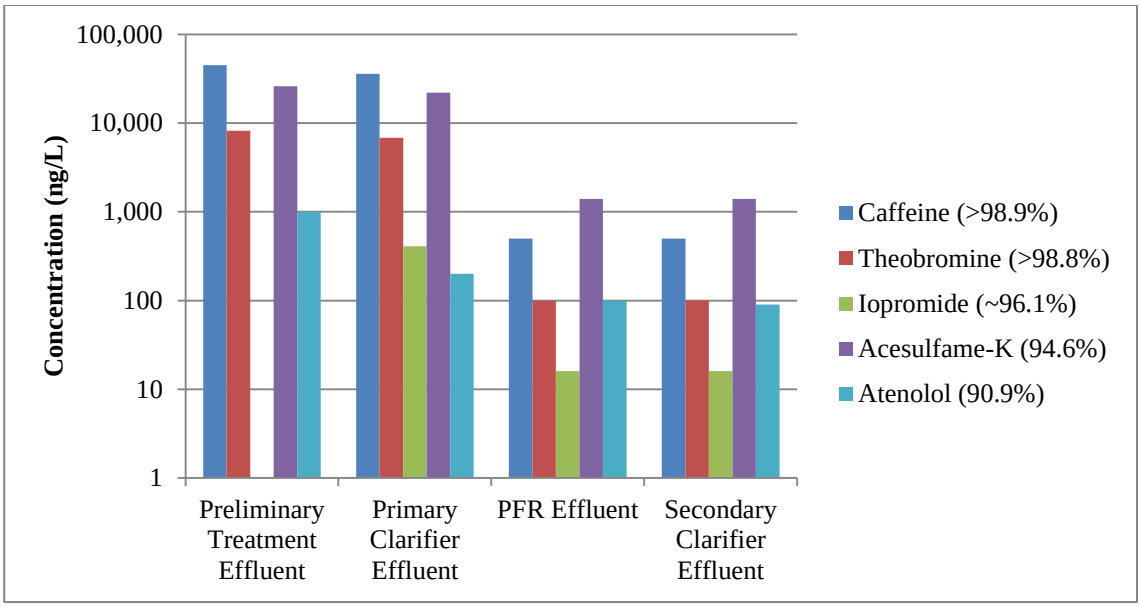

Figure 5-7: Indicator and Validator CECs with Removal Percentage Greater than 90%

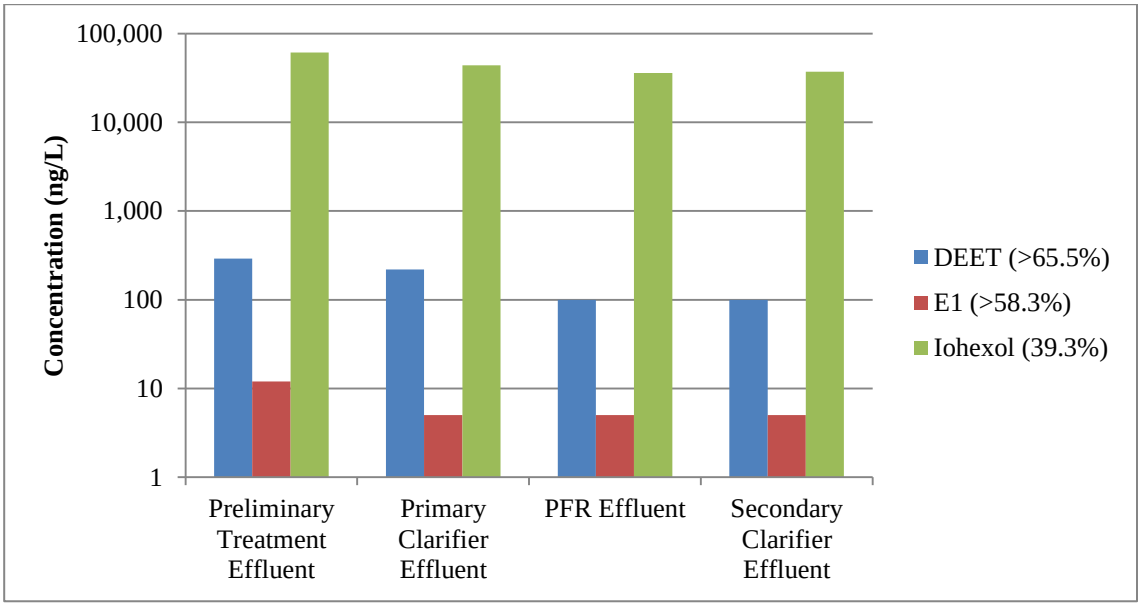

Figure 5-8: Indicator and Validator CECs with Removal Percentage between 30 and 90%

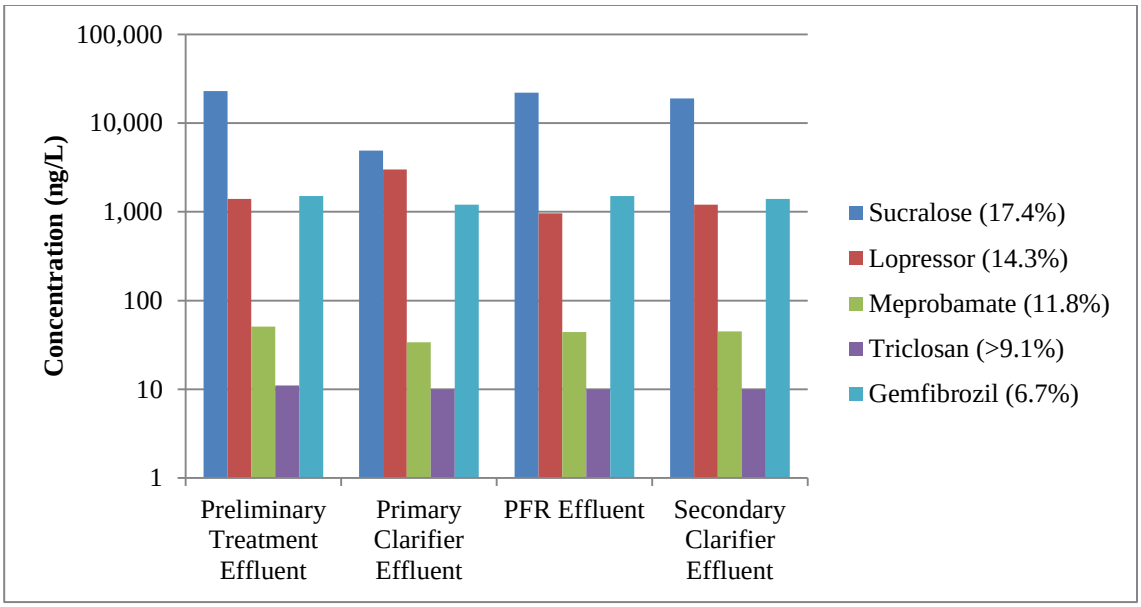

Figure 5-9: Indicator and Validator CECs with Removal Percentage between 0 and 30%

The removal percentages of each indicator CEC and its validation CEC were compared (Table 5-4). CECs with large negative removal percentages are not listed and were not included in the scope of this research. Furthermore, for CECs that have large negative removal percentages in any of the treatment processes (meprobamate, gemfibrozil, and sucralose); only the unit that had a positive removal percentage was calibrated in the model. As mentioned, these negative removal percentages can be attributed to a lack of multiple data sets or CECs converting back to their parent compounds (Jelić et al., 2012) or desorption of the compound (Verlicchi et al., 2012). Due to the complexity that this phenomenon would add to the model, these CECs were instead calibrated for the treatment process that showed positive removal percentages.

Due to budgetary constraints, CEC sampling was only done on one day (January 27, 2016). Consequently, the enhanced model was calibrated (CEC biodegradation and

adsorption constants were adjusted) using the average influent data for the month of January, 2016 (Table 5-5).

Table 5-4: Removal Percentages of Indicator and Validator CECs

		Removal Percentage				
		Prim. Clar.	PFR	Sec. Clar.	Plant	Sec. Dig.
Compound	**Class**	%	%	%	%	%
Meprobamate	Anti-Anxiety Indicator	33.3	-29.4	-2.3	11.8	31.0
Triclosan	Antibacterial Indicator	>9.1			>9.1	
Atenolol	Beta Blocker Indicator	79.8	50.0	10.0	90.9	100.0
E1	Hormone Validator	>58.3			>58.3	
Gemfibrozil	Lipid Regulator Indicator	20.0	-25.0	6.7	6.7	-63.6
DEET	Repellant Indicator	24.1	>54.5		>65.5	-114.3
Caffeine	Stimulant Indicator	20.0	>98.6		>98.9	
Theobromine	Caffeine Degradate Validator	17.1	>98.5		>98.8	
Sucralose	Sugar Substitute Indicator	78.7	-349.0	13.6	17.4	11.5
Acesulfame-K	Sugar Substitute Validator	15.4	93.6	0.0	94.6	2.7
Iopromide	X-Ray Contrast Agent Indicator		96.1	0.0		-10.7
Iohexol	X-Ray Contrast Agent Validator	27.9	18.2	-2.8	39.3	93.3

Table 5-5: Average Influent Conditions for January 2016

Influent Parameters	
Temperature	17.1°C
Influent Flow (split)	4.985 MGD
pH	7.44
TSS	161 mg/L
$cBOD_5$	263 mg/L
Ammonia	20.7 mg/L
DO	0.6 mg/L

5.2 Base Model

Preliminary steps of this research included the development, calibration, and validation of the base model. As mentioned, due to the size of the NWRF, the plant had to be divided in half (Table 4-1 and Figure 5-10).

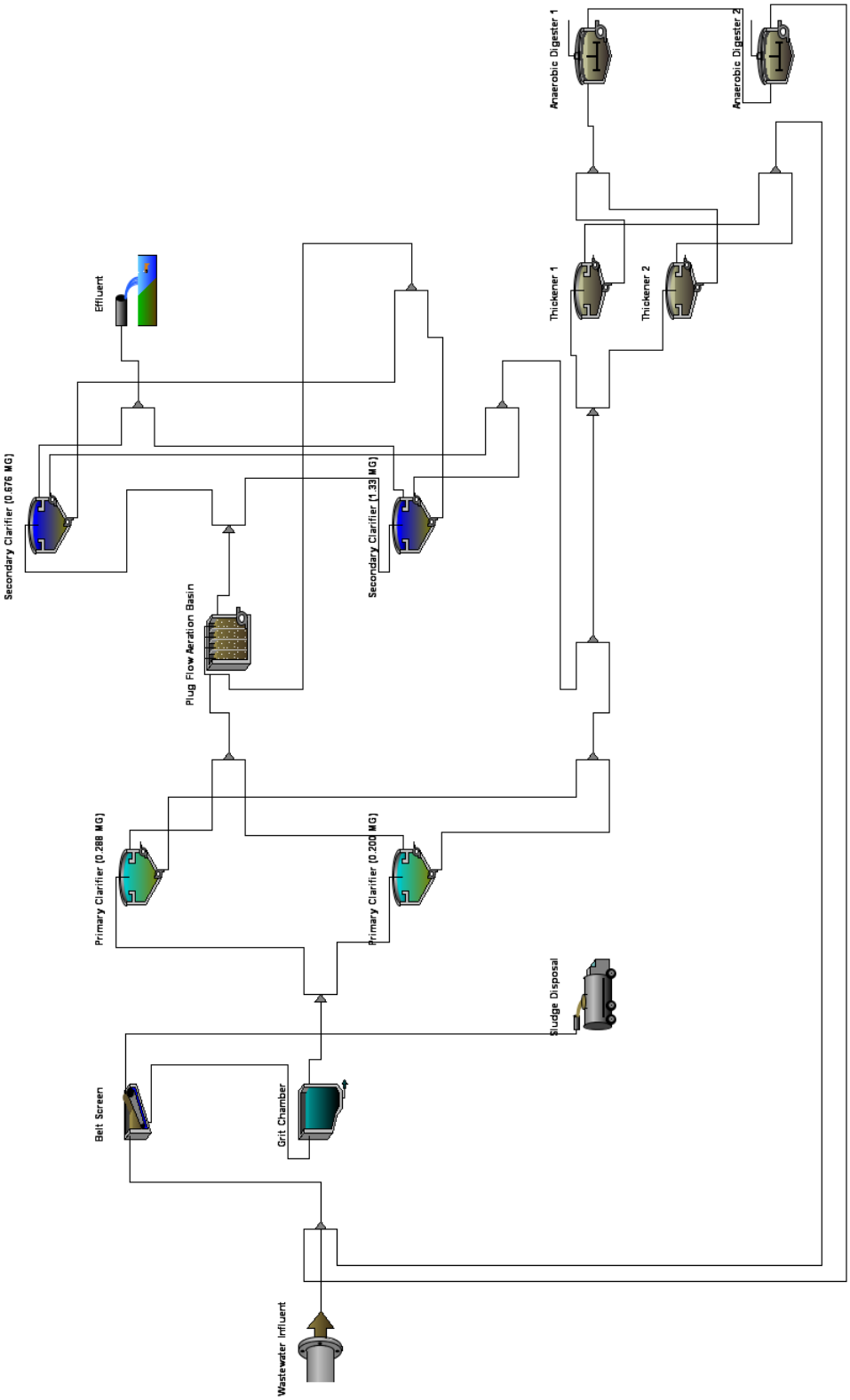

Figure 5-10: GPS-X Base Model Layout

In the GPS-X model, the influent passes through a bar screen and grit chamber before it is split to the two primary clarifiers (60% to the 0.288 million gallon (MG) clarifier and 40% to the 0.200 MG clarifier). The flow then combines into the PFR aeration basin, where it goes through three separate chambers in series. Next, the flow is split again to the secondary clarifiers (34% to the 0.676 MG clarifier and 66% to the 1.33 MG clarifier). The settled material from the primary clarifiers and some of the settled biomass, or waste activated sludge (WAS), from the secondary clarifiers are combined and split again (50%-50%) to the sludge thickeners. The remaining settled biomass, or return activated sludge (RAS), is recycled to the influent of the PFR. The secondary clarifier effluent is combined and released from the WWTP. From the thickeners, the thickened sludge goes through the two anaerobic digesters in series. The residual water from the thickeners and digesters is brought back to the front of the plant upstream of the belt screen.

5.2.1 Base Model Calibration

After the base model was developed, it was calibrated using daily NWRF cBOD, TSS, and ammonia data for the entire year of 2013. To analyze the accuracy of the model, measured and modeled concentrations of these three constituents, along with the 30-day moving average of the measured data, were plotted together (Figure 5-11 to Figure 5-13). The residual sum of squares (RSS) (Equation 5.1) and explained sum of squares (ESS) (Equation 5.1) were calculated for each constituent over the entire year and are displayed in the figures.

$$RSS = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$ **Equation 5.1**

where

n is the number of number of observations

y_i is the measured constituent concentration at day *i*, and

$\hat{y}_i$ is the modeled constituent concentration at day *i*.

$$ESS = \sum_{i=1}^{n} (\hat{y}_i - \bar{y})^2$$ **Equation 5.2**

where

$\bar{y}$ is the mean of the measured constituent concentration.

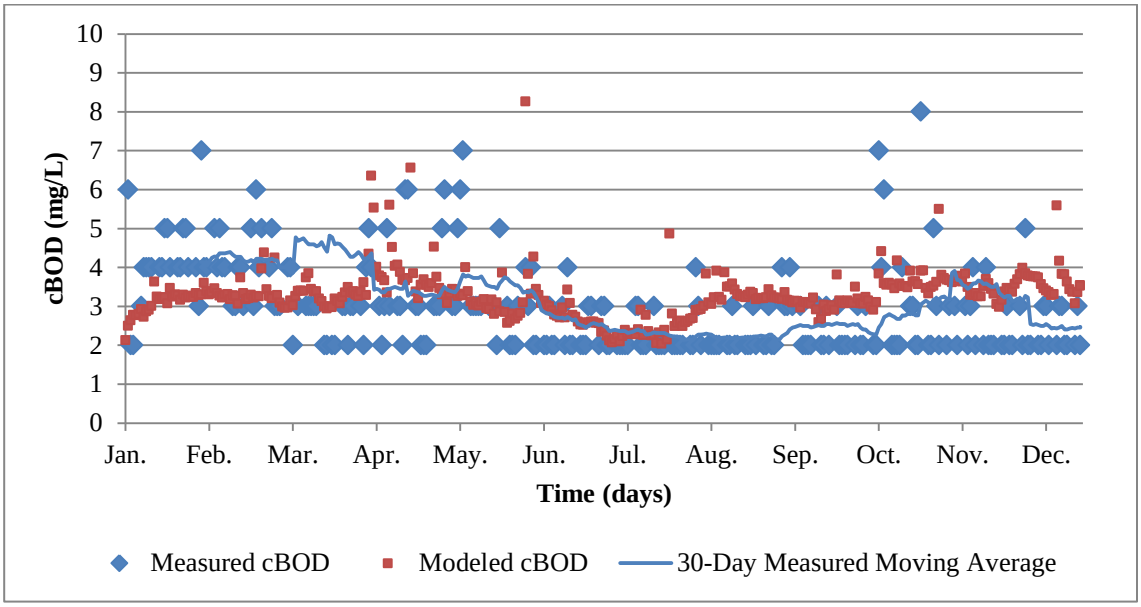

Figure 5-11: 2013 Measured and Modeled Effluent cBOD (RSS=1145.9 and ESS=153.5)

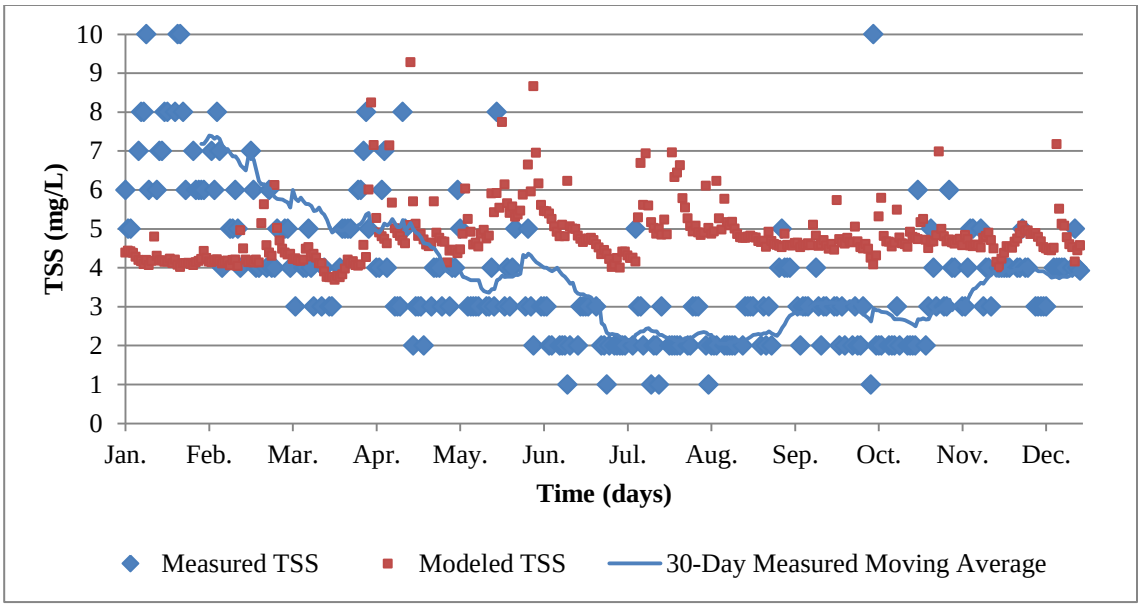

Figure 5-12: 2013 Measured and Modeled Effluent TSS (RSS=1724.4 and ESS=613.8)

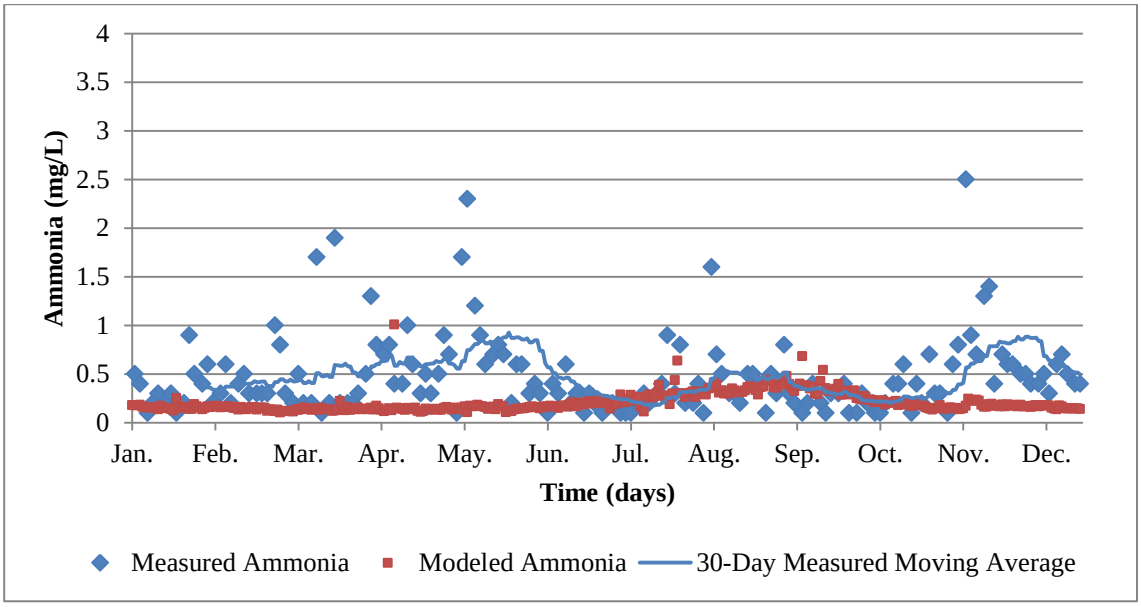

Figure 5-13: 2013 Measured and Modeled Effluent Ammonia (RSS=40.3 and ESS=29.7)

Modeled TSS is higher than measured TSS in the warmer months (Figure 5-12). Conversely, in 2012 data (the validator year), modeled TSS is lower than measured TSS in these months. However, adjusting settling characteristics to account for this resulted

in either the calibrated year *or* validated year showing accurate results, but not both. The same can be said for adjusting Arrhenius coefficients for cBOD and ammonia.

During calibration, because of a lack of data, several RAS and secondary clarifier WAS rates were analyzed. As expected, both parameters proved to have a significant influence on cBOD and TSS concentrations. After analyzing various RAS and WAS flows and slightly adjusting other model parameters (influent BOD and nutrient ratios, PFR ratios and stoichiometry, and settling characteristics), a RAS of 70% and secondary clarifier WAS of 4% of the total influent flow were found to result in the lowest combined RSS (cBOD=1145.9; TSS=1724.4; and ammonia=40.3) for all three constituents in the calibration year.

5.2.2 Base Model Validation

After adjustments were made for the base model calibration, the same parameters were used for base model validation. Although measured data from the validation year (2012) varied significantly, the modeled data generally provided reasonable results (RSS values: cBOD=1747.7; TSS=961.4; and ammonia=69.4) (Figure 5-14 to Figure 5-16). As mentioned, adjusting settling characteristics could result in the calibration year *or* validation year being more accurate, but not both. The settling characteristics used herein resulted in the lowest RSS for TSS between both calibration and validation years. Similarly, adjusting Arrhenius coefficients proved that the model could be calibrated to reduce RSS values for the calibration or validation year, but not both. Additionally, as cBOD is a function of RAS and secondary clarifier WAS rates, both could be adjusted to result in cBOD modeled data that lowered RSS.

In fact, calibration revealed that RAS and secondary clarifier WAS had the largest effect on effluent results. However, with no data to support changing these rates, 70% (RAS) and 4% (secondary clarifier WAS) were assumed. This research, as shown in *Sections 5.4.1* and *5.4.4*, analyzed plant efficiency under various RAS and WAS rates.

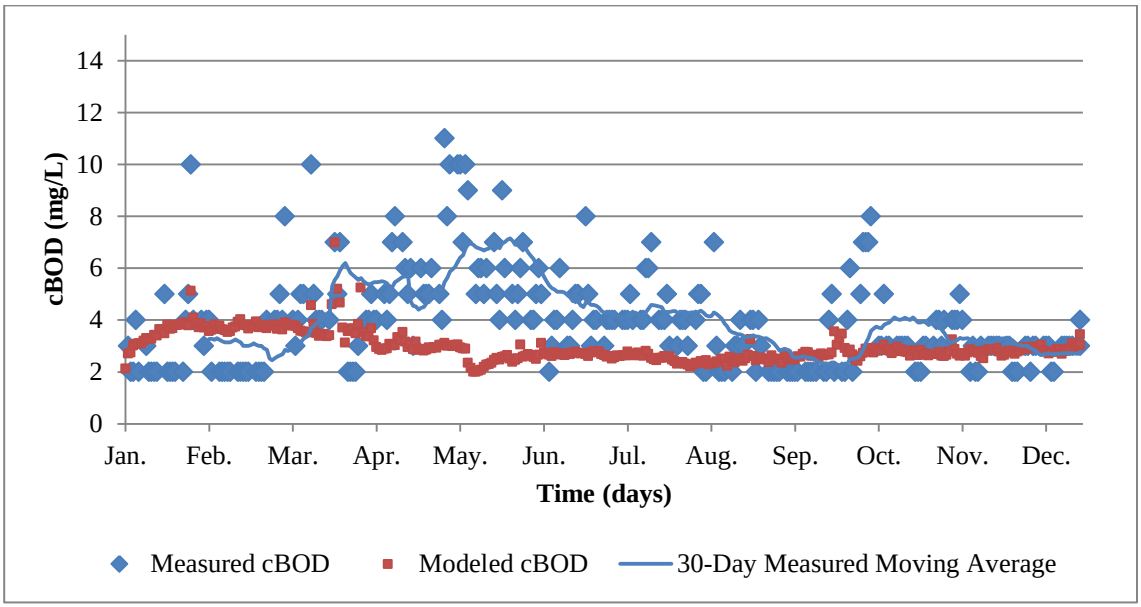

Figure 5-14: 2012 Measured and Modeled Effluent cBOD (RSS=1747.7 and ESS =500.1)

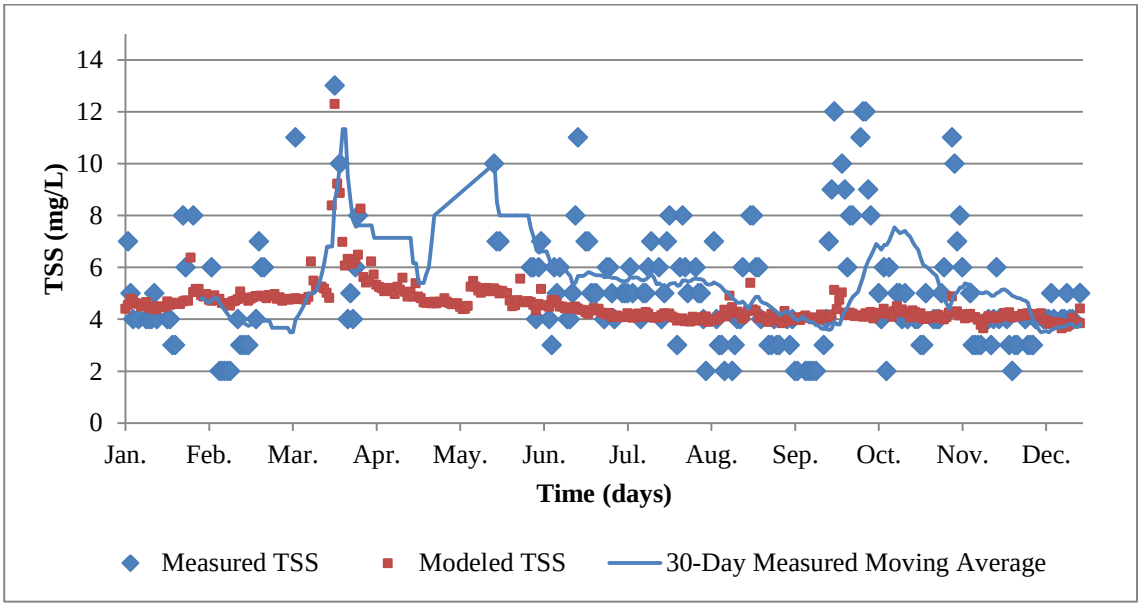

Figure 5-15: 2012 Measured and Modeled Effluent TSS (RSS=961.4 and ESS =317.7)

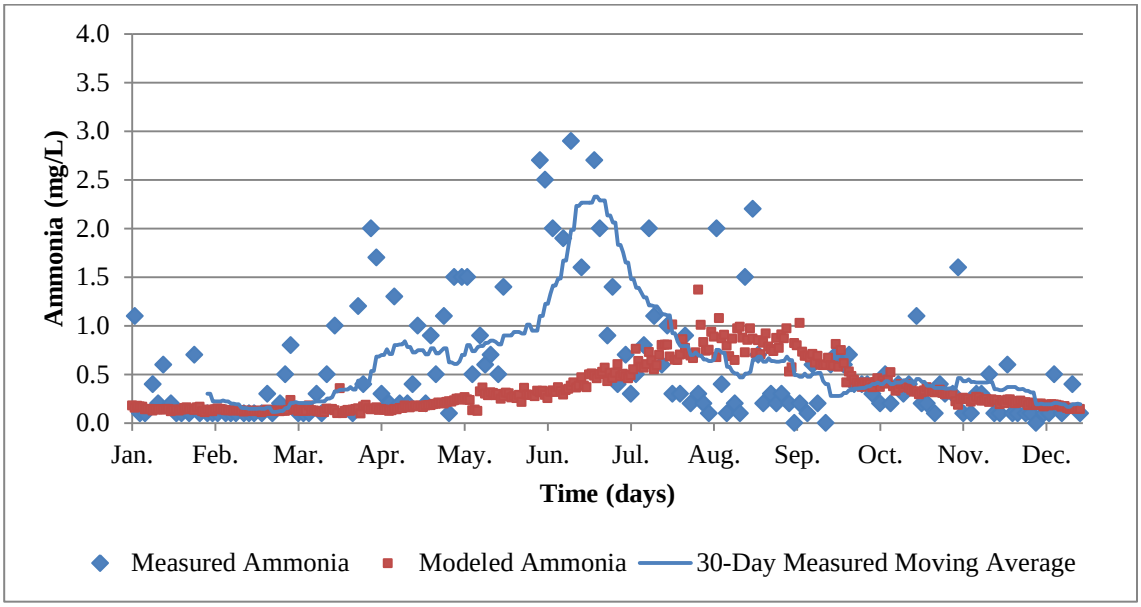

Figure 5-16: 2012 Measured and Modeled Effluent Ammonia (RSS=69.4 and ESS=40.4)

5.3 Enhanced Model

After base model calibration and validation, the MD tool was used to incorporate CECs and biodegradation and adsorption reactions and constants into the model. Because it allows for customizable state variables, the Carbon, Nitrogen, Phosphorus, Custom Components library (cnpiplib) was used. By coding some of the text files associated with this library, CEC names were entered into the model. GPS-X separates customizable state variables into soluble and particulate matter (Table 5-6).

Table 5-6: Customizable State Variables and Corresponding CECs

State Variable Name (Soluble)	Corresponding CEC (Soluble)	State Variable Name (Particulate)	Corresponding CEC (Particulate)
sza	Soluble E1	xza	Particulate E1
szb	Soluble atenolol	xzb	Particulate atenolol
szd	Soluble meprobamate	xzd	Particulate meprobamate
sze	Soluble triclosan	xze	Particulate triclosan
szf	Soluble gemfibrozil	xzf	Particulate gemfibrozil
szg	Soluble DEET	xzg	Particulate DEET
szh	Soluble caffeine	xzh	Particulate caffeine
szi	Soluble theobromine	xzi	Particulate theobromine
szj	Soluble sucralose	xzj	Particulate sucralose
szk	Soluble acesulfame-K	xzk	Particulate acesulfame-K
szl	Soluble iopromide	xzl	Particulate iopromide
szm	Soluble iohexol	xzm	Particulate iohexol

Most pharmaceuticals have solubility concentrations on the order of mg/L, while concentrations in wastewater are on the order of ng/L (Shraim et al., 2012). Therefore, plant influent CEC concentrations (before adsorption takes place) are assumed to be in the soluble form. During adsorption, the CECs move from soluble to particulate matter and, as shown in *Section 5.6*, are considerably removed during final sedimentation. Unless specifically noted as "particulate", all references to CECs in this research are meant as soluble CECs.

The next step in the model developer tool was to set up and populate the Stoichiometry Matrix (Appendix C: Stoichiometry Matrix). Then, Equation 2.2, Equation 2.3, and Equation 2.6 were modified to be entered into the Kinetic Equations section (Appendix D: Kinetic Equations and Equation 5.3 to Equation 5.5). For this case, the equations below are shown for E1 (sza). The three equations were used for every indicator and validator CEC. It should be noted that only state variables can be

used in the Kinetic Equations second. In GPS-X, VSS is a composite variable. Therefore, Equation 5.3 had to be modified to include only state variables.

$$X = k_{d_{E1}} \times sza \times VSS \qquad \textbf{Equation 5.3}$$

$$= k_{d_{E1}} \times sza \times \frac{(xs + xbh + xba + xsto + xbp + xbt + xgly + xi + xu)}{icv}$$

where

X is the sorbed CEC concentration (g/m^3)

k_{dE1} is the E1 partitioning coefficient (m^3/g)

sza is the soluble E1 concentration (g/m^3)

VSS is the volatile suspended solids concentration (g/m^3)

icv is the particulate COD to VSS ratio

xs is the slowly biodegradable substrate concentration (g/m^3)

xbh is the active heterotrophic biomass concentration (g/m^3)

xba is the active autotrophic biomass concentration (g/m^3)

xsto is the internal cell storage product concentration (g/m^3)

xbp is the active poly-phosphorus accumulating biomass concentration (g/m^3)

xbt is the polyhydroxyalkanoates concentration (g/m^3)

xgly is the stored glycogen concentration (g/m^3)

xi is the particulate inert organic material concentration (g/m^3), and

xu is the unbiodegradable particulates from cell decay concentration (g/m^3)

$$r_{des} = k_{des} \times xza$$ **Equation 5.4**

where

r_{des} is the rate of adsorption of particulate E1 ($m^3/g \cdot d$)

k_{des} is the desorption coefficient (1/d), and

xza is the particulate E1 concentration (g/m^3)

$$r_{bio} = -k_{bio_{E1}} \times sza \times xbh$$ **Equation 5.5**

where

r_{bio} is the rate of biodegradation of the CEC ($g/m^3 \cdot d$)

k_{bioE1} is the E1 biodegradation constant ($g/m^3 \cdot d$)

sza is the soluble E1 concentration (g/m^3), and

xbh is the active heterotrophic biomass concentration (g/m^3)

Next, because the biodegradation and sorption constants are not defined in the model, they were added using the Kinetic Parameters section (Appendix E: Kinetic Parameters). Here, sorption and biodegradation constants were defined and assigned values within the model.

During the enhanced model development, it was discovered that the PFR was able to handle the modified model fairly easily. However, when the same model was developed for the primary clarifiers, the model slowed significantly. For the secondary clarifiers, the model became nonresponsive. Due to the low removal percentages in the secondary clarifiers, (no indicator or validator CEC was removed more than 13.6% (Table 5-4)) they were not modeled in this research.

5.3.1 Enhanced Model Calibration and Validation

During enhanced model calibration, biodegradation was found to have a larger effect on CEC removal than adsorption. This is evidenced by the general trend of CEC biodegradation constants being larger than their partitioning constants (Table 4-2 and Table 4-3). Although VSS is greater than the active heterotrophic biomass (X_a) concentration (Figure 5-17) in each treatment process, it is not a large enough difference to offset the differences in biodegradation and adsorption constants.

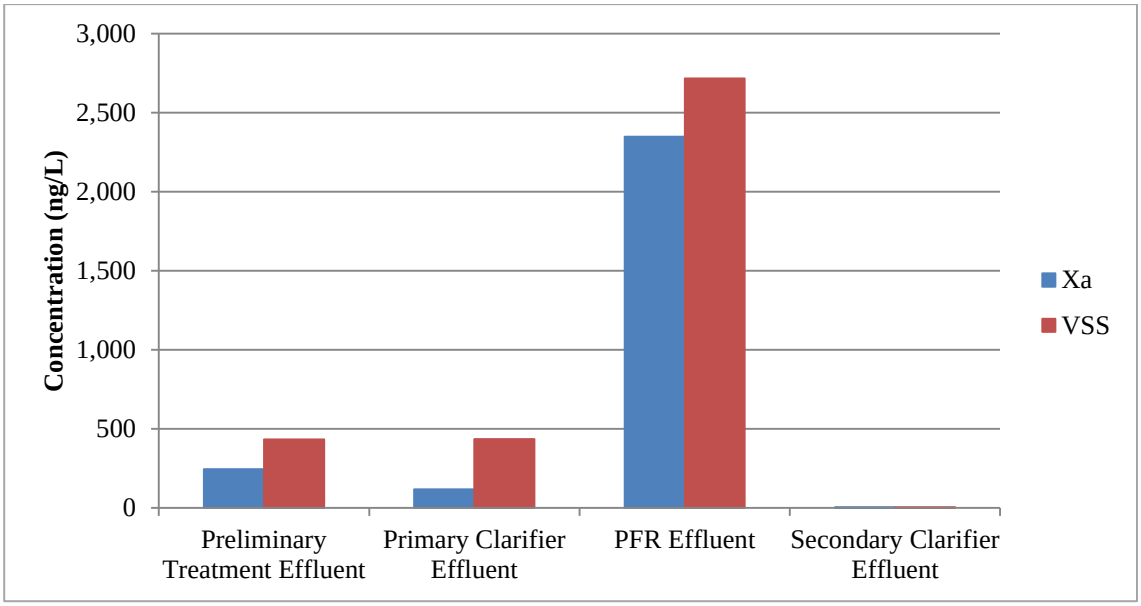

Figure 5-17: Modeled VSS and X_a Concentrations during Sampling

To calibrate the enhanced model, the biodegradation and adsorption constants were varied until modeled CEC concentrations matched measured concentrations. When possible, the constants were kept as close to literature values as possible. However, in some cases, this was not possible, as literature values resulted in effluent concentrations higher or lower than measured data (Table 5-7).

Table 5-7: Calibrated Biodegradation and Adsorption Constants

	k_{bio} (L/g-d)		K_d (L/kg)	
	Literature	**Modeled**	**Literature**	**Modeled**
Meprobamate	-	0	316.2-631.0	790.0 (Prim. Clar.)
Triclosan	1.2-3.6	1.2	1905-9550	1905.0
Atenolol	0.69-2.2	4.2	0.21-152	300.0
E1	162±25	162.0	170-362	170.0
Gemfibrozil	6.4-9.6	0.0 (Prim. Clar.)	10.0-1106	400.0 (Prim. Clar.)
DEET	-	1.5	58.9-1258.9	100.0
Caffeine	39.6-50.9	0.4 (Prim. Clar.) 40.0 (PFR)†	199.5-794.3	200.0
Theobromine	^	0.38 (Prim. Clar.) 38.0 (PFR) †	^	200.0
Sucralose	0.003-0.009	.0065 (Prim. Clar.)	66.6-1084.6	540.0 (Prim. Clar.)
Acesulfame-K	0.0448-0.0594	0.0613 (Prim. Clar.) 10.0 (PFR) †	42.5-704.3	170.0
Iopromide	1.6-2.5	7.5†	6.9-12	36.0†
Iohexol	1.8-2.4	0.8	-	0

† The calibrated constant was determined using removal efficiency rather than concentration.

As noted, PFR biodegradation constants for caffeine, theobromine, acesulfame-K, and iopromide were determined using PFR removal percentages rather than the actual concentration. Caffeine, theobromine, and acesulfame-K were removed more in the PFR than in the primary clarifiers while the influent data for iopromide was reported to be below MRL. Without developing an entirely new model for treatment processes with different biodegradation constants, there was no way to use different values for the primary clarifiers and PFR. Therefore, for caffeine, theobromine, and acesulfame-K, the model was first analyzed using primary clarifier constants. Then, k_{bio} was adjusted in a separate analysis until the modeled removal percentages closely matched the measured removal percentages. For iopromide, only one analysis was used to match the modeled PFR removal percentage with the measured PFR removal percentage.

Due to negative removal percentages in the PFR, biodegradation and adsorption constants for meprobamate, gemfibrozil, and sucralose were only determined for the

primary clarifiers. Throughout the remainder of the analyses, these three compounds are only analyzed in the primary clarifier.

Both E1 and triclosan had PFR, secondary clarifier, and effluent concentrations below the MRL. Therefore, the minimum literature biodegradation and adsorption constants that resulted in modeled effluent concentrations below the MRL were used.

The only calibration and validation CECs that perform the same throughout the NWRF are caffeine and theobromine. Because theobromine is a product of caffeine degradation (Asano et al., 1993), this is expected. Although sucralose and acesulfame-K are removed similarly in the primary clarifiers, acesulfame-K is more highly biodegraded in the PFR than sucralose. The partitioning coefficients for iohexol and iopromide are both well above each CEC's literature value. Iohexol, though, has a higher biodegradation constant than iopromide. From the constants in Table 5-7, concentrations of each CEC were plotted for each treatment process (Figure 5-18 to Figure 5-29).

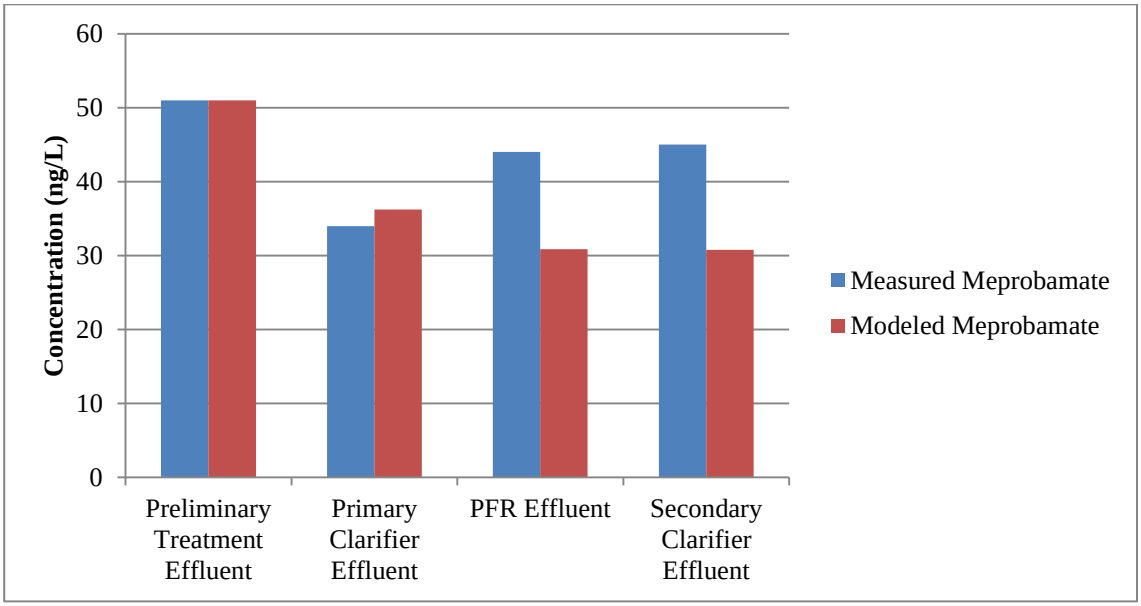

Figure 5-18: Enhanced Model Meprobamate Concentrations under Sampling Conditions

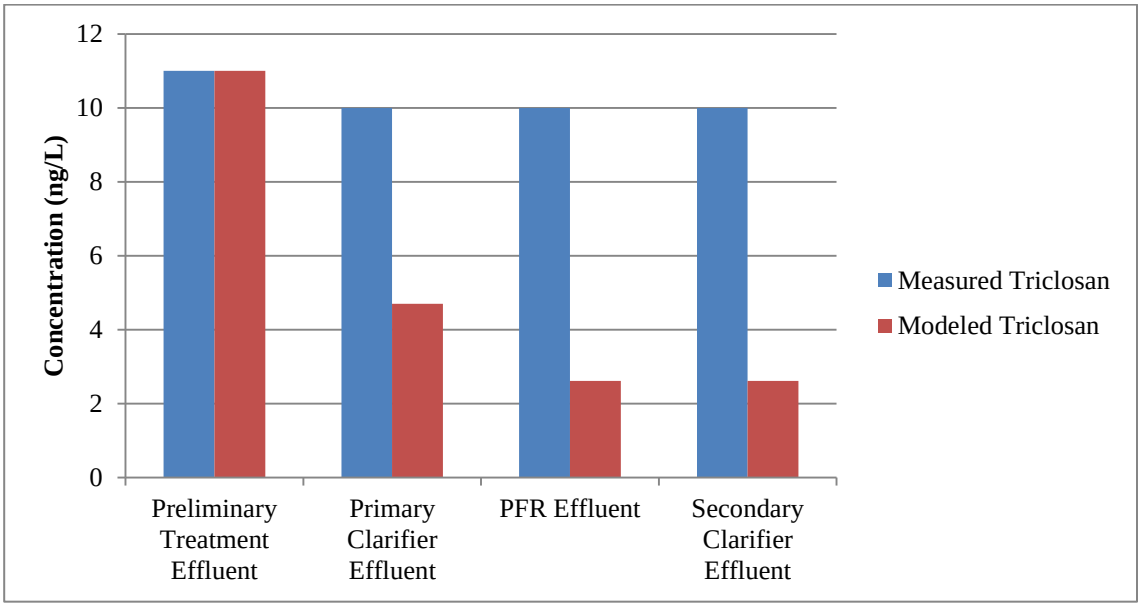

Figure 5-19: Enhanced Model Triclosan Concentrations under Sampling Conditions

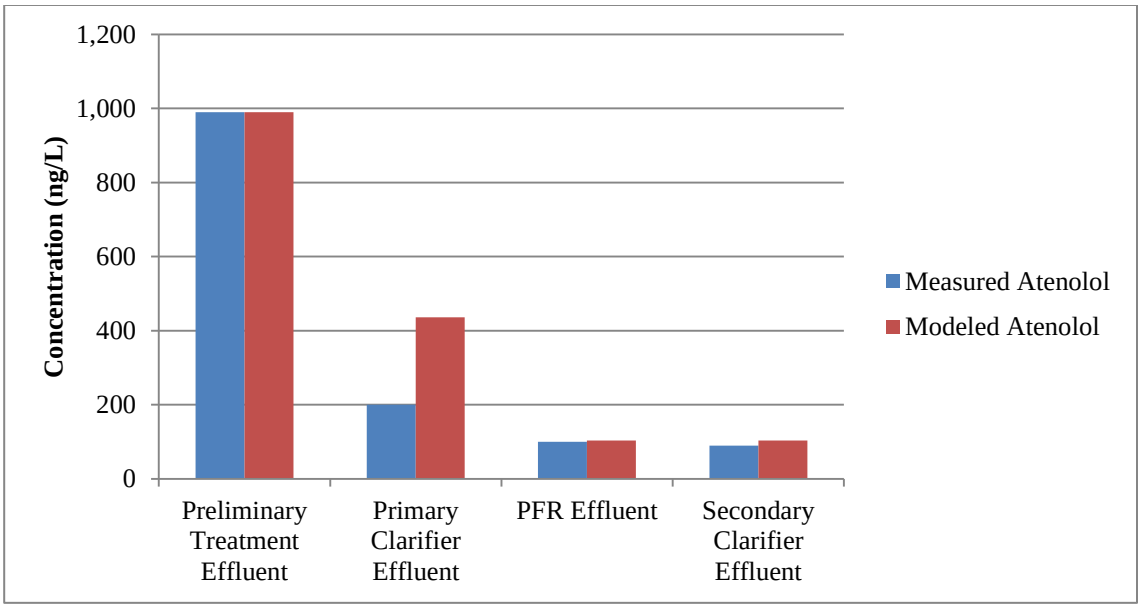

Figure 5-20: Enhanced Model Atenolol Concentrations under Sampling Conditions

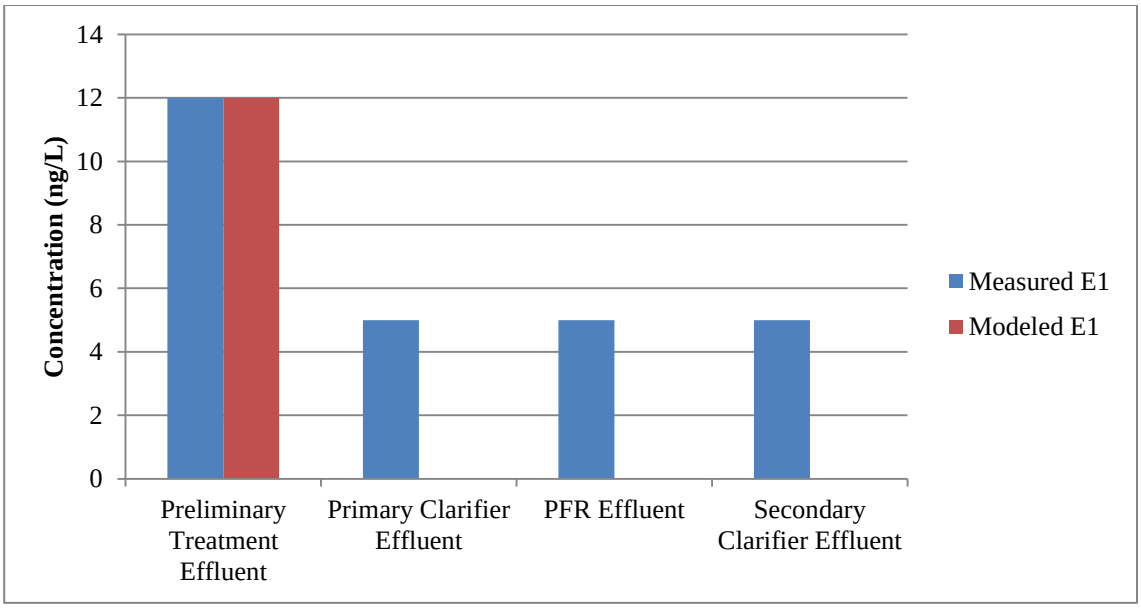

Figure 5-21: Enhanced Model E1 Concentrations under Sampling Conditions

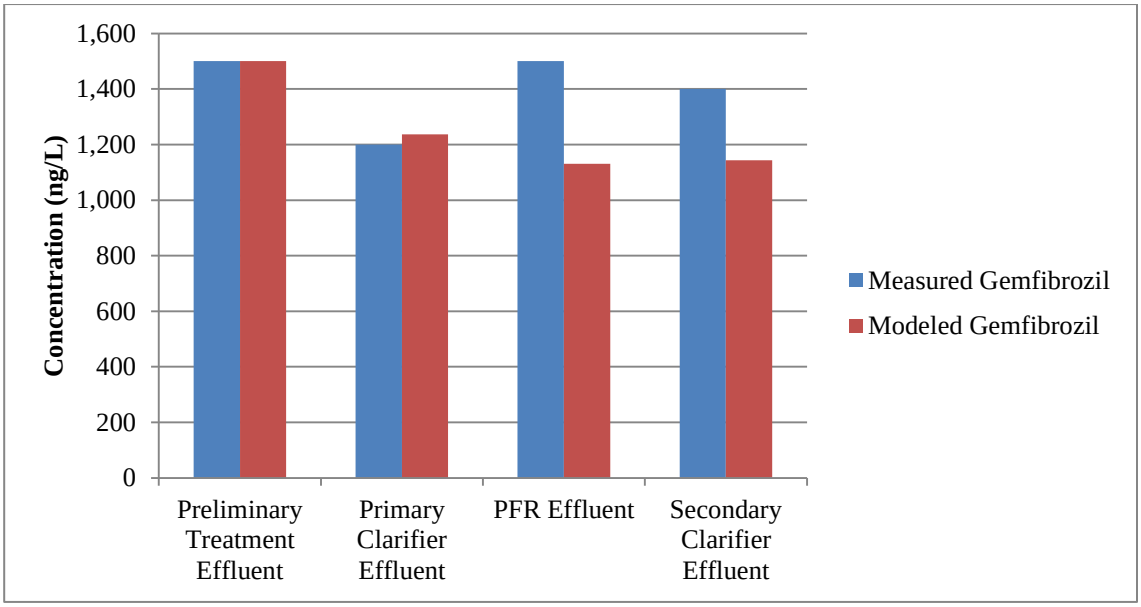

Figure 5-22: Enhanced Model Gemfibrozil Concentrations under Sampling Conditions

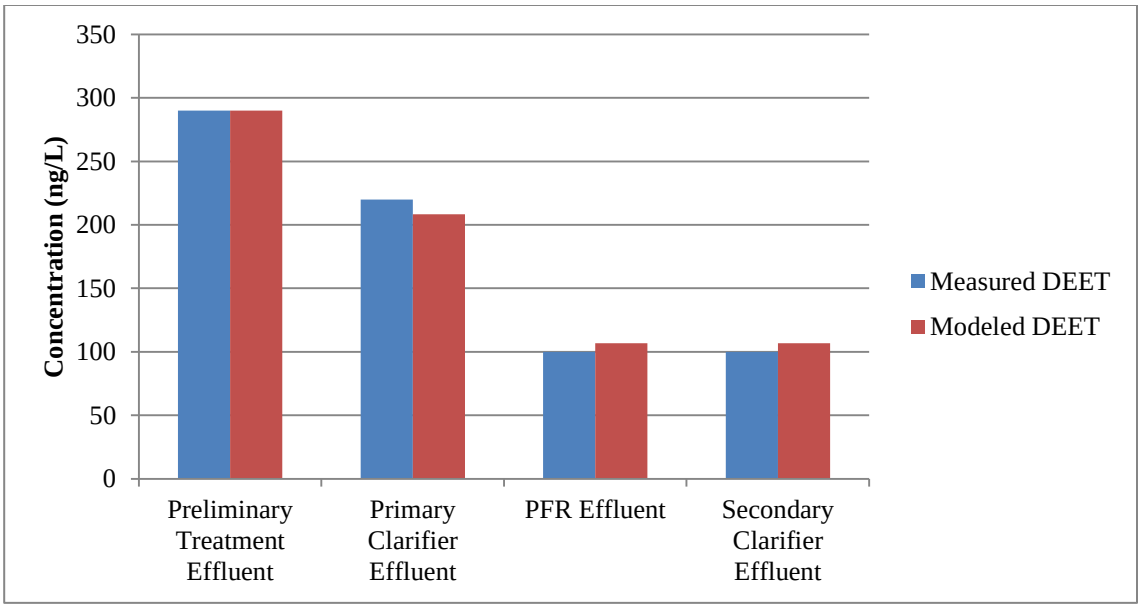

Figure 5-23: Enhanced Model DEET Concentrations under Sampling Conditions

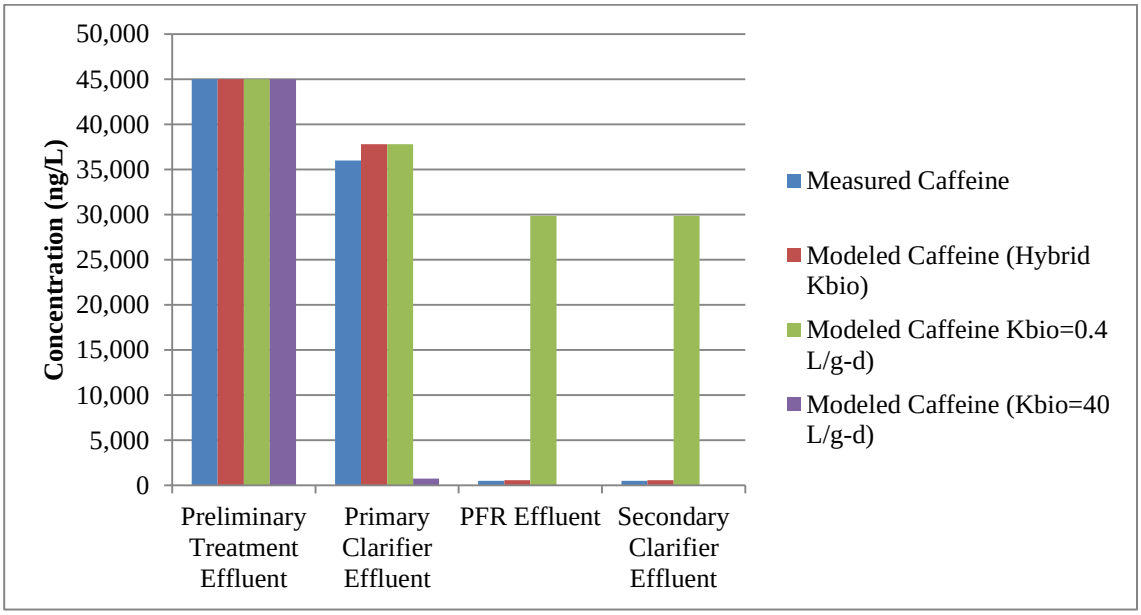

Figure 5-24: Enhanced Model Caffeine Concentrations under Sampling Conditions

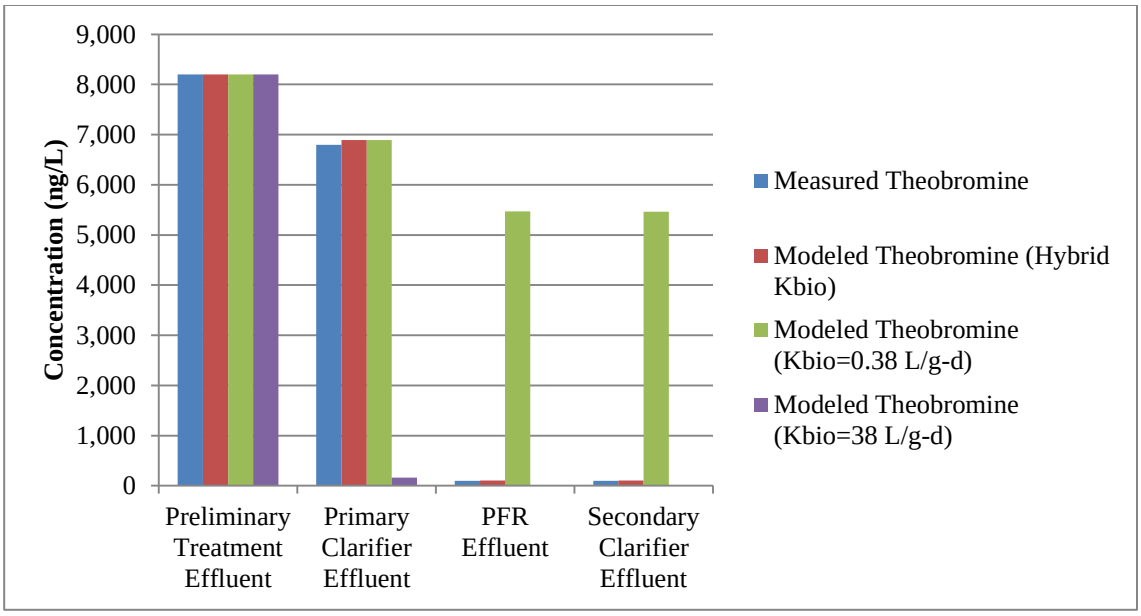

Figure 5-25: Enhanced Model Theobromine Concentrations under Sampling Conditions

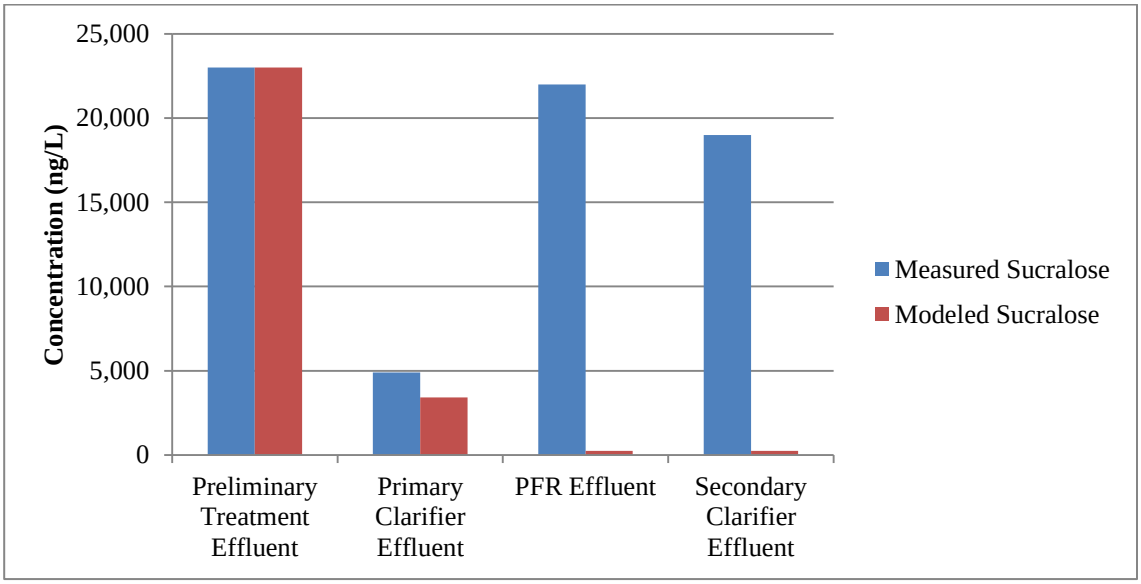

Figure 5-26: Enhanced Model Sucralose Concentrations under Sampling Conditions

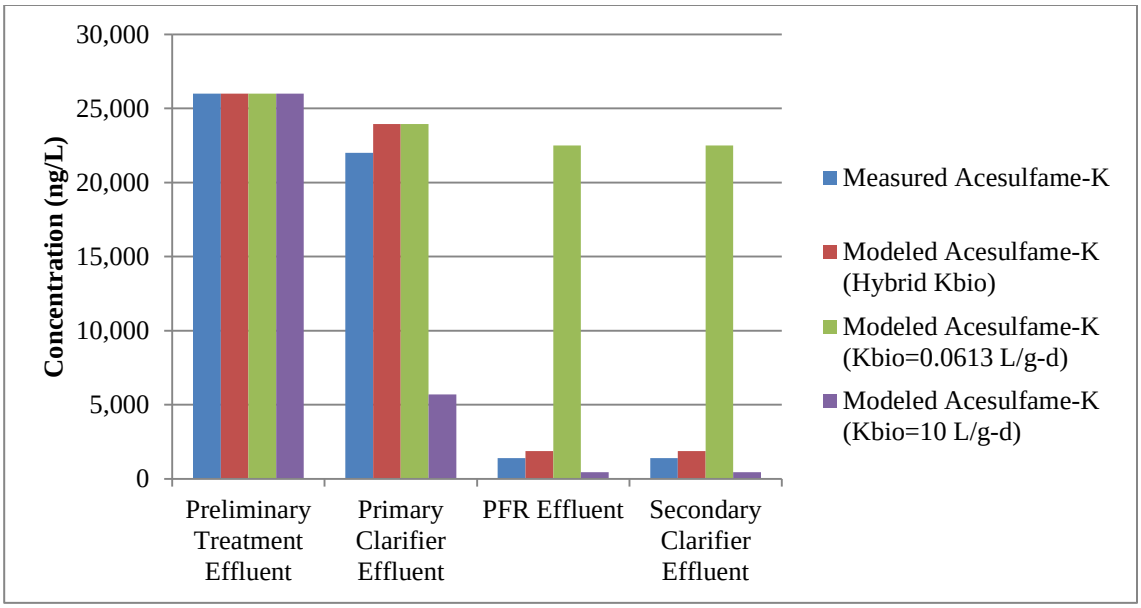

Figure 5-27: Enhanced Model Acesulfame-K Concentrations under Sampling Conditions

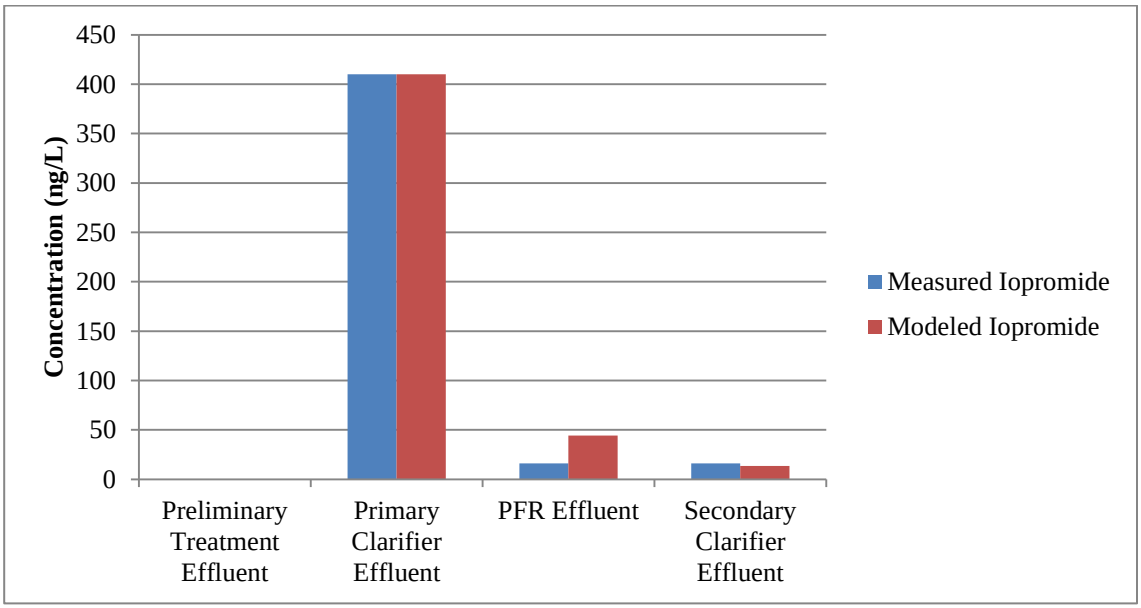

Figure 5-28: Enhanced Model Iopromide Concentrations under Sampling Conditions

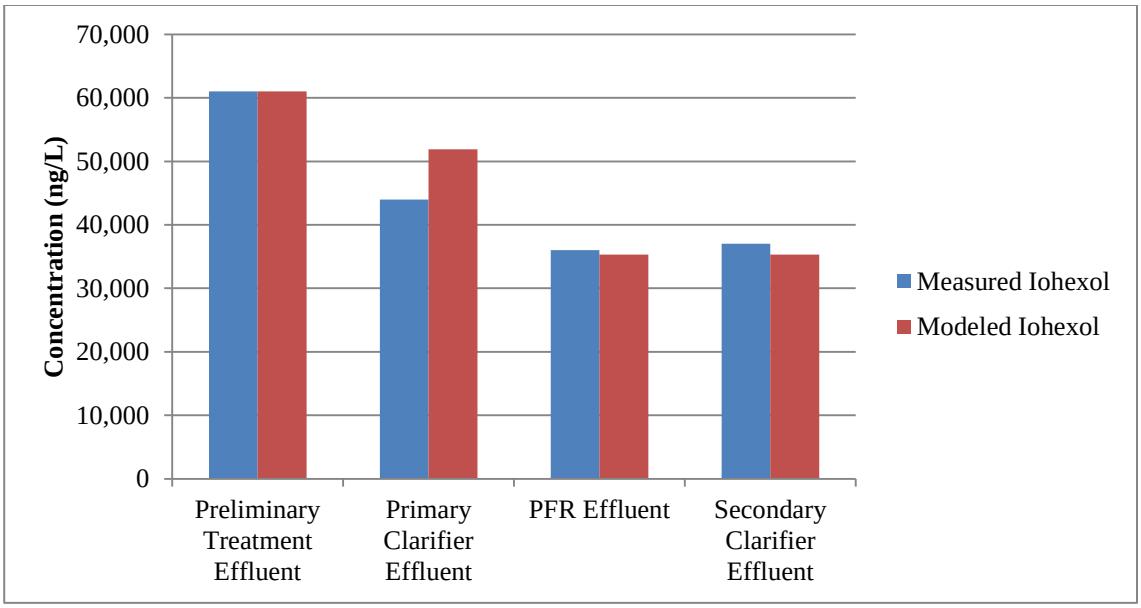

Figure 5-29: Enhanced Model Iohexol Concentrations under Sampling Conditions

Most CECs are removed predominantly by biodegradation. Generally, CECs are removed more in the PFR than in the primary clarifiers. Furthermore, CECs with higher removal percentages are more affected by biodegradation than by adsorption. While biodegradation and adsorption averages are similar in the primary clarifier, biodegradation becomes the dominant removal mechanism in the PFR (Table 5-8). The percent removed by biodegradation is calculated by dividing the concentration removed of a given CEC due to biodegradation by the total amount the CEC is removed (from biodegradation and adsorption) in each treatment process. The percent adsorption is the concentration removed due to adsorption divided by the total concentration removed.

Table 5-8: Enhanced Model Biodegradation vs. Adsorption during Sampling

CEC	Treatment Process	Percent of Total Removal		
		Biodegradation	Adsorption	Total
Meprobamate*	Primary Clarifier	0.0%	100.0%	100.0%
	PFR	0.0%	100.0%	100.0%
Triclosan	Primary Clarifier	34.4%	65.6%	100.0%
	PFR	69.5%	30.5%	100.0%
Atenolol	Primary Clarifier	90.3%	9.7%	100.0%
	PFR	98.9%	1.1%	100.0%
E1	Primary Clarifier	100.0%	0.0%	100.0%
	PFR	100.0%	0.0%	100.0%
Gemfibrozil*	Primary Clarifier	0.4%	99.6%	100.0%
	PFR	0.3%	99.7%	100.0%
DEET	Primary Clarifier	87.8%	12.2%	100.0%
	PFR	96.2%	3.8%	100.0%
Caffeine	Primary Clarifier	51.3%	48.7%	100.0%
	PFR	100.0%	0.0%	100.0%
Theobromine	Primary Clarifier	49.9%	50.1%	100.0%
	PFR	100.0%	0.0%	100.0%
Sucralose*	Primary Clarifier	0.9%	99.1%	100.0%
	PFR	1.9%	98.1%	100.0%
Acesulfame-K	Primary Clarifier	16.1%	83.9%	100.0%
	PFR	100.0%	0.0%	100.0%
Iopromide	Primary Clarifier	-	-	-
	PFR	100.0%	0.0%	100.0%
Iohexol	Primary Clarifier	100.0%	0.0%	100.0%
	PFR	100.0%	0.0%	100.0%
Average	Primary Clarifier	48.3%	51.7%	100.0%
	PFR	72.2%	27.8%	100.0%

* Modeled concentrations were used because measured concentrations showed negative removal percentages.

5.4 Expanded Model

After calibration of the enhanced model, the NWRF expansion was incorporated into the model, creating the expanded model. The only changes in the model from the current NWRF layout (Table 4-1) are the addition of an identical PFR (0.495 MG per chamber) and a secondary clarifier (1.33 MG). Because the PFR volume will increase by 100% and the final clarifier by 66%, an adjusted flowrate that is 75% greater than the most recent flowrate data is used. In keeping the other parameters constant (Table

5-5), CEC removal percentages for the expanded and enhanced model were compared (Figure 5-30 to Figure 5-41).

As mentioned, as part of the plant expansion, the NWRF will also incorporate UV disinfection as one of the last treatment processes. Unfortunately, GPS-X is unable to model UV disinfection. Like other oxidants, UV removal is largely dependent on concentration-time (or intensity-time in the case of UV) (Lee et al., 2009). In two studies, CEC removal percentage ranged from 1 to 90%, depending on the intensity-time provided by the UV lamps and the pH (Canonica et al., 2008; Kim et al., 2009).

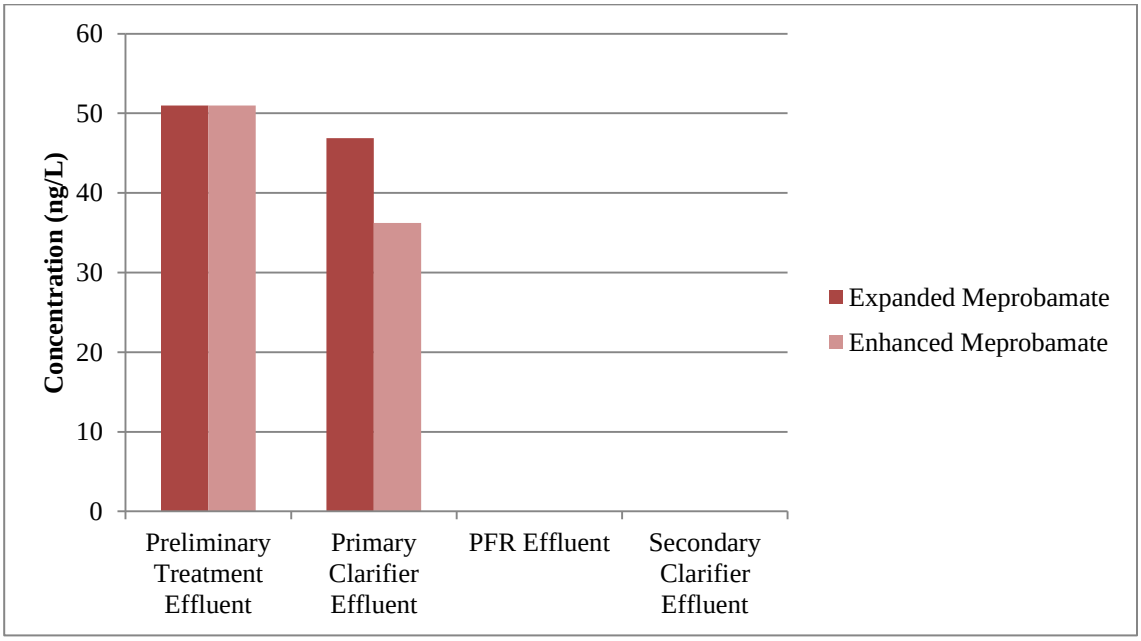

Figure 5-30: Expanded Model Meprobamate Concentrations under Sampling Conditions (Modified Flowrate)

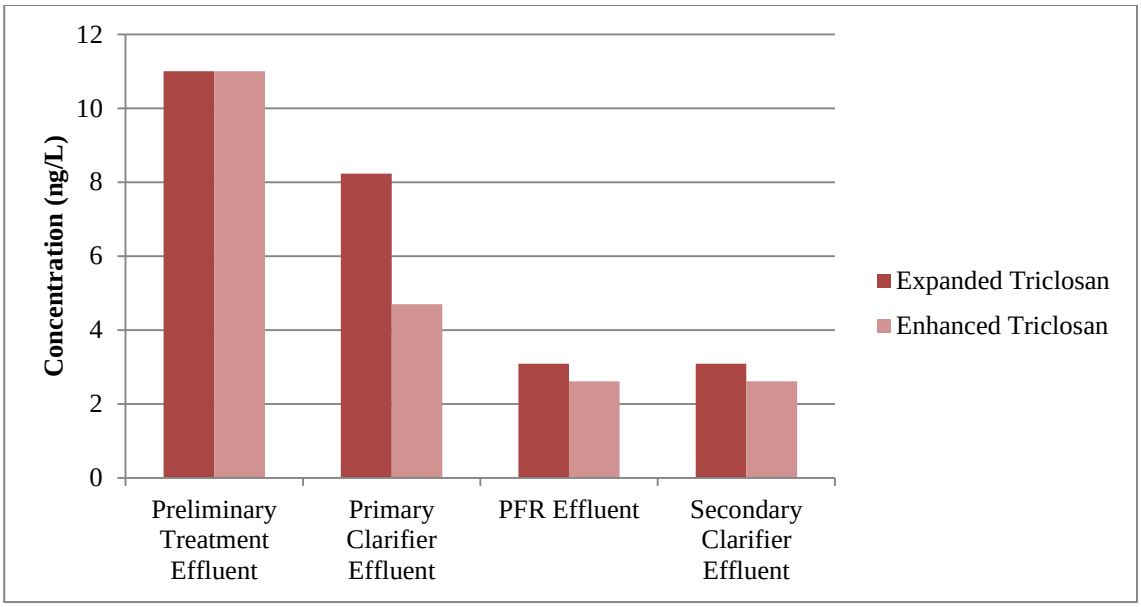

Figure 5-31: Expanded Model Meprobamate Concentrations under Sampling Conditions (Modified Flowrate)

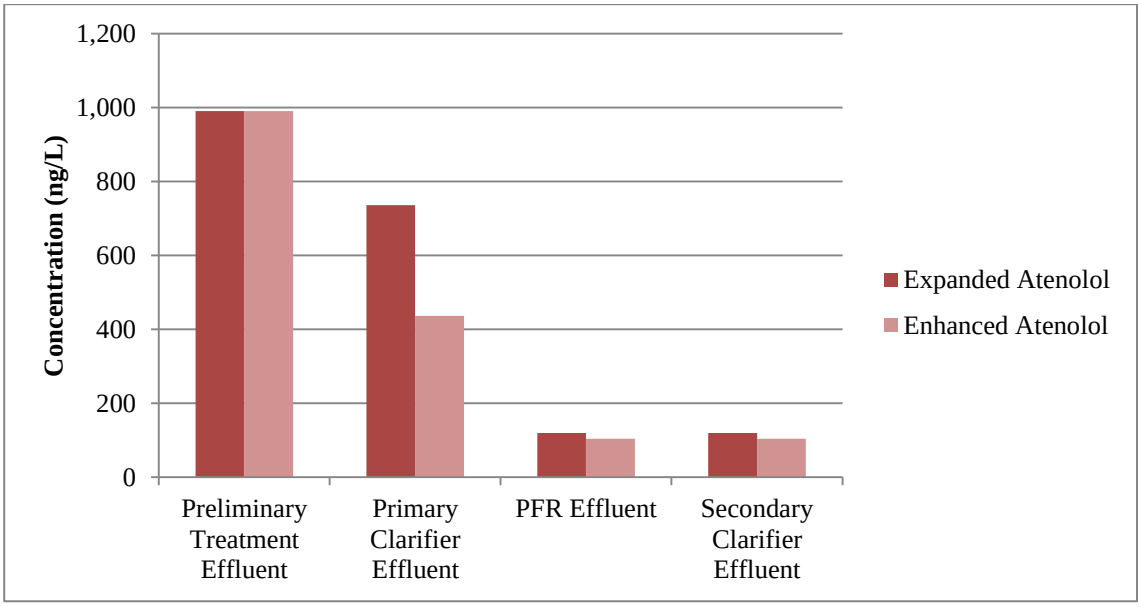

Figure 5-32: Expanded Model Atenolol Concentrations under Sampling Conditions (Modified Flowrate)

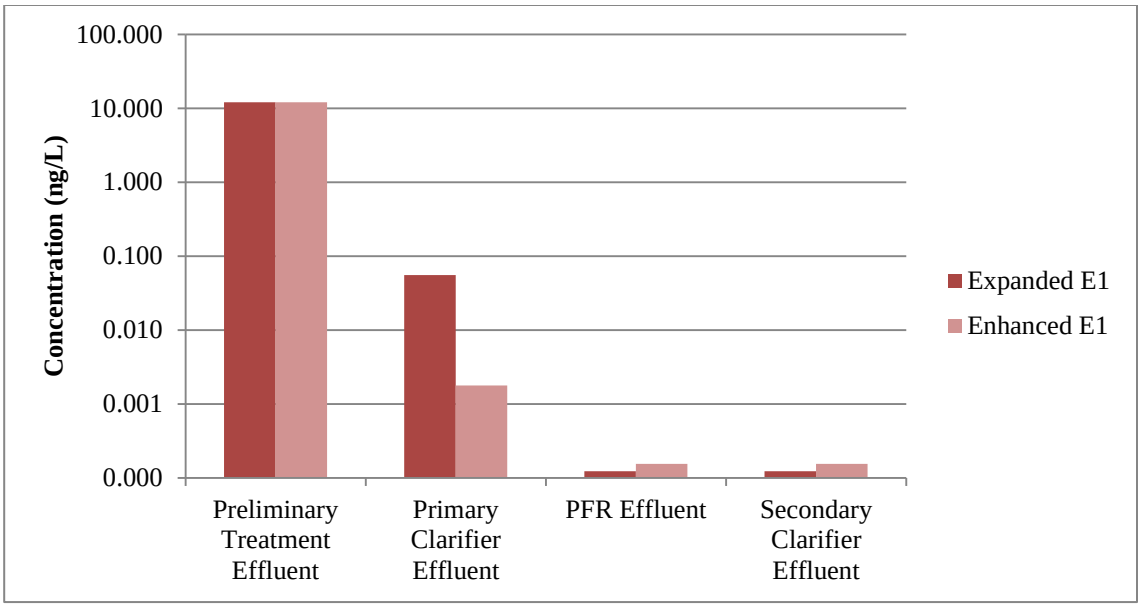

Figure 5-33: Expanded Model E1 Concentrations under Sampling Conditions (Modified Flowrate)

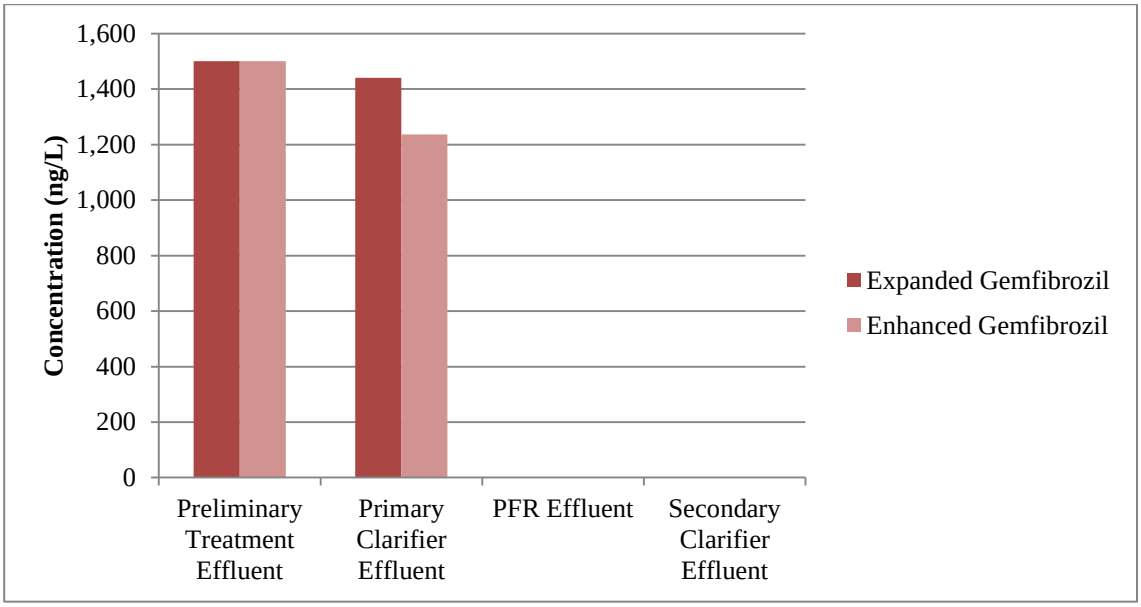

Figure 5-34: Expanded Model Gemfibrozil Concentrations under Sampling Conditions (Modified Flowrate)

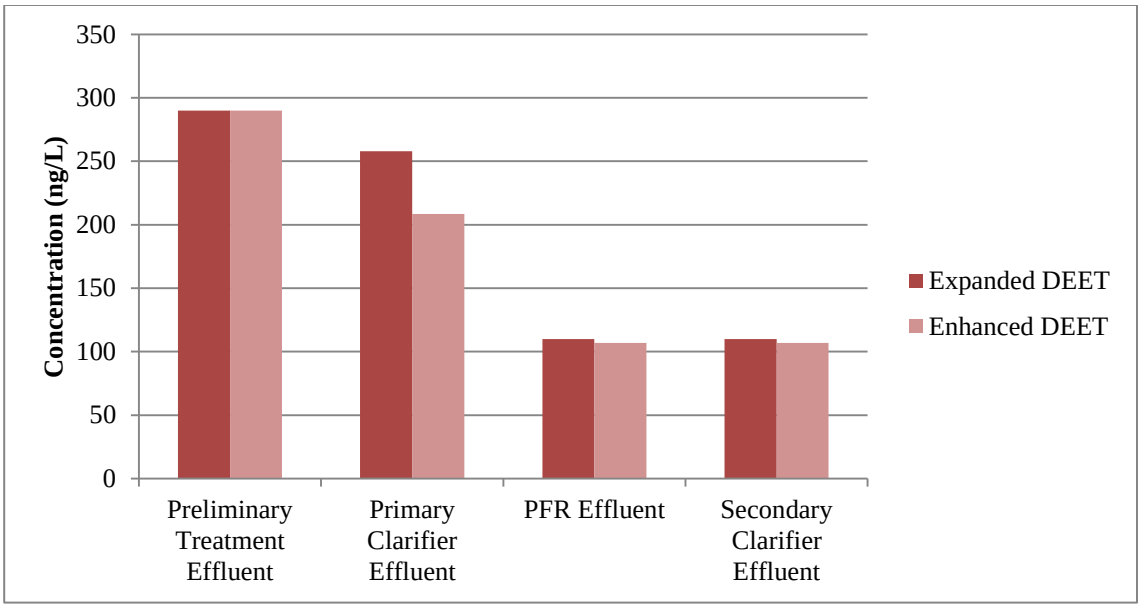

Figure 5-35: Expanded Model DEET Concentrations under Sampling Conditions (Modified Flowrate)

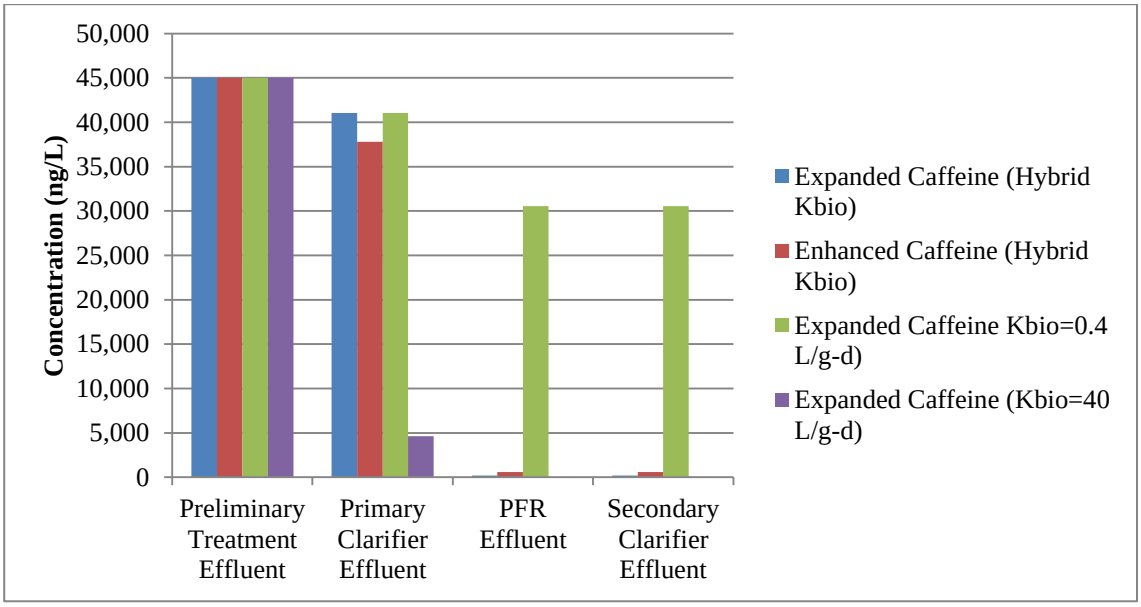

Figure 5-36: Expanded Model Caffeine Concentrations under Sampling Conditions (Modified Flowrate)

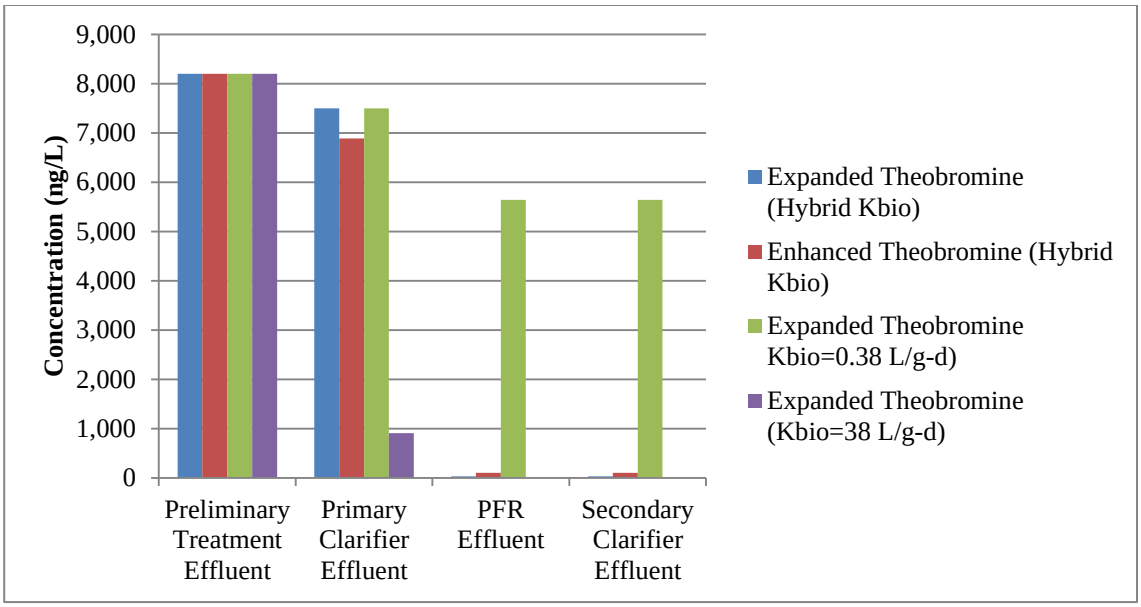

Figure 5-37: Expanded Model Theobromine Concentrations under Sampling Conditions (Modified Flowrate)

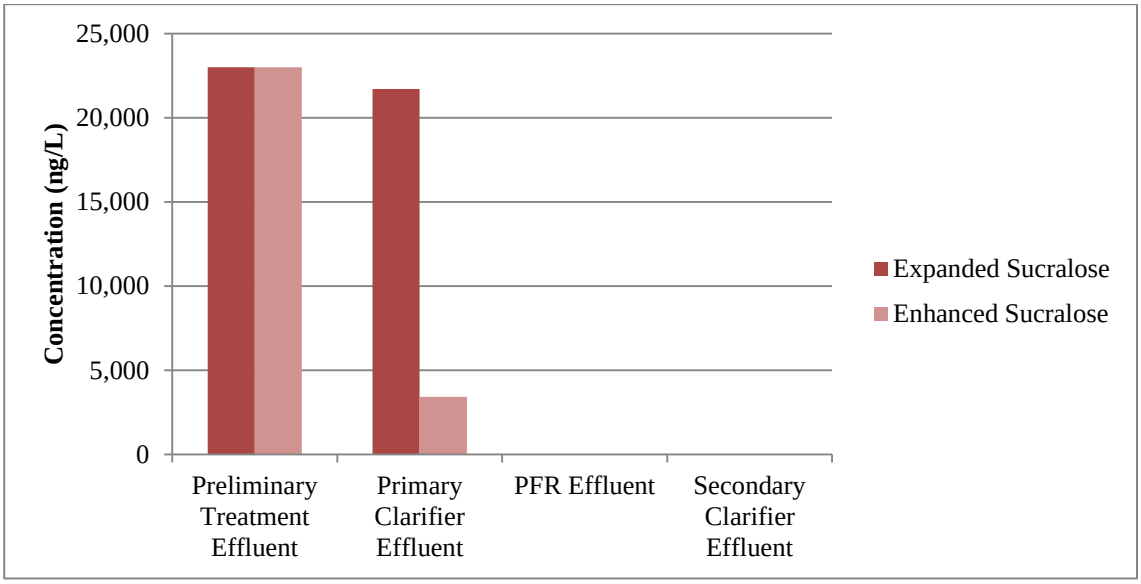

Figure 5-38: Expanded Model Sucralose Concentrations under Sampling Conditions (Modified Flowrate)

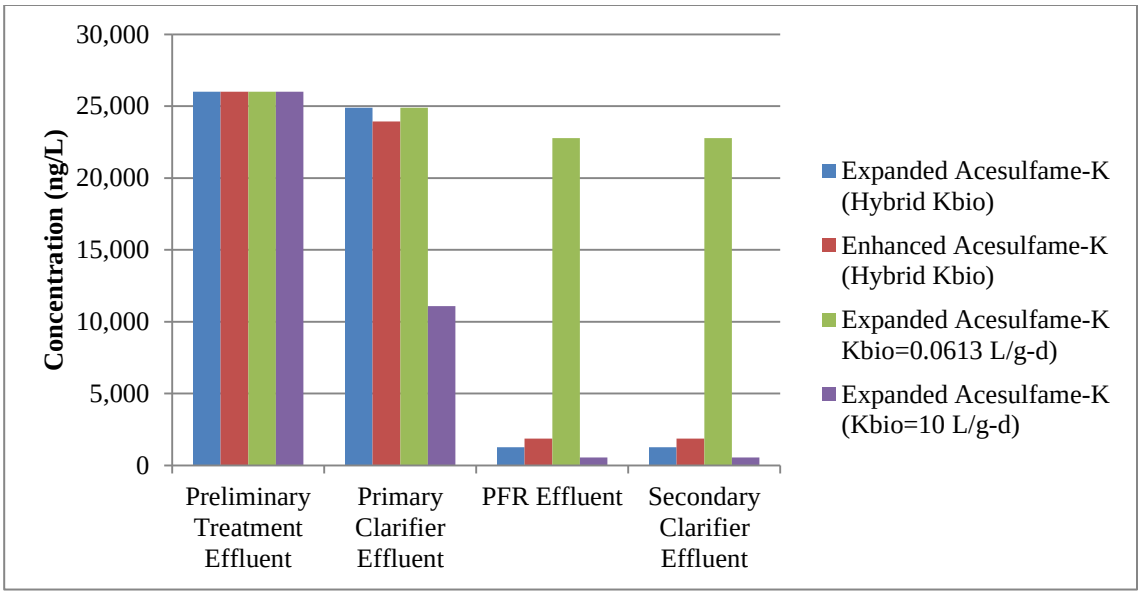

Figure 5-39: Expanded Model Acesulfame-K Concentrations under Sampling Conditions (Modified Flowrate)

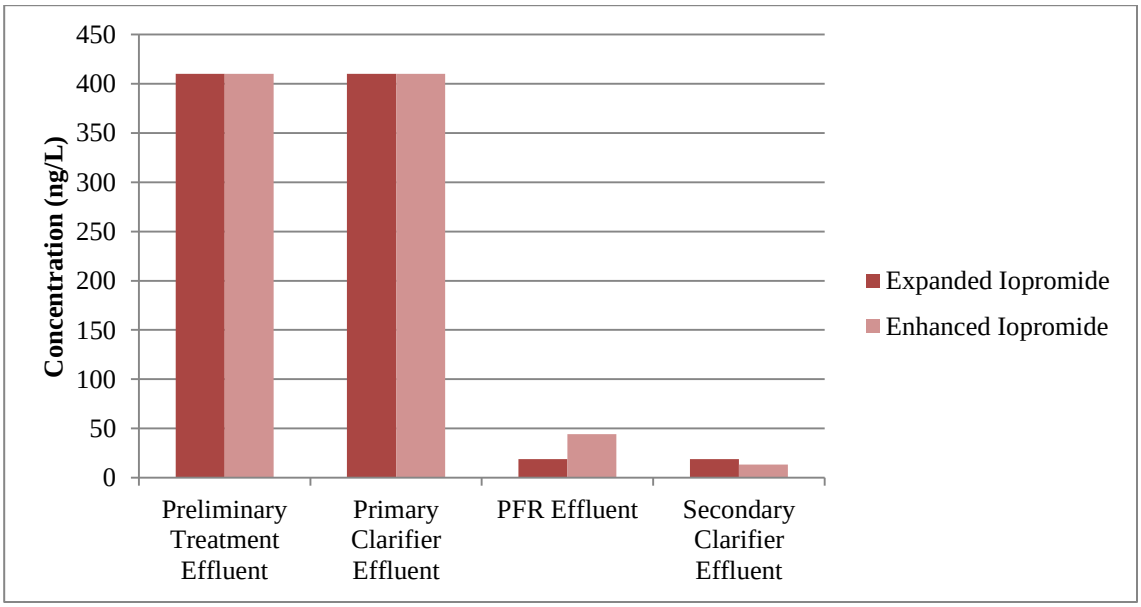

Figure 5-40: Expanded Model Iopromide Concentrations under Sampling Conditions (Modified Flowrate)

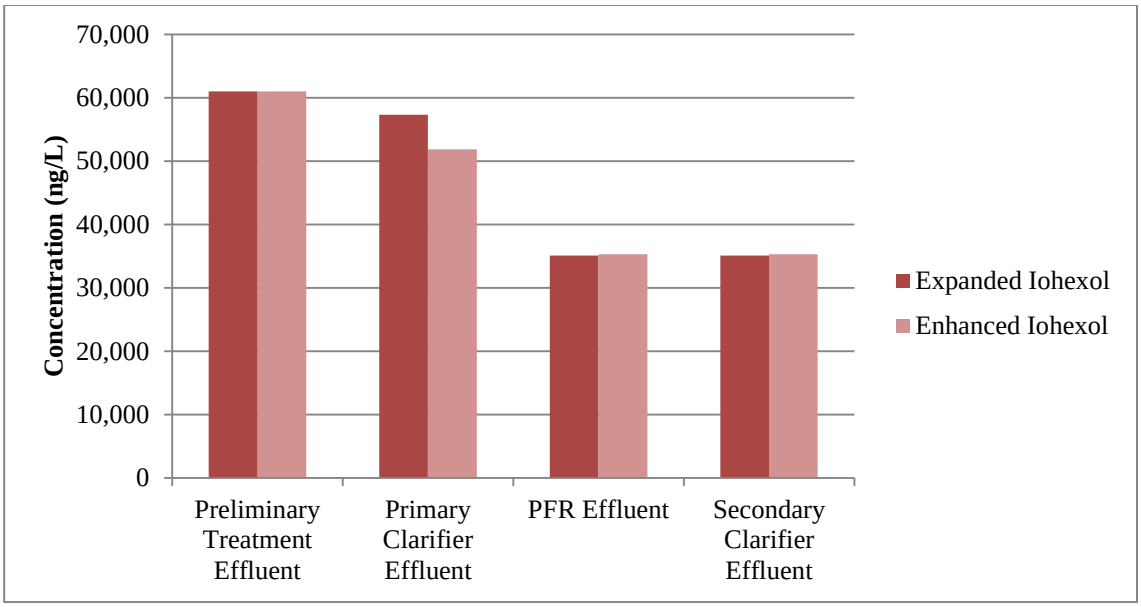

Figure 5-41: Expanded Model Iohexol Concentrations under Sampling Conditions (Modified Flowrate)

The expanded model has higher CEC concentrations in the primary clarifier effluent (Figure 5-30 to Figure 5-41). Because the expanded plant does not include an additional primary clarifier, it is likely that CEC concentrations are higher due to the increased flow rate per clarifier. In some cases, the additional PFR is able to compensate for the lack of an additional primary clarifier. Triclosan, atenolol, E1, DEET, caffeine, theobromine, iopromide, and iohexol all show similar, if not lower, concentrations in the expanded PFRs when compared to the enhanced PFR. When using 70% RAS for both the enhanced and expanded models, the primary clarifiers in both have similar VSS and X_a concentrations (Figure 5-42). In the PFR, expanded model VSS and X_a concentrations are noticeably larger. This implies that the rate of biodegradation and the amount of sorbed compound are larger in the expanded model PFRs, confirming the conclusions drawn from Figure 5-30 to Figure 5-41.

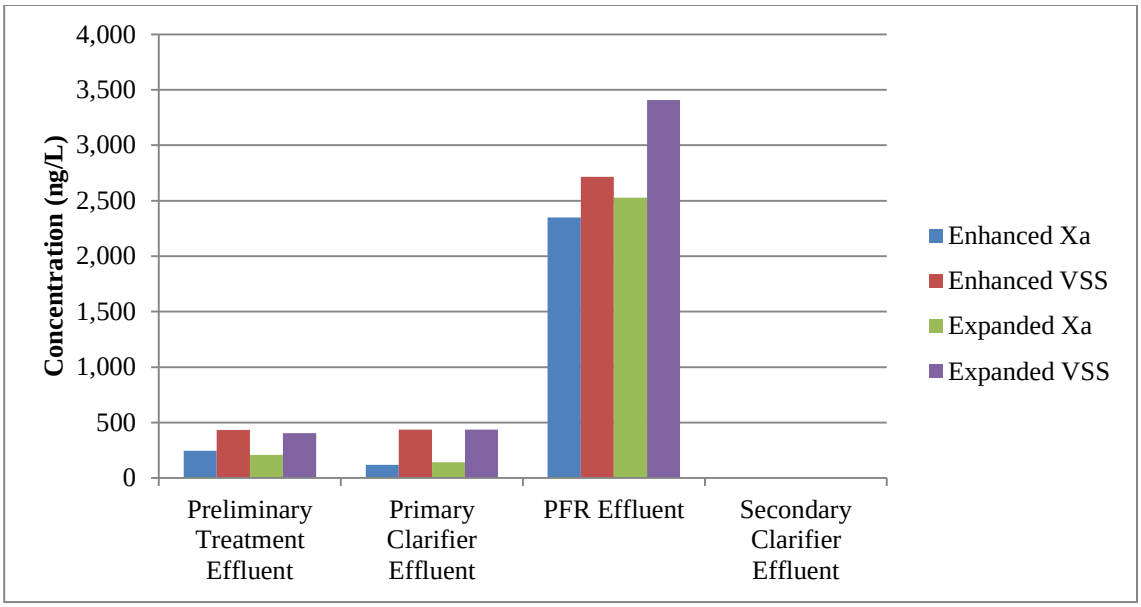

Figure 5-42: Expanded vs. Enhanced Model VSS and Xa Concentrations

Biodegradation and adsorption were compared in the primary clarifiers and the PFRs for the expanded model (Table 5-9). As with the enhanced model (Table 5-8), removal due to biodegradation and adsorption is roughly equal in the primary clarifier. Biodegradation in the PFRs becomes slightly higher in the expanded model because of the additional PFR. Because biodegradation is the primary removal mechanism (Table 5-8) in the PFRs, this is expected. VSS is over three times larger than X_a in the primary clarifiers (Figure 5-42). However, because biodegradation rates are typically larger than adsorption rates (Table 5-7), removal from biodegradation and adsorption are almost equal in the primary clarifiers. In the PFRs, VSS and X_a concentrations are closer together. This allows biodegradation to become the primary removal mechanism.

Table 5-9: Expanded Model Biodegradation vs. Adsorption in the Expanded Model

CEC	Treatment Process	Percent of Total Removal		
		Biodegradation	Adsorption	Total
Meprobamate*	Primary Clarifier	0.1%	99.9%	100.0%
	PFR	0.1%	99.9%	100.0%
Triclosan	Primary Clarifier	33.2%	66.8%	100.0%
	PFR	76.7%	23.3%	100.0%
Atenolol	Primary Clarifier	90.4%	9.6%	100.0%
	PFR	100.0%	0.0%	100.0%
E1	Primary Clarifier	100.0%	0.0%	100.0%
	PFR	100.0%	0.0%	100.0%
Gemfibrozil*	Primary Clarifier	0.0%	100.0%	100.0%
	PFR	0.0%	100.0%	100.0%
DEET	Primary Clarifier	90.5%	9.5%	100.0%
	PFR	100.0%	0.0%	100.0%
Caffeine	Primary Clarifier	56.1%	43.9%	100.0%
	PFR	100.0%	0.0%	100.0%
Theobromine	Primary Clarifier	54.9%	45.1%	100.0%
	PFR	100.0%	0.0%	100.0%
Sucralose*	Primary Clarifier	1.2%	98.8%	100.0%
	PFR	2.4%	97.6%	100.0%
Acesulfame-K	Primary Clarifier	19.8%	80.2%	100.0%
	PFR	100.0%	0.0%	100.0%
Iopromide	Primary Clarifier	-	-	-
	PFR	100.0%	0.0%	100.0%
Iohexol	Primary Clarifier	100.0%	0.0%	100.0%
	PFR	100.0%	0.0%	100.0%
Average	Primary Clarifier	49.7%	50.3%	100.0%
	PFR	73.3%	26.7%	100.0%

* Modeled concentrations were used because measured concentrations showed negative removal percentages.

After comparing the enhanced and expanded model with parameters from the day of sampling, the expanded model was then extrapolated and examined over an entire year (Figure 5-43 to Figure 5-54). With the exception of flow (which is 75% higher in the expanded model), influent data from 2013 is used in the analysis of the daily expanded model. With the exception of meprobamate, gemfibrozil, and sucralose, the model output predicts the expected CEC concentration when the NWRF is expanded.

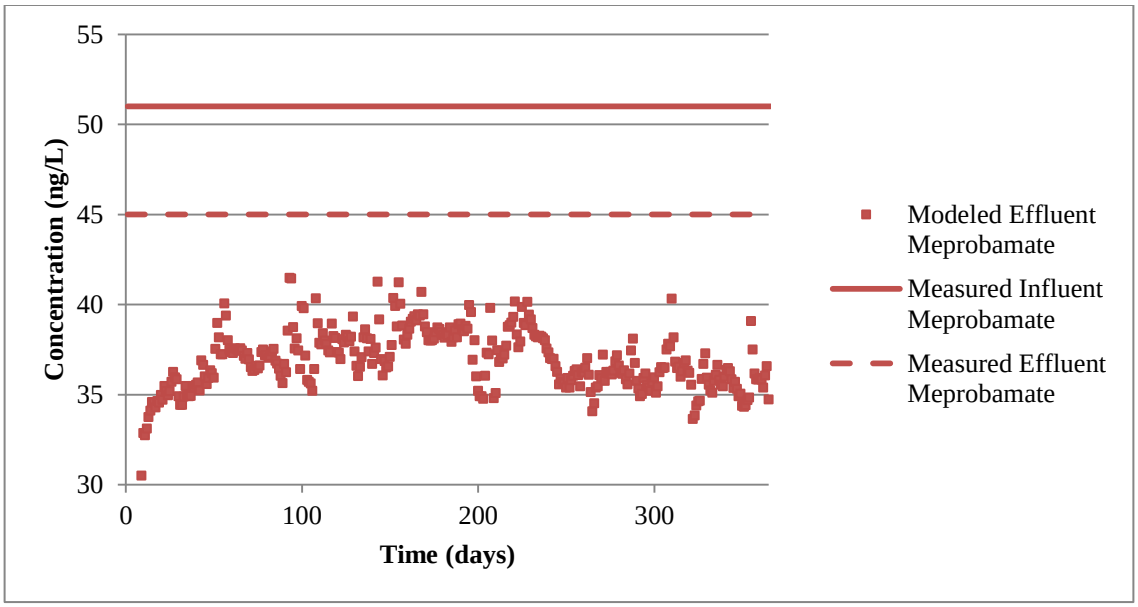

Figure 5-43: Expanded Extrapolated Meprobamate Concentrations
* Due to negative removal percentage in the PFR, the CEC was only calibrated in the primary clarifiers.

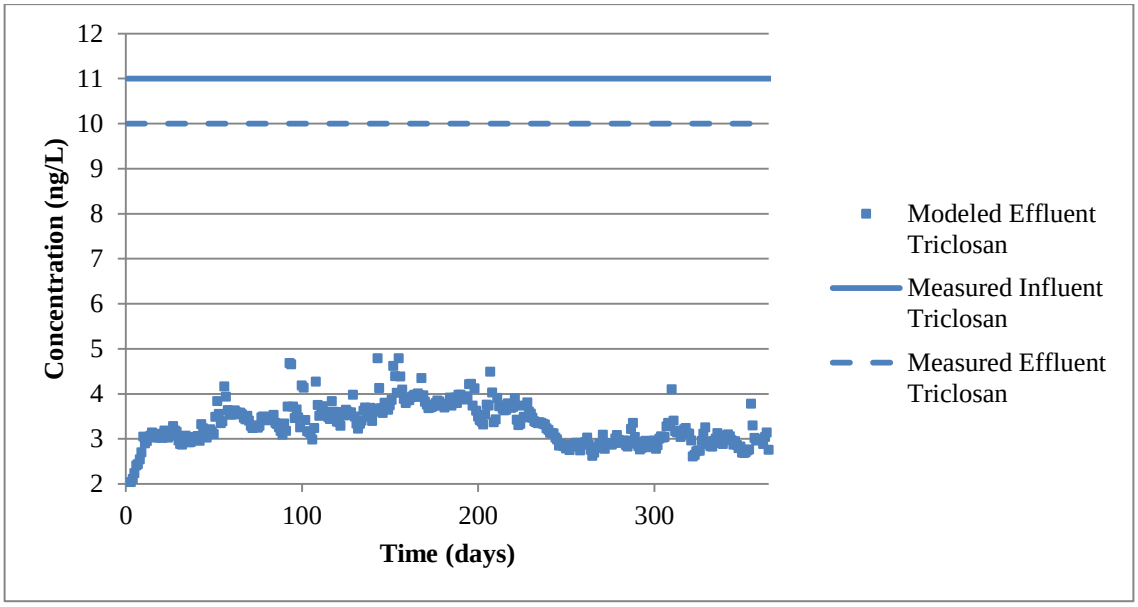

Figure 5-44: Expanded Extrapolated Triclosan Concentrations
* Measured effluent concentration was below the MRL.

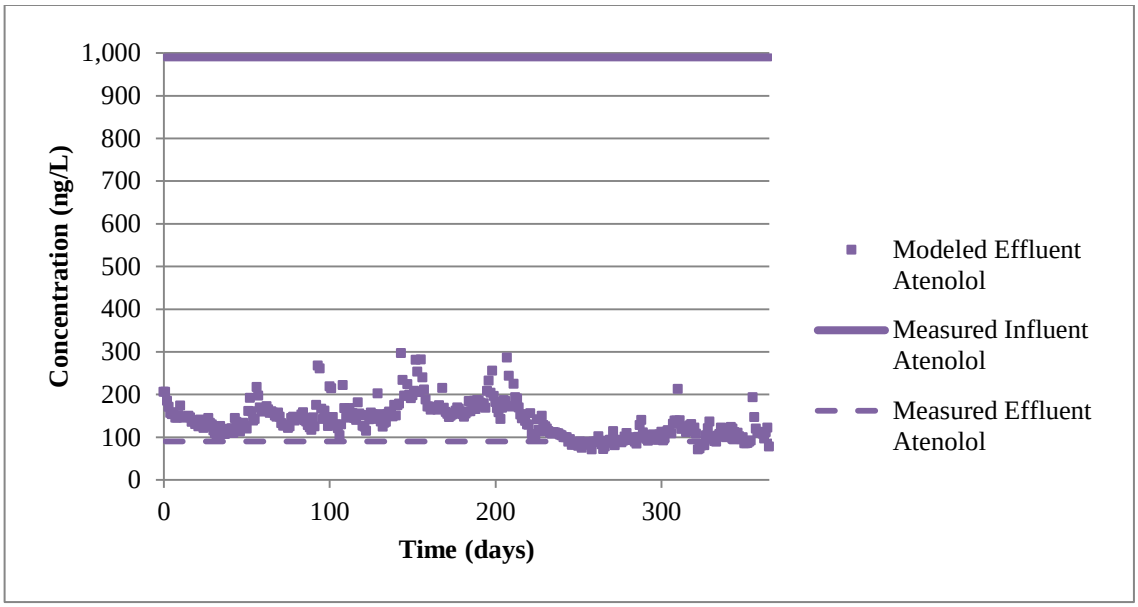

Figure 5-45: Expanded Extrapolated Atenolol Concentrations

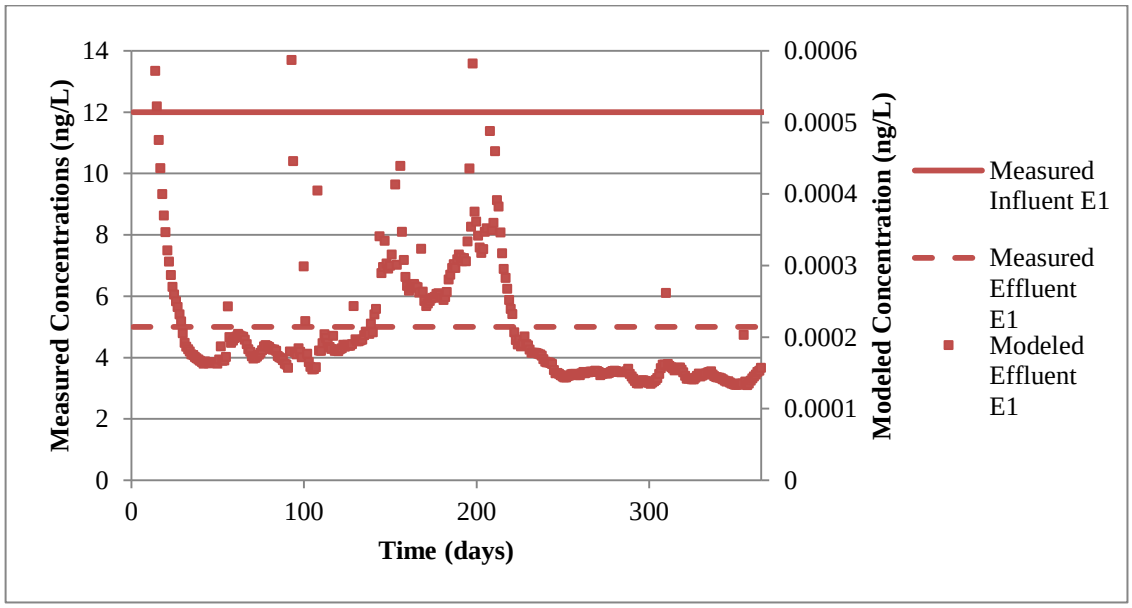

Figure 5-46: Expanded Extrapolated E1 Concentrations

* Measured effluent concentration was below the MRL.

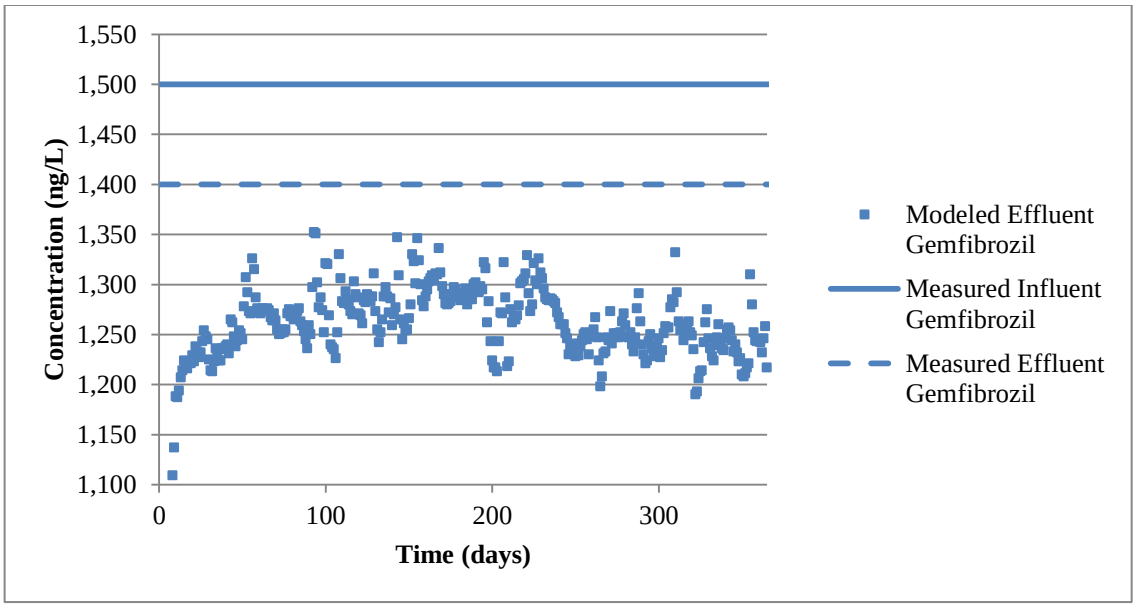

Figure 5-47: Expanded Extrapolated Gemfibrozil Concentrations

* Due to negative removal percentage in the PFR, the CEC was only calibrated in the primary clarifiers.

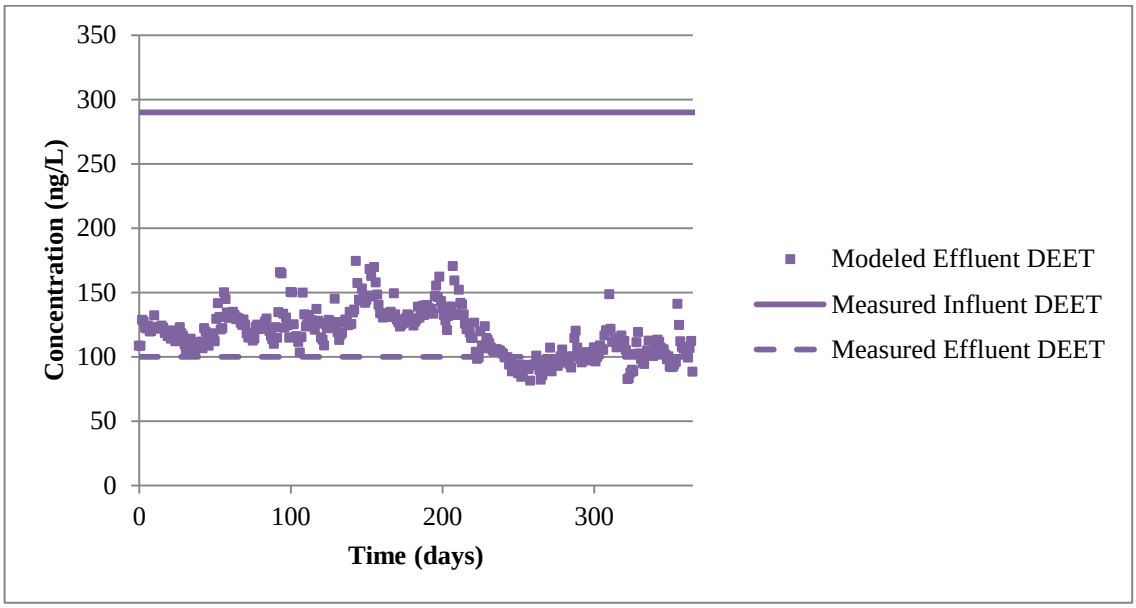

Figure 5-48: Expanded Extrapolated DEET Concentrations

* Measured effluent concentration was below the MRL.

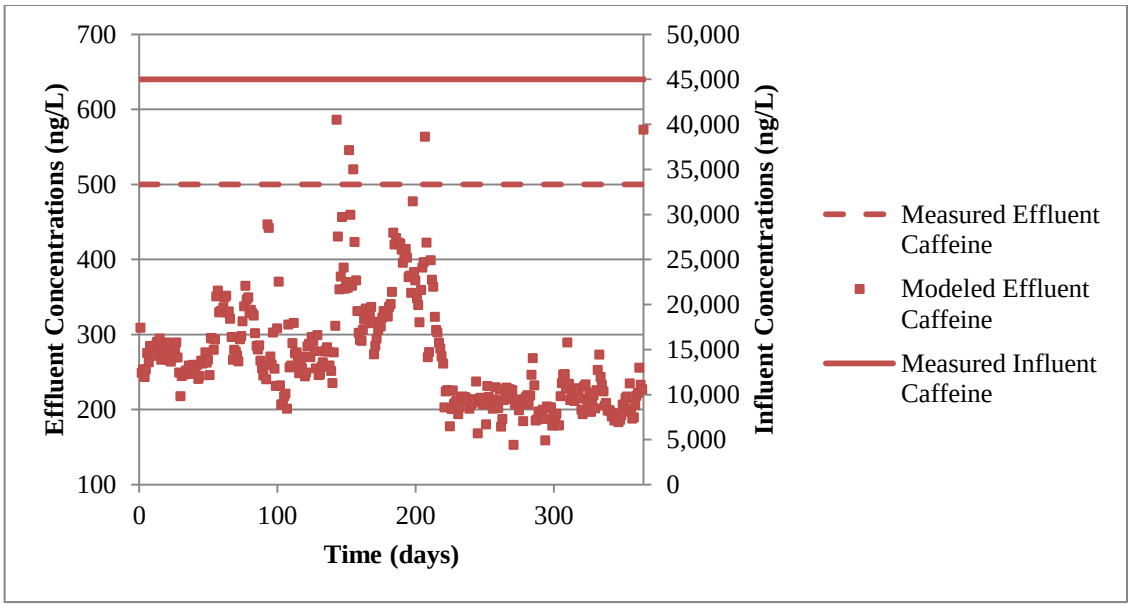

Figure 5-49: Expanded Extrapolated Caffeine Concentrations

* Measured effluent concentration was below the MRL.

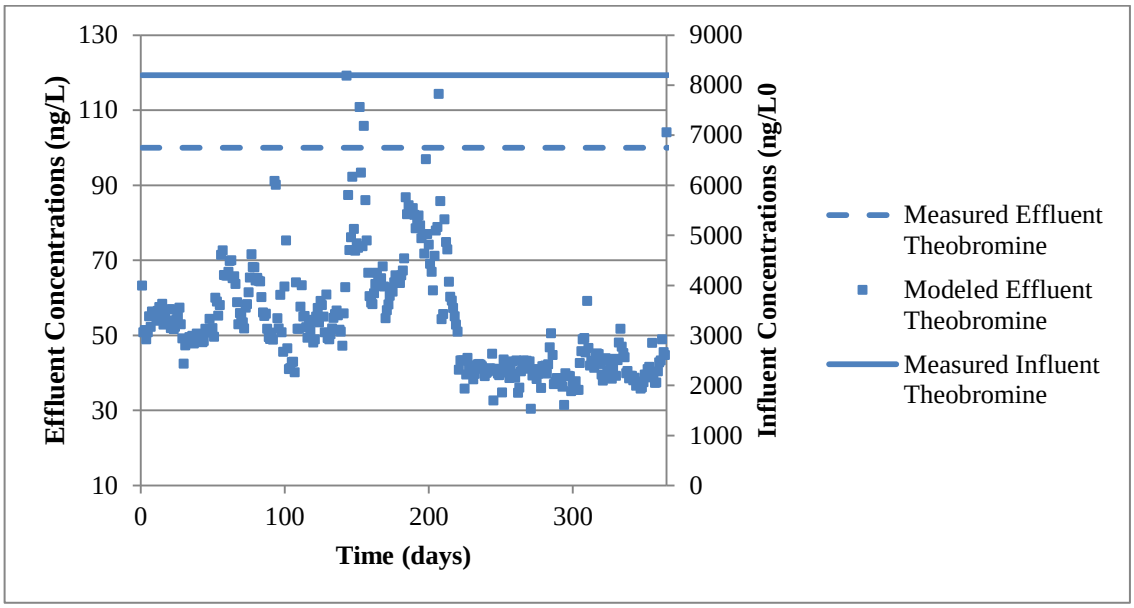

Figure 5-50: Expanded Extrapolated Theobromine Concentrations

* Measured effluent concentration was below the MRL.

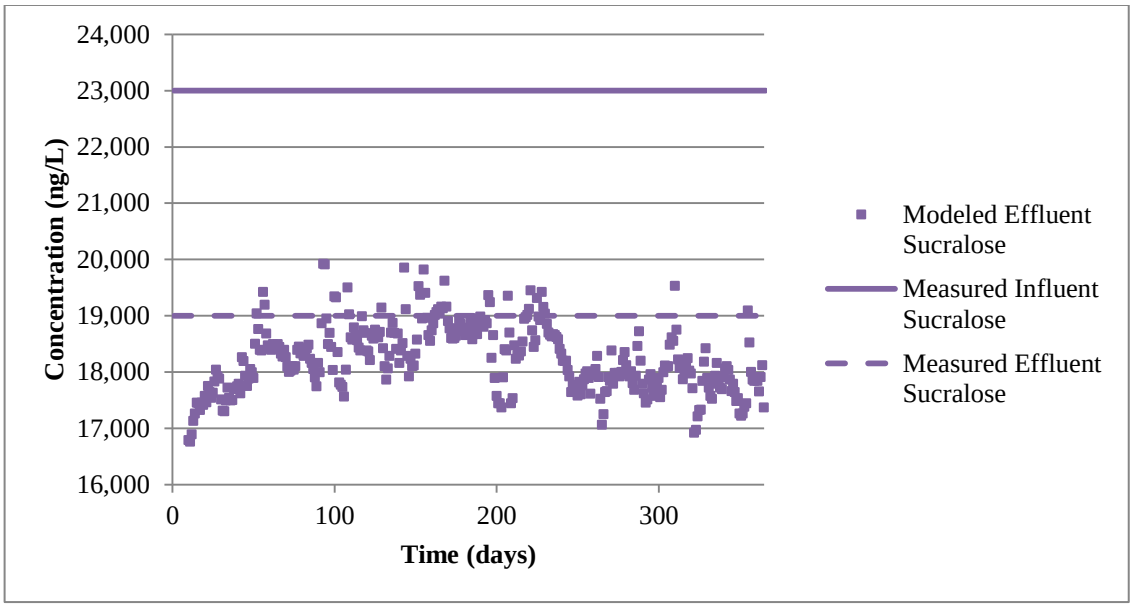

Figure 5-51: Expanded Extrapolated Sucralose Concentrations

* Due to negative removal percentage in the PFR, the CEC was only calibrated in the primary clarifiers.

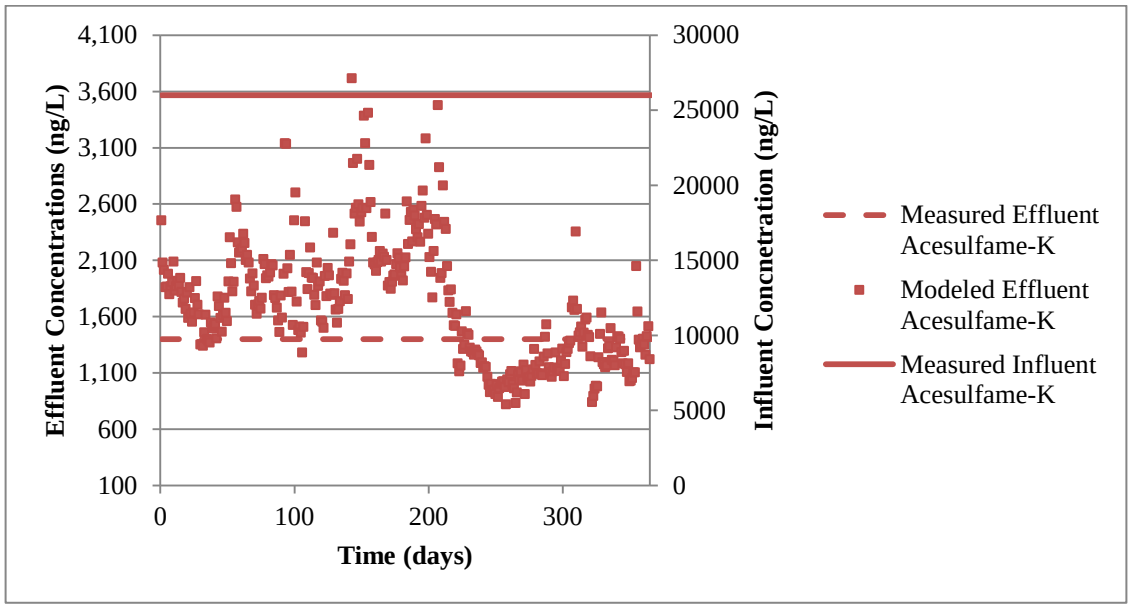

Figure 5-52: Expanded Extrapolated Acesulfame-K Concentrations

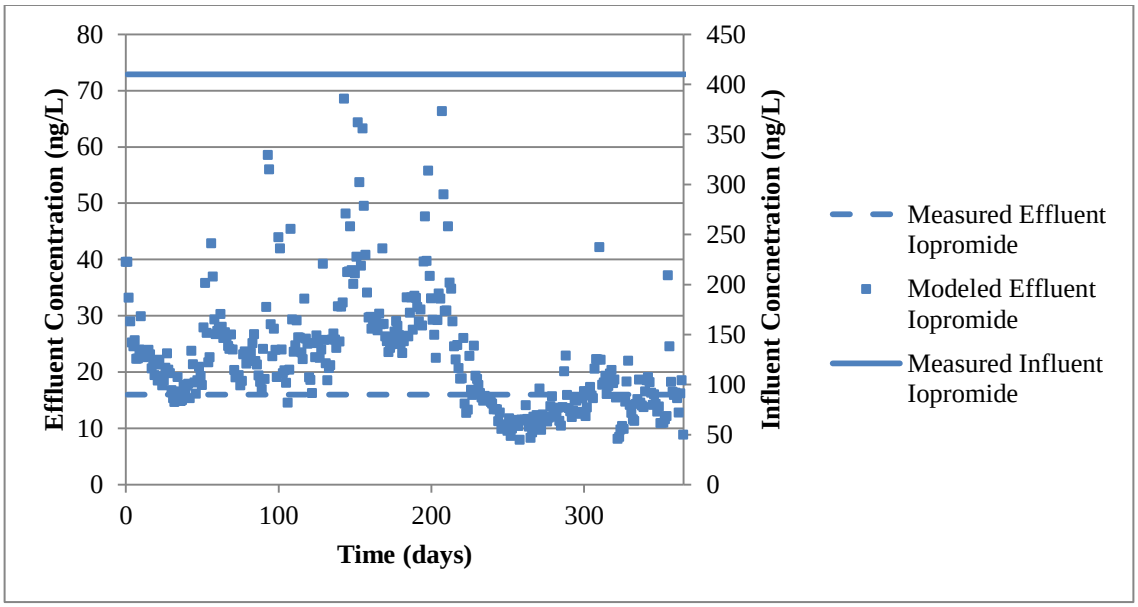

Figure 5-53: Expanded Extrapolated Iopromide Concentrations

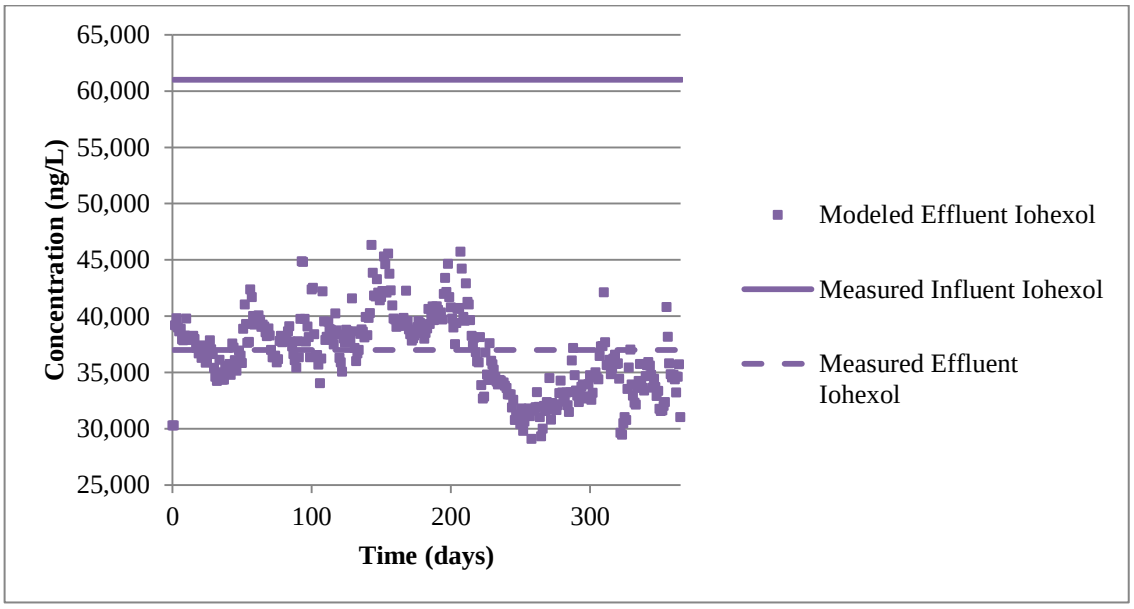

Figure 5-54: Expanded Extrapolated Iohexol Concentrations

Modeled CECs have similar removal patterns throughout the entire year of modeling. Most CECs reach their maximum concentration sometime in the middle of the year and decrease around 230 days. It should be noted that this assumes the same influent concentration of each CEC throughout the entire year. Because calibrated

biodegradation and adsorption constants were only found in the primary clarifier for meprobamate, gemfibrozil, and sucralose, these CECs have higher removals in the expanded model than in the measured data (each CEC had negative plant removal percentages). Although they have varying removal percentages, each CEC decreases in concentration around a time of 230 days. This is likely due to increasing VSS and X_a concentrations at this time (Figure 5-55 to Figure 5-56), as well as an increase in water temperature (Figure 5-57).

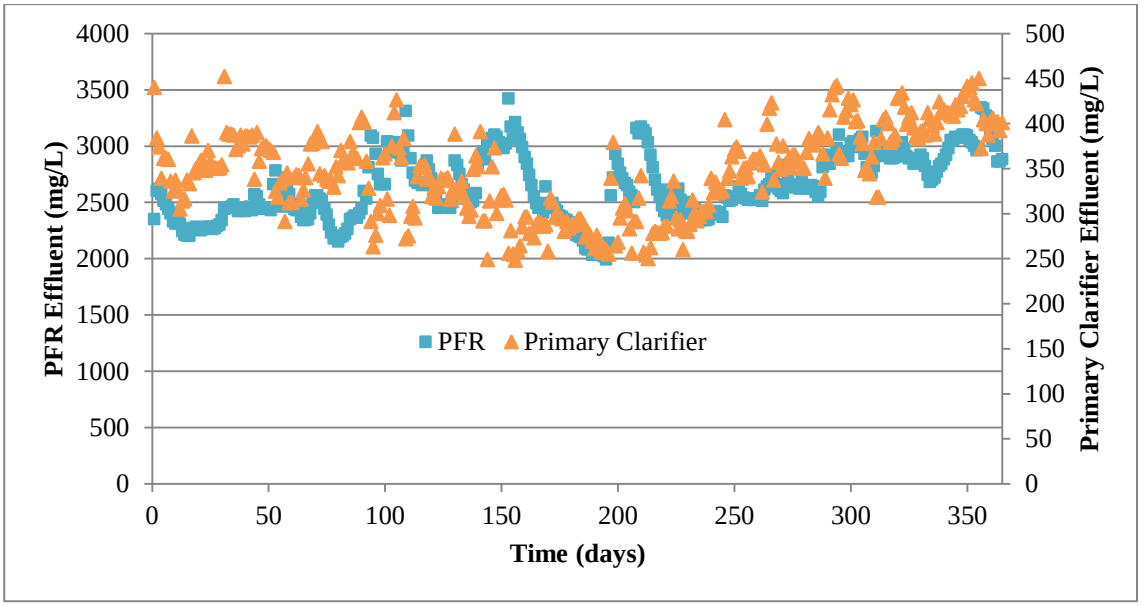

Figure 5-55: Expanded Model Primary Clarifier and PFR VSS Concentrations

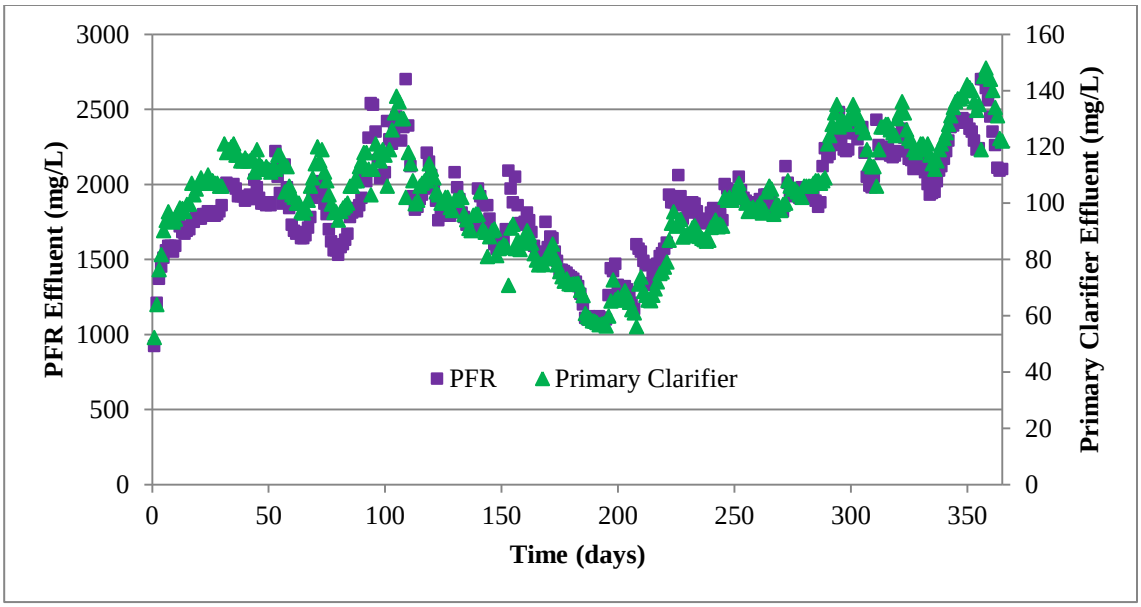

Figure 5-56: Expanded Model Primary Clarifier and PFR X_a Concentrations

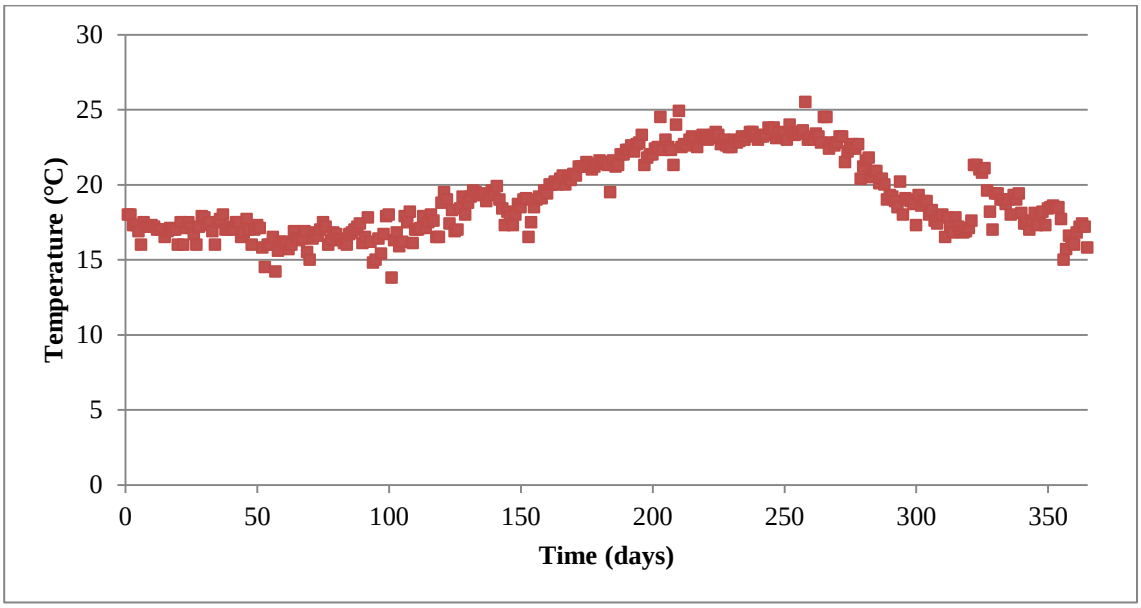

Figure 5-57: Daily Water Temperature

5.4.1 RAS Analysis

After analyzing the expanded plant with the estimated RAS from base model calibration (70%), VSS, X_a, and the CECs were analyzed with varying RAS rates. In this case, RAS is equal to the total recycle flow divided by the total influent flowrate

and comes from the settled solids in the secondary clarifiers. Because RAS does not require physical alteration of the plant, it is a reasonable change that can be made to the plant. While primary clarifier VSS and X_a decrease with increasing RAS, PFR concentrations increase (Figure 5-58 to Figure 5-59). Because RAS is pumped from the settled solids area in the secondary clarifiers to the influent of the PFR, concentrations in the PFR increase as the RAS flow increases. Both VSS and X_a have a greater rate of change at lower RAS rates. In the primary clarifier, both decrease at approximately equal rates of change. In the PFRs, VSS increases at a greater rate than X_a as RAS increases. As RAS approaches 100%, it has less effect on concentration. As RAS increases, plant effluent VSS increases and X_a decreases (Figure 5-60).

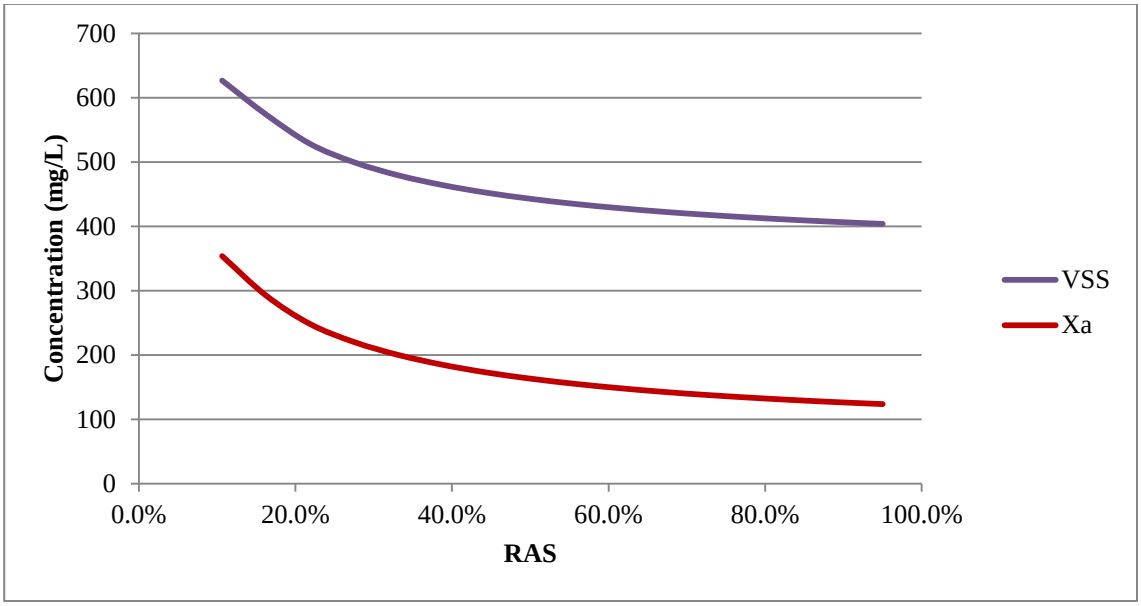

Figure 5-58: Primary Clarifier VSS and X_a with Varying RAS

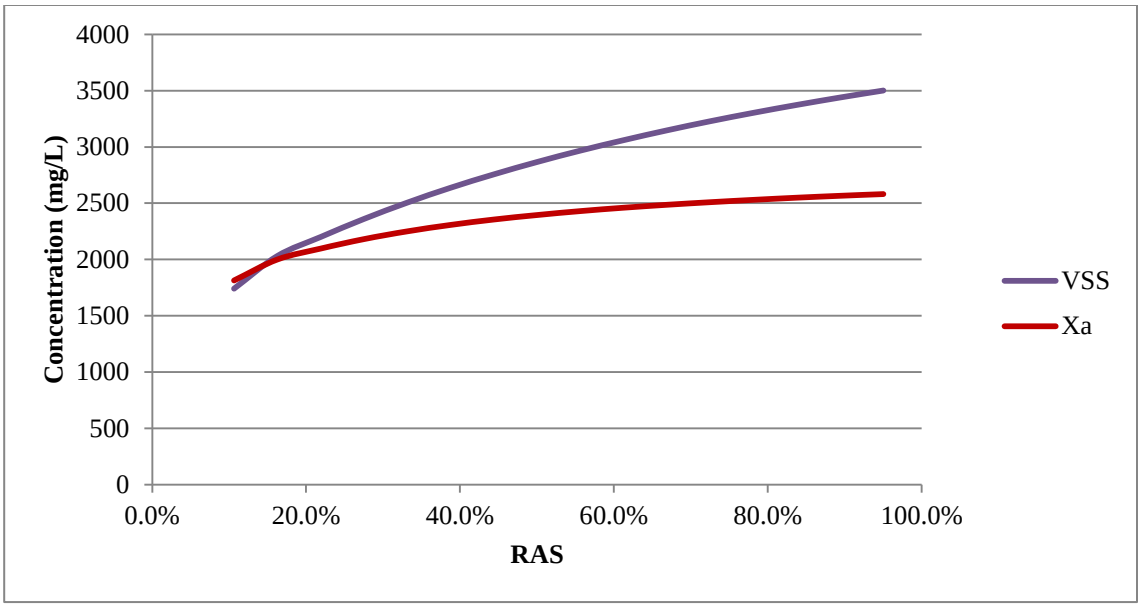

Figure 5-59: PFR VSS and X_a with Varying RAS

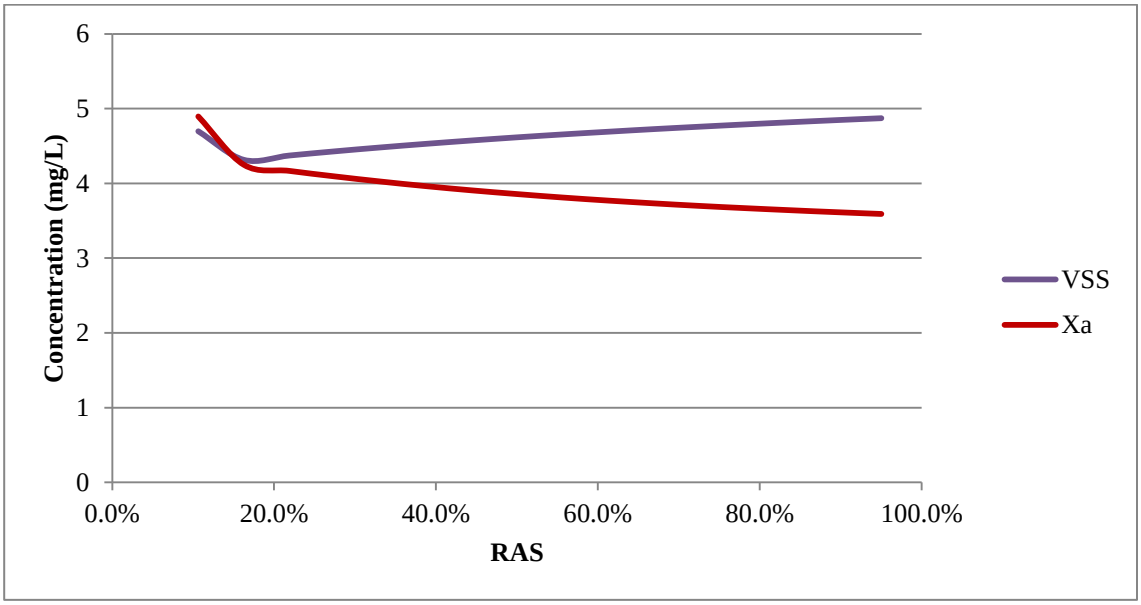

Figure 5-60: Plant Effluent VSS and X_a with Varying RAS

The decrease in VSS and X_a in the primary clarifiers results in a higher concentration of CECs as RAS increases (Figure 5-61 to Figure 5-63). Because VSS and X_a increase in the PFRs, most CECs have increased removal percentages (Figure

5-64 to Figure 5-66). Due to the small differences in removal percentage, the CECs have been grouped in ranges.

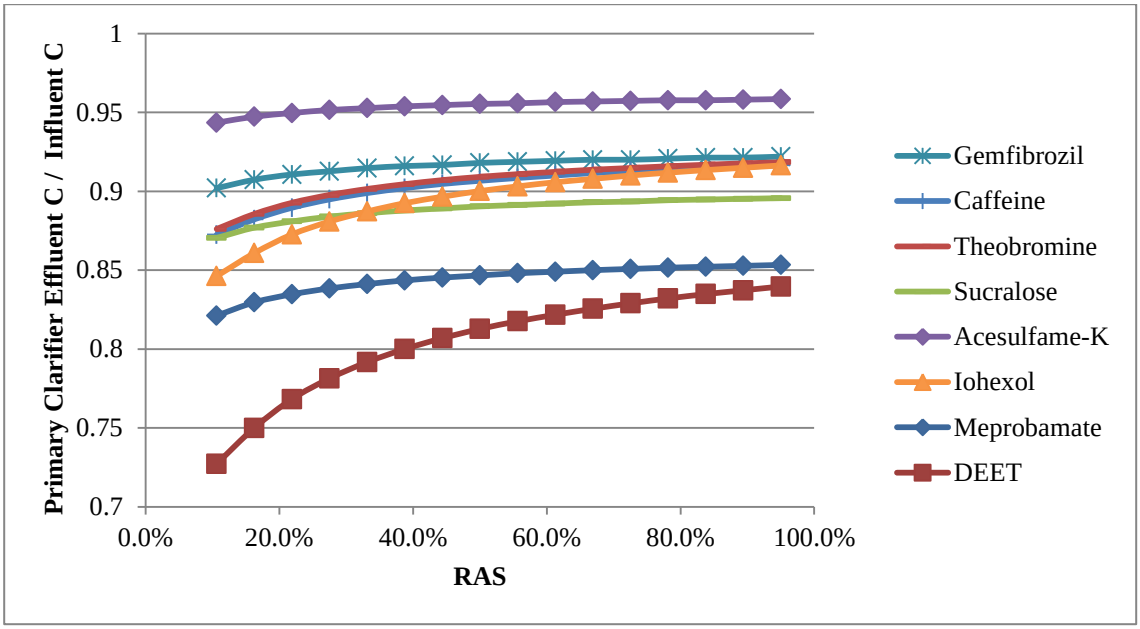

Figure 5-61: Primary Clarifier CEC Removal with Varying RAS (0-30% Removal)

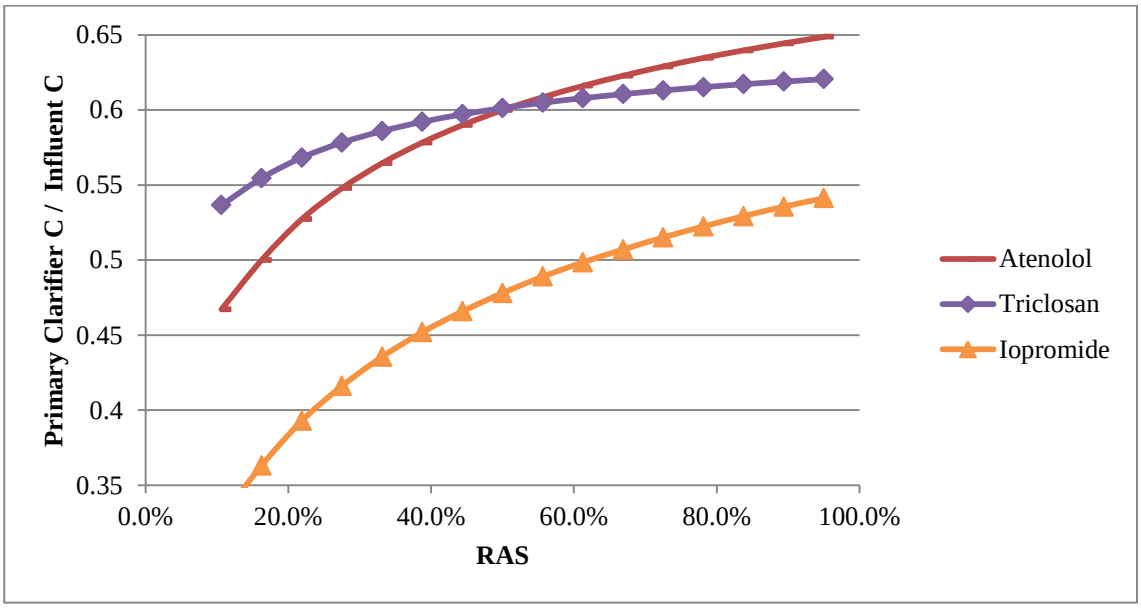

Figure 5-62: Primary Clarifier CEC Removal with Varying RAS (35-65% Removal)

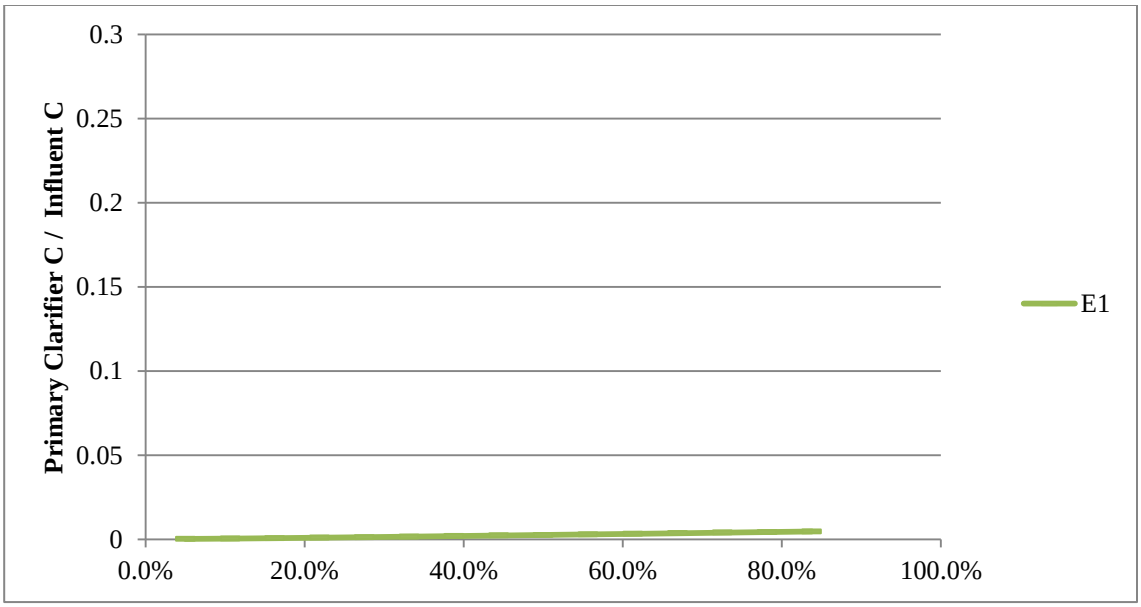

Figure 5-63: Primary Clarifier CEC Removal with Varying RAS (70-100% Removal)

Each CEC has a lower removal percentage in the primary clarifiers as RAS increases (Figure 5-61 to Figure 5-63). Acesulfame-K, gemfibrozil, caffeine, theobromine, iohexol, sucralose, and meprobamate do not have significant removal changes after about 50% RAS. DEET, atenolol, triclosan, and iopromide have a greater rate of decreasing removal at low RAS but start to level off as RAS approaches 100%.

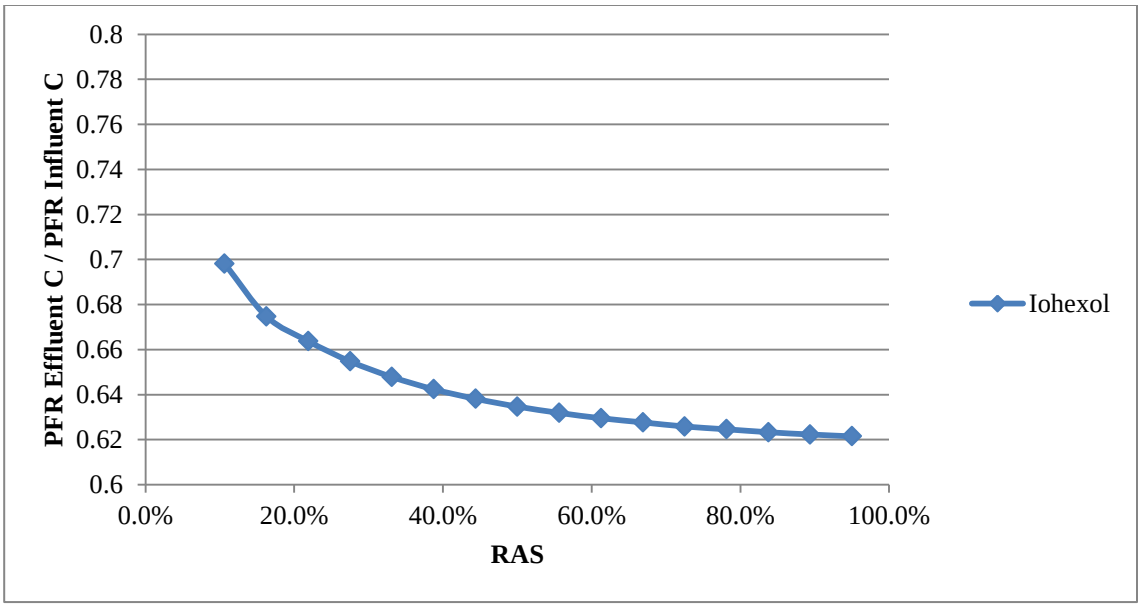

Figure 5-64: PFR CEC Removal with Varying RAS (20-40% Removal)

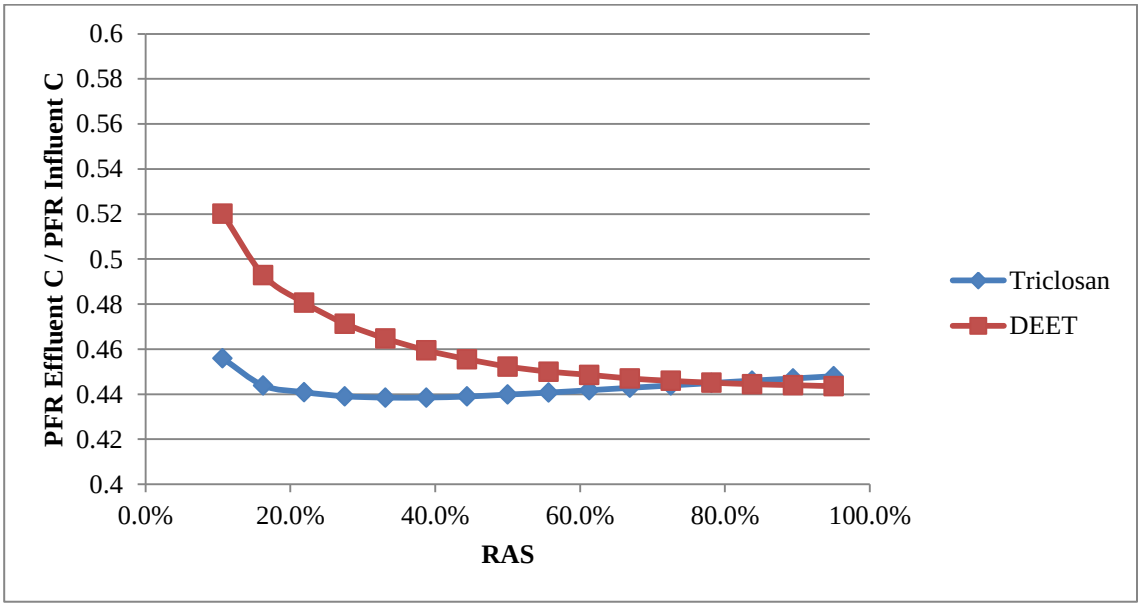

Figure 5-65: PFR CEC Removal with Varying RAS (40-60% Removal)

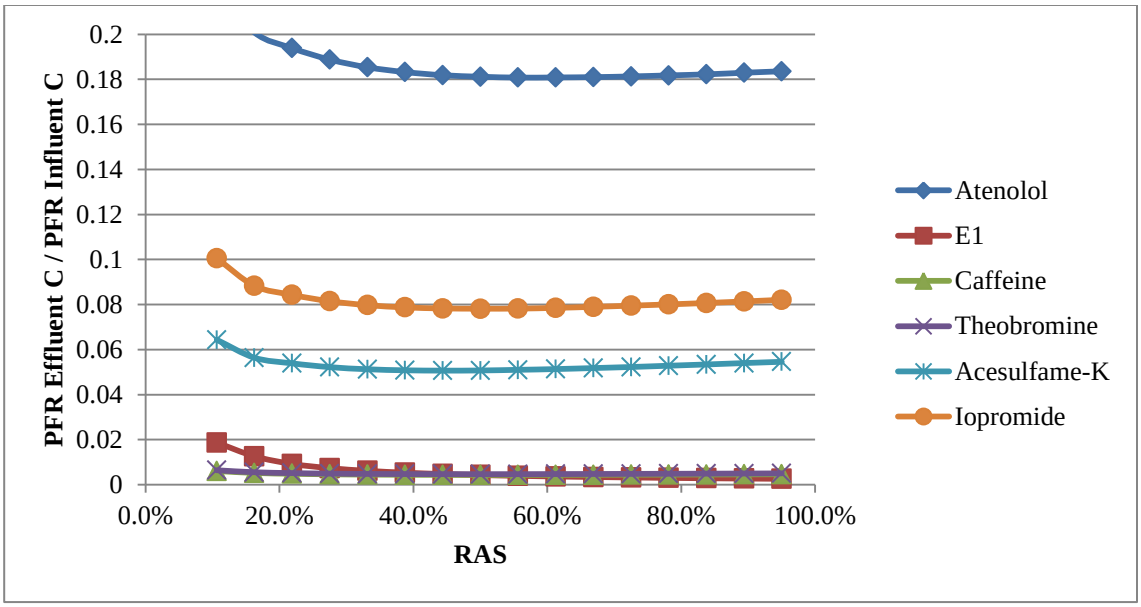

Figure 5-66: PFR CEC Removal with Varying RAS (80-100% Removal)

In the PFRs, iohexol has the greatest increase in removal percentage (~8%) of any CEC modeled (Figure 5-64). Triclosan, atenolol, iopromide, acesulfame-K, E1, caffeine, and theobromine do not show any considerable removal change above a RAS of about 30%. However, some of these CECs (triclosan, atenolol, iopromide, and acesulfame-K), display gradually smaller removal percentages as RAS approaches 100%.

Ultimately, due to the decreased removal percentage in the primary clarifiers and the increased removal percentages in the PFR, RAS proved to have a small effect on the total plant CEC removal. CECs that are equally removed in the primary clarifiers and the PFRs (atenolol and triclosan) tend to decrease in removal percentage as RAS increases. CECs with reliance on the PFR for removal (iohexol, DEET, and acesulfame-K) behave the opposite, as RAS increased, the CEC's removal percent also increased (Figure 5-67 to Figure 5-68).

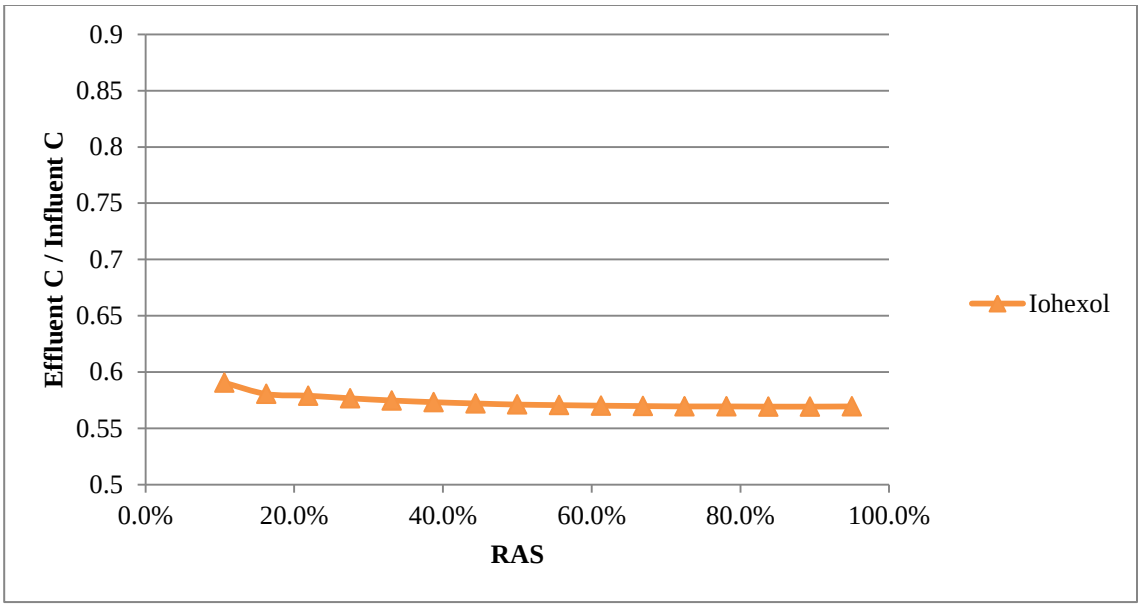

Figure 5-67: Plant CEC Removal with Varying RAS (10-50% Removal)

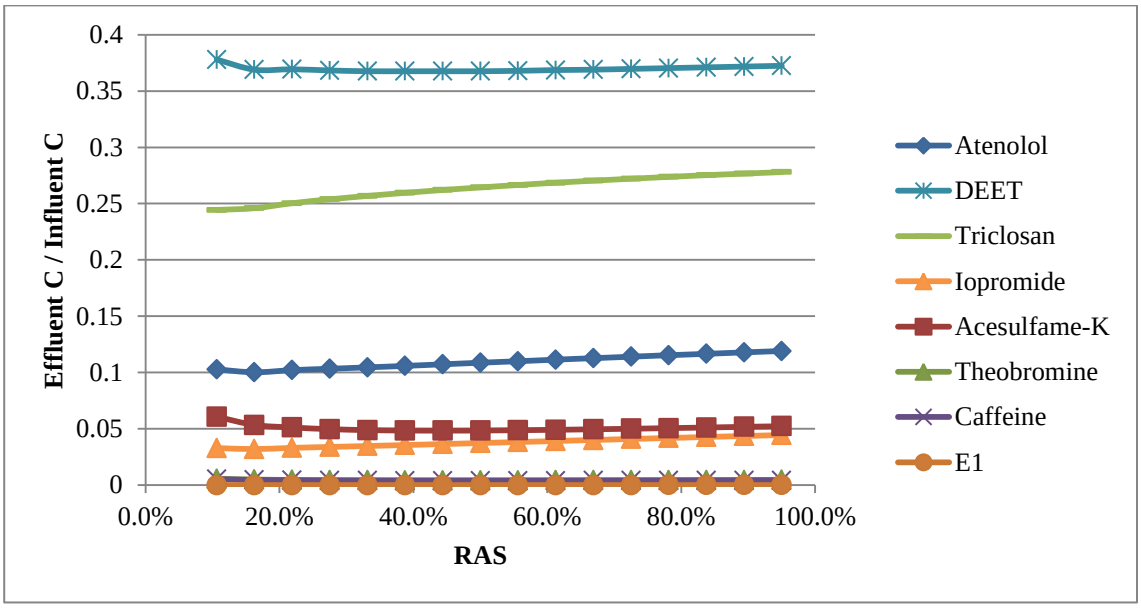

Figure 5-68: Plant CEC Removal with Varying RAS (60-100% Removal)

To further analyze RAS effects, other plant effluent parameters were compared. Variability in RAS has a larger effect on TSS than it does cBOD or TKN (Figure 5-69). While cBOD and ammonia stay relatively constant with increasing RAS, TSS increases.

Similar to VSS, TSS in the RAS stream causes an increase in concentration in both the PFR and the plant effluent.

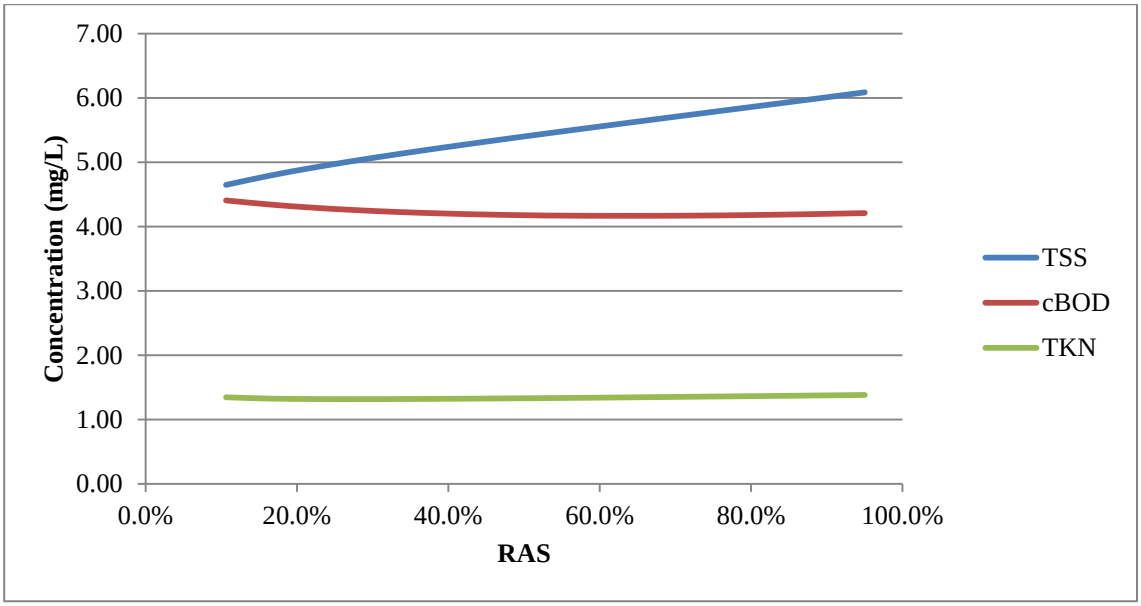

Figure 5-69: Plant Effluent TSS, cBOD, and TKN with Varying RAS

5.4.2 Primary Clarifier Volume Analysis

Next, primary clarifier volume's effect on CEC removal was examined. The analysis was completed for primary clarifier volume ranging from 57% to 200% of the size of the current primary clarifiers. In general, primary clarifier has a larger effect on CEC removal than RAS. First, the removal percentages of the primary clarifiers were analyzed. Although primary clarifier, PFR, and plant effluent VSS and X_a decrease with increasing primary clarifier volume (Figure 5-70 to Figure 5-72), CEC removal percentage in the primary clarifier increase due to the increased HRT (Figure 5-73). With increased HRT, CECs have longer time to biodegrade.

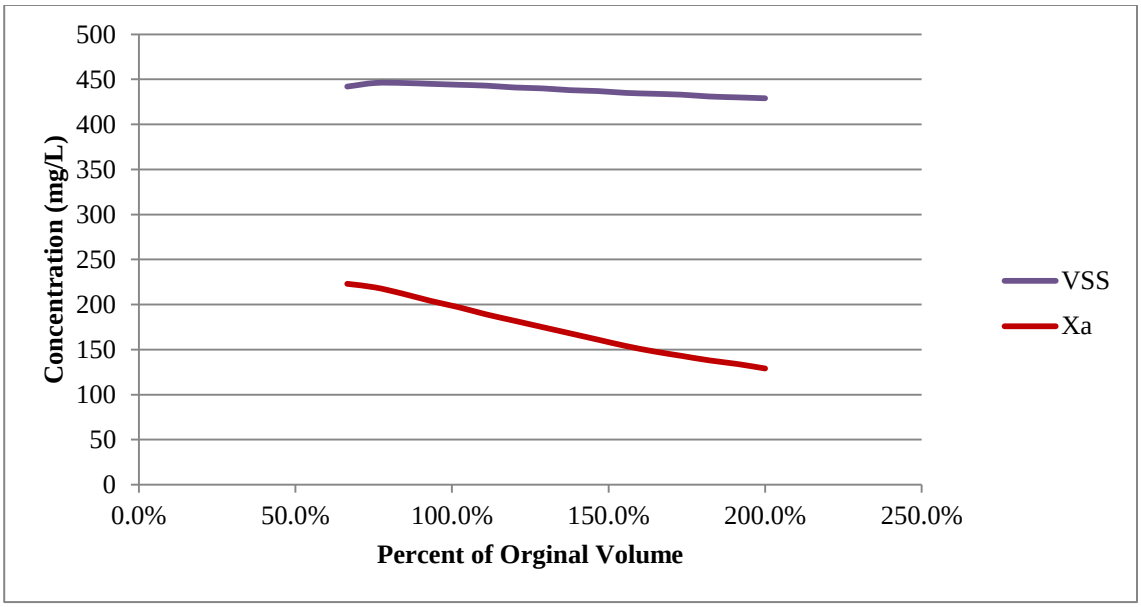

Figure 5-70: Primary Clarifier VSS and X_a with Varying Primary Clarifier Volume

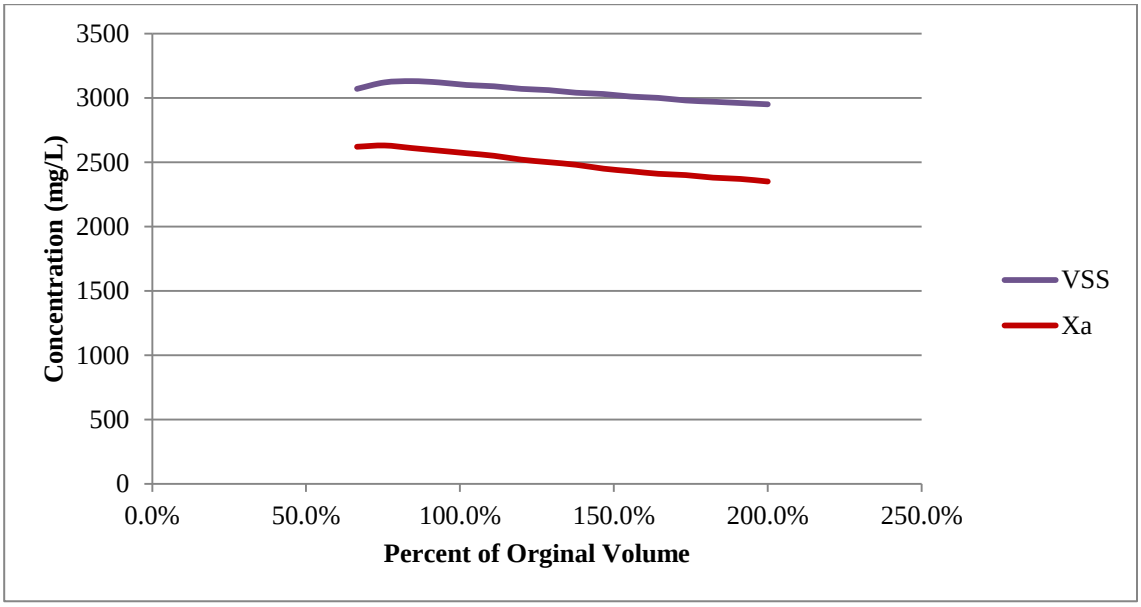

Figure 5-71: PFR VSS and X_a with Varying Primary Clarifier Volume

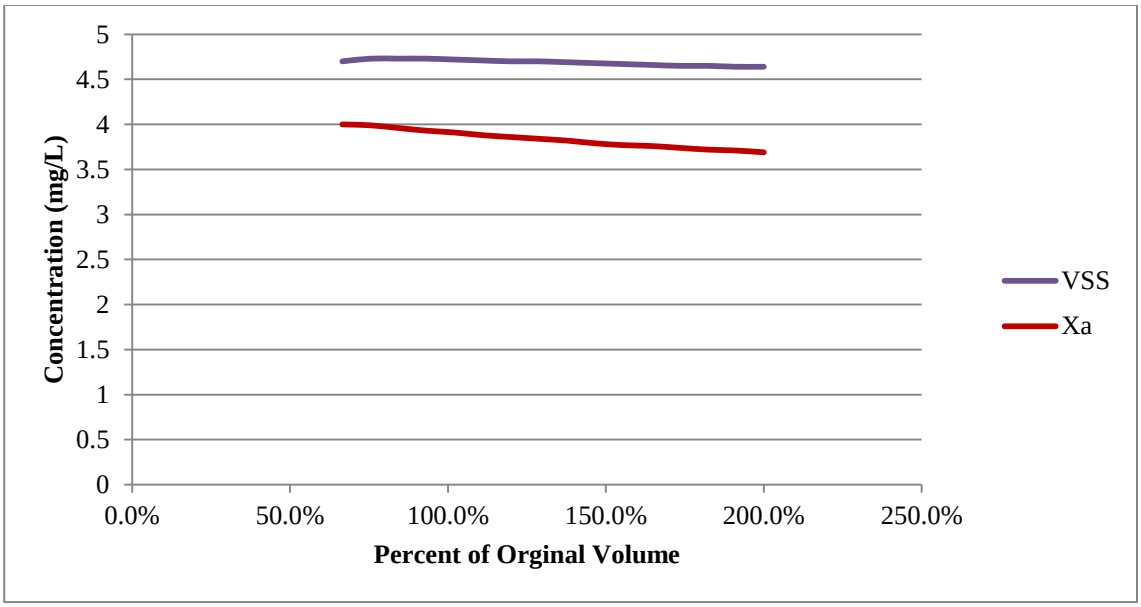

Figure 5-72: Effluent VSS and X_a with Varying Primary Clarifier Volume

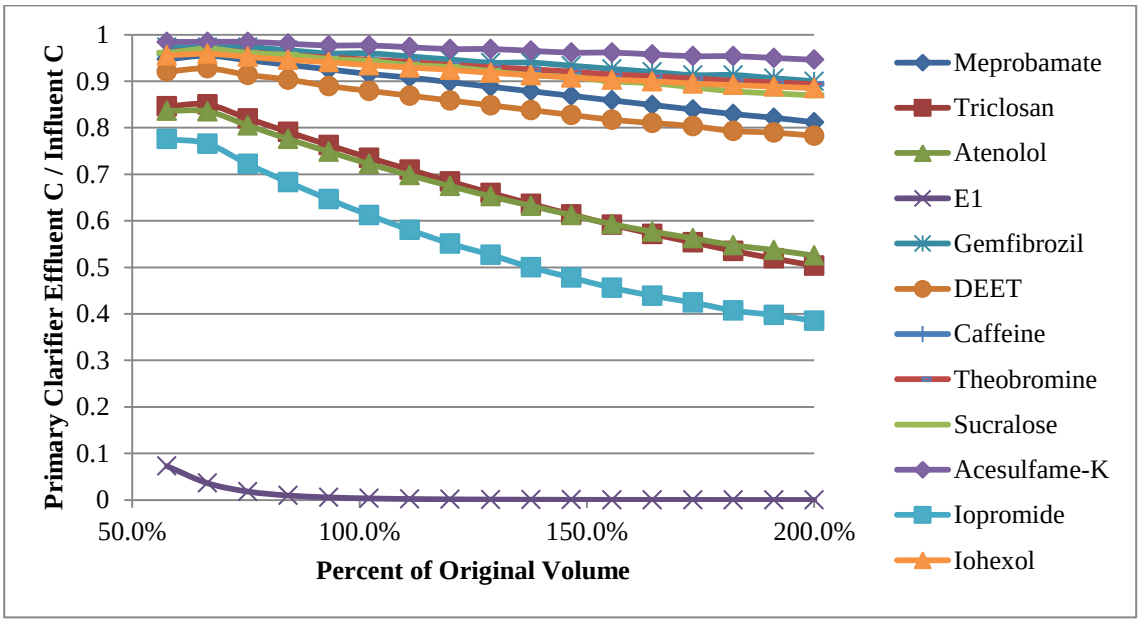

Figure 5-73: Primary Clarifier CEC Removal with Varying Primary Clarifier Volume

Each modeled CEC decreases in primary clarifier effluent concentration as primary clarifier volume increases (Figure 5-73). As expected, CECs that are more removed in the primary clarifiers (sucralose, triclosan, and iopromide) were more

influenced by primary clarifier volume. However, even CECs that are initially removed primarily by the PFR (Figure 5-7) experience at least some increase in removal percentage as volume increases. Next, the PFR was analyzed under varying primary clarifier volumes (Figure 5-74 to Figure 5-75).

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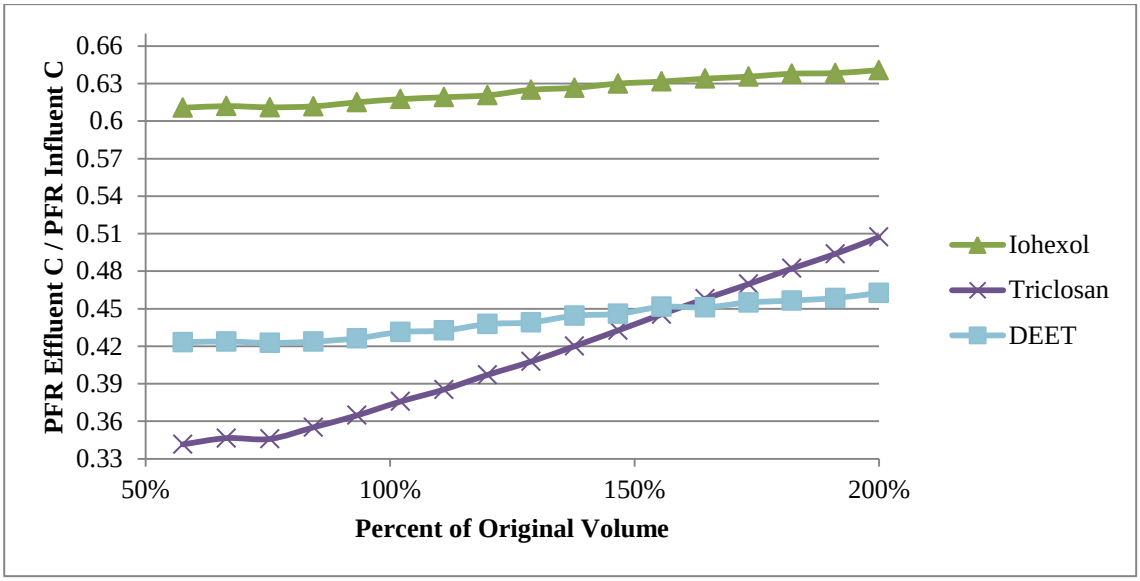

Figure 5-74: PFR CEC Removal with Varying Primary Clarifier Volume (33-67% Removal)

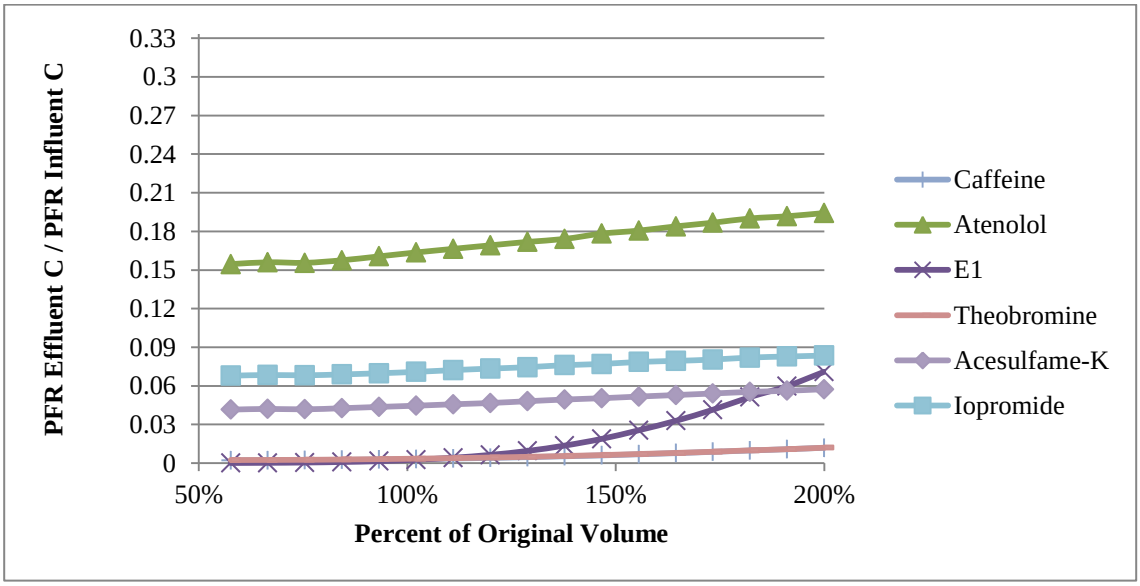

Figure 5-75: PFR CEC Removal with Varying Primary Clarifier Volume (67-100% Removal)

As primary clarifier volume increases, the removal percentages of iohexol, DEET, atenolol, iopromide, acesulfame-K, theobromine, and caffeine slightly decrease. Meanwhile, triclosan and DEET's removal percentages both decrease by about 10%. In general, as the volume of the primary clarifier increases, the percent removal observed in the PFR decreases. This can be attributed to two reasons. First, there are lower concentrations of VSS and X_a in the PFR, as they are being more removed in the primary clarifiers (Figure 5-71). Second, because the primary clarifiers are also removing higher percentages of CECs, there is a lower concentration entering the PFR (Figure 5-73). Biodegradation and adsorption are first-order with respect to CEC concentration and X_a and VSS concentrations, respectively. Because of this relationship, removal rates decrease. Although the PFR removal decreases, because of the increased primary clarifier removal, the overall plant removal for most CECs increases with increased primary clarifier volume (Figure 5-76 to Figure 5-77).

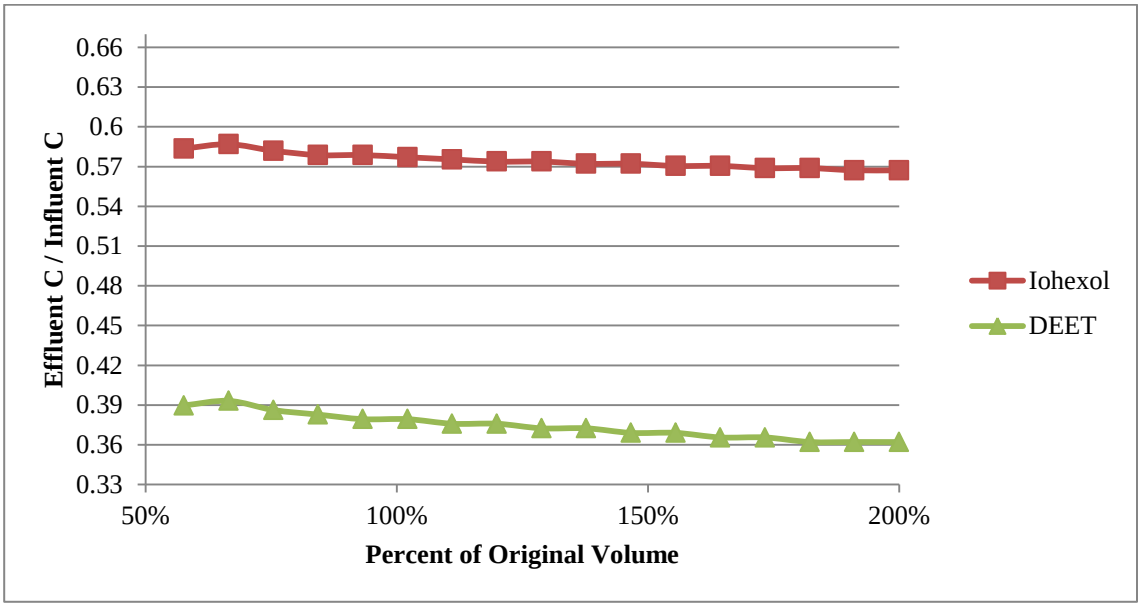

Figure 5-76: Plant CEC Removal with Varying Primary Clarifier Volume (33-67% Removal)

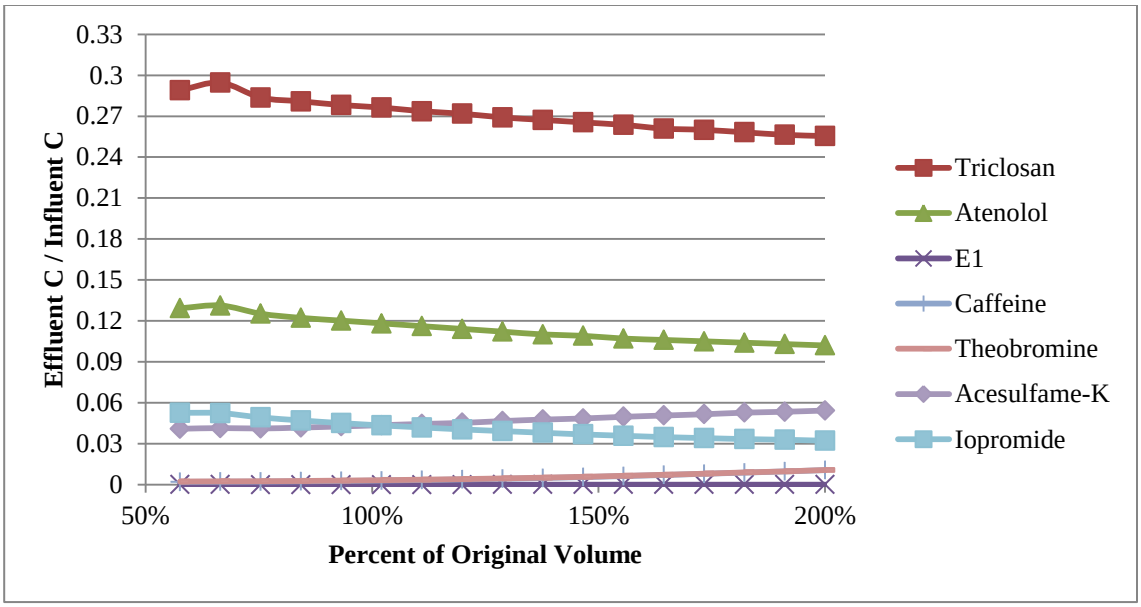

Figure 5-77: Plant CEC Removal with Varying Primary Clarifier Volume (67-100% Removal)

Although the difference is small, as the primary clarifier volume increases, CEC removal increases. Interestingly, though, the removal percentage for each CEC increases at approximately the same rate. This indicates that, while biodegradation and adsorption constants are important factors in determining the removal percentage of each CEC, primary clarifier HRT helps to improve removal, regardless of the biodegradation and adsorption rates. However, as primary clarifier volume is doubled, most CEC removal percentages increase only by 3 to 4%.

5.4.3 Primary Clarifier WAS Analysis

The next operational modification analyzed was the primary clarifier waste activated sludge (WAS) (defined as waste flowrate divided by plant flowrate) rates. During calibration, a primary clarifier WAS of 0.095% was used (0.0083 MGD).

Analysis indicated that primary clarifier WAS has minimal effect on VSS, X_a, and thus, on CEC removal (Figure 5-78 to Figure 5-80).

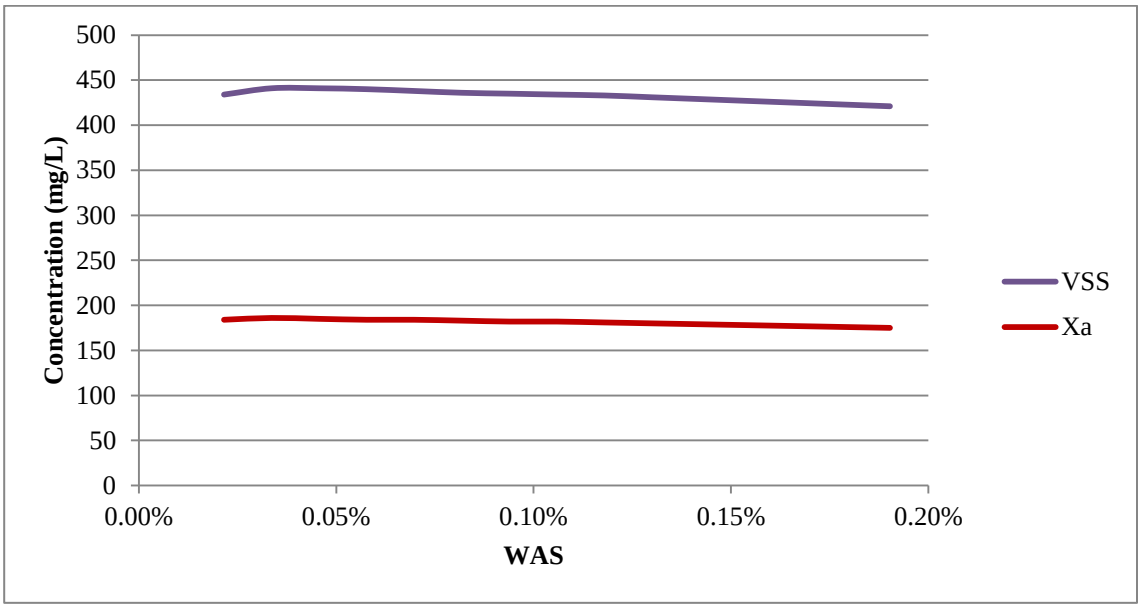

Figure 5-78: Primary Clarifier VSS and X_a with Varying Primary Clarifier WAS

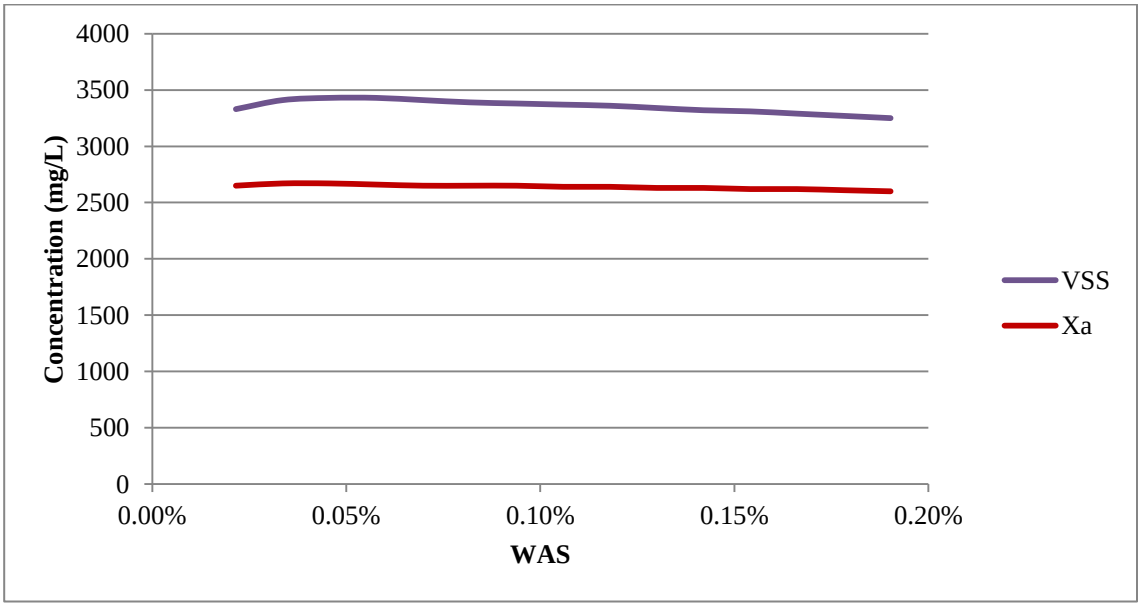

Figure 5-79: PFR VSS and X_a with Varying Primary Clarifier WAS

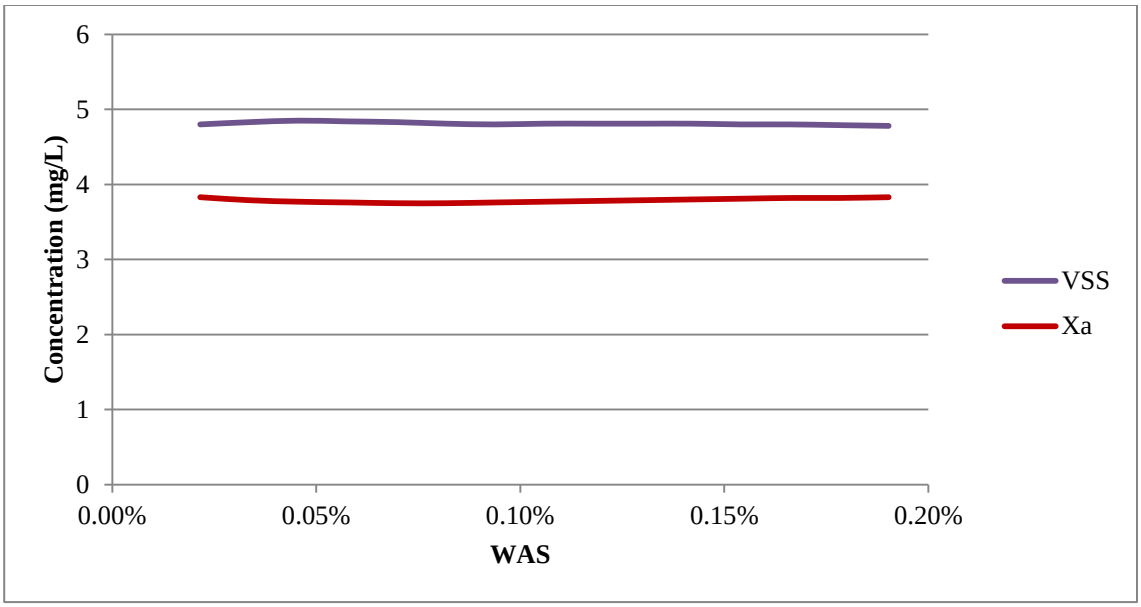

Figure 5-80: Effluent VSS and X_a with Varying Primary Clarifier WAS

Due to the small decrease of VSS and X_a in the primary clarifiers and PFRs, CEC removal percentages slightly decrease with increased WAS. Due to the small removal percentage decrease in the primary clarifiers and PFRs, only the effluent removal change is shown (Figure 5-81 to Figure 5-82). Each CEC modeled experiences a slight decrease in removal percentage as primary clarifier WAS increases.

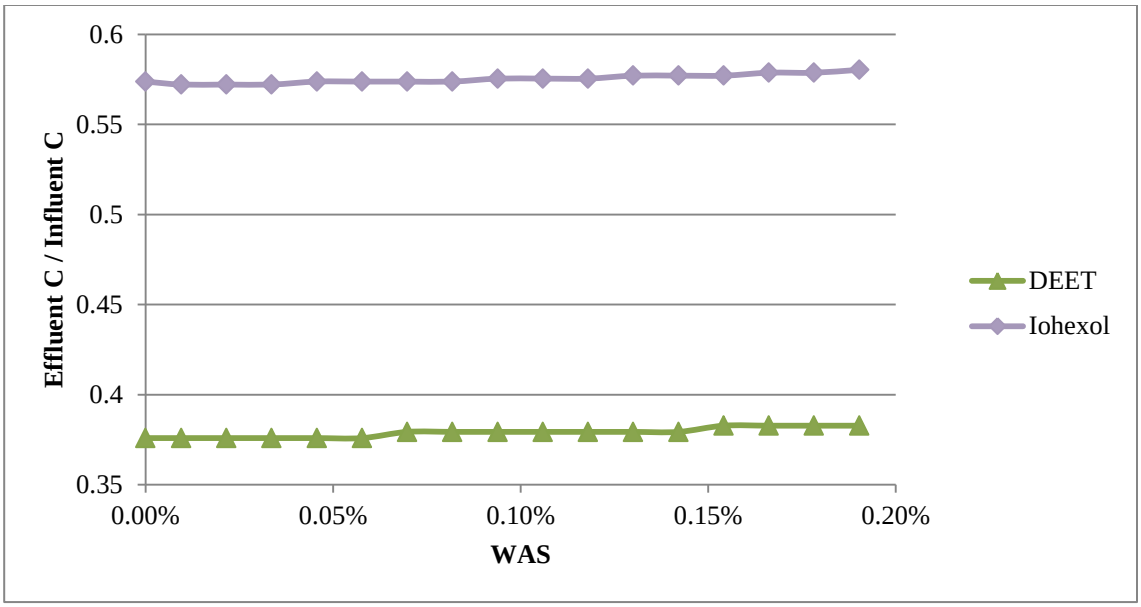

Figure 5-81: Plant CEC Removal with Varying Primary Clarifier WAS (40-65% Removal)

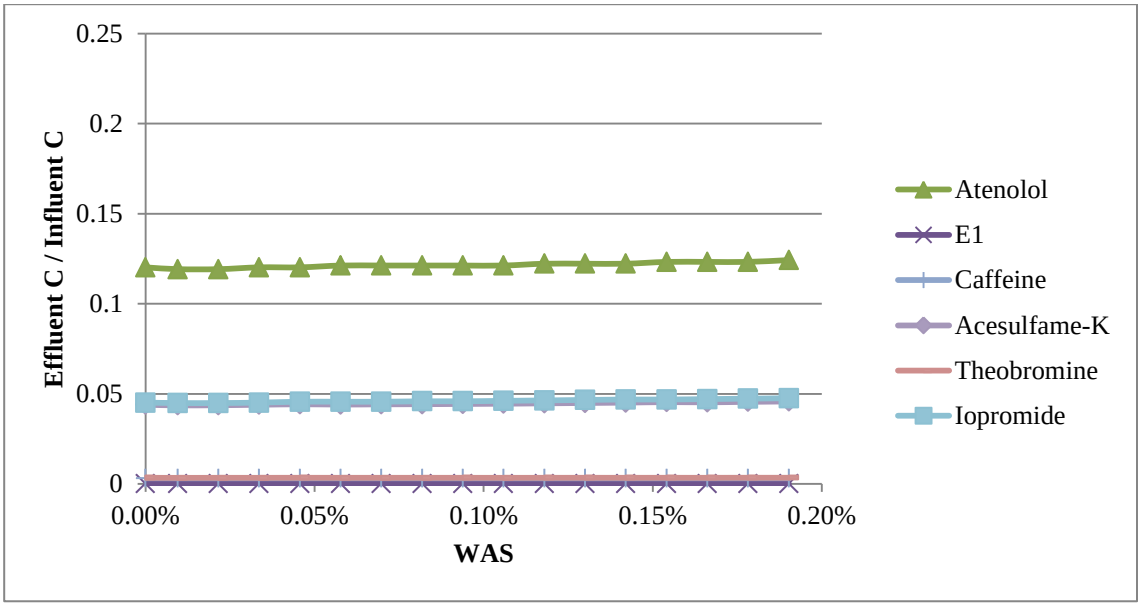

Figure 5-82: Plant CEC Removal with Varying Primary Clarifier WAS (75-100% Removal)

5.4.4 Secondary Clarifier WAS Analysis

The next variable analyzed was the secondary clarifier WAS. Because the SRT in the PFR is a function of the wastage flowrate (Figure 5-83), secondary clarifier WAS has a large effect on CEC concentrations.

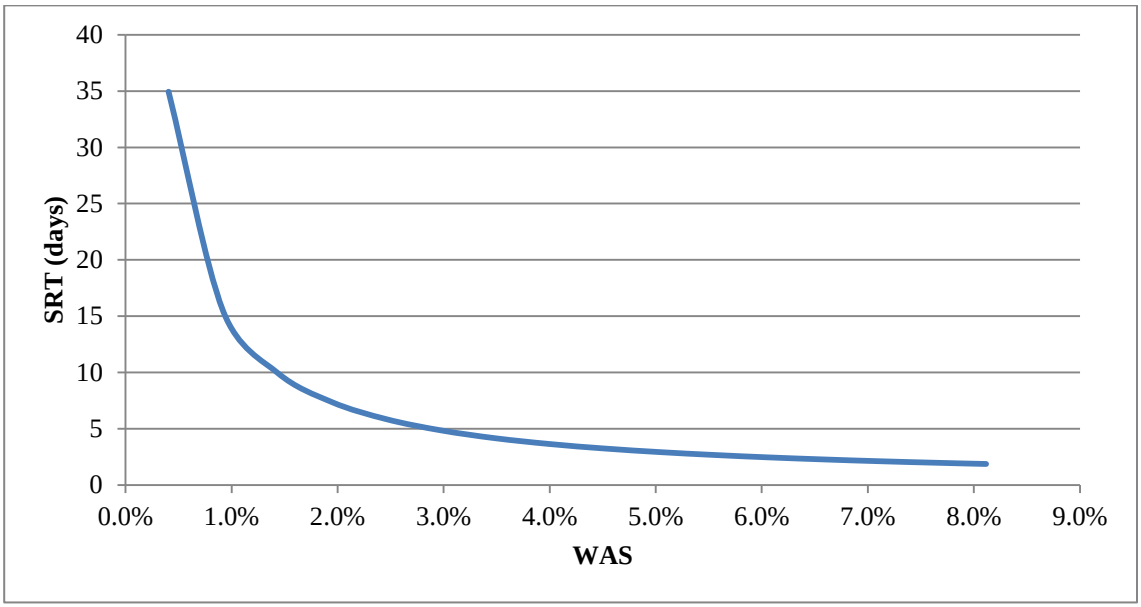

Figure 5-83: SRT vs. Secondary Clarifier WAS

The SRT in the current NWRF layout (base model) is about 8 days. In the expanded model, this SRT is achieved with a WAS of approximately 2% of the influent flow. In the primary clarifier, as secondary clarifier WAS increases, VSS and X_a increase (Figure 5-84). However, the rate of increase is smaller after a WAS of about 4.5%. Interestingly, PFR VSS and X_a increase until WAS reaches this 4.5%. After this point, VSS and X_a begin to decrease with increased WAS (Figure 5-85). This indicates a critical point for WAS, and thus SRT. As will be shown, a secondary clarifier WAS in this range allows for optimal removal of CECs (Figure 5-91 to Figure 5-93). Furthermore, plant effluent VSS and X_a levels off at a WAS of about 4.5% (Figure 5-86). Past this point, effluent concentrations do not decrease significantly.

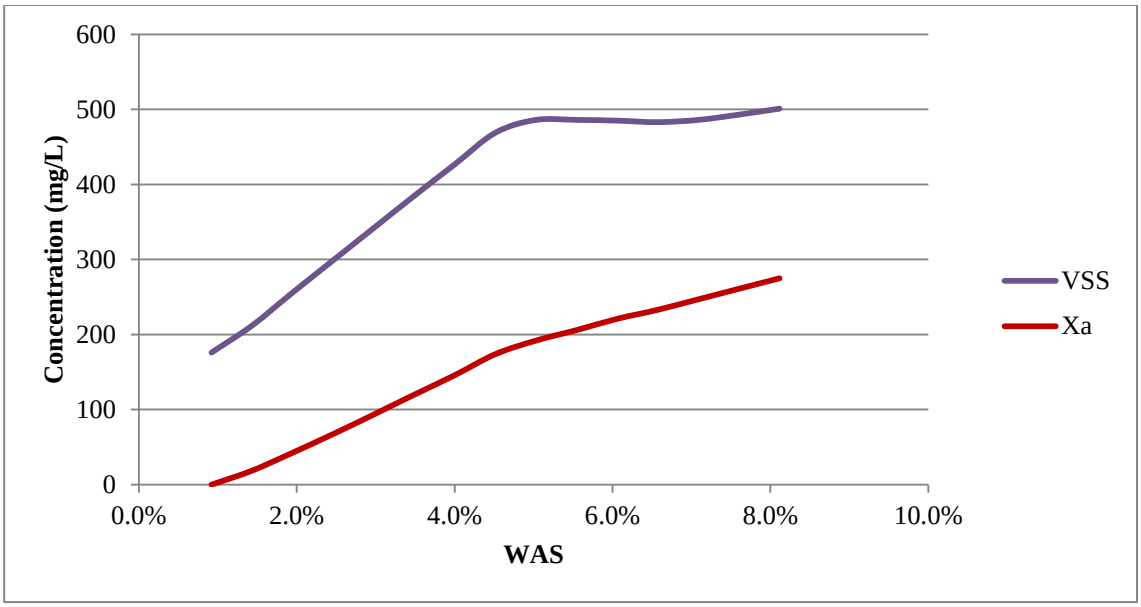

Figure 5-84: Primary Clarifier VSS and X_a with Varying Secondary Clarifier WAS

Figure 5-85: PFR VSS and X_a with Varying Secondary Clarifier WAS

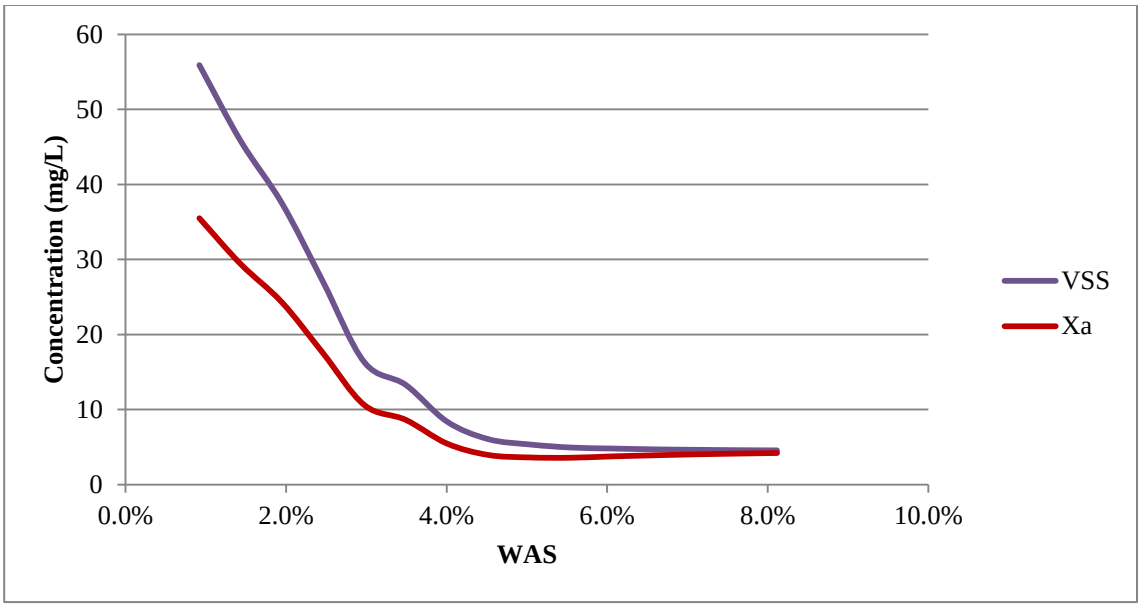

Figure 5-86: Effluent VSS and X_a with Varying Secondary Clarifier WAS

Due to the increased VSS and X_a, secondary clarifier WAS is influential on CEC removal in the primary clarifiers. Almost every CEC experiences increased removal as WAS increases (Figure 5-87).

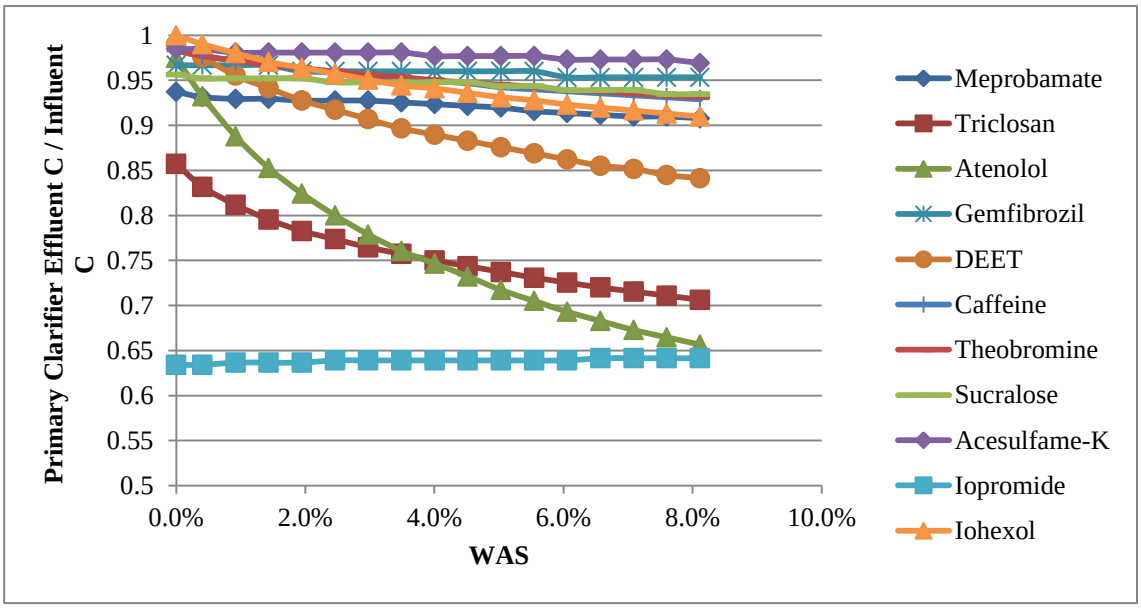

Figure 5-87: Primary Clarifier CEC Removal with Varying Secondary Clarifier WAS

Each CEC modeled (with the exception of iopromide) experiences increased primary clarifier removal percentage as secondary clarifier WAS increases. As WAS approaches 0%, several CECs approach 0% removal. However, some CECs experience an increase of about 10-15% in removal percentage as WAS approaches 8%. While primary clarifier removal is increased, PFR removal decreases with increased WAS (Figure 5-88 to Figure 5-90). After WAS reaches about 4.5%, VSS and X_a decrease, resulting in decreased CEC removal percentages in the PFR (Figure 5-85).

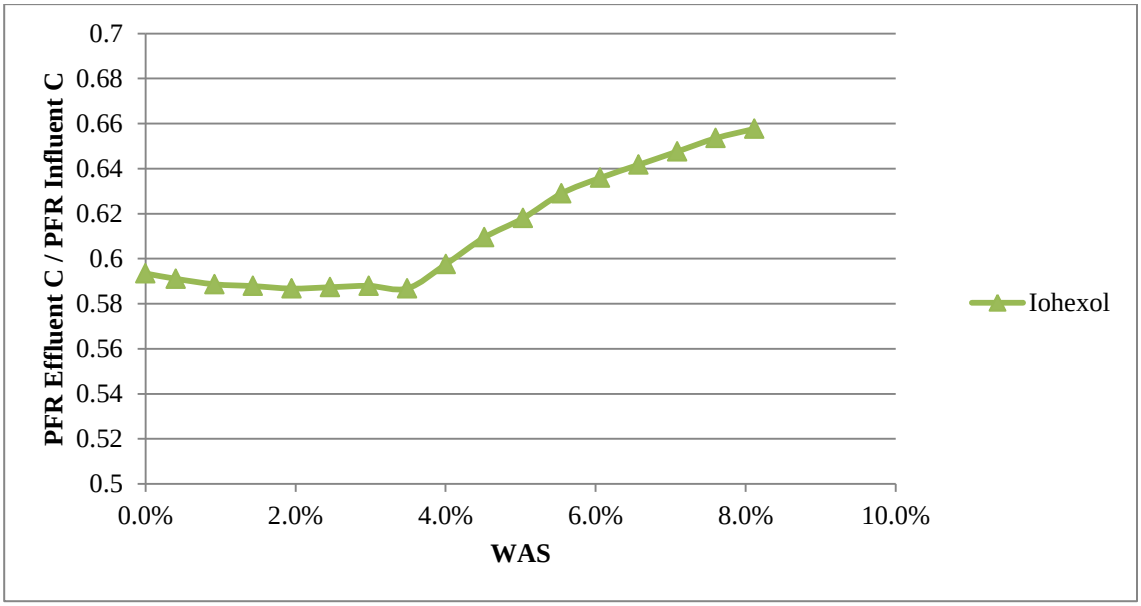

Figure 5-88: PFR CEC Removal with Varying Secondary Clarifier WAS (30-50% Removal)

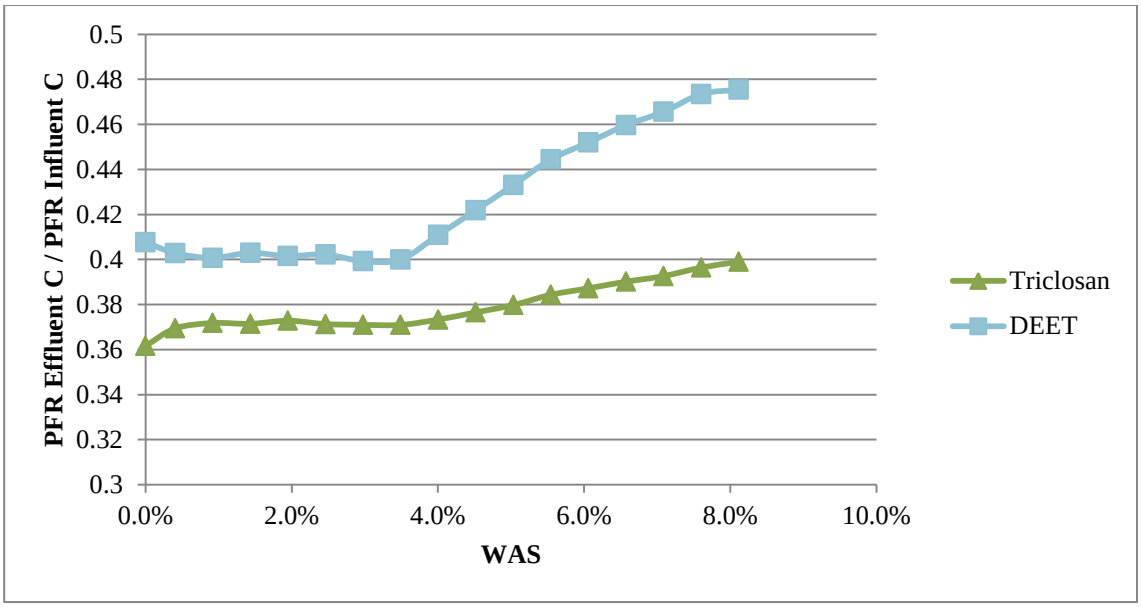

Figure 5-89: PFR CEC Removal with Varying Secondary Clarifier WAS (50-70% Removal)

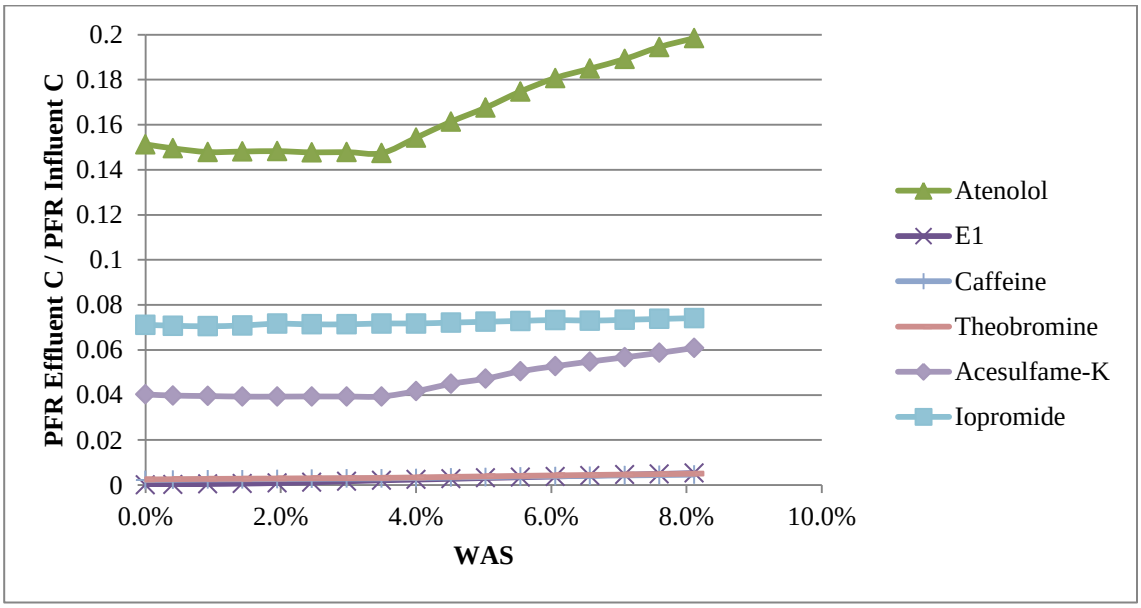

Figure 5-90: PFR CEC Removal with Varying Secondary Clarifier WAS (80-100% Removal)

For each CEC modeled, PFR CEC removal is relatively unchanged until WAS reaches 3.5 to 4%. At this point, removal percentages for iohexol, DEET, and atenolol decrease by 5% or more. Triclosan and acesulfame-K decrease in removal percentage

by about 2%. For this reason, 4.5% is considered a critical point for WAS, which corresponds to a SRT of 4.2 days. It is this range that plant CEC removal is optimum (Figure 5-91 to Figure 5-93).

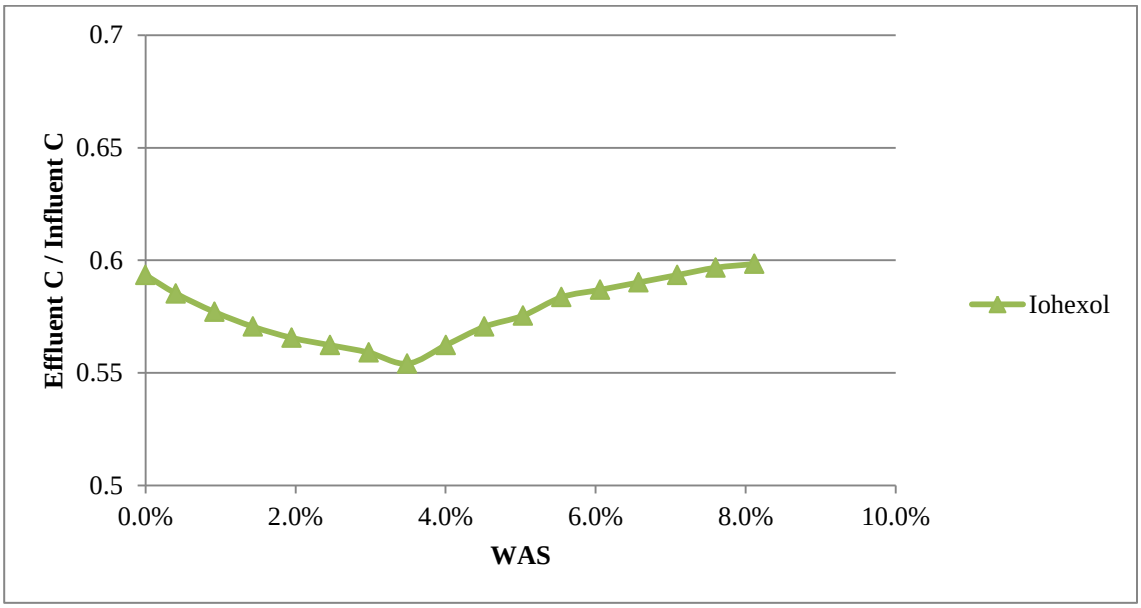

Figure 5-91: Plant CEC Removal with Varying Secondary Clarifier WAS (30-70% Removal)

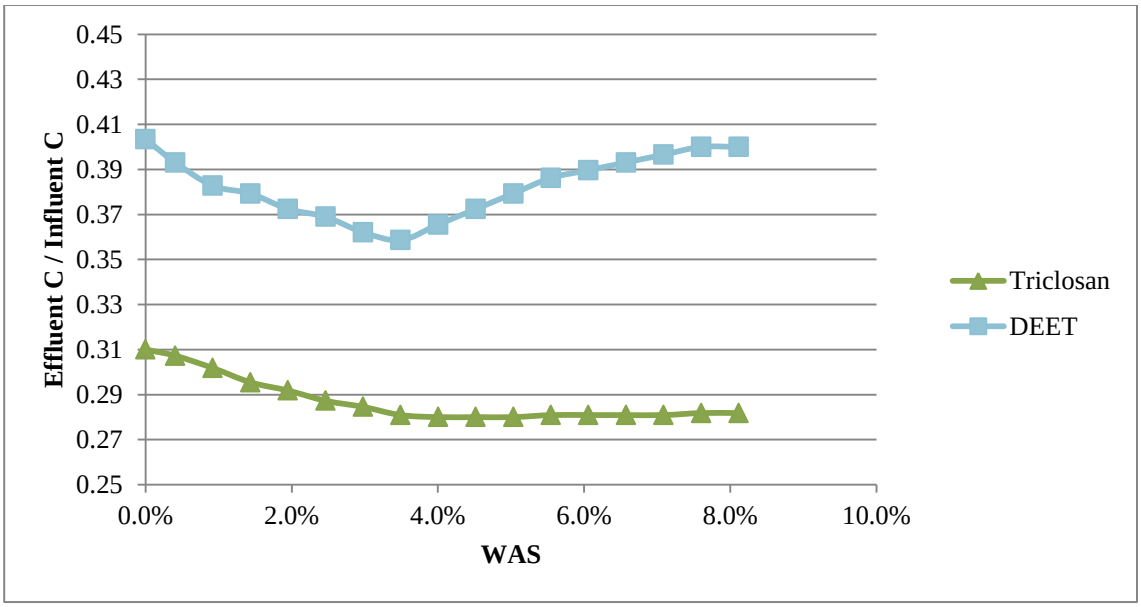

Figure 5-92: Plant CEC Removal with Varying Secondary Clarifier WAS (55-75% Removal)

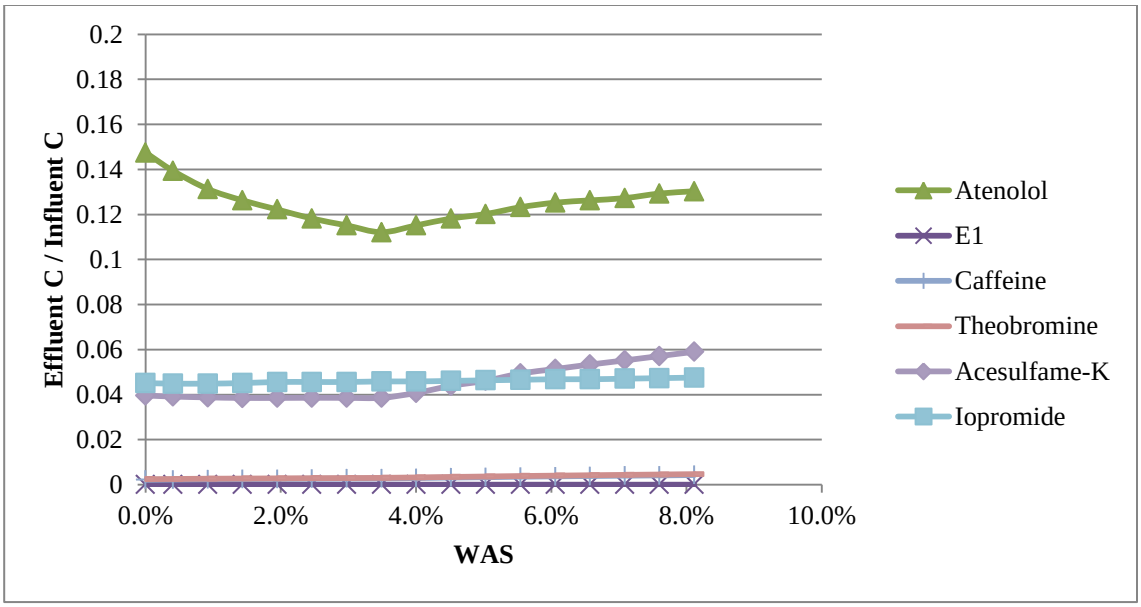

Figure 5-93: Plant CEC Removal with Varying Secondary Clarifier WAS (80-100% Removal)

The critical secondary clarifier WAS range for CEC removal is between 2 and 5% (Figure 5-91 to Figure 5-93). This critical WAS can also be seen when analyzing TSS, cBOD, and TKN (Figure 5-94). As shown, all three of these parameters reach a near-minimum point in this range. In this range, most CECs experience maximum removal. Secondary clarifier WAS proved to be the operational change that had the largest effect on CEC removal. Iohexol and DEET experience up to 5% change in removal percentage as WAS varies. Compared with RAS and primary clarifier volume, this is a significant effect. Because WAS is an operational parameter, adjusting WAS to control CEC concentrations is a feasible consideration.

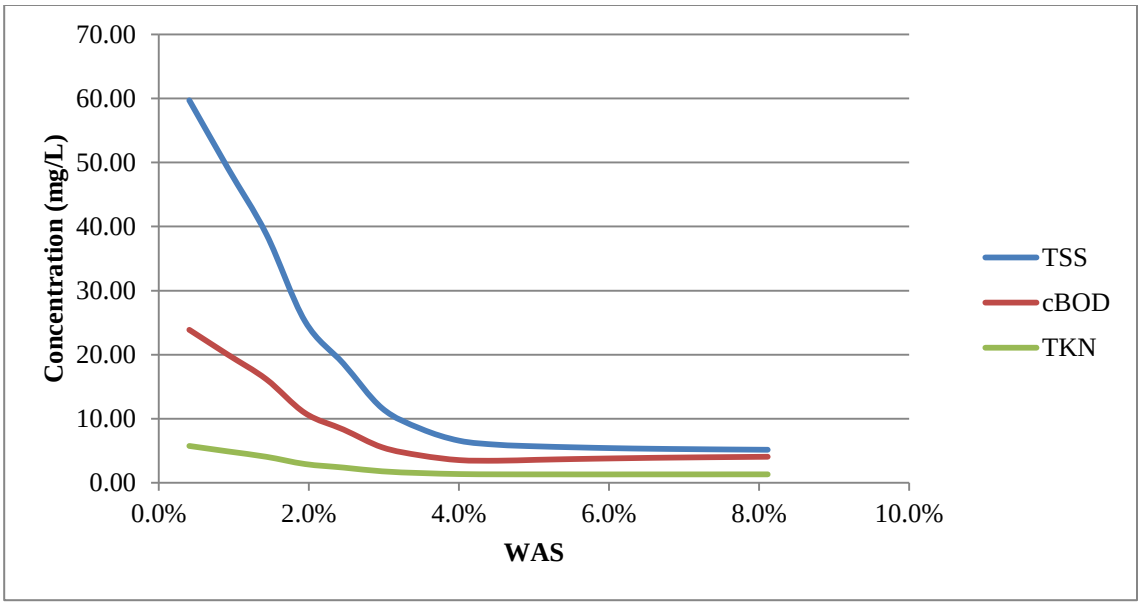

Figure 5-94: Plant Effluent TSS, cBOD, and TKN with Varying Secondary Clarifier WAS

5.5 Advanced Model

After the analysis of several parameters in the expanded model, the advanced model was developed by replacing the PFRs with membrane bioreactors (MBRs). The MBRs are modeled using the same volume as the PFRs, and each has three chambers. Unlike the PFRs in GPS-X, MBRs use internal recycle as their RAS. Rather than have a line from the settled matter in the secondary clarifier like with the PFR, the MBR recycles from the third chamber to the first. Furthermore, with the PFRs, WAS flow from the secondary clarifiers controls the SRT in the reactors. With the MBR, pumped flow from the MBR (WAS) itself controls the SRT (Figure 5-95).

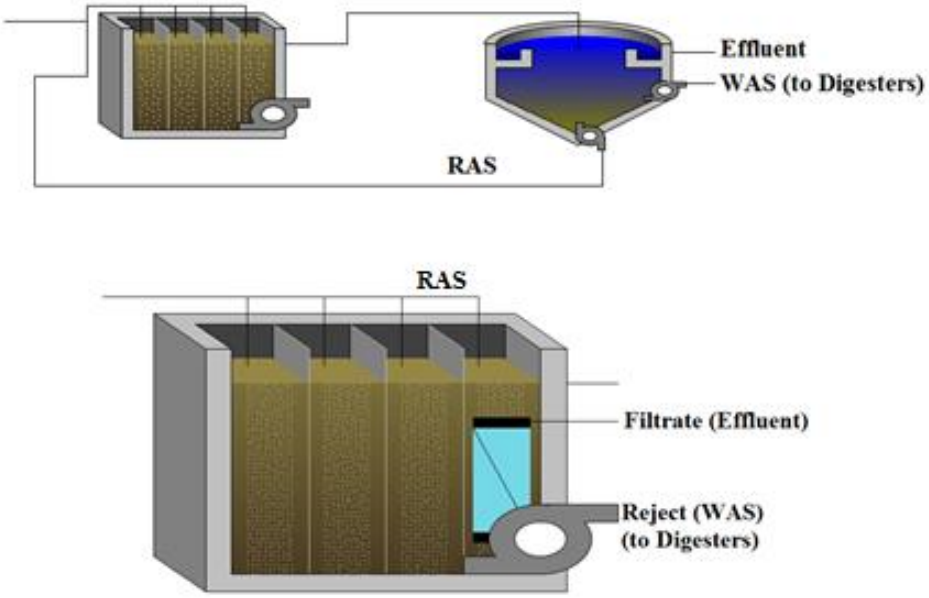

Figure 5-95: PFR vs. MBR Effluent, RAS, and WAS in GPS-X

Because the NWRF does not currently have MBRs, the first step in modeling was to evaluate the sensitivity of CEC removals to changes in RAS and WAS. WAS from the secondary clarifier was also examined but had minimal effect on CEC removal. This is due to the fact that the secondary clarifier only receives filtrate water. Therefore, even the settled solid concentrations in the secondary clarifier are low. After the analysis of RAS and WAS, the optimized advanced plant could be analyzed and compared to the enhanced plant.

5.5.1 MBR WAS Analysis

As mentioned, WAS is one of the controlling factors in SRT. In the MBR, WAS is defined as the waste flowrate per MBR divided by the influent flowrate to each MBR. As WAS increases, SRT decreases (Figure 5-96).

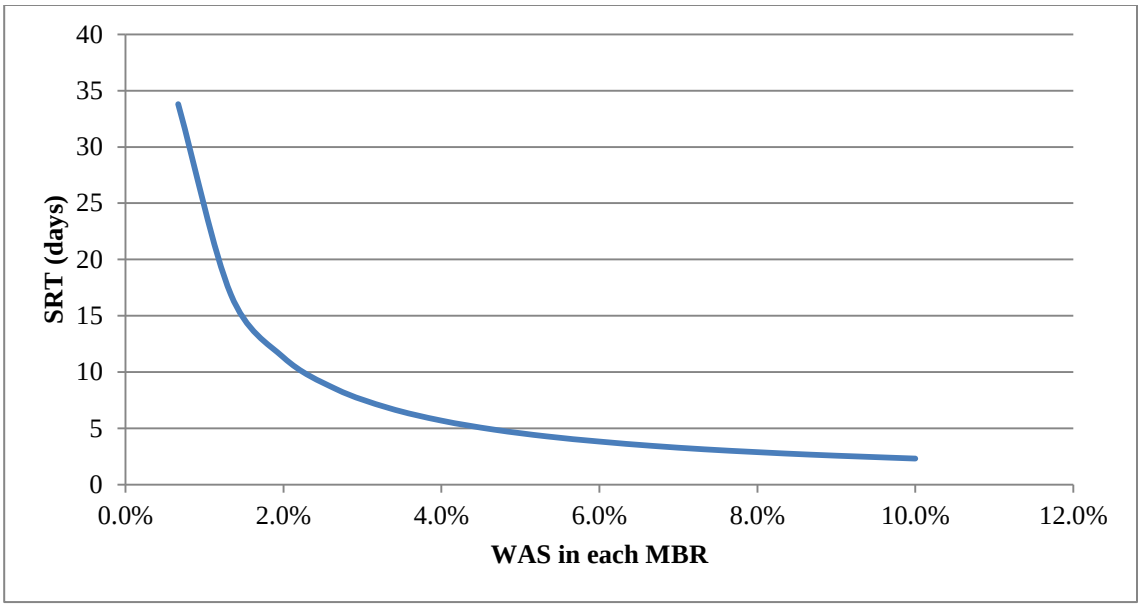

Figure 5-96: SRT vs. MBR WAS

In the primary clarifier, as WAS increases, X_a also increases. VSS reaches a maximum point at a WAS of 2%. After this point, it decreases until WAS reaches approximately 6%. As WAS approaches 10%, VSS slightly increases (Figure 5-97).

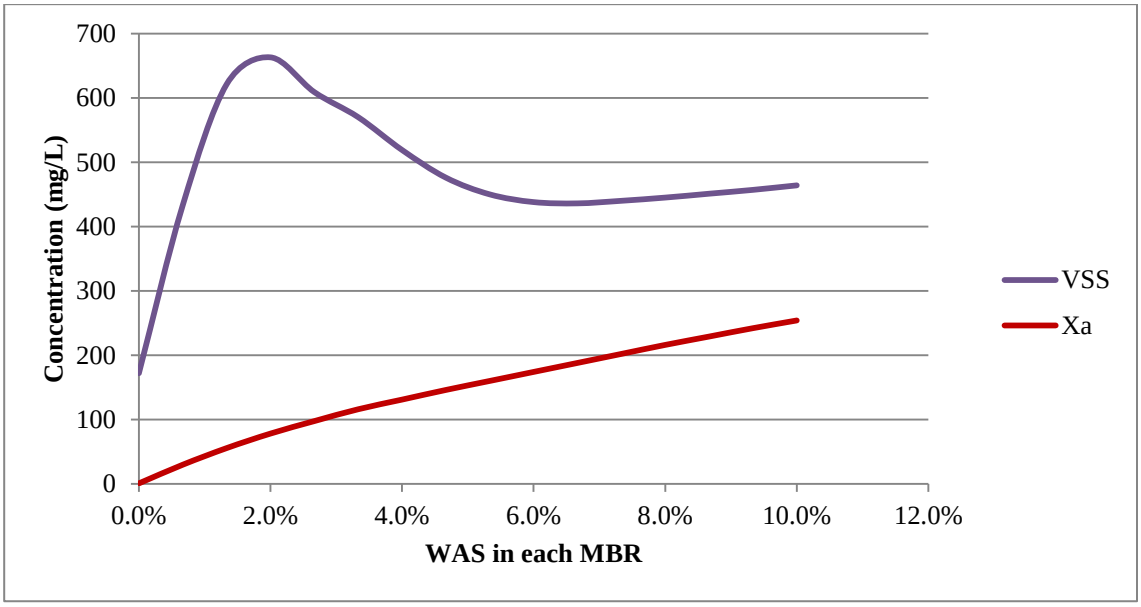

Figure 5-97: Primary Clarifier VSS and X_a with Varying MBR WAS

MBR WAS follows a similar VSS and X_a concentration pattern to secondary clarifier WAS with a PFR (Figure 5-84). In the MBRs, both RAS and WAS streams have equal concentrations. Furthermore, these streams are equal to the concentrations found in the third chamber of the MBR. During WAS variation, all three chambers follow the same VSS and X_a trends, so chambers one and two are not shown.

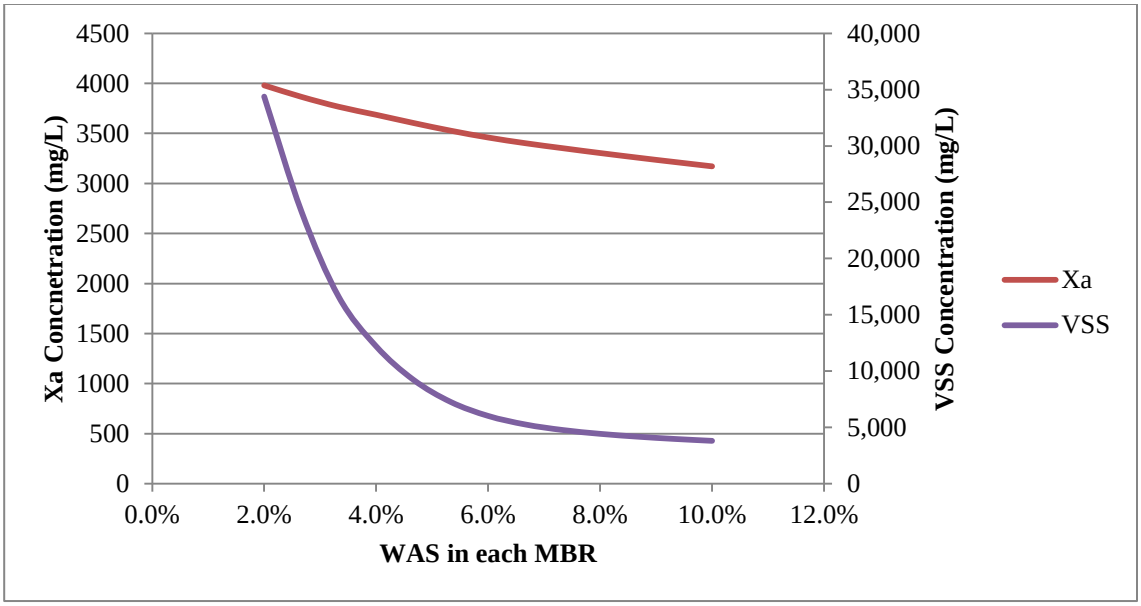

Figure 5-98: MBR RAS and WAS Streams VSS and X_a with Varying MBR WAS

While X_a decrease is gradual, VSS decreases exponentially with increased WAS. The dramatic decrease in VSS is likely the cause of the maximum point found in the primary clarifiers. At low WAS, because the VSS is largely removed by the membrane (Figure 5-99), higher concentrations are entering the RAS and WAS streams. As WAS leaves the PFR and is sent through the digesters and then to the front of the plant, the high concentrations at lower rates cause the primary clarifier to spike (Figure 5-97).

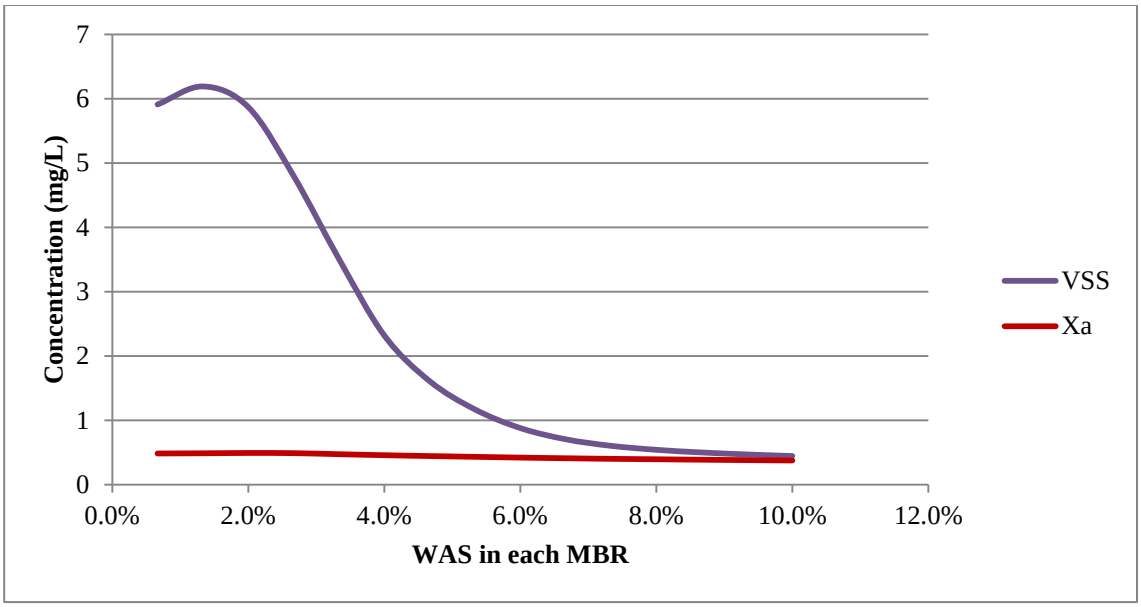

Figure 5-99: MBR Filtrate VSS and X_a with Varying MBR WAS

The membrane in the MBR largely removes VSS and X_a (Figure 5-99). The *filtrate* concentrations are within the same order of magnitude as the *plant effluent* concentrations when the PFR is used. Because filtrate concentrations are so low, the secondary clarifier is now essentially a polishing clarifier (Figure 5-100).

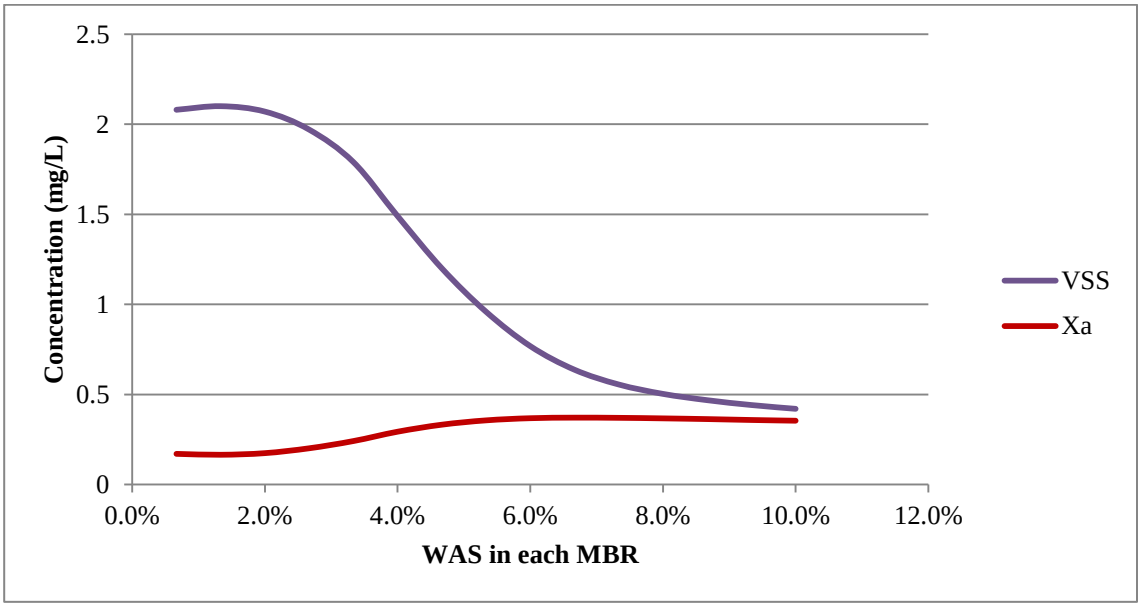

Figure 5-100: Effluent VSS and X_a with Varying MBR WAS

Due to the increased concentrations of VSS and X_a in primary clarifiers, CECs experience higher removal in the primary clarifiers as WAS increases (Figure 5-101). Removal patterns in the primary clarifiers are similar to those when PFRs are used and WAS from the secondary clarifiers increases (Figure 5-87).

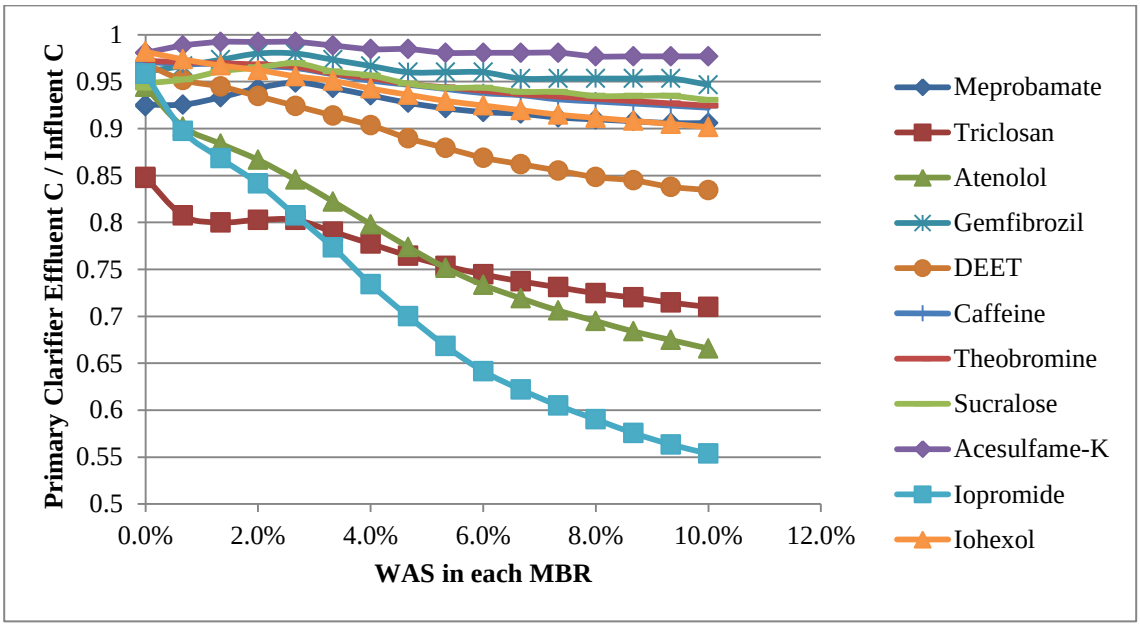

Figure 5-101: Primary Clarifier CEC Removal with Varying MBR WAS

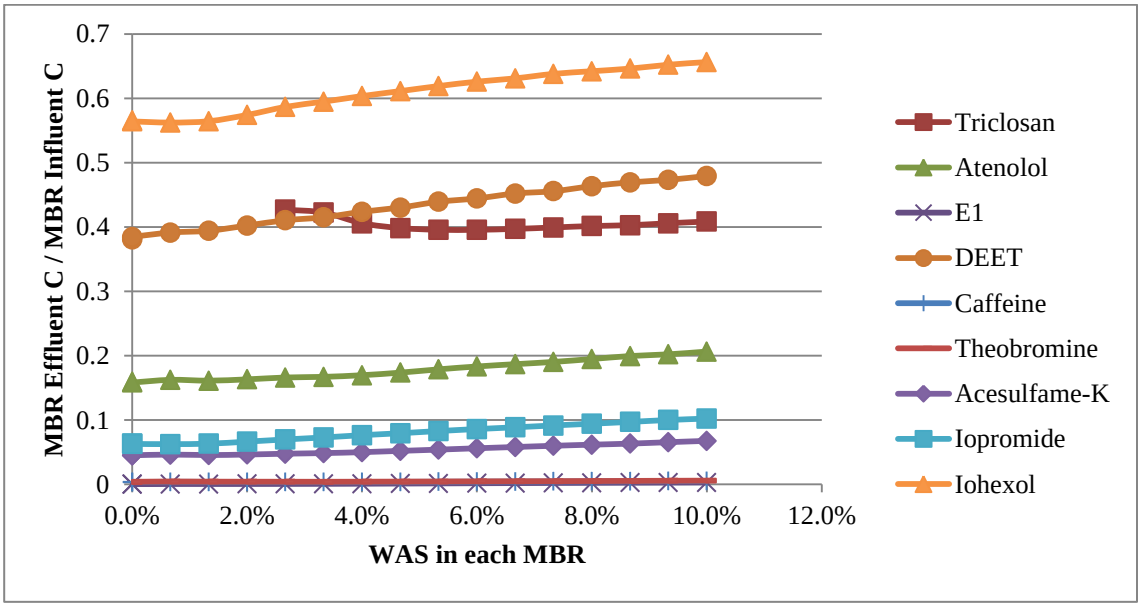

Figure 5-102: MBR CEC Removal with Varying MBR WAS

Because VSS and X_a decrease in the MBRs as WAS increases, CEC removal decreases (Figure 5-102). Iohexol and DEET experience close to 10% decrease in removal percentage, while atenolol, iopromide, and acesulfame-K about 5% change. In general, the rate at which MBR removal decreases is smaller than the rate which primary clarifier removal increases.

Finally, the overall plant removal was analyzed. Because primary clarifier removal increases and MBR removal decreases, overall removal was relatively constant (Figure 5-103). Although gradual, CECs tend to experience change in removal percentage after WAS reaches about 5%, corresponding to a SRT of about 4.5 days. Although MBR removal percentages do not fluctuate as much as primary clarifier percentages, because more removal occurs in the MBRs, plant removal change is small (only up to 3% for DEET and iohexol).

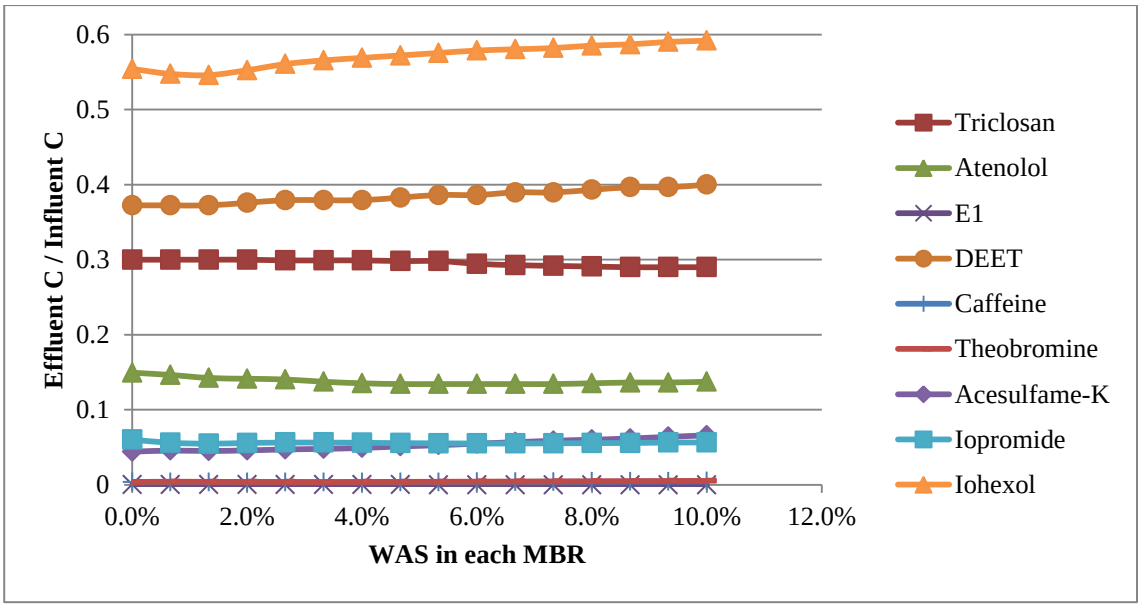

Figure 5-103: Plant CEC Removal with Varying MBR WAS

5.5.2 MBR RAS Analysis

In MBRs, RAS can be as high as four times (400%) larger than the influent flow (Davis, 2010). To ensure that the optimized RAS was chosen, it was analyzed from 100 to 800% in each MBR. In the primary clarifiers, RAS has little effect on VSS and X_a concentrations (Figure 5-104).

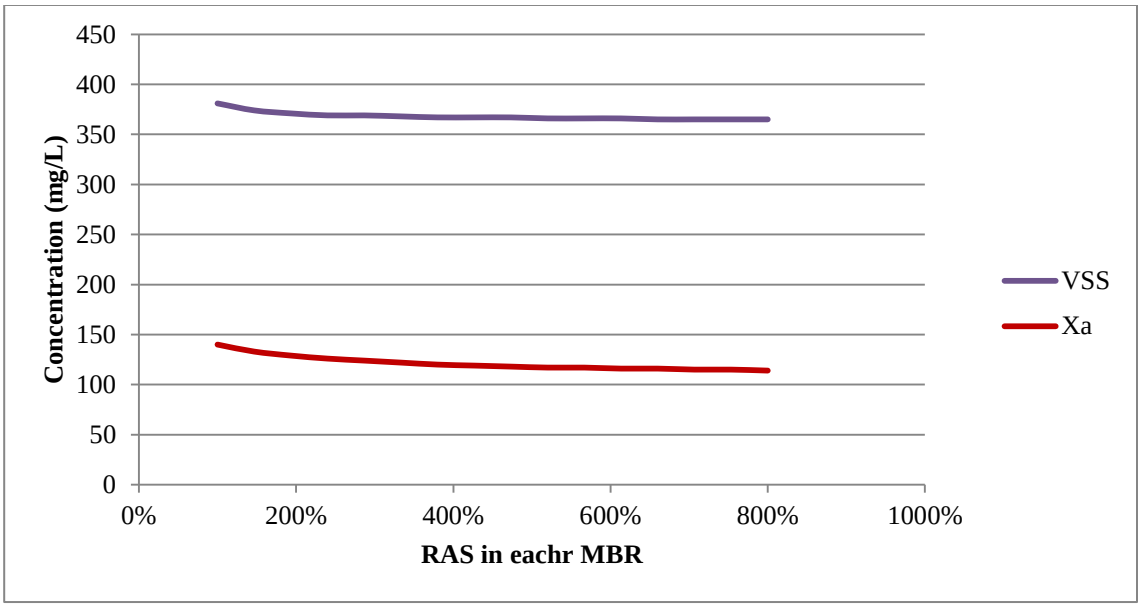

Figure 5-104: Primary Clarifier VSS and X_a with Varying RAS

Unlike in varying WAS analysis, VSS and X_a concentrations in each MBR chamber display different patterns as RAS increases. While VSS and X_a in the first two chambers increase with increasing RAS, concentrations in the third chamber decreased (Figure 5-105). Because RAS is pumped from the last chamber to the first, as RAS increases, a higher mass loading is sent from the effluent to the MBR to the influent. While this decreases concentrations in the third chamber, it increases concentrations in the first and second.

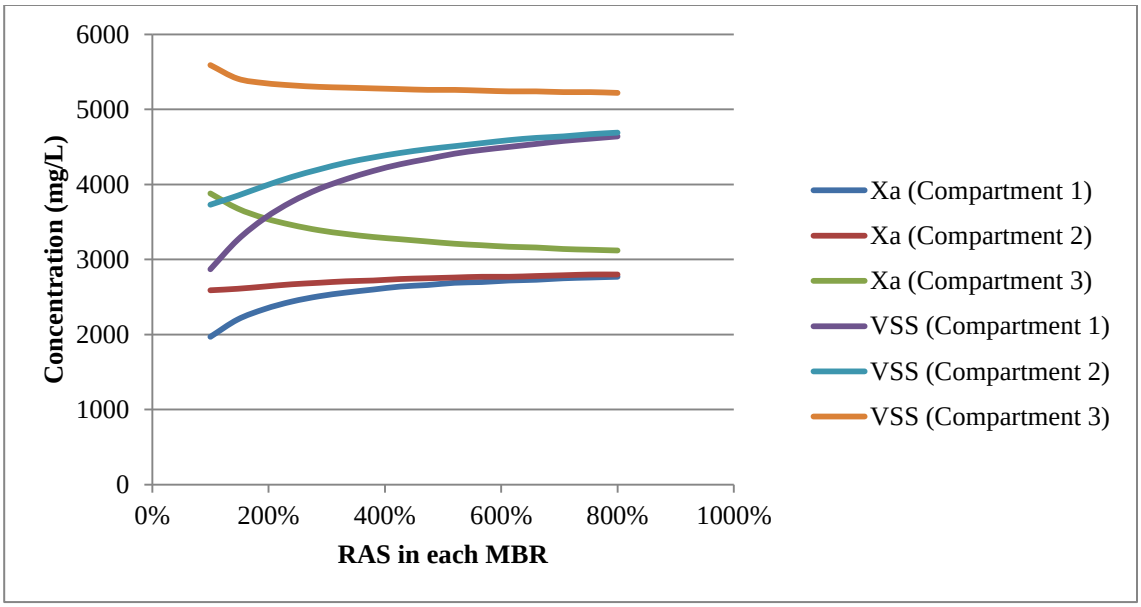

Figure 5-105: MBR VSS and X_a with Varying RAS

Similar to the primary clarifiers, RAS has little effect on filtrate and plant effluent concentrations. Furthermore, because the membrane treats the water to low VSS and X_a concentrations, the secondary clarifier acts only as a polishing tank, without significant removal (Figure 5-106 to Figure 5-107).

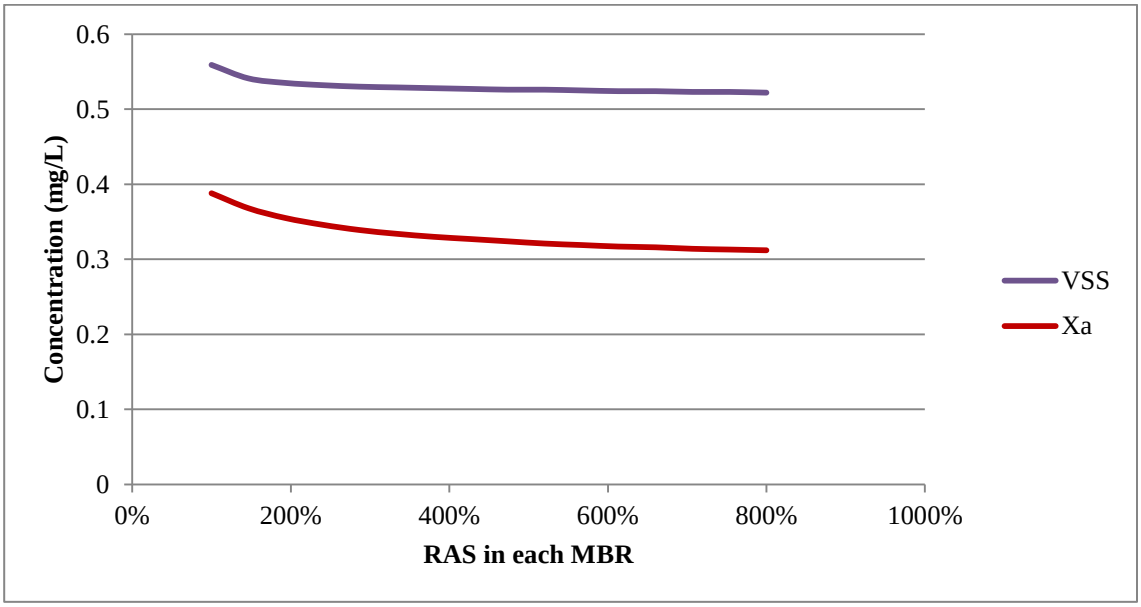

Figure 5-106: MBR Filtrate VSS and X_a with Varying RAS

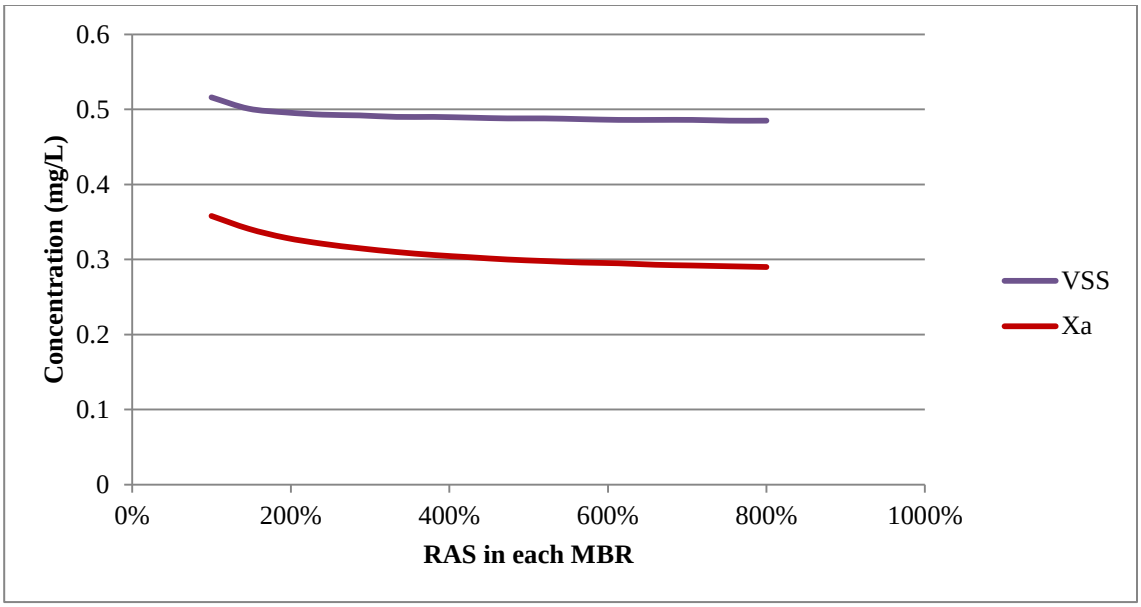

Figure 5-107: Effluent VSS and X_a with Varying RAS

Due to the small change in removal percentages in the primary clarifiers and MBRs, CEC data is not shown. In both, CEC removal slightly decreases as RAS increases. The same is true for overall plant removal. Although the change is small, as RAS increases, CEC removal decreases (Figure 5-108).

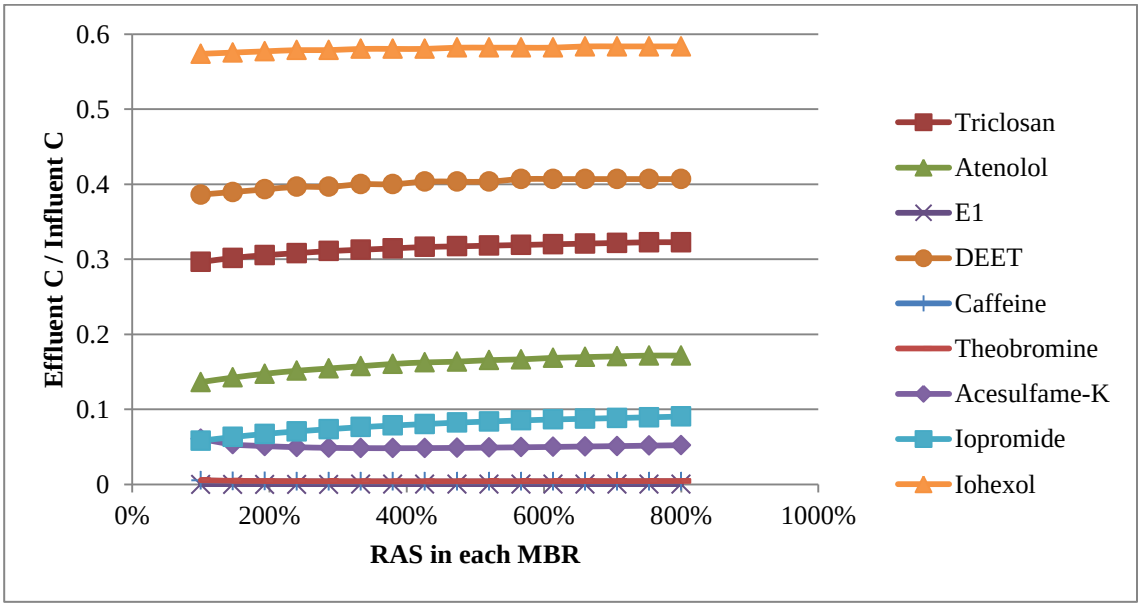

Figure 5-108: Plant CEC Removal with Varying RAS

At lower RAS rates, CEC removal increases at a larger rate than it does as RAS approaches 800% (Figure 5-108). Regardless of the removal percentage, each CEC tends to decrease in removal percentage at relatively the same rate. As with the expanded model RAS, there is a balance between other constituents and CECs. As RAS increases, plant effluent VSS and X_a decrease but CEC concentrations increase. However, the change in removal percentage is small (<3% for most CECs) even as RAS approaches 800%.

5.6 Expanded and Advanced Model Comparisons

After sensitivity analyses were completed for the enhanced and advanced models, the two were compared to determine the improvement of MBRs in the removal of CECs at the NWRF. First, using these analyses, optimized WAS and RAS rates were determined for each model. These rates (shown below) were selected based on CEC removal as well as effluent VSS and X_a concentrations, attempting to find a balance between the parameters. The optimized parameters are as follows:

- Expanded model:
    - Primary Clarifier WAS: 0.1%
    - Secondary Clarifier WAS: 4%
    - RAS: 70%
- Advanced model:
    - Primary Clarifier WAS: 0.1%
    - Secondary Clarifier WAS: 4%
    - MBR WAS: 5%

- RAS: 200%

With these parameters, the models were compared using sampling data (with modified flowrate). First, VSS and X_a concentrations were analyzed throughout the plant (Figure 5-109). The expanded model has larger concentrations of VSS and X_a in the preliminary and primary clarifier effluents. Secondary clarifier WAS is less concentrated in the advanced model because of the high removal from the membrane in the MBR. For this reason, because WAS is eventually returned to the front of the NWRF, preliminary and primary clarifier effluent VSS and X_a concentrations are lower in the advanced model. However, as mentioned, even when WAS approached 0%, there was not a significant increase in VSS or X_a concentrations (Figure 5-103).

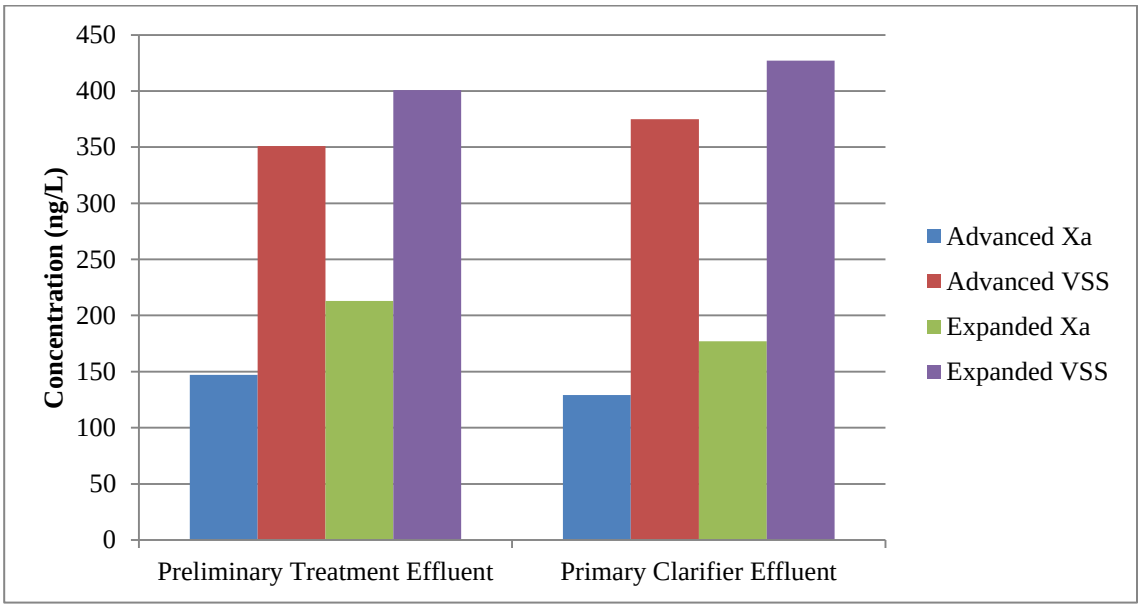

Figure 5-109: Preliminary and Primary Clarifier Advanced vs. Expanded X_a and VSS under Sampling Conditions (Modified Flowrate)

Next, VSS and X_a were analyzed in the PFR, MBR, and plant effluents. While expanded model concentrations are relatively stable throughout the PFR, concentrations

in the MBR (advanced model) increase by chamber. The averages of the three chambers for VSS and X_a in both models are:

- Advanced model X_a: 2820 mg/L
- Advanced model VSS: 4393.33 mg/L
- Expanded model X_a: 2646.67 mg/L
- Expanded model VSS: 3360 mg/L

There is just a small difference in the X_a concentrations between the advanced and expanded models. The advanced model VSS concentration, meanwhile, is about 30% larger than the expanded model.

Although it is difficult to tell in the graph, expanded model plant effluent VSS and X_a concentrations are approximately ten times larger than concentrations in the advanced model (Figure 5-110). This can be attributed to the membrane, which removes VSS and X_a to concentrations of less than 1 mg/L.

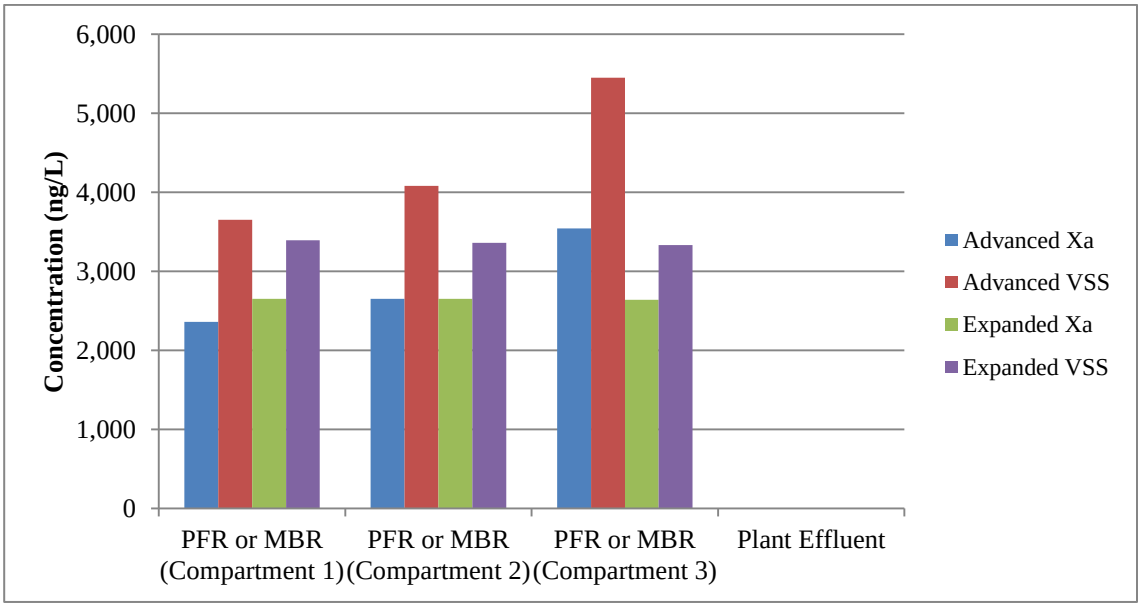

Figure 5-110: MBR or PFR Advanced vs. Expanded X_a and VSS under Sampling Conditions (Modified Flowrate)

Because of the higher concentrations of VSS and X_a in the primary clarifiers, the expanded model primary clarifiers typically remove CECs slightly better than the advanced model primary clarifiers. PFR and MBR removal percentages are similar for the two models. Despite the higher levels of X_a in the MBRs, CEC removal does not change significantly (Figure 5-111 to Figure 5-122).

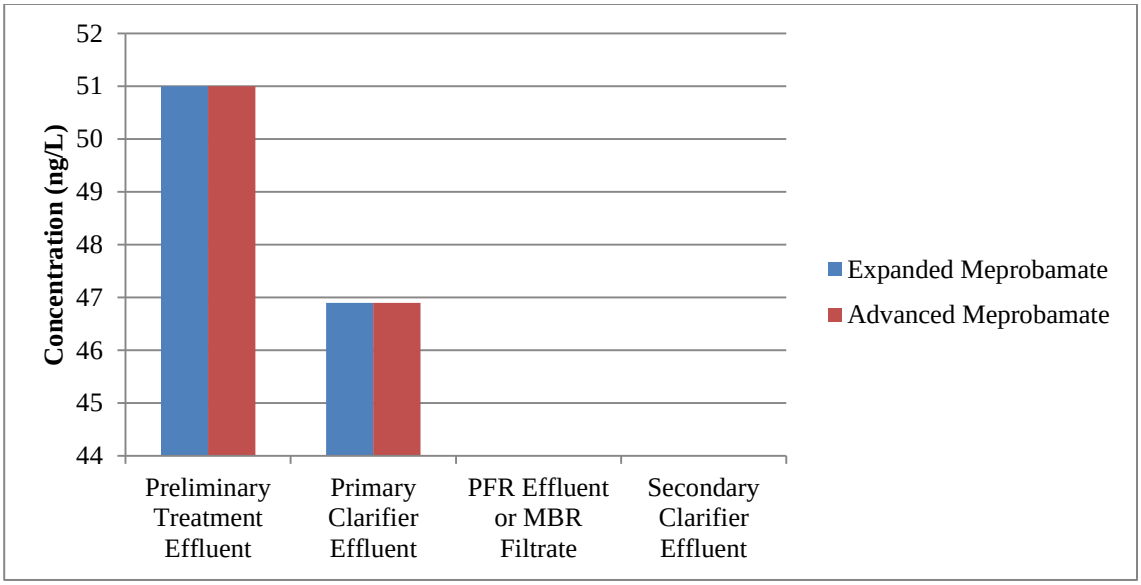

Figure 5-111: Expanded vs. Advanced Meprobamate under Sampling Conditions (Modified Flowrate)

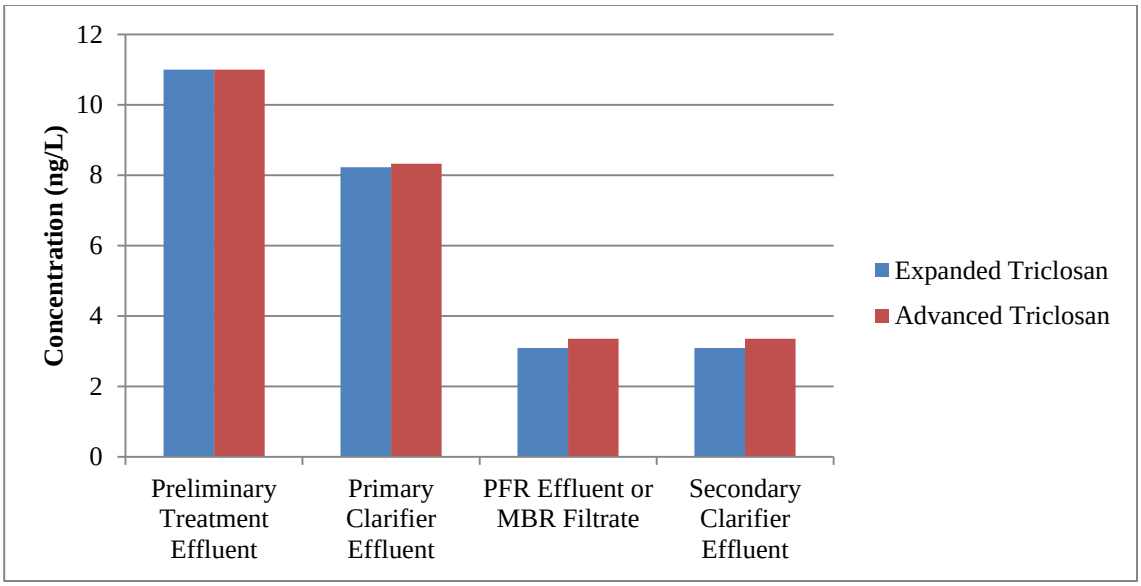

Figure 5-112: Expanded vs. Advanced Triclosan under Sampling Conditions (Modified Flowrate)

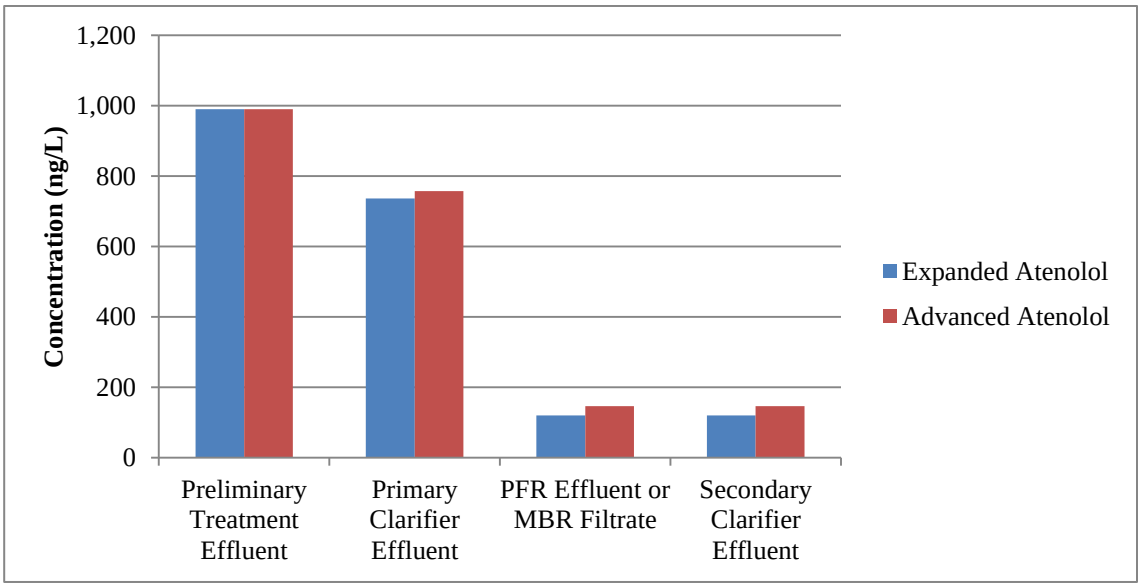

Figure 5-113: Expanded vs. Advanced Atenolol under Sampling Conditions (Modified Flowrate)

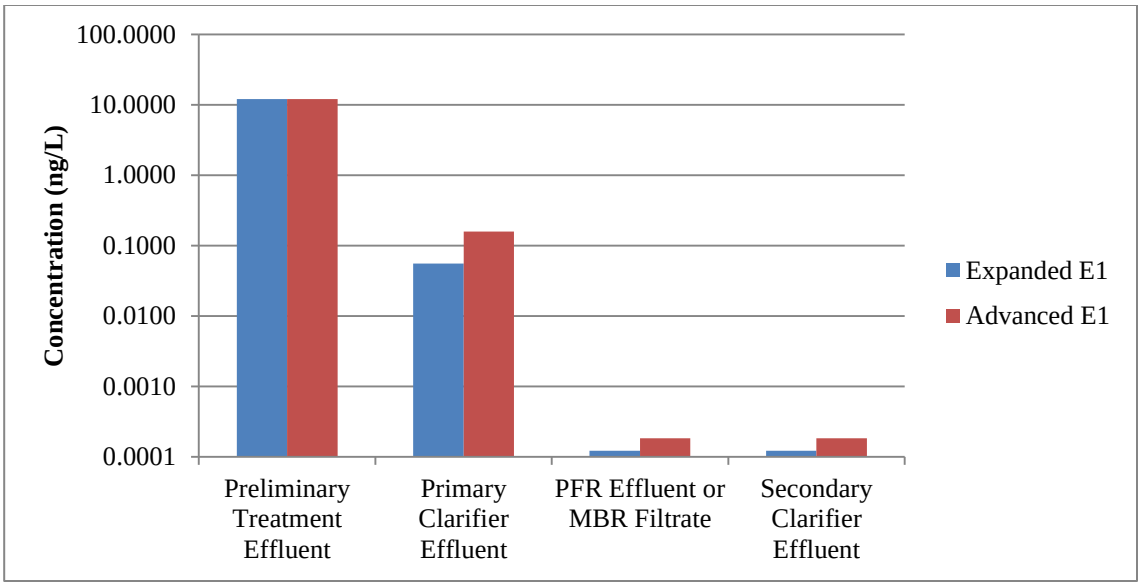

Figure 5-114: Expanded vs. Advanced E1 under Sampling Conditions (Modified Flowrate)

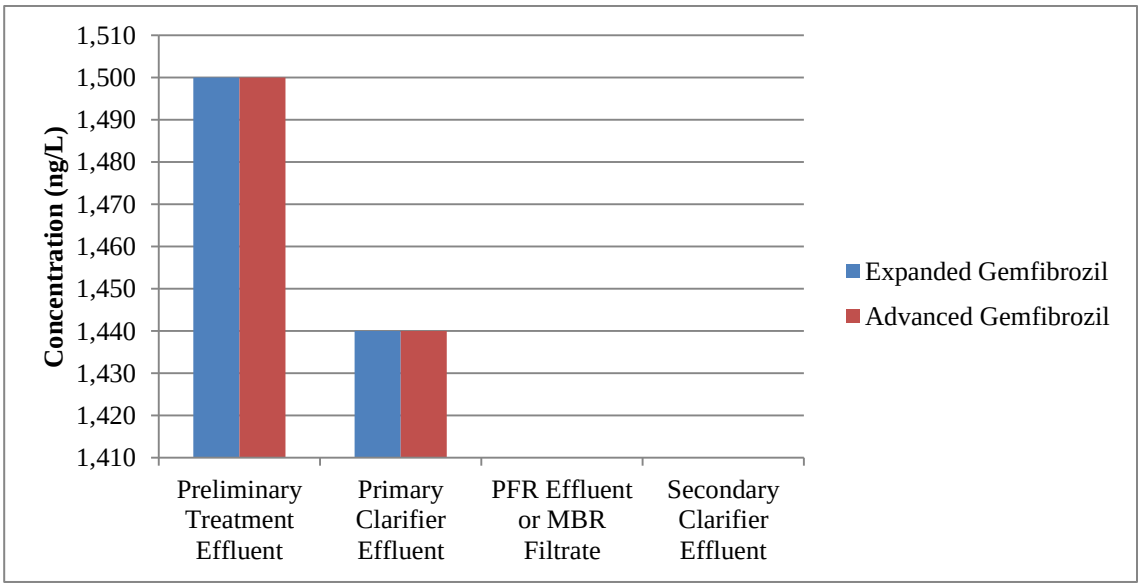

Figure 5-115: Expanded vs. Advanced Gemfibrozil under Sampling Conditions (Modified Flowrate)

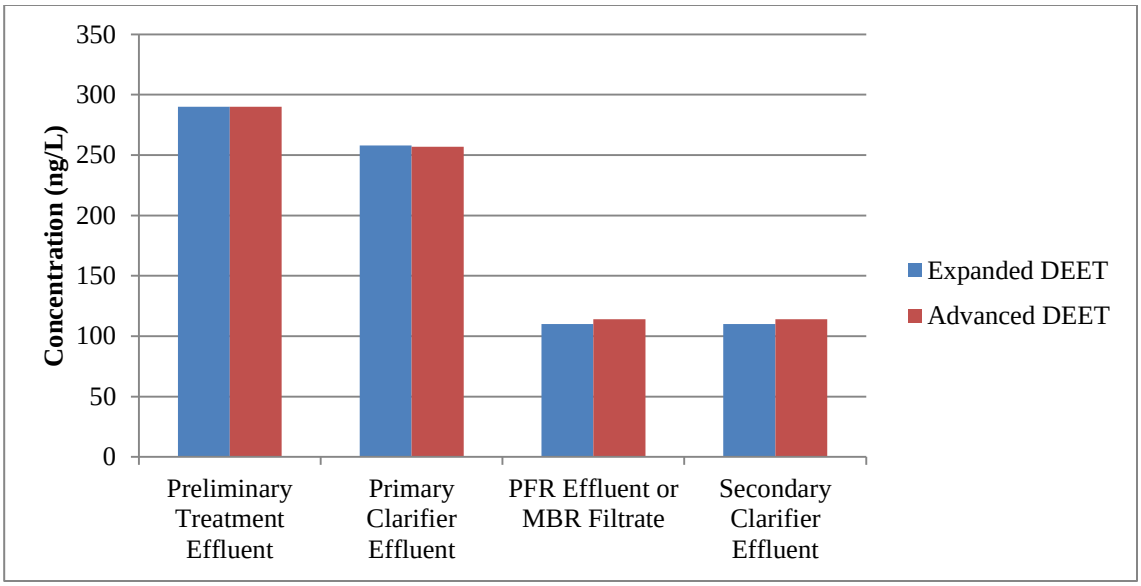

Figure 5-116: Expanded vs. Advanced DEET under Sampling Conditions (Modified Flowrate)

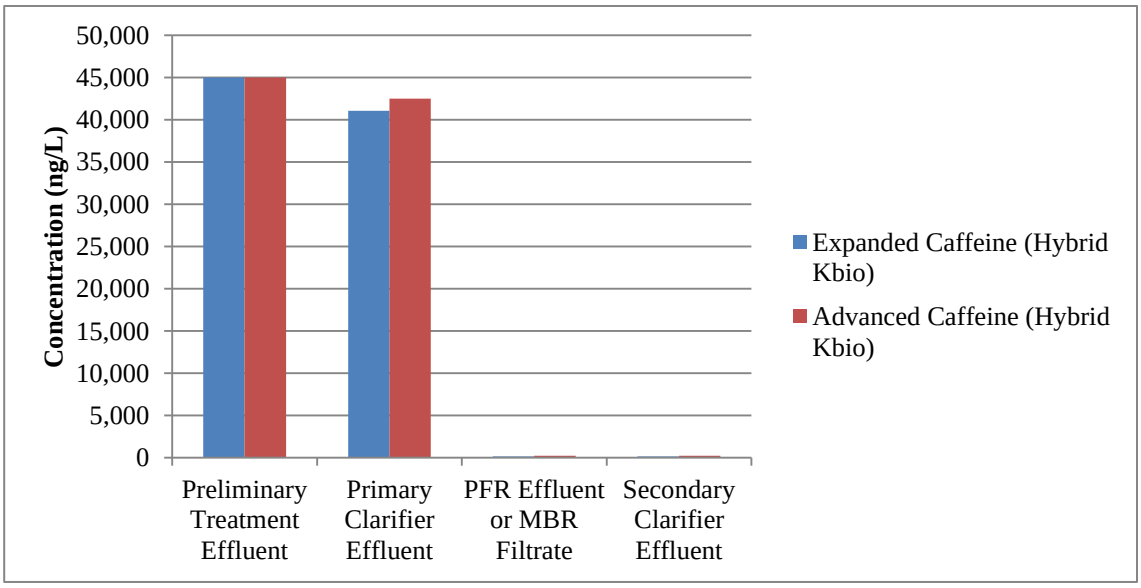

Figure 5-117: Expanded vs. Advanced Caffeine under Sampling Conditions (Modified Flowrate)

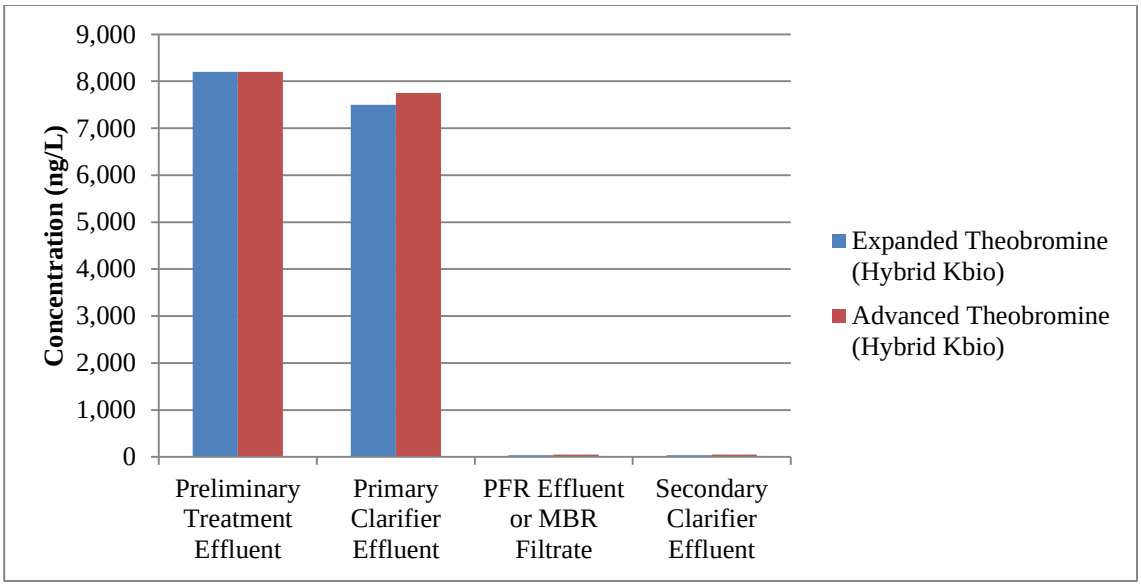

Figure 5-118: Expanded vs. Advanced Theobromine under Sampling Conditions (Modified Flowrate)

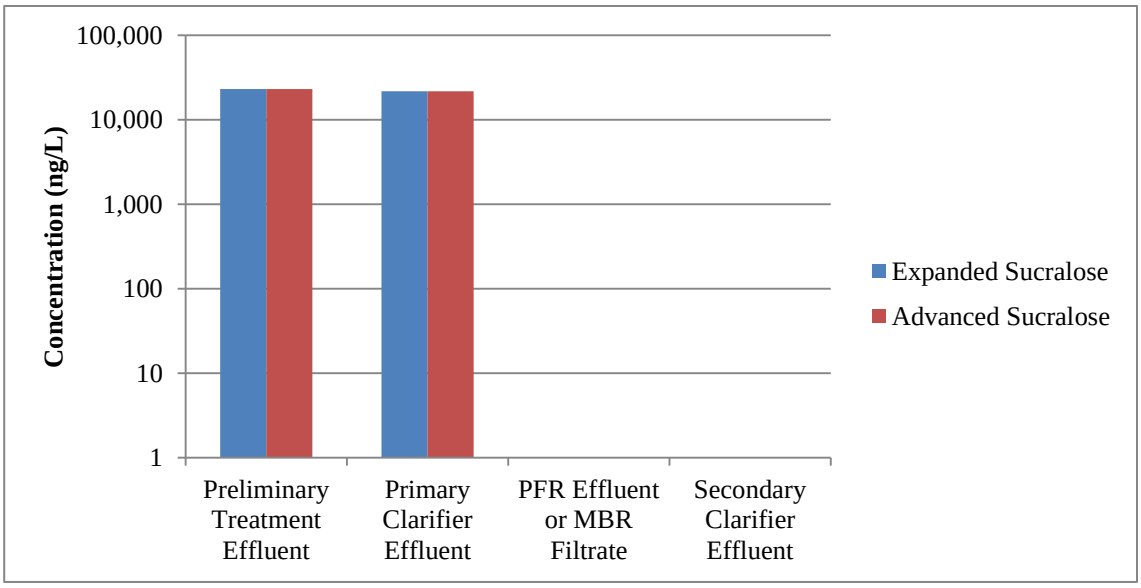

Figure 5-119: Expanded vs. Advanced Sucralose under Sampling Conditions (Modified Flowrate)

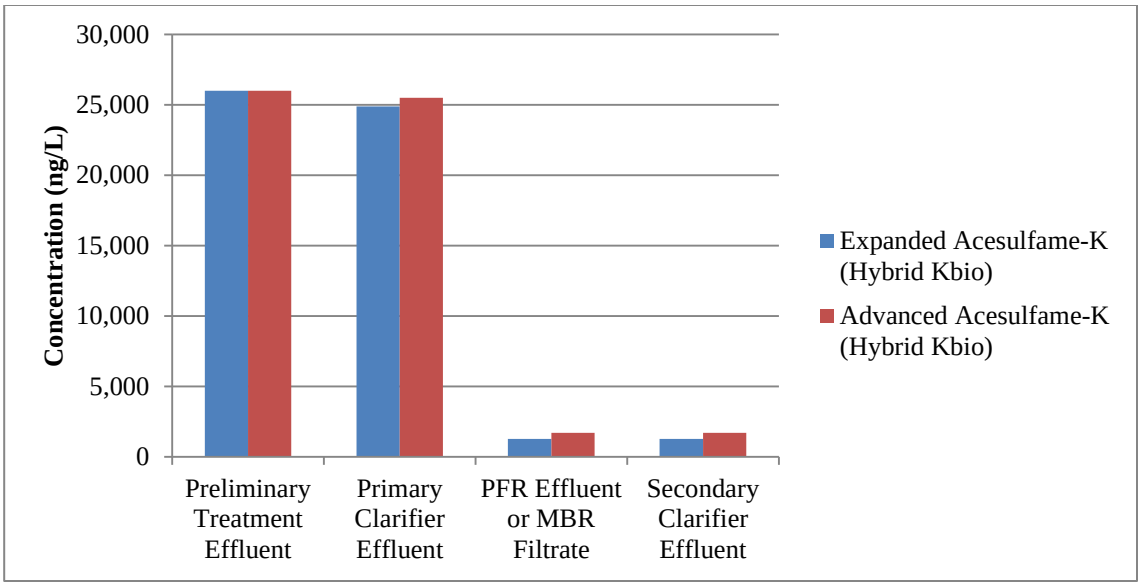

Figure 5-120: Expanded vs. Advanced Acesulfame-K under Sampling Conditions (Modified Flowrate)

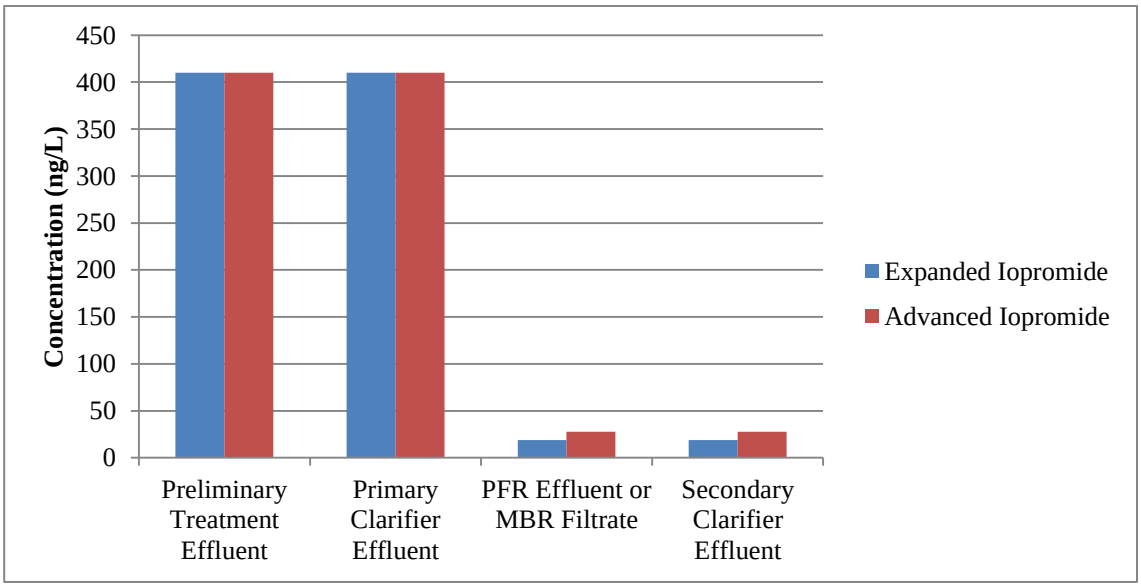

Figure 5-121: Expanded vs. Advanced Iopromide under Sampling Conditions (Modified Flowrate)

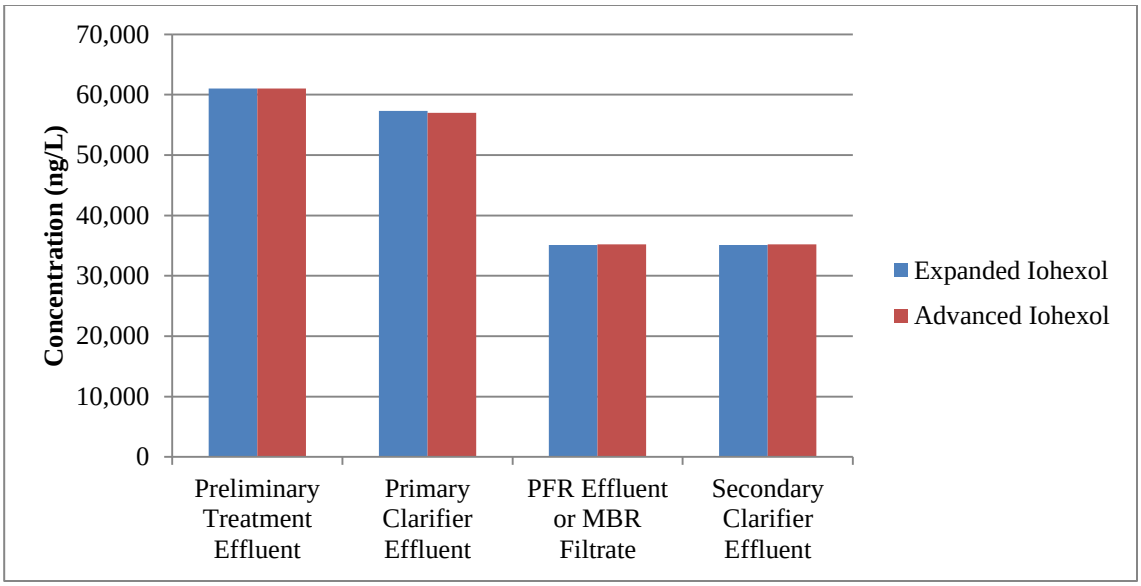

Figure 5-122: Expanded vs. Advanced Iohexol under Sampling Conditions (Modified Flowrate)

There is no significant difference in CEC removal between the expanded and advanced models. In the MBR membranes, GPS-X only removes soluble compounds when they are inert. Because the CECs are not inert in the model, they are not removed by the membrane. For micro- and ultrafiltration membranes, pore size is on the order of 100 times larger than most CECs. However, some removal may take place due to sorption to the membrane (Lee et al., 2009). Therefore, although removal varies, actual CEC concentrations might be expected to be lower than levels determined in the advanced model.

While modeled soluble CECs are not shown to decrease through the membrane, advanced model particulate CECs are removed to lower concentrations than expanded model concentrations. Although effluent particulate CEC concentrations in the expanded model are small, advanced model filtrate *and* plant concentrations are approximately ten times smaller. Even without the secondary clarifiers, the advanced model is still better at removing particulate CECs (Figure 5-123 to Figure 5-134).

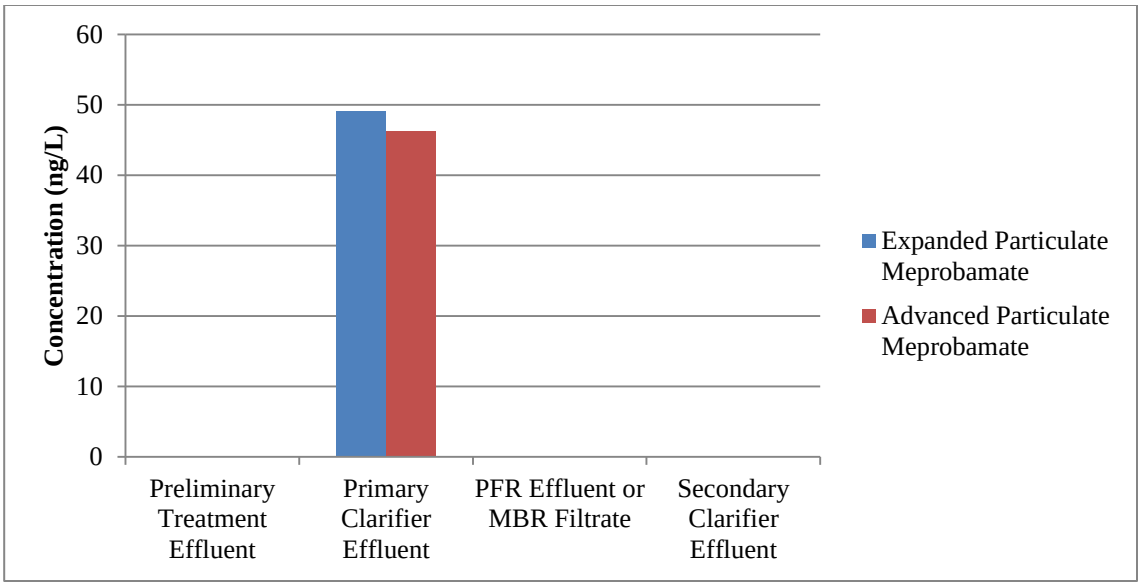

Figure 5-123: Expanded vs. Advanced Particulate Meprobamate under Sampling Conditions (Modified Flowrate)

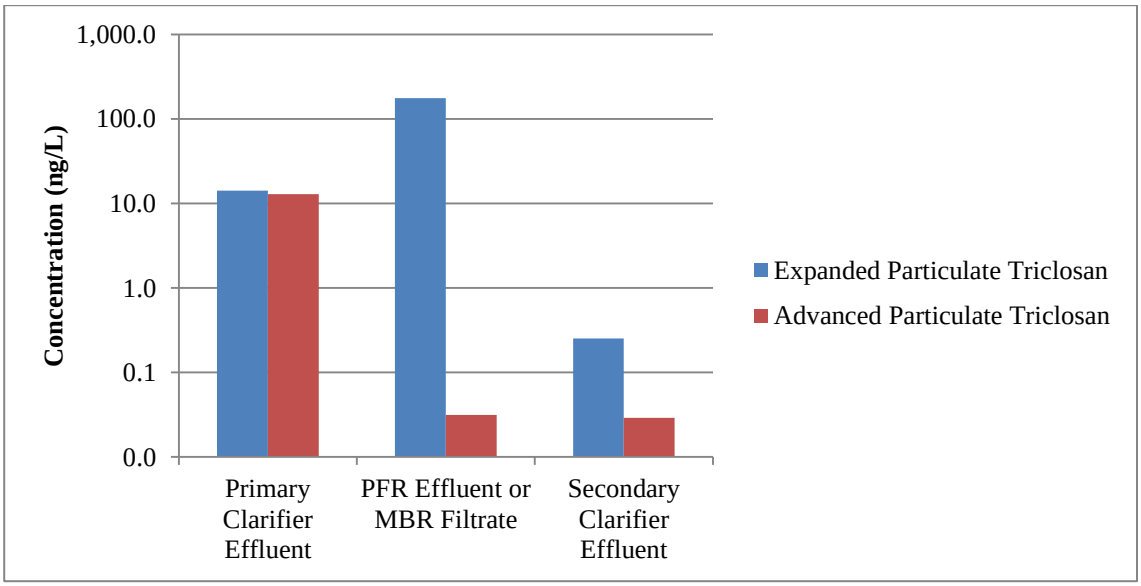

Figure 5-124: Expanded vs. Advanced Particulate Triclosan under Sampling Conditions (Modified Flowrate)

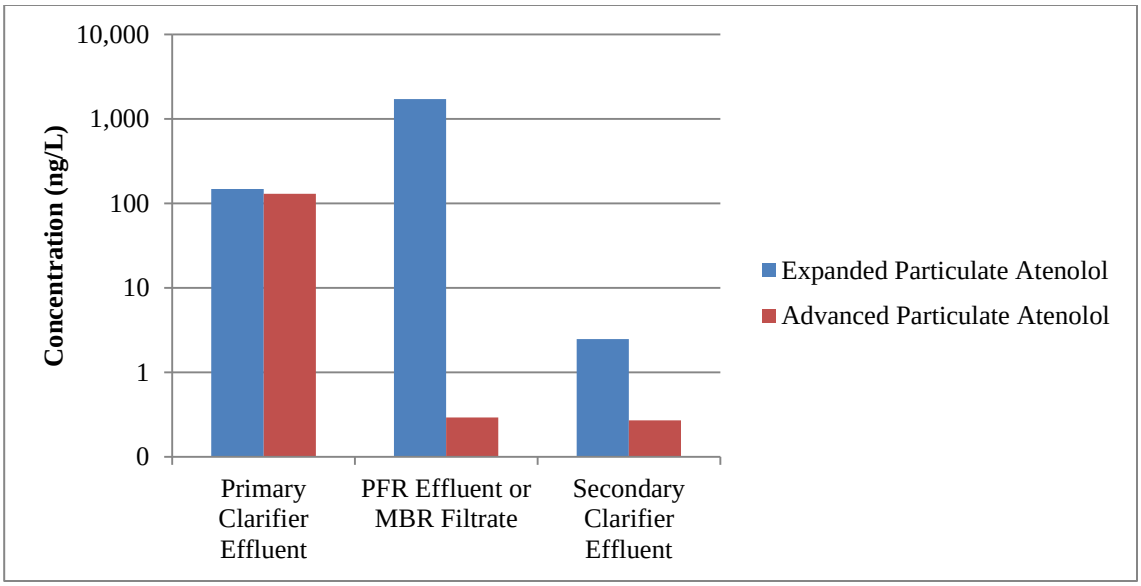

Figure 5-125: Expanded vs. Advanced Particulate Atenolol under Sampling Conditions (Modified Flowrate)

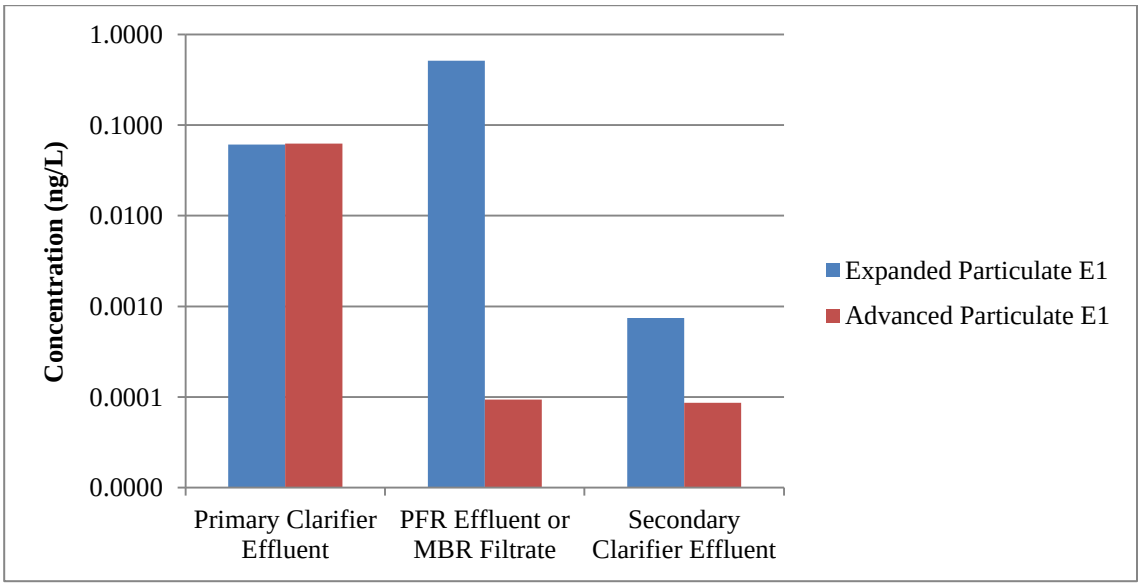

Figure 5-126: Expanded vs. Advanced Particulate E1 under Sampling Conditions (Modified Flowrate)

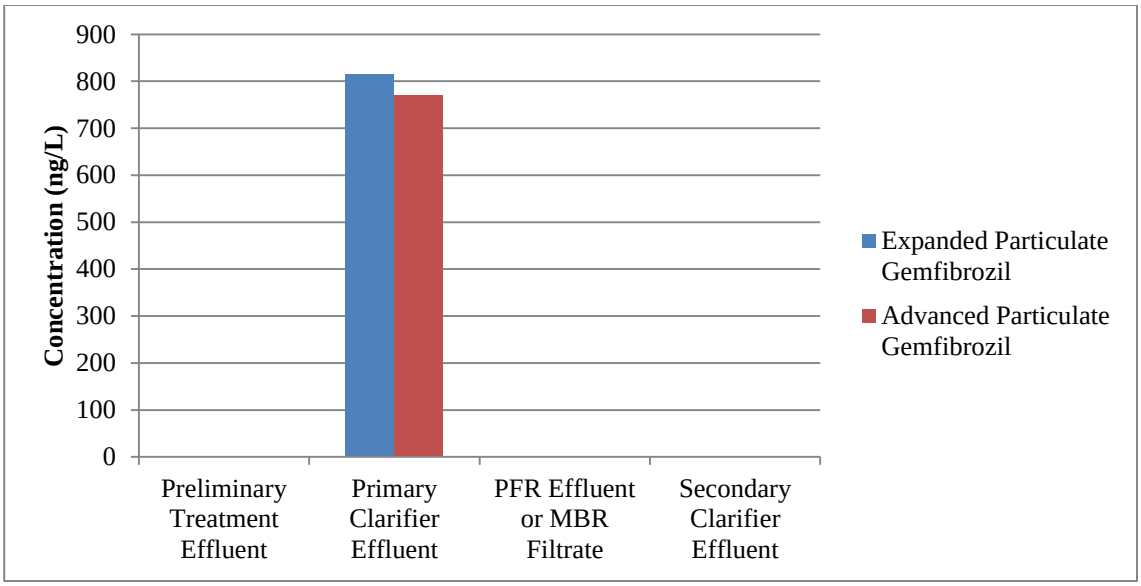

Figure 5-127: Expanded vs. Advanced Particulate Gemfibrozil under Sampling Conditions (Modified Flowrate)

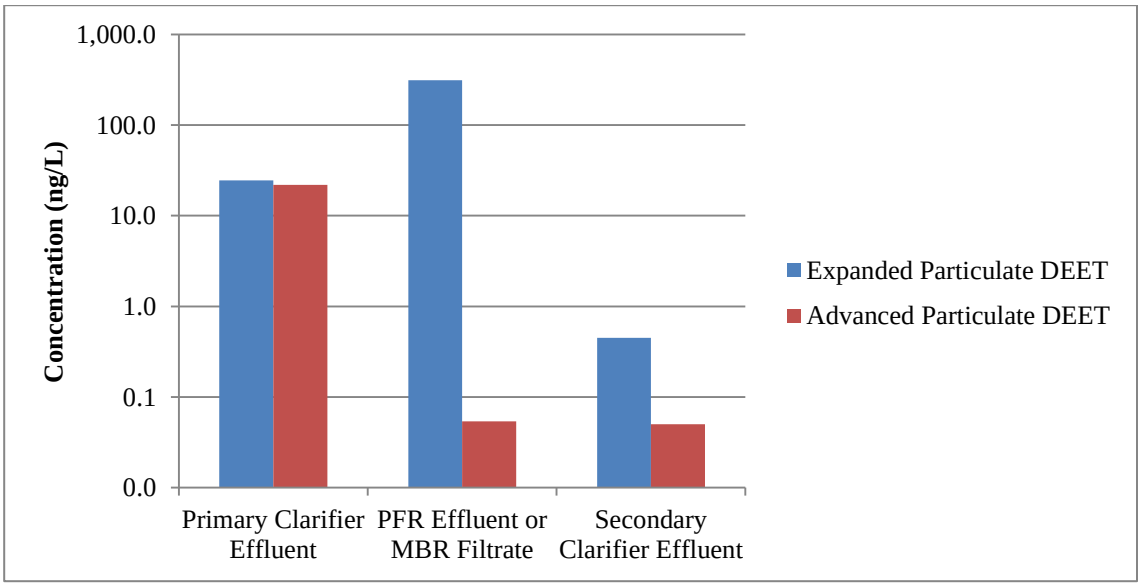

Figure 5-128: Expanded vs. Advanced Particulate DEET under Sampling Conditions (Modified Flowrate)

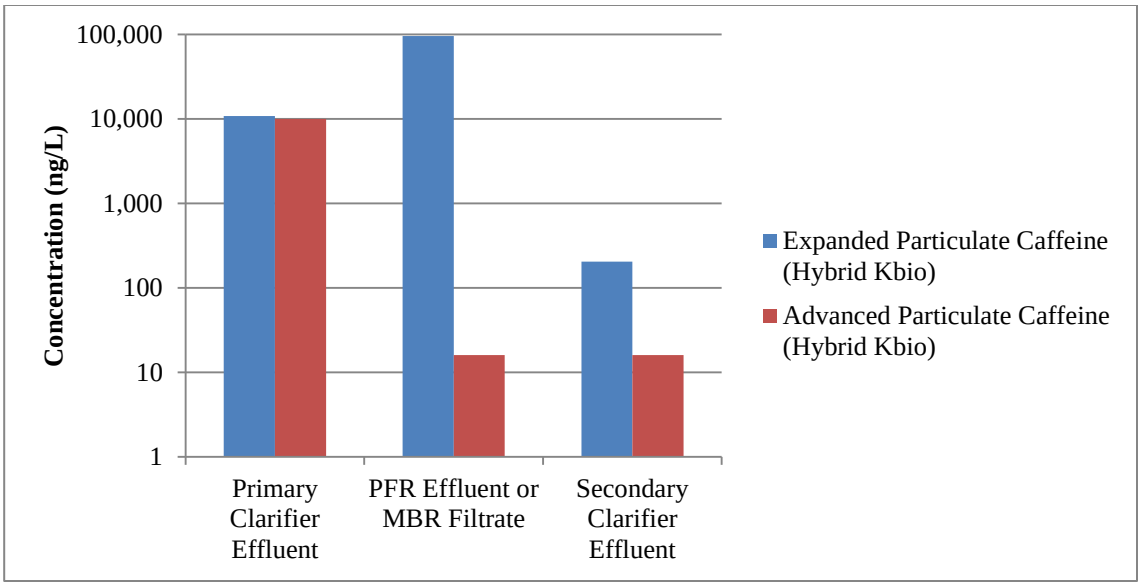

Figure 5-129: Expanded vs. Advanced Particulate Caffeine under Sampling Conditions (Modified Flowrate)

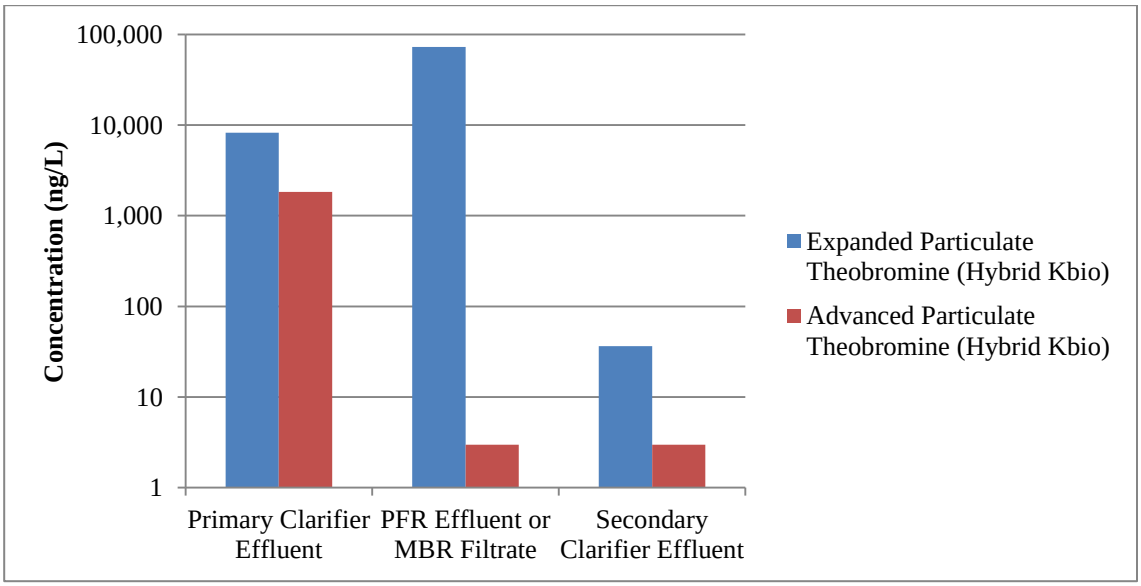

Figure 5-130: Expanded vs. Advanced Particulate Theobromine under Sampling Conditions (Modified Flowrate)

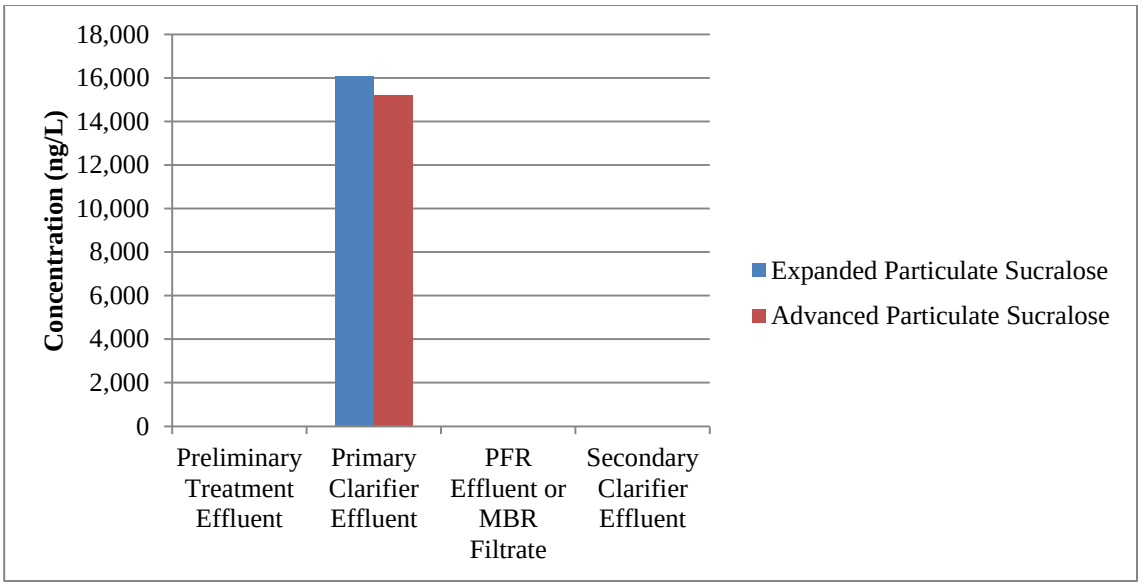

Figure 5-131: Expanded vs. Advanced Particulate Sucralose under Sampling Conditions (Modified Flowrate)

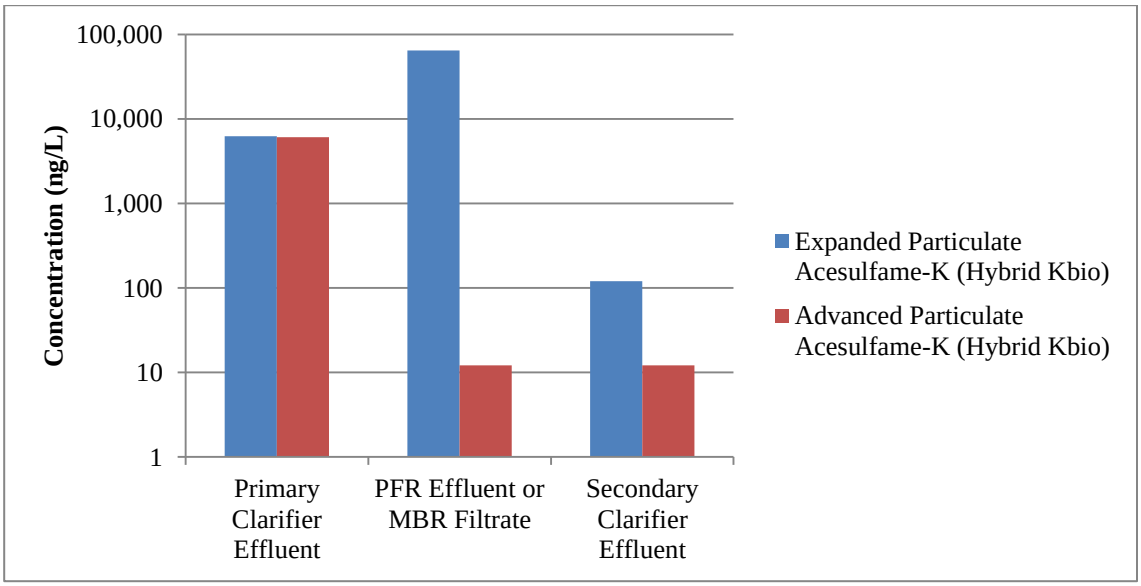

Figure 5-132: Expanded vs. Advanced Particulate Acesulfame-K under Sampling Conditions (Modified Flowrate)

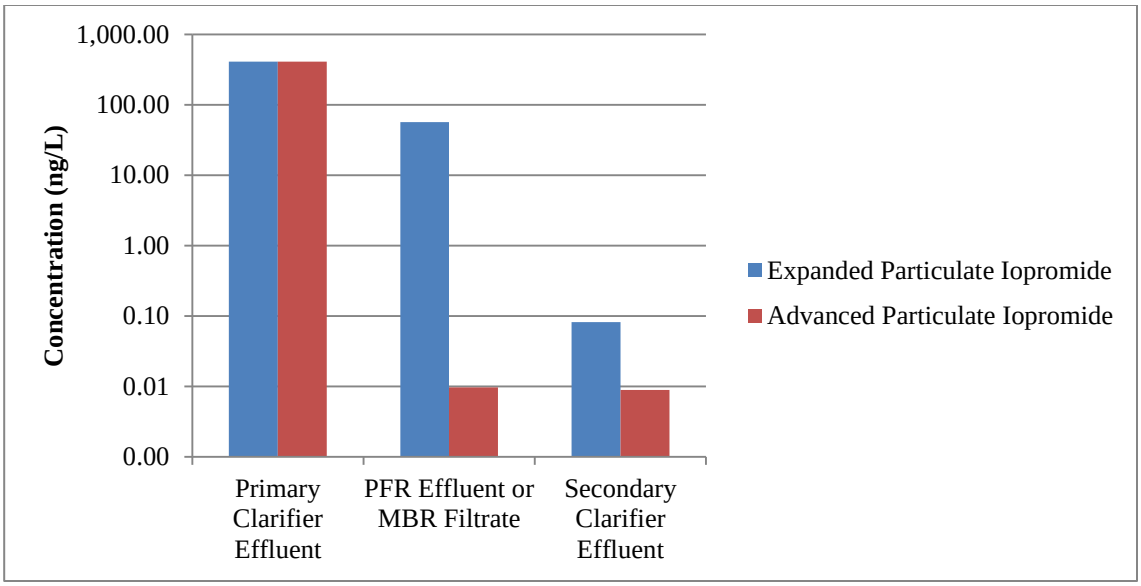

Figure 5-133: Expanded vs. Advanced Particulate Iopromide under Sampling Conditions (Modified Flowrate)

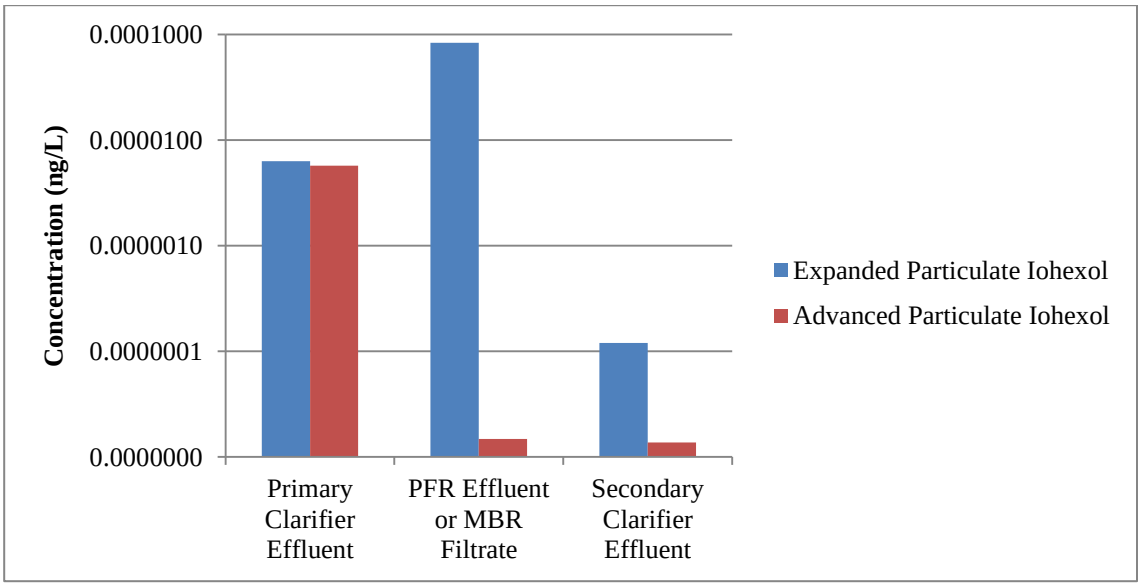

Figure 5-134: Expanded vs. Advanced Particulate Iohexol under Sampling Conditions (Modified Flowrate)

Next, soluble CEC data was extrapolated to analyze concentrations throughout an entire year. Again, influent data (except an increased flowrate) from 2013 was used as the influent data in the extrapolated advanced model. Flowrate, as mentioned earlier, is 75% higher than the base model flowrate. Both the advanced and expanded CEC

concentrations are graphed (Figure 5-135 to Figure 5-146). The expanded model typically outperforms the advanced model for CEC removal. However, as mentioned, GPS-X does not account for removal of soluble CECs in the membrane. Therefore, advanced model concentrations could be expected to be lower than model prediction.

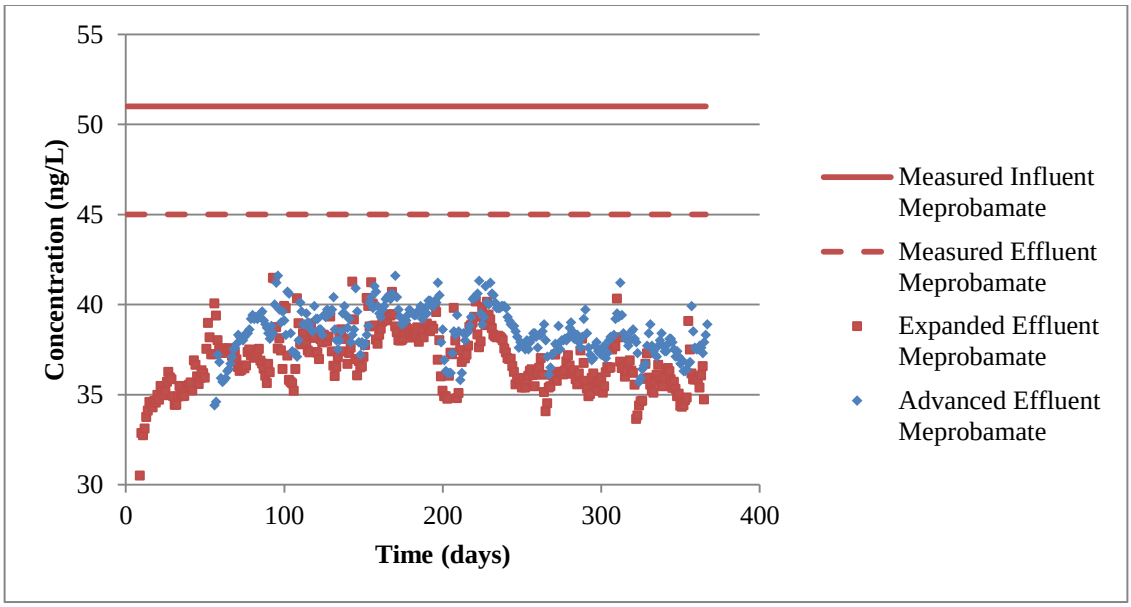

Figure 5-135: Expanded vs. Advanced Extrapolated Meprobamate

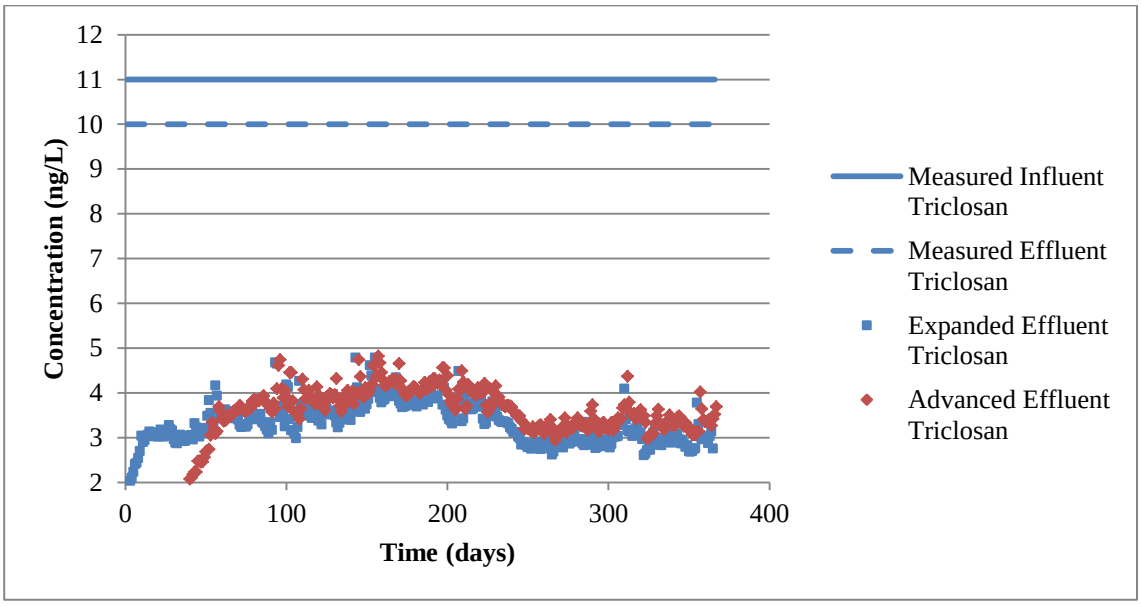

Figure 5-136: Expanded vs. Advanced Extrapolated Triclosan

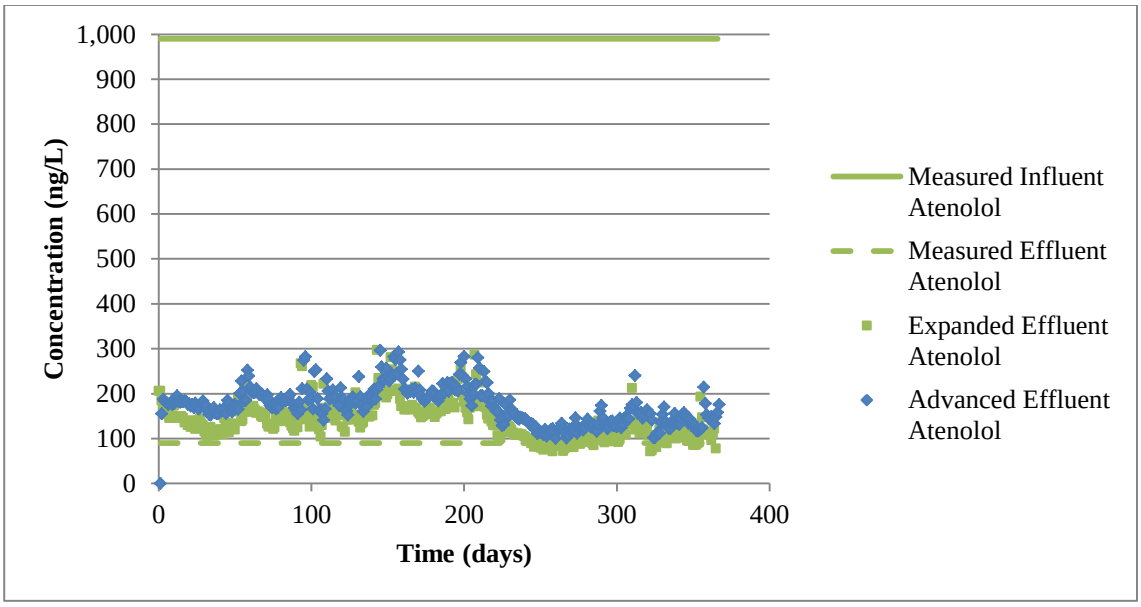

Figure 5-137: Expanded vs. Advanced Extrapolated Atenolol

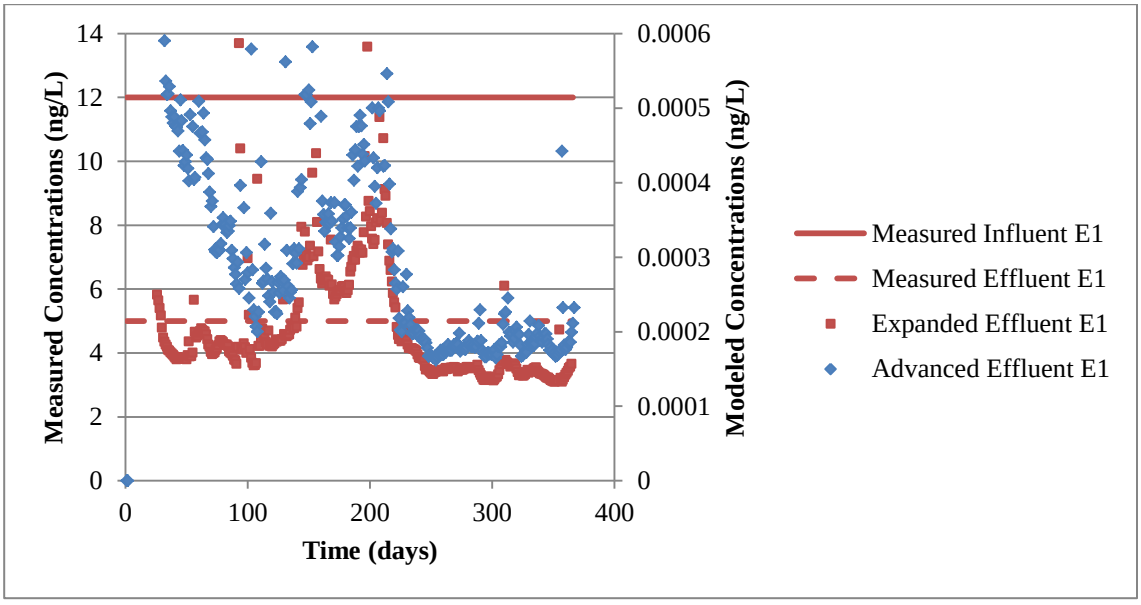

Figure 5-138: Expanded vs. Advanced Extrapolated E1

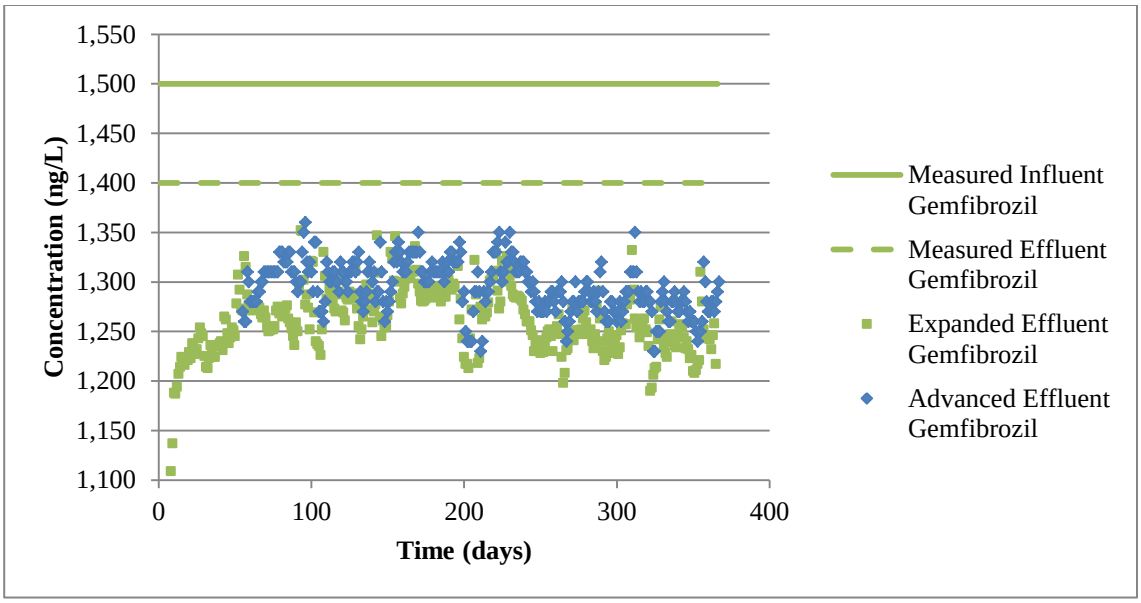

Figure 5-139: Expanded vs. Advanced Extrapolated Gemfibrozil

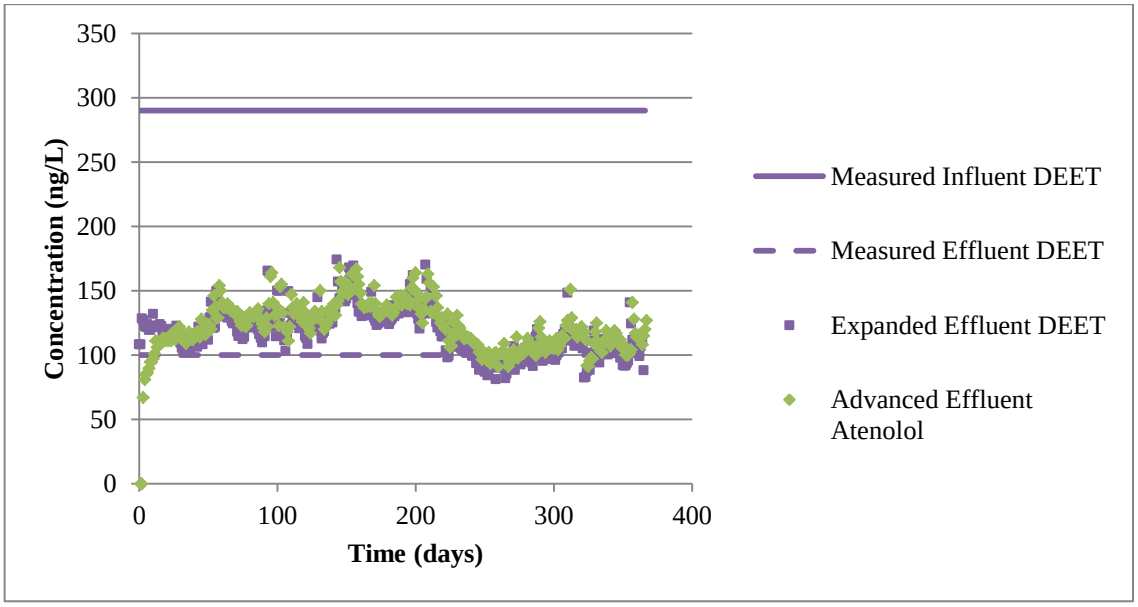

Figure 5-140: Expanded vs. Advanced Extrapolated DEET

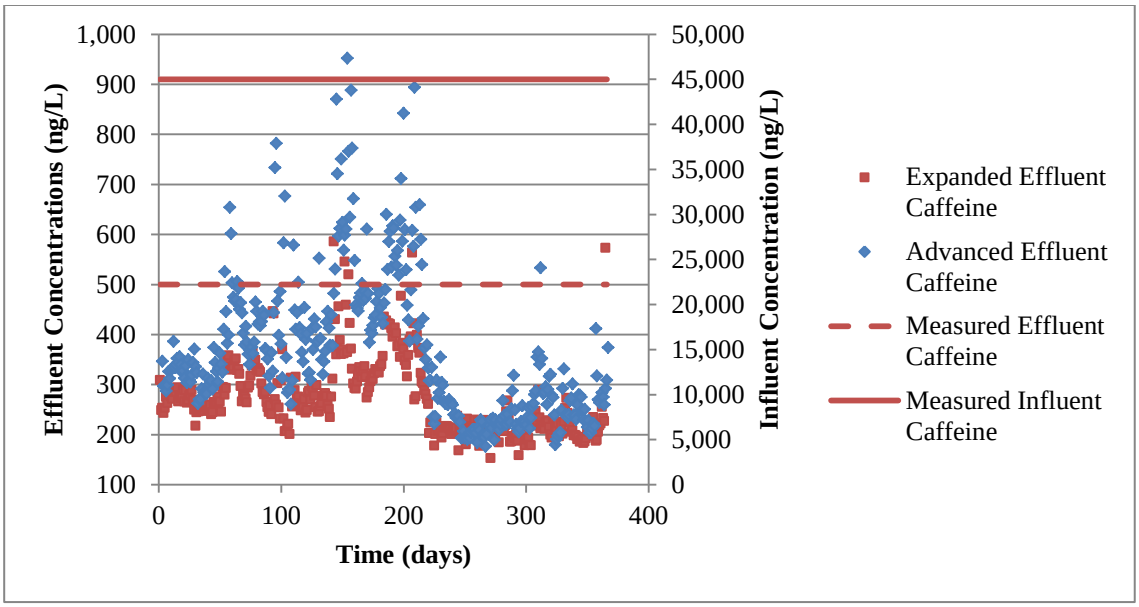

Figure 5-141: Expanded vs. Advanced Extrapolated Caffeine

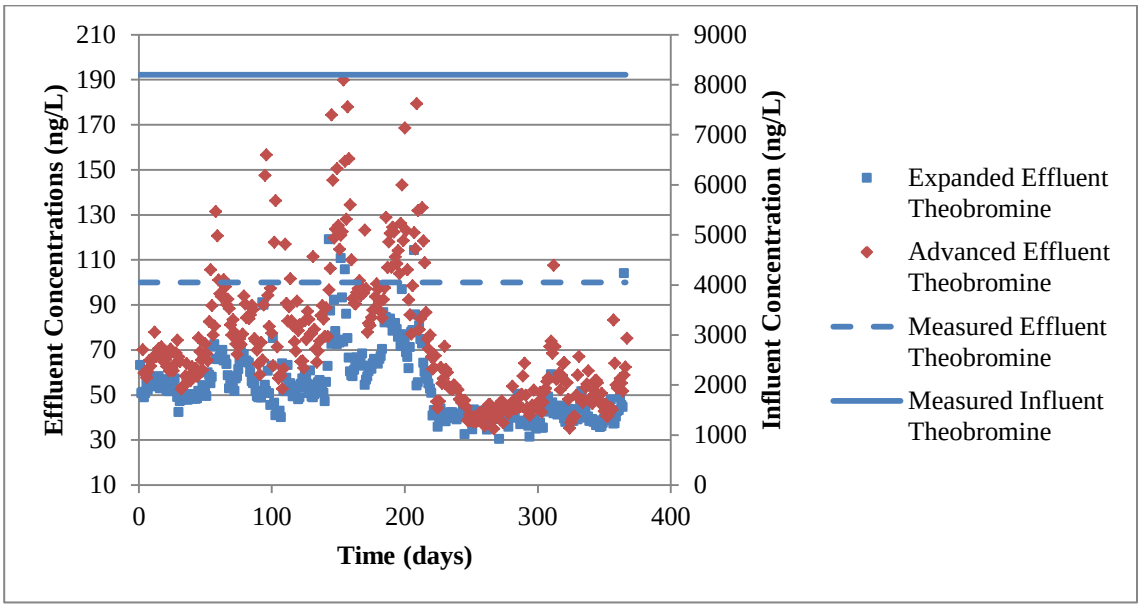

Figure 5-142: Expanded vs. Advanced Extrapolated Theobromine

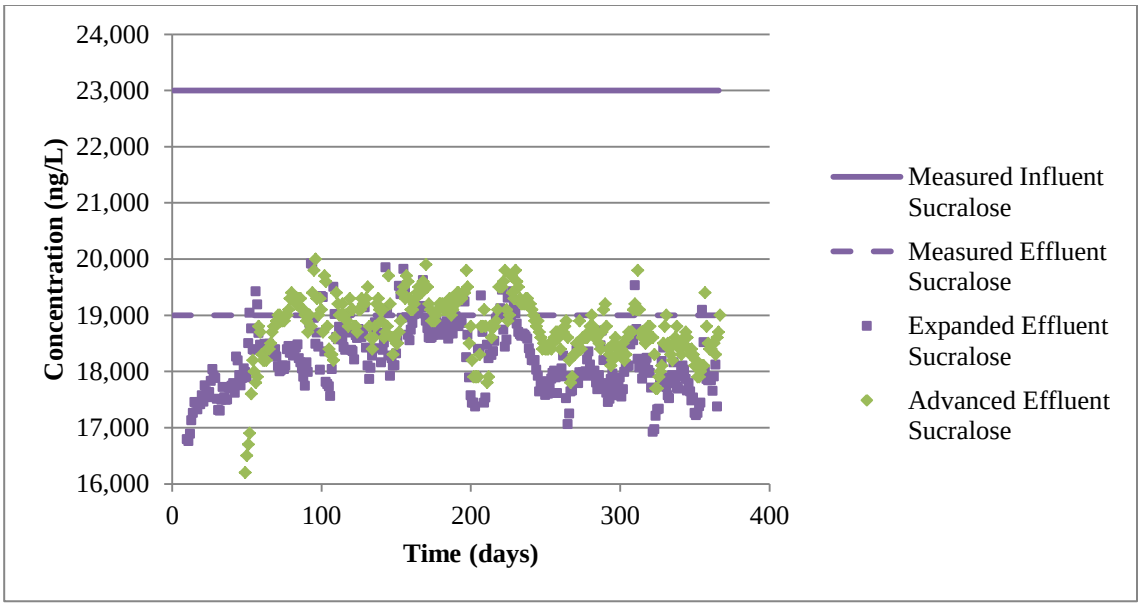

Figure 5-143: Expanded vs. Advanced Extrapolated Sucralose

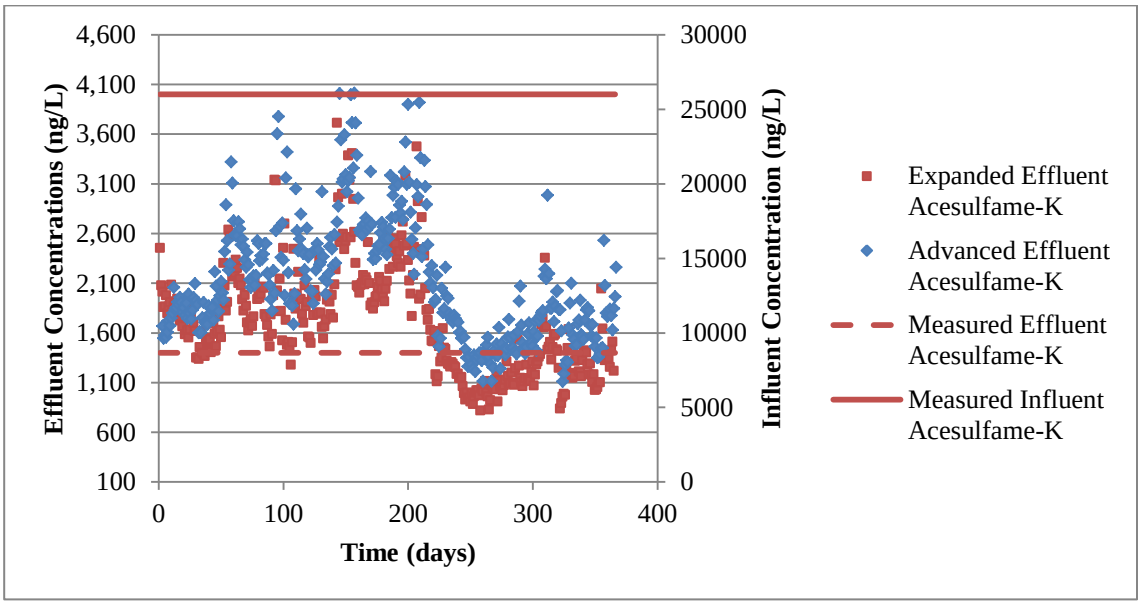

Figure 5-144: Expanded vs. Advanced Extrapolated Acesulfame-K

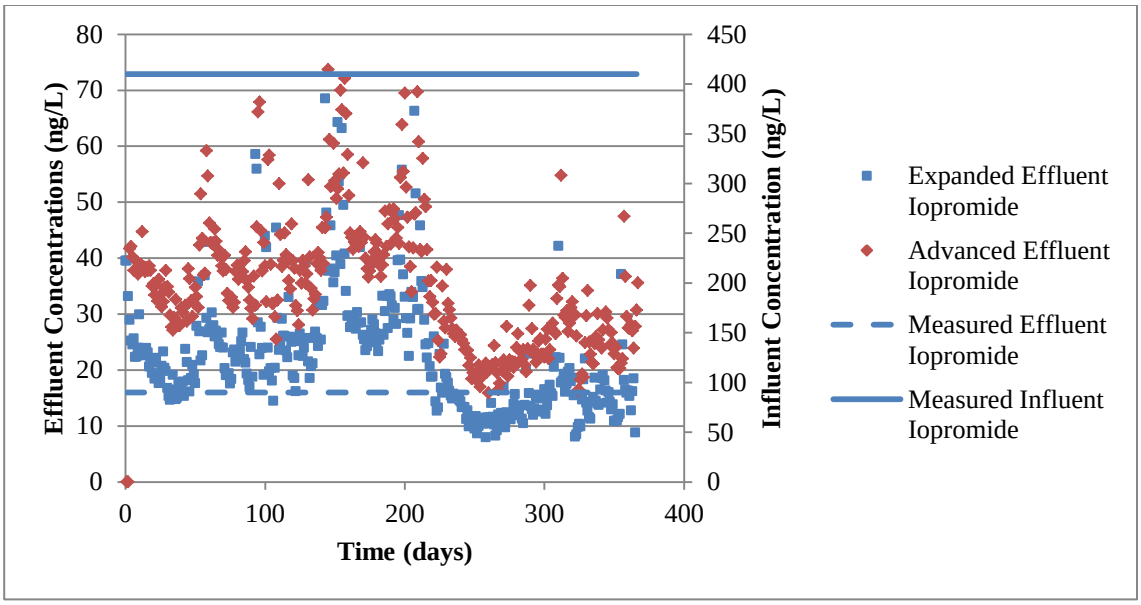

Figure 5-145: Expanded vs. Advanced Extrapolated Iopromide

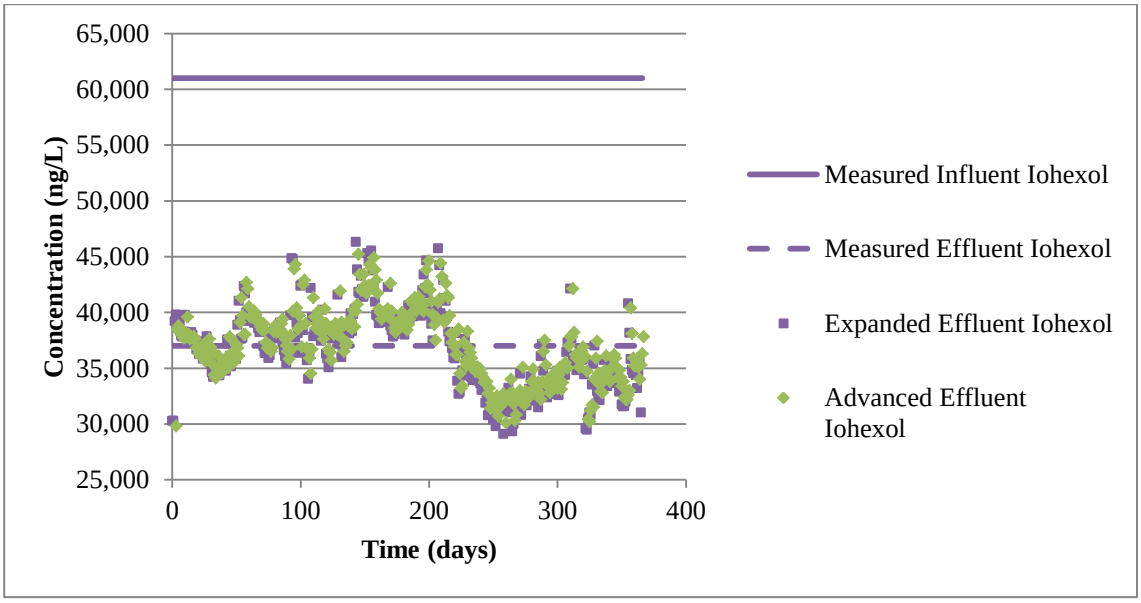

Figure 5-146: Expanded vs. Advanced Extrapolated Iohexol

CECs that rely on biodegradation for removal (atenolol, DEET, caffeine, theobromine, and iohexol) typically perform equally in the advanced and expanded models. As mentioned earlier, meprobamate, gemfibrozil, and sucralose rate constants were only calibrated for the primary clarifiers. These compounds, though, are typically

less removed in the advanced model due to their dependence on adsorption. These trends show the importance of biodegradation in the advanced model. Because VSS concentrations are lower (Figure 5-109), the advanced model relies more heavily on biodegradation.

Chapter 6: Conclusion

With the rise in popularity of direct and indirect water reuse, CECs are of growing concern to both ecosystems and human consumption. Because direct and indirect reuse can include wastewater effluent application to natural streams, lakes, irrigated land, and even water treatment plants, it is desirable to understand CEC concentrations and removal patterns throughout WWTPs. Due to the wide range of WWTP characteristics, CEC removal varies greatly and can be difficult to predict without knowledge and information of the specific plant. This research uses a stochastic model to analyze CEC removal through the various treatment processes at the NWRF. Using the commercial software GPS-X, CECs are analyzed with varying RAS, WAS, SRTs, and HRTs. GPS-X incorporates the use of the model developer tool, which uses matrix format to model the relationships between model parameters and CECs that are added to the model. This research evaluates operational effects at the NWRF on CEC removal. Additionally, it analyzes the use of MBRs instead of PFRs and evaluates advanced treatment options for CEC removal.

CECs are primarily removed from wastewater by biodegradation and adsorption to biosolids. At low CEC concentrations, both biodegradation and adsorption are first-order reactions with respect to X_a and VSS concentrations, respectively. While most reclamation facilities use CAS, other treatment techniques include MBRs, RO and other membrane processes, and UV disinfection. In the NWRF, CECs are most significantly removed in the primary clarifiers and the PFR. Because of the high concentrations of X_a and VSS, these treatment processes are able to remove CECs. Of 98 CECs analyzed, only 38 are larger than the MRL in one or more of the treatment processes.

Furthermore, influent and effluent indicator CEC concentrations are well below MTT levels. There are some general trends from biodegradation and adsorption that can be seen from CEC removal:

- CECs that are predominantly removed in the PFR (caffeine, theobromine, iopromide, and acesulfame-K) are heavily biodegraded in the PFR and experience removal from both biodegradation and adsorption in the primary clarifiers. These CECs have the highest removal percentages (>94%) of all indicator and validator CECs in the study.
- CECs that are mostly removed in the primary clarifiers (sucralose, meprobamate, and gemfibrozil) rely on adsorption in both the primary clarifiers and the PFR. These CECs have the lowest removal percentages (<30%) of modeled CECs in the NWRF.
- CECs that show steady and equal removal through both the primary clarifiers and the PFR (atenolol, iohexol, DEET) tend to favor biodegradation in both treatment processes. These CECs have removal percentages between 39 and 91% from the NWRF.

RAS and WAS are operational effects that can help reduce CEC concentrations in WWTPs. However, as with most engineered processes, there is a balance between CEC concentrations and plant performance for others contaminants. As mentioned, biodegradation and adsorption are first-order rates with respect to X_a and VSS. Therefore, at higher levels of X_a and VSS, CEC removal rates increase. RAS has varying effects on removal. While some CECs experience increased removal with

increasing RAS, other CECs decrease in removal. CECs that rely more heavily on biodegradation for removal tend to increase in removal percentage as RAS increases. However, RAS has a small effect on overall CEC removal, with each CEC experiencing less than 4% change in removal percentage.

Because it controls SRT, secondary clarifier WAS has a larger effect on CEC removal than RAS. Interestingly, there seems to be a clear critical point with WAS flowrate. As WAS approaches 4 to 5%, removal percentage of each CEC is optimized. This confirms current literature (Clara et al., 2005a; Monteith et al., 2008; Jelić et al., 2012) that suggests that critical SRT (and consequentially WAS) can be determined to optimize CEC removal. In these studies, as SRT increases, CEC removal increases but generally reaches a maximum percentage. In the model, at this critical WAS, plant effluent VSS and X_a reach a low point and are maintained with increasing WAS. Unlike RAS, there is a clear optimum WAS rate in which CEC removal is maximized and plant effluent VSS and X_a are minimized. For these reasons, adjustment of the secondary clarifier WAS is a more viable operational change to the NWRF for CEC removal.

In GPS-X, MBRs do not significantly increase soluble removal percentages of any of the CECs modeled. However, because of the membrane filter, particulate CECs are removed approximately ten times greater in the MBRs than they are in the PFRs and secondary clarifiers of the expanded model. Although particulate removal depends on the membrane used, Clara et al. (2005b) and Radjenović et al. (2006) confirm that particulate matter is detained by an ultrafiltration membrane, resulting in negligible concentrations of suspended solids in the effluent. In this research, modeled MBR

filtrate VSS and X_a concentrations are also about ten times smaller than expanded model plant effluent concentrations, eliminating the need for the secondary clarifiers.

Changes in WAS or RAS in the MBRs did not show a large effect on modeled CEC removal. In contrast, literature finds that increased SRT (decreased WAS) increases CEC removal. Longer SRTs result in diversified biomass, allowing for higher removal (Kimura et al., 2007; Radjenović et al., 2009). This research did not account for biomass diversification, which could be a reason that increased SRTs only slightly increase CEC removal. Although GPS-X does not show the removal of soluble CECs with the membrane, several studies (Kimura et al., 2005; Lee et al., 2009; Sipma et al., 2010; Snyder et al., 2007) show that CEC removal is a function of the type of membrane used, pressure, flux, and molecular weight of the CEC. Furthermore, UV disinfection removal depends on intensity-time values and can be as large as 90% (Canonica et al., 2008; Kim et al., 2009). So, although modeled MBR removal is similar to PFR removal, AT techniques, if properly applied, can help to remove CECs in WWTPs. This is in agreement with literature information, confirming that AT processes can increase CEC removal when compared to CAS systems.

As mentioned, both influent and effluent CEC concentrations in the NWRF are below MTT levels. The models in this research suggest that the plant expansion (even with increased flowrate) might slightly decrease removal percentages of CECs, but not at a level that should cause concern. If concentrations do rise to levels approaching the MTT, WAS could be an effective parameter to increase removal percentage of the overall plant. Several studies (Clara et al., 2005a; Monteith et al., 2008; Jelić et al., 2012) show that determining critical SRT (which is controlled by WAS) can enhance

CEC removal in CAS systems. MBRs, though, have the potential to increase removal percentage greater than operational changes can. As mentioned, CECs that are sorbed to biomass (particulate CECs) can be expected to be smaller in effluent concentrations if MBRs are utilized. Furthermore, research suggests that soluble CECs can experience higher removal depending on the type of membrane used.

The following is a summary of limitations that are also noted throughout the paper:

- CECs were only collected during one sampling day. In order to better evaluate removal, more data from various months of the year is desirable.
- CEC analysis did not indicate whether the CEC was ionized or neutral. This could have some effect on removal in the plant.
- GPS-X, while extensive and robust for suspended and attached growth processes, does not allow for the modeling of some AT processes, like UV disinfection and membrane filtration. Furthermore, CEC removal mechanisms are not able to be modeled in the digesters.
- MBR membranes do not remove soluble matter in GPS-X. The model does not allow for the input of size, pressure, or other characteristics needed for membrane filtration.

Based on the mentioned limitations and on the research as a whole, the following recommendations are made:

- If possible, more sampling should be completed. Seasonal and even daily variations of CECs are possible and more data would allow for a more finely calibrated mode.
- Because of the lack of model capability for AT processes and the wide range of removal percentages, pilot or bench-scale testing is likely the most ideal option for understanding removal through AT processes.
- In CAS processes, sampling and analysis of CECs only in the primary clarifiers and PFRs can save time and money. These unit processes account for the majority of removal in CAS WWTPs.

As direct and indirect water reuse becomes increasingly popular, information regarding CEC removal in WWTPs is needed. This research helps to understand CEC removal in the NWRF. Using a stochastic model, it is able to evaluate and quantify the key removal mechanisms in CAS treatment processes, operational improvements to increase CEC removal, and the use and benefit of AT processes in WWTPs.

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Appendix A: NWRF Typical Wastewater Parameters

Date	Flow (MGD)	Infl. Temp. (°C)	Infl. pH	Infl. TSS (mg/L)	Infl. $cBOD_5$ (mg/L)	Infl. NH_3-N (mg/L)	Infl. DO (mg/L)	Effl. Temp. (°C)	Effl. pH	Effl. TSS (mg/L)	Effluent $cBOD_5$ (mg/L)	Effl. NH_3-N (mg/L)	Effl. DO (mg/L)
1/1/12	8.445	18.2	7.4	164	265	27.8	1.2	17.8	7.2	7	3	1.1	7.2
1/2/12	9.033	15.6	7.5	208	253		1.5	15.0	7.3	5	2		6.5
1/3/12	8.968	15.5	7.6	136	232		1.3	15.0	7.2	4	2	0.1	6.4
1/4/12	8.842	15.7	7.7	112	214		1.4	14.9	7.3	20	4		6.3
1/5/12	8.867	15.8	7.6	156	222	26.7	1.5	15.5	7.3	4	2	0.1	6.5
1/6/12	8.671	15.8	7.5				1.1	15.7	7.3				6.3
1/7/12	8.853	15.2	7.6				1.7	15.3	7.4				7.0
1/8/12	9.116	15.4	7.5	216	234	29.8	1.3	15.4	7.3	4	3	0.4	6.3
1/9/12	8.749	15.5	7.7	140	227		1.5	14.8	7.3	4	2		6.3
1/10/12	8.586	15.3	7.6	144	227		1.3	15.0	7.2	4	2	0.2	6.3
1/11/12	8.739	15.8	7.8	160	239		1.3	15.3	7.3	5	2		6.1
1/12/12	8.603	15.0	7.7	136	245	26.6	1.4	13.1	7.4	4	2	0.6	6.9
1/13/12	8.953	15.3	7.7				1.4	14.3	7.3				6.5
1/14/12	8.941	15.1	7.5				1.4	14.9	7.1				6.9
1/15/12	8.931	15.1	7.5	180	202	27.6	1.4	15.1	7.3	29	5	0.2	6.5
1/16/12	9.485	15.3	7.7	160	255		1.6	15.5	7.3	4	2		6.6
1/17/12	9.085	15.4	7.7	152	237		1.3	14.2	7.3	4	2	0.1	6.4
1/18/12	9.346	15.4	7.8	196	242		1.4	14.6	7.3	3	2		6.7
1/19/12	9.147	15.8	7.8	160	323	23.6	1.4	15.0	7.3	3	2	0.1	6.5
1/20/12	9.039	15.7	7.7				1.5	15.2	7.0				6.5
1/21/12	8.960	14.6	7.7				1.7	14.0	7.3				6.8
1/22/12	9.173	15.0	7.7	164	259	25.7	1.6	14.7	7.1	8	2	0.1	6.6
1/23/12	9.299	15.1	7.7	160	251		2.5	15.0	7.3	6	4		6.6
1/24/12	9.256	15.3	7.7	204	248		1.3	15.0	7.1	16	5	0.7	6.6
1/25/12	14.085	13.6	7.8	132	179		2.4	14.1	7.3	36	10		6.3
1/26/12	10.003	15.1	7.8	212	205	38.8	1.4	14.3	7.3	8	4	0.1	6.8
1/27/12	10.357	15.1	7.7				1.6	14.8	7.3				6.4
1/28/12	10.301	14.0	7.5				1.8	14.5	7.1				6.5
1/29/12	9.557	15.4	7.6	164	276	31.0	1.5	15.1	7.3	12	4	0.1	6.5
1/30/12	9.431	15.2	7.5	210	268		1.2	15.3	7.3	14	3		6.4
1/31/12	9.584	16.0	7.4	264	299		1.0	16.0	7.3	16	4	0.1	5.9
2/1/12	9.040	15.8	7.7	164	261		1.0	15.7	7.2	18	4		6.1
2/2/12	9.045	15.8	7.7	144	238	29.4	1.2	15.5	7.3	6	2	0.1	6.7
2/3/12	9.665	15.7	7.5				0.9	15.9	7.3				6.7

2/4/12	9.177	14.7	7.6				1.2	14.6	7.5				6.9
2/5/12	9.392	15.1	7.6	172	240	28.6	1.4	14.8	7.4	2	2	0.1	6.9
2/6/12	9.006	15.4	7.6	160	251		1.4	14.9	7.3	2	2		6.9
2/7/12	9.050	15.7	7.7	164	235		1.5	15.2	7.2	2	2	0.1	6.6
2/8/12	9.005	15.1	7.7	156	218		1.6	14.3	7.2	2	2		6.8
2/9/12	8.885	15.1	7.7	160	244	28.9	1.6	14.2	7.2	2	2	0.1	6.6
2/10/12	9.276	14.8	7.7				1.6	14.4	7.2				7.0
2/11/12	9.326	13.8	7.4				1.5	13.0	7.0				6.0
2/12/12	9.461	14.2	7.6	180	282	21.1	1.3	13.1	7.2	4	2	0.1	6.5
2/13/12	9.993	14.0	7.7	196	242		1.4	13.0	7.3	3	2		6.7
2/14/12	9.425	14.6	7.7	144	212		1.6	13.7	7.1	3	2	0.1	6.6
2/15/12	9.647	15.0	7.6	156	213		1.7	15.2	7.2	3	2		6.4
2/16/12	9.361	15.1	7.8	164	229	23.0	1.8	14.9	7.2	3	2	0.1	7.0
2/17/12	9.612	15.0	7.7				1.9	15.0	7.3				6.8
2/18/12	9.760	14.3	7.6				1.6	14.7	7.4				6.9
2/19/12	9.722	15.1	7.5	252	309	22.4	1.7	15.5	7.2	4	2	0.1	6.9
2/20/12	9.722	14.8	7.6	176	205		1.6	14.4	7.2	7	2		6.6
2/21/12	9.621	14.9	7.6	120	204		1.7	15.0	7.2	6	2	0.3	6.9
2/22/12	9.502	15.3	7.6	180	233		1.7	15.4	7.2	6	2		6.5
2/23/12	9.532	15.4	7.5	168	228	26.6	1.5	15.8	7.0	14	4	0.1	6.5
2/24/12	9.912	14.7	7.6				1.5	15.0	7.0				6.6
2/25/12	9.811	14.9	7.5				2.0	15.3	7.3				6.5
2/26/12	9.724	15.4	7.5	160	227	21.9	1.9	15.4	7.1	12	4	0.2	7.9
2/27/12	9.418	15.4	7.6	152	236		1.3	15.1	7.1	26	4		6.2
2/28/12	9.612	15.4	7.6	216	287		1.9	15.6	7.1	81	5	0.5	6.7
2/29/12	9.253	15.8	7.5	156	241		1.3	15.9	7.2	30	4		5.3
3/1/12	9.413	15.9	7.5	151	281	38.6	1.9	16.1	7.1	21	8	0.8	6.3
3/2/12	9.350	15.4	7.6				1.1	15.5	7.2				6.4
3/3/12	9.288	14.9	7.6				1.5	15.0	7.3				6.5
3/4/12	9.401	15.9	7.5	184	255	21.7	1.3	16.1	7.1	31	4	0.1	6.3
3/5/12	9.436	15.7	7.4	132	249		1.2	16.0	7.1	11	3		6.2
3/6/12	9.319	15.5	7.6	248	279		1.2	15.6	7.1	28	4	0.1	6.3
3/7/12	9.214	16.2	7.6	228	252		1.2	16.3	7.1	22	5		6.3
3/8/12	9.204	15.0	7.6	180	223	37.1	1.1	14.3	7.2	17	5	0.1	6.3
3/9/12	9.097	15.7	7.6				1.2	15.1	7.2				6.8
3/10/12	9.416	15.3	7.5				1.6	15.5	7.3				6.6
3/11/12	13.343	14.4	7.4	196	220	21.9	1.3	15.0	7.1	148	10	0.3	5.6
3/12/12	11.011	15.9	7.7	200	197		1.2	15.7	7.2	18	5		6.2
3/13/12	10.276	16.0	7.7	260	230		1.2	16.8	7.3	15	4	0.1	6.2
3/14/12	10.121	16.1	7.7	304	256		1.4	17.0	7.2	21	4		6.2

3/15/12	10.105	16.3	7.6	164	234	26.4	1.3	17.5	7.2	15	4	0.5	6.2
3/16/12	10.035	16.5	7.5				1.2	17.7	7.3				6.4
3/17/12	9.650	15.0	7.5				1.4	17.0	7.3				6.3
3/18/12	9.127	16.0	7.5	164	242	24.8	1.4	17.0	7.2	48	4	1.0	6.4
3/19/12	17.167	14.5	7.1	252	134		0.5	15.3	7.2	334	28		5.2
3/20/12	19.212	14.7	7.6	200	165		3.3	14.6	7.2	13	7	3.6	5.8
3/21/12	14.985	15.0	7.6	336	247		1.9	15.2	7.3	16	5		6.4
3/22/12	14.090	14.5	7.6	176	144	17.2	1.1	14.9	7.2	10	7	3.3	6.2
3/23/12	12.189	15.4	7.7				1.3	15.7	7.3				6.6
3/24/12	10.750	15.1	7.6				1.5	15.2	7.3				6.7
3/25/12	11.491	16.1	7.6	132	202	21.6	1.3	17.8	7.4	4	2	0.1	6.7
3/26/12	11.583	16.7	7.6	148	217		1.1	17.4	7.2	5	2		6.6
3/27/12	11.283	16.9	7.6	130	215		1.5	17.8	7.1	4	2	1.2	6.4
3/28/12	11.441	16.4	7.4	388	245		0.8	17.5	7.2	6	2		6.1
3/29/12	11.883	17.2	7.6	136	221	28.4	1.5	18.0	7.3	8	3	0.4	6.3
3/30/12	14.604	17.2	7.6				1.4	18.1	7.2				6.0
3/31/12	9.667	17.1	7.5				1.4	17.1	7.2				6.2
4/1/12	9.799	17.5	7.5	164	205	25.6	1.6	19.0	7.0	34	4	2.0	6.2
4/2/12	9.616	18.8	7.5	148	197		1.2	20.0	7.2	16	4		5.8
4/3/12	11.339	18.1	7.5	172	212		1.2	18.6	7.2	14	5	1.7	6.0
4/4/12	10.048	18.5	7.7	192	173		1.2	19.0	7.3	20	4		6.1
4/5/12	9.521	18.4	7.5	156	186	26.7	1.2	18.8	7.2	16	4	0.3	6.0
4/6/12	9.473	18.3	7.5				0.7	18.8	7.2				6.1
4/7/12	9.449	17.2	7.5				1.4	18.5	7.2				6.2
4/8/12	9.229	17.5	7.4	168	216	24.6	1.2	17.8	7.2	31	5	0.2	5.8
4/9/12	9.399	17.8	7.5	156	198		1.2	18.3	7.3	30	4		5.8
4/10/12	9.265	18.0	7.5	144	245		1.3	18.6	7.2	21	5	1.3	5.7
4/11/12	9.270	18.1	7.5	160	232		1.2	18.7	7.2	26	7		5.9
4/12/12	9.189	18.0	7.5	140	226	28.9	1.1	19.1	7.3	132	8	0.2	5.6
4/13/12	10.168	20.0	7.8				1.0	20.8	7.2				5.7
4/14/12	9.935	19.7	7.4				1.2	20.7	7.1				5.8
4/15/12	11.353	19.0	7.4	184	227	23.5	1.1	20.3	7.0	37	7	0.2	6.3
4/16/12	9.781	20.1	7.6	140	187		1.0	20.4	7.2	64	6		6.0
4/17/12	9.375	20.1	7.6	148	185		1.3	20.7	7.2	33	5	0.4	5.9
4/18/12	9.541	20.3	7.5	144	195		1.2	21.5	7.3	61	6		5.8
4/19/12	9.447	20.2	7.6	160	186	23.9	1.4	20.8	7.3	22	3	1.0	5.9
4/20/12	10.953	19.9	7.5				1.3	20.2	7.2				5.6
4/21/12	9.628	19.9	7.5				1.3	20.6	7.2				5.3
4/22/12	9.532	20.4	7.5	136	202	28.0	1.2	20.6	7.3	40	6	0.2	5.7
4/23/12	9.227	20.5	7.4	140	207		1.2	21.0	7.3	49	5		6.0

4/24/12	9.297	20.6	7.5	152	216		1.3	21.2	7.2	20	5	0.9	5.9
4/25/12	9.454	20.9	7.5	148	216		1.2	21.9	7.2	41	5		5.5
4/26/12	9.370	21.1	7.4	148	203	24.5	1.3	22.0	7.1	74	6	0.5	5.5
4/27/12	9.436	21.0	7.4				1.3	22.5	7.0				5.6
4/28/12	9.432	20.6	7.4				1.5	22.2	7.3				5.8
4/29/12	9.601	21.2	7.3	144	224	25.2	1.3	22.6	7.1	43	5	1.1	6.0
4/30/12	9.586	21.3	7.4	172	245		0.9	22.1	7.1	21	4		5.8
5/1/12	9.977	21.3	7.4	168	213		1.1	22.9	7.1	112	11	0.1	5.6
5/2/12	9.713	21.2	7.5	172	210		1.0	22.4	7.1	56	8		5.6
5/3/12	9.500	21.8	7.4	144	224	27.4	1.3	23.2	7.1	79	10	1.5	5.5
5/4/12	9.414	21.8	7.3				0.9	22.6	7.1				5.5
5/5/12	9.554	21.7	7.3				1.2	23.7	7.2				5.6
5/6/12	9.573	22.1	7.3	176	236	26.8	1.0	24.0	7.1	118	10	1.5	5.3
5/7/12	9.173	21.6	7.3	140	223		1.2	22.3	7.0	79	10		5.6
5/8/12	8.945	21.5	7.3	140	221		1.1	22.3	7.1	34	7	1.5	5.5
5/9/12	8.892	21.8	7.3	148	210		1.1	22.6	7.2	81	10		5.3
5/10/12	8.758	22.3	7.1	580	217	21.3	1.3	22.7	6.6	155	9	0.5	5.0
5/11/12	9.774	21.1	7.4				1.1	21.7	7.2				5.6
5/12/12	9.782	21.5	7.3				1.2	22.1	7.2				5.7
5/13/12	9.014	22.0	7.1	148	216	23.3	1.0	22.9	7.0	40	5	0.9	5.5
5/14/12	8.727	21.6	7.2	132	221		1.1	22.6	7.1	27	6		5.5
5/15/12	8.466	21.9	7.2	148	219		1.1	23.0	7.1	18	6	0.6	5.4
5/16/12	9.033	22.1	7.3	188	214		1.1	23.2	7.1	20	5		5.5
5/17/12	9.326	22.2	7.3	128	207	25.2	1.0	23.1	7.0	25	6	0.7	5.4
5/18/12	9.132	22.0	7.2				1.1	23.2	7.0				5.7
5/19/12	8.989	22.3	7.0				1.1	23.7	7.0				5.8
5/20/12	9.539	21.5	7.1	180	225	31.4	1.1	22.0	7.1	10	7	0.5	5.8
5/21/12	9.238	22.3	7.1	156	235		0.8	22.9	7.0	7	5		6.0
5/22/12	9.093	22.6	7.2	152	219		1.1	23.3	7.1	7	4	1.4	5.8
5/23/12	9.198	22.3	7.2	116	203		0.8	23.7	7.0	32	9		5.7
5/24/12	9.326	22.2	7.3	152	222	33.5	1.2	23.8	6.9	44	6	4.1	5.3
5/25/12	9.488	22.7	7.2				1.2	24.5	6.9				5.5
5/26/12	8.891	22.5	7.1				1.1	23.7	6.9				5.8
5/27/12	8.365	22.9	7.1	196	231	29.7	1.0	25.1	6.9	20	5	2.8	5.7
5/28/12	8.598	22.1	7.2	152	230		1.3	24.5	7.0	12	4		5.9
5/29/12	8.993	22.9	7.3	272	253		0.9	24.4	7.1	10	5	4.2	5.4
5/30/12	11.202	22.6	7.4	124	194		1.2	23.9	7.0	12	6		5.4
5/31/12	8.785	22.4	7.3	140	223	29.1	1.0	23.6	7.0	13	7	2.6	5.7
6/1/12	8.485	22.6	7.3				1.4	23.4	7.0				5.5
6/2/12	9.087	22.7	7.3				1.1	23.6	7.1				5.8

6/3/12	9.186	23.4	7.1	140	196	25.4	1.0	25.0	7.0	6	4	7.2	5.7
6/4/12	8.739	23.2	7.3	124	189		1.4	24.6	7.0	6	4		5.7
6/5/12	8.448	23.8	7.1	108	202		1.2	25.1	6.8	4	5	2.7	5.6
6/6/12	9.259	22.9	7.2	176	236		1.2	24.3	7.0	6	6		5.7
6/7/12	10.750	22.2	7.1	200	251	26.0	1.4	23.8	7.1	7	5	2.5	5.8
6/8/12	8.985	23.3	7.2				1.0	24.5	7.1				5.7
6/9/12	8.980	23.3	7.2				1.1	25.3	7.1				5.9
6/10/12	8.922	23.5	7.1	140	201	25.2	1.2	26.2	7.0	4	2	2.0	5.7
6/11/12	9.621	23.4	7.0	184	157		1.1	25.1	7.0	3	3		5.7
6/12/12	9.683	23.3	7.2	128	217		1.8	24.8	6.9	6	4	4.6	5.8
6/13/12	9.444	23.2	7.1	159	217		1.9	24.6	7.0	5	4		5.8
6/14/12	9.139	23.5	7.1	176	231	23.4	1.6	25.2	6.9	6	6	1.9	5.8
6/15/12	9.088	23.6	7.2				1.5	25.5	7.0				5.7
6/16/12	9.010	23.8	7.1				1.9	25.9	7.0				5.9
6/17/12	8.890	24.2	7.1	132	236	23.9	1.8	26.5	7.0	4	3	2.9	5.9
6/18/12	8.912	23.5	7.1	176	259		1.5	25.5	6.9	4	3		5.7
6/19/12	9.061	23.6	7.1	176	238		1.9	25.4	6.9	5	4	3.9	5.7
6/20/12	9.124	24.0	7.1	164	243		1.4	25.4	6.9	8	5		5.6
6/21/12	8.947	23.7	7.2	148	232	33.2	1.2	25.1	6.9	11	5	1.6	5.5
6/22/12	8.852	23.6	7.2				1.0	25.4	7.0				5.4
6/23/12	8.869	24.3	7.2				1.1	26.7	7.1				5.4
6/24/12	8.627	25.0	7.1	132	252	34.1	1.0	25.6	7.1	7	8	16.3	5.6
6/25/12	8.496	24.7	7.1	124	227		1.2	26.5	6.8	7	5		5.1
6/26/12	8.822	24.6	7.2	132	272		1.0	26.6	6.9	5	3	2.7	5.2
6/27/12	9.106	25.0	7.1	144	225		1.0	26.8	7.0	5	4		5.7
6/28/12	8.941	25.1	7.1	152	253	29.0	1.0	26.6	7.0	5	4	2.0	5.6
6/29/12	9.076	25.5	7.0				1.0	26.7	7.0				5.6
6/30/12	8.697	24.8	7.1				1.1	26.6	7.0				5.3
7/1/12	8.680	25.1	7.1	132	208	21.5	1.0	27.3	7.1	4	3	0.9	5.4
7/2/12	8.652	24.7	7.1	124	195		1.2	27.0	7.0	6	4		5.7
7/3/12	8.887	25.2	7.2	128	186		0.9	26.4	7.1	6	4	1.4	5.6
7/4/12	8.567	25.2	7.1	108	196		1.2	27.2	7.0	5	4		5.4
7/5/12	8.604	24.8	7.2	108	217	34.2	1.1	26.8	7.1	4	4	0.4	5.5
7/6/12	8.747	25.2	7.2				0.9	26.9	7.2				5.7
7/7/12	8.667	25.3	7.3				1.2	27.0	7.2				5.5
7/8/12	8.589	25.0	7.1	140	252	26.3	1.0	26.5	7.1	5	4	0.7	5.3
7/9/12	8.625	25.0	7.2	160	229		0.9	26.9	7.3	5	4		5.6
7/10/12	8.973	25.3	7.2	180	280		1.2	26.8	7.2	5	4	0.3	5.4
7/11/12	8.834	25.6	7.3	148	212		0.8	26.7	7.2	6	5		5.5
7/12/12	8.500	25.8	7.3	132	230	37.1	1.0	27.0	7.2	5	4	0.5	5.3

7/13/12	8.616	25.4	7.3				1.0	27.1	7.2				5.3
7/14/12	8.840	25.7	7.2				1.2	27.6	7.1				5.5
7/15/12	8.412	25.9	7.1	152	242	27.5	1.1	27.6	7.1	4	4	0.8	5.4
7/16/12	8.685	25.8	6.6	168	225		0.7	27.1	7.2	5	4		5.2
7/17/12	8.772	25.7	7.3	136	305		1.2	27.2	7.1	5	6	2.0	5.6
7/18/12	8.763	25.9	7.2	140	214		1.1	27.2	7.1	6	6		5.5
7/19/12	8.479	25.8	7.2	172	216	25.1	1.0	27.5	7.1	7	7	1.1	5.7
7/20/12	8.453	26.3	7.3				0.9	27.6	7.1				5.7
7/21/12	8.491	26.3	7.2				1.1	28.1	7.1				5.1
7/22/12	8.533	26.5	7.1	132	243	29.9	1.0	28.6	7.0	6	4	0.6	5.2
7/23/12	8.756	26.3	7.2	148	212		0.9	27.6	7.1	4	4		6.0
7/24/12	8.911	26.0	7.3	120	203		1.1	27.5	7.1	5	4	1.0	5.4
7/25/12	8.708	26.1	7.2	128	218		0.9	27.7	7.1	7	5		5.5
7/26/12	8.636	26.0	7.2	136	190	37.0	0.8	27.5	7.1	8	3	0.3	5.3
7/27/12	8.574	26.2	7.1				1.1	27.7	7.1				5.5
7/28/12	8.538	26.7	7.2				1.0	28.5	7.1				5.5
7/29/12	8.259	27.1	7.1	146	203	28.8	1.0	28.8	7.1	3	3	0.3	5.3
7/30/12	8.404	26.6	7.3	151	208		1.1	27.7	7.1	6	4		5.5
7/31/12	8.565	26.4	7.2	140	205		1.1	28.3	7.2	8	4	0.9	5.4
8/1/12	8.296	26.7	7.2	132	191		1.0	28.7	7.1	6	4		5.3
8/2/12	8.430	26.5	7.2	204	219	30.4	1.1	28.3	7.0	5	3	0.2	5.4
8/3/12	8.217	26.5	7.2				1.0	28.1	7.1				5.1
8/4/12	8.664	26.8	7.2				1.1	28.6	7.2				5.2
8/5/12	8.472	27.2	7.1	124	210	38.9	0.9	28.5	7.1	6	4	0.3	5.0
8/6/12	8.293	26.8	7.2	144	225		0.9	28.1	7.2	5	5		5.2
8/7/12	8.646	26.6	7.2	160	207		1.1	28.2	7.1	5	5	0.2	5.1
8/8/12	8.371	26.6	7.3	172	219		0.9	28.4	7.2	4	2		5.3
8/9/12	8.638	27.2	7.1	132	191	25.9	1.0	28.5	7.0	2	2	0.1	5.5
8/10/12	8.227	26.9	7.2				1.0	28.3	7.1				5.5
8/11/12	8.467	27.0	7.2				0.9	27.7	7.2				5.5
8/12/12	8.489	27.2	7.1	180	226	22.7	0.8	28.5	7.0	7	7	2.0	5.0
8/13/12	8.304	26.7	7.2	148	255		1.1	27.9	7.1	4	3		5.5
8/14/12	8.599	26.5	7.2	172	198		1.0	27.7	7.1	3	2	0.4	5.5
8/15/12	8.806	26.6	7.2	136	218		1.1	27.7	7.1	3	2		5.4
8/16/12	9.322	26.3	7.3	168	162	28.7	1.0	27.3	7.0	2	2	0.1	5.4
8/17/12	8.657	26.5	7.3				0.9	27.5	7.0				5.6
8/18/12	10.740	26.7	7.3				0.9	27.5	7.1				5.6
8/19/12	9.457	27.0	7.2	172	236	22.3	0.8	27.5	7.0	2	2	0.2	5.0
8/20/12	8.867	26.8	7.3	148	227		1.2	27.4	7.0	3	3		5.6
8/21/12	9.114	26.6	7.1	136	211		0.9	27.8	6.9	4	3	0.1	5.5

8/22/12	8.979	26.7	7.2	148	230		1.1	27.8	7.0	4	4		5.6
8/23/12	8.481	26.6	7.1	160	227	25.7	1.1	27.4	6.9	6	3	1.5	5.6
8/24/12	8.763	26.8	7.1				1.0	27.5	7.0				5.4
8/25/12	9.263	26.7	7.2				1.0	28.1	7.0				5.5
8/26/12	12.063	26.2	7.2	152	176	24.0	1.3	27.2	7.0	8	4	2.2	5.4
8/27/12	9.271	26.7	7.2	160	202		1.2	27.7	7.0	8	4		5.4
8/28/12	9.241	26.0	7.2	140	146		1.5	27.8	6.9	6	2	0.7	5.3
8/29/12	8.604	26.4	7.2	133	291		1.2	27.6	7.0	6	4		5.6
8/30/12	8.806	26.9	7.3	118	203	31.1	0.9	27.7	7.0	4	3	0.2	5.5
8/31/12	8.673	26.5	7.2				1.0	28.0	7.2				5.6
9/1/12	8.553	26.8	7.0				1.3	28.7	6.9				5.8
9/2/12	8.328	26.2	7.1	125	186	28.6	1.6	29.0	7.0	3	2	0.3	5.9
9/3/12	9.176	27.1	6.9	136	218		1.3	28.7	6.9	3	2		5.4
9/4/12	8.763	26.6	7.2	160	213		1.2	28.3	7.0	4	2	0.2	5.5
9/5/12	8.566	27.1	7.2	148	215		1.1	28.4	7.0	3	2		5.9
9/6/12	8.798	27.1	7.2	140	189	30.4	1.2	28.3	6.9	3	2	0.3	5.7
9/7/12	8.321	27.0	7.2				0.6	28.4	6.6				5.6
9/8/12	9.530	26.0	6.9				1.2	27.0	6.9				5.7
9/9/12	8.795	25.5	7.1	176	241	24.8	1.2	27.4	6.8	4	2	0.2	6.3
9/10/12	8.460	26.7	7.2	148	219		0.5	27.3	7.0	3	2		5.7
9/11/12	8.715	26.6	7.2	156	190		0.8	27.2	7.0	4	2	0.0	5.8
9/12/12	8.623	26.8	7.3	160	217		0.5	27.2	7.0	2	2		6.0
9/13/12	8.785	26.1	7.3	152	254	34.6	1.2	26.3	7.1	2	2	0.2	6.1
9/14/12	8.481	25.8	7.2				1.1	25.2	7.0				5.6
9/15/12	8.744	25.5	7.0				1.1	25.6	6.9				5.6
9/16/12	8.873	25.6	7.0	132	238	32.7	1.2	26.0	6.8	2	2	0.1	5.2
9/17/12	8.605	26.2	7.2	128	272		1.3	26.5	7.0	2	2		5.6
9/18/12	8.620	25.7	7.3	148	184		1.3	26.1	7.0	2	2	0.6	5.9
9/19/12	8.432	25.5	7.2	144	230		1.2	26.2	7.0	2	2		5.7
9/20/12	8.688	25.8	7.3	160	218	37.2	1.3	26.3	7.1	2	2	0.2	5.8
9/21/12	8.504	25.7	7.2				1.4	26.6	7.0				5.8
9/22/12	9.011	25.7	7.3				1.3	27.0	7.0				5.7
9/23/12	8.680	25.8	7.0	176	232	33.8	1.3	26.5	6.7	3	2	0.0	5.4
9/24/12	8.652	25.6	7.2	120	239		1.1	26.6	7.0	4	2		5.5
9/25/12	8.706	25.8	7.2	140	224		1.2	26.4	7.0	7	4	0.6	5.5
9/26/12	8.942	25.7	7.2	192	258		1.0	26.7	7.0	9	5		5.3
9/27/12	11.251	25.0	7.3	140	292	29.6	1.4	25.4	6.8	12	2	0.7	5.6
9/28/12	8.970	25.6	7.4				1.1	26.4	7.1				5.4
9/29/12	10.029	24.7	7.3				1.0	25.5	7.1				5.3
9/30/12	10.818	24.1	7.3	124	200	32.6	1.1	25.4	7.0	10	2	0.6	5.0

10/1/12	8.761	25.3	7.4	132	236		1.0	25.6	7.2	9	2		5.4
10/2/12	8.635	25.1	7.5	128	203		1.2	25.0	7.1	6	4	0.7	5.5
10/3/12	8.940	24.9	7.5	188	282		1.3	25.5	7.1	8	6		5.4
10/4/12	8.808	24.8	7.5	192	197	32.4	1.2	25.1	7.0	8	2	0.4	5.5
10/5/12	8.478	24.6	7.4				1.1	23.9	7.1				5.6
10/6/12	8.554	23.8	7.5				1.6	23.0	7.2				5.6
10/7/12	8.598	23.9	7.3	148	247	30.5	1.3	23.2	7.0	11	5	0.4	5.0
10/8/12	8.504	23.7	7.4	124	267		1.2	23.1	7.1	12	7		5.5
10/9/12	8.788	23.9	7.5	148	289		1.4	23.7	7.1	12	7	0.4	5.4
10/10/12	8.469	23.7	7.5	152	239		1.3	23.5	7.0	9	7		5.6
10/11/12	8.944	24.1	7.4	144	266	26.2	1.3	23.9	7.0	8	8	0.3	5.6
10/12/12	8.301	24.2	7.3				1.3	24.6	7.1				5.6
10/13/12	8.695	23.7	7.4				1.2	24.2	7.3				5.5
10/14/12	8.692	24.1	7.4	144	245	26.0	1.4	24.1	7.0	5	3	0.2	5.6
10/15/12	8.562	23.5	7.4	144	237		1.4	24.2	7.0	4	3		5.8
10/16/12	9.105	24.5	7.5	164	304		1.3	24.2	7.1	6	5	0.5	5.9
10/17/12	8.671	23.7	7.5	196	261		1.5	24.2	7.1	2	3		5.8
10/18/12	8.729	23.7	7.5	172	228	40.3	1.5	23.0	7.0	6	3	0.2	6.0
10/19/12	8.367	23.2	7.5				1.5	23.0	7.1				5.8
10/20/12	8.950	23.5	7.4				1.5	23.7	7.1				5.8
10/21/12	9.277	24.2	7.3	148	219	30.2	1.4	25.1	7.0	5	3	0.4	5.7
10/22/12	8.826	23.9	7.5	164	247		1.3	24.3	7.3	5	3		5.7
10/23/12	9.086	24.0	7.5	184	248		1.3	24.2	7.3	4	3	0.3	5.7
10/24/12	8.718	24.0	7.4	148	247		1.2	24.3	7.0	5	3		5.5
10/25/12	8.760	23.6	7.5	172	232	28.9	1.1	23.1	7.3	4	3	0.4	5.7
10/26/12	8.233	23.0	7.5				1.2	21.4	7.2				5.9
10/27/12	8.990	22.8	7.4				1.3	21.5	7.1				5.6
10/28/12	8.813	23.0	7.4	144	217	32.7	1.3	22.8	7.0	4	2	1.1	5.5
10/29/12	8.352	22.7	7.4	184	232		1.1	22.3	7.1	4	2		5.8
10/30/12	8.602	23.0	7.4	168	291		1.3	22.6	7.0	3	2	0.2	5.8
10/31/12	7.953	23.1	7.5	136	250		1.2	22.8	7.3	3	3		6.0
11/1/12	8.356	23.1	7.5	148	220	35.5	1.6	23.0	7.3	5	3	0.2	6.0
11/2/12	8.184	23.3	7.5				2.0	23.5	7.3				6.5
11/3/12	8.435	23.4	7.5				1.5	22.5	7.1				6.1
11/4/12	8.430	23.2	7.3	164	241	29.5	2.3	22.9	7.0	4	3	0.1	7.0
11/5/12	8.322	23.0	7.5	152	242		1.8	22.4	7.3	4	4		6.5
11/6/12	8.329	23.0	7.5	140	249		1.8	22.6	7.3	4	4	0.4	6.6
11/7/12	8.196	22.5	7.5	144	205		2.3	22.7	7.0	5	3		7.0
11/8/12	8.172	22.8	7.5	136	202	33.8	1.4	22.4	7.2	6	4	0.3	5.2
11/9/12	8.465	22.8	7.4				1.3	23.2	7.3				5.8

11/10/12	8.924	22.8	7.5				1.2	23.0	7.3				5.6
11/11/12	10.523	21.1	7.3	148	220	27.9	1.3	21.5	7.0	11	4	0.3	5.0
11/12/12	8.750	21.5	7.6	128	222		1.3	21.0	7.1	10	4		6.0
11/13/12	8.871	21.9	7.6	280	218		1.3	21.8	7.3	7	4	1.6	5.8
11/14/12	8.400	21.8	7.6	160	221		1.4	21.2	7.2	8	5		6.1
11/15/12	8.598	21.9	7.5	168	234	33.9	1.1	21.2	7.3	6	4	0.1	6.0
11/16/12	8.136	21.7	7.5				1.5	21.3	7.1				6.3
11/17/12	8.488	21.2	7.3				1.3	21.0	7.0				6.3
11/18/12	8.637	21.4	7.4	188	265	28.6	1.5	21.2	7.0	5	2	0.1	5.7
11/19/12	8.272	21.8	7.5	164	239		1.2	21.5	7.4	3	3		6.0
11/20/12	8.298	22.0	7.5	136	234		1.2	22.2	7.3	3	2	0.3	6.0
11/21/12	8.064	21.4	7.5	168	262		1.4	21.8	7.3	3	2		6.2
11/22/12	7.575	21.3	7.4	128	234	25.8	1.2	21.6	7.3	3	3	0.3	6.1
11/23/12	7.232	21.0	7.4				1.4	20.5	7.2				5.5
11/24/12	8.234	20.8	7.5				1.3	20.0	7.1				5.2
11/25/12	8.437	21.2	7.4	172	242	29.8	1.5	20.8	7.0	4	3	0.5	5.9
11/26/12	8.181	20.5	7.5	152	265		1.2	19.8	7.1	3	3		6.4
11/27/12	8.393	20.9	7.5	116	229		1.7	19.5	7.5	4	3	0.1	6.3
11/28/12	8.296	20.8	7.5	140	259		0.8	19.9	7.3	6	3		6.4
11/29/12	8.356	22.0	7.5	240	233	31.3	1.2	20.0	7.2	4	3	0.1	6.2
11/30/12	8.263	21.0	7.4				0.9	20.8	7.3				6.2
12/1/12	8.482	20.8	7.5				0.6	21.0	7.4				6.1
12/2/12	8.298	21.2	7.3	124	229	30.7	0.8	21.5	7.0	4	3	0.6	5.4
12/3/12	8.617	20.7	7.4	140	211		0.5	21.2	7.1	3	3		6.1
12/4/12	8.178	21.0	7.5	152	235		0.4	20.7	7.1	2	2	0.1	6.1
12/5/12	8.253	20.9	7.4	216	233		0.6	20.3	7.1	3	2		6.1
12/6/12	8.278	21.0	7.6	160	239	31.7	0.6	20.7	7.3	3	2	0.1	6.0
12/7/12	8.300	20.2	7.6				0.4	20.2	7.3				6.0
12/8/12	8.491	20.2	7.5				0.8	20.2	7.1				6.0
12/9/12	8.397	20.0	7.5	140	206	32.3	0.5	19.9	7.1	4	3	0.1	5.2
12/10/12	8.595	20.0	7.5	200	223		0.5	18.3	7.4	3	3		6.3
12/11/12	8.474	19.9	7.6	120	231		0.7	18.7	7.4	3	2	0.1	6.2
12/12/12	8.524	19.8	7.5	168	239		0.7	18.8	7.2	3	3		6.1
12/13/12	8.342	20.0	7.5	160	254	28.1	0.4	18.9	7.1	4	3	0.0	6.4
12/14/12	8.345	19.9	7.4				0.4	18.9	7.1				6.1
12/15/12	8.571	19.4	7.5				1.3	19.0	7.1				5.3
12/16/12	7.987	20.0	7.3	136	206	25.8	0.9	20.0	7.0	4	3	0.1	5.6
12/17/12	7.998	19.7	7.6	152	219		0.7	19.3	7.1	4	3		6.1
12/18/12	7.724	19.9	7.5	148	204		1.7	19.5	7.1	4	3	0.1	6.8
12/19/12	7.932	19.8	7.5	124	212		0.8	19.6	7.2	5	2		6.2

12/20/12	7.776	19.0	7.4	116	239	29.2	0.4	17.5	7.3	4	2	0.5	6.6
12/21/12	7.623	18.8	7.4				1.0	17.8	7.1				6.1
12/22/12	7.675	18.7	7.4				1.0	18.2	7.2				6.6
12/23/12	7.258	19.0	8.5	120	208	30.3	0.6	18.3	7.1	4	3	0.1	6.3
12/24/12	7.759	17.9	7.3	144	244		0.9	17.3	7.1	4	3		6.3
12/25/12	7.489	17.0	7.5	156	239		0.4	15.8	7.2	5	3		6.5
12/26/12	7.737	17.7	7.5	148	204		1.0	15.3	7.2	4	3		6.9
12/27/12	8.399	17.4	7.5	140	211	30.2	0.8	15.4	7.2	4	3	0.4	6.7
12/28/12	7.970	17.7	7.5				1.1	16.3	7.1				6.6
12/29/12	7.956	17.1	7.5				1.0	16.0	7.5				6.3
12/30/12	7.853	17.5	7.4	136	247	28.0	0.8	16.4	7.0	5	4	0.1	6.4
12/31/12	9.318	16.2	7.3	148	211		0.8	16.0	7.1	5	3		6.7
1/1/13	8.173	18.0	7.8	172	280		0.8	16.0	7.0	6	6	0.5	5.5
1/2/13	8.193	17.3	7.5	124	246		0.4	16.4	7.2	5	2		6.4
1/3/13	8.037	17.3	7.6	164	239	29.6	0.8	16.5	7.2	5	2	0.4	6.5
1/4/13	7.906	16.9	7.6				0.8	16.4	7.2				6.6
1/5/13	7.888	16.0	7.4				0.4	17.0	7.3				5.7
1/6/13	7.805	17.5	7.3	144	182	32.8	0.7	17.4	7.1	7	3	0.1	5.5
1/7/13	8.153	17.2	7.6	136	202		0.8	16.5	7.2	8	4		6.5
1/8/13	7.920	17.2	7.5	148	251		0.8	16.6	7.1	8	4	0.2	6.5
1/9/13	8.229	17.3	7.6	168	238		0.9	17.0	7.1	10	4		6.3
1/10/13	9.778	17.2	7.5	112	211	24.2	0.4	17.8	7.3	6	4	0.3	6.4
1/11/13	8.588	17.0	7.5				0.6	17.0	7.3				6.0
1/12/13	8.377	17.0	7.4				0.5	16.0	7.0				6.1
1/13/13	8.471	17.0	7.5	148	240	29.7	0.8	15.4	7.1	6	4	0.2	6.3
1/14/13	8.395	16.5	7.6	152	227		0.4	15.5	6.8	7	4		6.6
1/15/13	8.373	16.9	7.7	248	237		0.9	15.7	7.5	7	5	0.3	6.2
1/16/13	8.529	17.1	7.7	136	248		0.7	16.0	7.2	8	5		6.4
1/17/13	8.250	17.0	7.6	160	245	39.3	0.6	16.4	7.1	8	4	0.1	6.4
1/18/13	8.480	17.0	7.7				0.9	16.5	7.2				6.4
1/19/13	8.133	16.0	7.3				1.4	17.0	7.1				5.0
1/20/13	8.007	17.5	7.5	132	246	32.7	0.4	17.9	7.0	8	4	0.2	5.3
1/21/13	8.283	16.0	7.6	164	225		0.5	16.0	7.0	10	4		5.4
1/22/13	8.258	17.1	7.7	204	258		0.8	16.4	7.0	10	5	0.9	6.2
1/23/13	8.254	17.5	7.6	148	237		0.7	17.4	7.1	8	5		6.3
1/24/13	8.196	17.1	7.7	132	230	36.1	0.8	16.9	7.0	6	4	0.5	6.3
1/25/13	8.144	16.7	7.6				0.9	16.5	7.0				6.4
1/26/13	8.354	16.0	7.5				0.5	16.0	7.1				5.4
1/27/13	8.441	17.2	7.5	144	232	27.3	0.7	17.7	7.0	7	4	0.4	5.7
1/28/13	8.558	17.9	7.5	136	242		0.4	18.3	7.0	6	3		6.4

1/29/13	8.917	17.8	7.6	240	377		0.8	18.2	7.0	6	7	0.6	6.1
1/30/13	8.404	17.3	7.7	140	256		0.5	16.8	7.4	6	4		6.4
1/31/13	8.196	17.5	7.5	136	256	29.2	0.4	17.2	7.1	6	4	0.2	6.2
2/1/13	8.192	16.9	7.5				0.7	16.3	6.9				6.5
2/2/13	8.324	16.0	7.6				0.9	17.0	6.9				5.6
2/3/13	8.413	17.5	7.4	148	228	29.8	0.4	17.5	7.0	7	5	0.3	5.3
2/4/13	8.335	17.7	7.5	160	237		0.8	17.8	6.9	6	4		6.2
2/5/13	8.174	18.0	7.6	148	259		0.3	17.0	6.8	8	5	0.6	6.0
2/6/13	8.289	17.0	7.6	168	239		0.8	18.0	7.1	7	4		5.6
2/7/13	8.366	17.0	7.6	184	251	32.8	0.7	18.3	7.2	4	4	0.2	6.1
2/8/13	8.059	17.2	7.6				0.4	17.6	7.0				6.3
2/9/13	8.389	17.0	7.4				0.4	16.5	7.3				5.6
2/10/13	8.370	17.5	7.5	144	254	24.1	1.8	17.9	6.9	5	3	0.4	6.1
2/11/13	8.028	17.5	7.6	168	206		1.3	17.0	6.8	5	3		6.6
2/12/13	10.104	16.5	7.5	236	251		1.5	16.8	6.7	6	4	0.5	5.7
2/13/13	8.910	16.8	7.7	144	219		1.2	16.3	7.0	5	4		6.6
2/14/13	8.330	17.7	7.7	136	239	28.6	0.8	17.2	6.9	4	3	0.3	6.2
2/15/13	8.241	17.0	7.6				1.0	16.4	7.0				6.5
2/16/13	8.351	16.0	7.6				0.9	17.0	7.2				5.6
2/17/13	8.250	17.0	7.5	128	238	24.9	1.2	18.0	7.3	14	5	0.3	6.2
2/18/13	8.472	17.3	7.6	152	232		0.9	17.1	6.8	7	3		6.4
2/19/13	8.277	17.1	7.5	152	261		1.4	17.3	6.8	6	6	0.3	6.1
2/20/13	10.676	15.8	7.3	168	203		1.3	16.1	6.8	4	4		6.2
2/21/13	11.774	14.5	7.5	156	193	20.7	1.3	14.7	6.6	4	5	0.3	6.5
2/22/13	9.166	16.0	7.6				2.3	15.0	6.9				6.4
2/23/13	8.827	16.0	7.5				3.6	15.0	7.1				5.7
2/24/13	8.743	16.5	7.5	124	177	24.4	1.4	16.0	6.6	4	4	1.0	6.5
2/25/13	12.989	14.2	7.2	228	171		1.3	16.1	6.9	6	5		5.2
2/26/13	10.122	15.6	7.7	144	155		1.1	14.5	6.8	4	3	0.8	6.7
2/27/13	9.440	16.2	7.7	140	173		1.3	15.4	6.8	4	3		6.5
2/28/13	8.982	16.2	7.7	172	198	29.7	1.4	15.8	6.8	5	3	0.3	6.4
3/1/13	8.775	16.1	7.6				1.3	16.0	6.9				6.6
3/2/13	8.668	15.7	7.5				1.6	15.7	6.6				6.8
3/3/13	8.799	16.0	7.6	96	196	29.5	1.9	17.0	7.0	5	4	0.2	6.5
3/4/13	8.546	16.9	7.6	140	202		1.3	17.1	6.9	5	4		6.3
3/5/13	8.682	16.4	7.6	120	225		1.4	15.9	6.9	4	2	0.5	6.5
3/6/13	8.606	16.3	7.6	140	239		1.5	16.3	6.8	16	24		6.5
3/7/13	8.556	16.4	7.6	160	264	34.5	1.5	16.8	6.7	3	3	0.2	6.2
3/8/13	8.592	16.9	7.6				1.5	17.0	7.0				6.3
3/9/13	9.207	15.5	7.5				1.4	17.0	6.7				5.7

3/10/13	9.220	15.0	7.6	140	267	25.5	1.6	16.0	7.4	4	3	0.2	5.5
3/11/13	8.673	16.4	7.7	124	190		1.5	15.9	7.0	4	3		6.2
3/12/13	8.865	16.8	7.6	208	226		1.4	16.6	6.9	5	3	1.7	6.3
3/13/13	8.659	16.6	7.6	116	197		1.5	17.1	6.9	4	3		6.6
3/14/13	8.389	17.0	7.5	148	190	31.6	1.6	17.7	7.0	3	3	0.1	6.5
3/15/13	8.424	17.5	7.4				1.3	18.3	7.0				6.5
3/16/13	7.979	17.2	7.4				1.3	18.5	6.7				6.5
3/17/13	7.693	16.0	7.6	136	182	32.2	2.3	17.0	7.1	3	2	0.2	6.5
3/18/13	7.709	16.3	7.4	140	226		1.5	16.8	6.9	4	2		6.4
3/19/13	7.743	16.8	7.4	128	207		1.3	17.2	7.0	11	14	1.9	6.3
3/20/13	7.550	16.7	7.5	104	256		1.5	17.0	7.0	3	2		6.6
3/21/13	7.824	16.4	7.3	156	227	38.7	1.3	16.2	7.0	3	2	0.2	6.5
3/22/13	7.730	16.3	7.5				1.6	16.3	7.1				6.3
3/23/13	7.918	16.1	7.3				1.4	16.1	6.9				5.4
3/24/13	8.217	16.0	7.5	192	267	36.8	1.8	15.5	7.1	4	3	0.2	5.2
3/25/13	8.672	16.7	7.6	124	245		1.4	15.9	7.0	5	3		6.4
3/26/13	8.460	16.8	7.5	168	233		1.3	16.5	6.9	5	2	0.2	6.6
3/27/13	8.567	17.0	7.6	140	231		1.3	16.4	6.9	5	3		6.6
3/28/13	8.294	17.2	7.5	204	282	30.7	1.4	17.5	6.8	5	3	0.3	6.5
3/29/13	8.216	17.4	7.4				1.3	17.8	6.9				6.3
3/30/13	8.220	16.1	7.2				1.6	16.9	6.8				5.7
3/31/13	9.373	16.5	7.4	172	209	29.1	1.5	16.3	6.7	6	3	0.5	5.9
4/1/13	8.630	17.8	7.5	152	220		1.3	18.2	6.9	6	2		6.4
4/2/13	12.731	16.2	7.5	188	178		1.2	16.4	6.9	7	4	1.3	6.3
4/3/13	18.473	14.8	7.6	120	172		1.7	14.9	6.8	8	5		6.7
4/4/13	15.595	15.0	7.6	100	173	26.2	1.5	13.9	6.8	5	4	0.8	7.1
4/5/13	10.770	16.4	7.7				1.5	16.3	7.0				6.7
4/6/13	10.124	15.4	7.6				1.5	16.0	7.0				6.4
4/7/13	9.999	16.7	7.5	156	253	26.6	1.6	17.5	6.9	4	3	0.7	6.4
4/8/13	9.858	17.9	7.5	124	243		1.1	18.8	7.1	4	2		6.1
4/9/13	9.592	18.0	7.6	200	188		1.2	19.0	7.1	6	3	0.8	6.1
4/10/13	15.726	13.8	7.4	156	162		1.8	15.7	7.0	7	5		5.6
4/11/13	11.868	16.3	7.7	100	303	41.5	1.2	15.4	7.0	4	3	0.4	6.7
4/12/13	10.251	16.8	7.6				1.0	16.6	7.1				6.6
4/13/13	9.950	15.9	7.5				1.3	15.6	6.9				6.1
4/14/13	9.870	16.2	7.5	136	209	22.8	1.3	16.0	6.9	3	3	0.4	6.2
4/15/13	9.661	17.9	7.5	108	203		1.2	18.8	7.1	3	3		6.4
4/16/13	9.506	17.5	7.5	152	254		1.0	17.9	7.0	3	2	1.0	6.1
4/17/13	10.715	18.2	7.4	156	158		1.1	18.8	6.9	8	6		6.3
4/18/13	21.197	16.1	7.7	136	139	24.2	2.0	15.3	6.9	5	6	0.6	6.4

4/19/13	11.724	17.0	7.6				1.3	16.5	7.0				6.7
4/20/13	10.487	17.0	7.6				1.5	18.1	6.9				5.9
4/21/13	9.965	17.1	7.5	112	158	21.7	1.3	17.7	7.0	2	3	0.3	6.6
4/22/13	10.290	17.9	7.5	116	244		1.1	18.8	7.0	3	3		6.5
4/23/13	10.022	17.1	7.6	124	242		1.2	16.7	7.0	3	2	0.5	6.4
4/24/13	9.707	17.5	7.5	152	223		1.2	17.3	7.5	3	2		6.7
4/25/13	9.611	18.0	7.5	160	227	24.3	1.1	18.2	7.0	2	2	0.3	6.5
4/26/13	9.818	17.6	7.4				1.1	17.8	7.0				6.4
4/27/13	12.328	16.5	7.5				1.4	17.0	6.9				5.9
4/28/13	10.298	16.5	7.5	132	173	18.7	1.3	19.5	6.9	3	3	0.5	6.3
4/29/13	10.051	18.8	7.5	160	184		1.2	19.9	7.0	4	3		6.3
4/30/13	9.879	19.5	7.5	148	176		1.9	20.5	7.1	4	3	0.9	6.3
5/1/13	9.874	19.0	7.4	164	208		1.0	20.6	6.9	4	5		6.4
5/2/13	8.574	17.4	7.6	132	212	20.8	1.2	17.3	7.1	3	6	0.7	6.2
5/3/13	9.405	18.3	7.3				1.0	17.8	6.9				6.6
5/4/13	9.443	16.9	7.4				1.5	17.0	7.0				6.5
5/5/13	9.395	17.0	7.5	140	212	24.9	1.2	17.5	7.0	3	3	0.1	5.5
5/6/13	9.258	18.4	7.4	116	176		1.0	19.3	7.0	4	3		6.4
5/7/13	9.534	19.2	7.4	132	207		1.1	20.1	6.9	4	5	1.7	6.3
5/8/13	10.349	18.0	7.4	280	196		0.9	21.0	7.0	6	6		6.2
5/9/13	12.995	18.8	7.6	168	194	19.7	1.2	19.4	6.8	5	7	2.3	6.2
5/10/13	10.960	19.2	7.5				1.1	19.9	6.9				6.4
5/11/13	10.166	19.6	7.4				1.2	20.5	6.9				6.8
5/12/13	9.446	19.5	7.4	112	203	23.1	1.1	20.6	6.9	3	3	1.2	6.1
5/13/13	9.703	19.3	7.3	132	178		1.2	20.3	6.9	3	3		6.3
5/14/13	9.522	19.3	7.4	128	171		1.1	20.9	6.9	3	3	0.9	6.3
5/15/13	10.359	19.4	7.4	156	157		0.9	20.6	6.9	3	3		6.2
5/16/13	10.480	18.9	7.4	216	216	24.6	1.2	19.8	6.9	3	3	0.6	6.0
5/17/13	9.795	19.3	7.4				1.1	20.0	6.9				6.1
5/18/13	9.883	19.6	7.4				1.1	21.7	6.9				6.4
5/19/13	12.273	19.5	7.4	264	172	23.1	1.1	21.7	6.9	3	3	0.7	6.2
5/20/13	10.970	19.9	7.4	128	132		1.0	21.4	6.8	3	3		6.2
5/21/13	12.313	19.0	7.5	132	137		1.2	19.9	6.9	4	3	0.8	6.3
5/22/13	11.349	18.4	7.5	124	119		0.8	19.2	6.9	3	2		6.3
5/23/13	16.890	17.3	7.1	212	140	30.6	1.0	18.8	6.9	8	5	0.7	5.1
5/24/13	12.487	18.2	7.5				1.1	19.2	7.0				6.5
5/25/13	11.162	17.9	7.4				1.2	19.5	7.0				6.3
5/26/13	10.583	17.3	7.5	104	148	24.8	1.1	18.0	7.0	3	3	0.2	6.3
5/27/13	11.111	18.0	7.4	128	170		1.4	19.3	7.1	4	2		6.2
5/28/13	10.470	18.7	7.3	136	169		1.3	20.2	6.9	3	2	0.6	6.0

5/29/13	10.671	18.5	7.3	144	161		1.4	20.0	6.9	4	2		6.2
5/30/13	10.965	19.0	7.4	152	171	25.8	1.4	20.3	7.0	5	3	0.6	6.3
5/31/13	12.052	19.1	7.4				1.3	20.6	6.9				6.3
6/1/13	26.641	16.5	7.3				2.9	18.0	6.9				6.0
6/2/13	13.584	17.5	7.4	84	119	15.3	1.6	19.5	7.1	14	4	0.3	6.3
6/3/13	12.014	18.5	7.5	124	133		1.5	19.7	6.9	3	3		6.9
6/4/13	19.054	19.0	7.3	140	87		2.7	19.5	7.1	5	4	0.4	5.9
6/5/13	14.720	19.2	7.4	120	128		1.1	20.0	7.0	3	2		5.5
6/6/13	12.728	19.1	7.4	124	198	17.5	1.2	20.1	7.1	2	2	0.3	6.1
6/7/13	11.391	19.6	7.4				1.4	20.7	7.1				6.2
6/8/13	11.091	19.4	7.3				1.2	21.2	7.0				6.1
6/9/13	11.238	20.0	7.4	112	132	19.9	1.3	21.3	7.0	3	2	0.1	5.9
6/10/13	11.206	20.0	7.3	120	143		1.0	21.4	7.1	3	2		6.2
6/11/13	10.961	20.2	7.3	116	137		1.0	21.9	7.1	3	3	0.4	6.2
6/12/13	10.559	20.0	7.3	140	151		1.0	22.2	7.1	2	2		6.0
6/13/13	10.256	20.4	7.3	140	173	18.6	1.1	22.7	7.0	2	2	0.3	5.9
6/14/13	10.018	20.6	7.3				1.1	22.9	6.9				6.0
6/15/13	10.794	20.0	7.1				1.1	21.6	6.9				6.1
6/16/13	10.035	20.5	7.2	164	166	18.3	1.0	22.5	6.7	2	3	0.6	6.2
6/17/13	13.555	20.3	7.2	128	127		1.1	21.8	6.9	2	2		5.9
6/18/13	10.600	20.7	7.3	132	275		0.8	22.0	6.9	2	4	0.2	6.1
6/19/13	10.499	20.6	7.3	180	126		1.0	22.3	7.0	1	2		6.0
6/20/13	10.507	21.2	7.3	148	153	20.5	1.0	22.5	7.1	2	2	0.3	6.1
6/21/13	10.102	21.2	7.3				0.9	23.4	7.1				6.3
6/22/13	9.921	21.2	7.2				1.0	23.2	7.1				6.1
6/23/13	9.742	21.5	7.2	144	174	17.7	1.1	23.1	7.1	2	2	0.1	6.4
6/24/13	9.951	21.3	7.2	128	154		1.0	23.1	7.0	3	2		6.1
6/25/13	10.031	21.0	7.2	152	156		1.1	23.0	7.0	3	2	0.3	6.1
6/26/13	10.086	21.2	7.2	140	160		0.9	23.1	7.1	3	3		6.0
6/27/13	9.951	21.4	7.2	144	175	18.5	1.0	23.8	7.0	3	3	0.2	6.1
6/28/13	9.717	21.6	7.3				1.2	23.8	7.1				6.1
6/29/13	9.545	21.5	7.1				1.2	23.4	7.0				6.6
6/30/13	9.117	21.5	7.1	156	132	26.2	1.2	23.2	7.0	3	2	0.1	6.0
7/1/13	9.406	21.3	7.2		147		0.9	22.6	7.1		3		6.0
7/2/13	9.158	19.5	7.1	152	104		0.8	20.2	7.0	2	3	0.2	5.8
7/3/13	8.865	21.6	7.1	124	133		0.8	23.0	7.1	2	2		5.1
7/4/13	8.407	21.2	7.2	132	152	17.5	1.1	23.4	7.0	1	2	0.2	5.8
7/5/13	8.633	21.3	7.2	128			1.1	22.8	7.0	2			5.7
7/6/13	9.079	22.0	7.2				1.0	23.2	7.0				5.8
7/7/13	8.490	22.0	7.1	116	122	31.9	0.9	24.8	7.0	2	2	0.1	5.8

7/8/13	9.532	22.3	7.0	152	130		0.9	24.1	6.9	2	2		5.9
7/9/13	9.503	22.3	7.0	136	185		0.6	24.3	6.9	2	2	0.1	5.9
7/10/13	9.285	22.6	7.2	120	127		1.0	24.8	6.9	2	2		5.7
7/11/13	9.154	22.2	7.1	128	152	28.5	1.0	24.3	6.9	2	2	0.1	5.6
7/12/13	9.221	22.7	7.0				0.8	24.4	6.9				5.7
7/13/13	9.002	22.8	7.1				0.9	24.2	6.9				5.7
7/14/13	11.575	23.3	6.9	272	132	24.1	0.8	24.5	6.9	2	3	0.2	5.7
7/15/13	14.467	21.3	6.8	296	170		1.6	22.1	6.8	5	3		5.5
7/16/13	11.535	21.8	7.2	136	103		1.4	22.6	6.9	3	2	0.3	6.2
7/17/13	14.980	22.0	7.2	140	109		1.5	23.0	7.0	3	2		6.1
7/18/13	11.424	22.0	7.2	144	176	20.5	1.6	23.3	7.0	2	2	0.2	6.2
7/19/13	10.432	22.4	7.2				1.5	23.8	7.1				6.0
7/20/13	10.153	22.5	7.2				1.3	24.5	7.1				6.0
7/21/13	9.873	24.5	7.2	140	124	24.6	1.3	25.5	7.1	1	3	0.3	6.1
7/22/13	10.297	22.3	7.1	112	160		1.0	24.4	7.1	2	2		5.8
7/23/13	10.028	23.0	7.2	96	59		1.6	24.5	6.9	2	2	0.4	5.5
7/24/13	11.020	22.5	7.0	152	168		1.2	24.0	6.8	1	2		5.8
7/25/13	9.985	22.3	7.2	216	155	27.4	1.0	24.4	7.0	3	2	0.9	5.8
7/26/13	23.781	21.3	6.8				2.4	22.2	6.7				5.1
7/27/13	14.430	24.0	7.1				1.2	25.1	7.0				5.9
7/28/13	12.932	24.9	7.4	88	110	23.7	1.1	25.3	7.1	2	2	0.3	5.7
7/29/13	13.398	22.5	7.3	104	103		1.2	23.7	7.1	2	2		5.9
7/30/13	14.008	22.7	7.2	92	93		1.1	24.0	7.0	2	2	0.8	6.1
7/31/13	11.882	22.6	7.3	92	168		0.9	24.5	7.0	2	2		5.9
8/1/13	11.393	23.0	7.3	108	195	20.5	1.2	24.3	7.0	2	2	0.2	6.0
8/2/13	10.851	23.2	7.2				0.9	24.8	7.0				5.9
8/3/13	10.509	23.1	7.2				1.0	24.8	6.9				5.9
8/4/13	10.279	22.5	7.1	116	176	25.1	1.1	24.9	6.9	2	2	0.2	6.0
8/5/13	10.767	23.1	7.1	124	195		1.0	24.8	7.0	2	2		6.0
8/6/13	10.392	23.3	7.1	132	211		1.0	25.1	7.0	3	4	0.4	5.7
8/7/13	10.293	23.1	7.1	140	198		1.0	24.9	7.0	3	3		5.5
8/8/13	10.403	23.0	7.1	196	243	20.8	0.9	24.3	6.9	3	2	0.1	5.7
8/9/13	13.234	23.1	7.0				1.2	24.2	6.8				5.9
8/10/13	10.410	23.3	7.2				1.3	24.2	6.9				5.9
8/11/13	10.185	23.5	7.1	108	191	24.3	1.1	24.6	7.0	2	2	1.6	5.9
8/12/13	10.500	23.3	7.1	104	199		1.1	24.7	7.0	1	2		5.6
8/13/13	13.672	22.7	6.9	176	181		1.1	23.8	6.9	2	2	0.7	5.2
8/14/13	11.269	23.0	7.2	108	151		1.1	23.7	6.9	2	2		5.8
8/15/13	10.694	22.6	7.2	124	198	22.1	1.1	23.8	7.0	2	2	0.5	5.9
8/16/13	12.756	22.5	7.3				1.2	23.9	7.0				5.7

8/17/13	11.270	22.5	7.2				1.2	24.0	7.0				5.9
8/18/13	11.061	23.0	7.2	104	238	23.3	1.1	24.5	7.0	2	2	0.3	5.9
8/19/13	11.315	22.8	7.2	112	206		1.1	23.9	7.0	2	2		5.9
8/20/13	10.912	22.9	7.2	120	189		1.0	24.3	7.0	2	3	0.3	5.9
8/21/13	10.612	23.2	7.2	120	198		0.8	24.5	7.0	2	2		5.9
8/22/13	10.437	23.0	7.2	132	203	19.0	0.8	24.5	6.7	2	2	0.2	5.9
8/23/13	10.424	23.2	7.2				0.9	24.8	7.0				5.8
8/24/13	10.425	23.5	7.2				1.0	25.0	7.0				6.0
8/25/13	10.490	23.5	7.2	112	216	24.9	1.0	25.2	7.0	2	2	0.5	5.8
8/26/13	10.506	23.3	7.1	148	258		1.1	24.8	6.9	3	2		5.9
8/27/13	10.385	23.0	7.2	140	221		0.9	24.7	7.0	3	2	0.5	5.8
8/28/13	10.330	23.2	7.2	200	212		0.8	24.5	7.0	3	3		5.7
8/29/13	10.108	23.2	7.2	136	222	19.8	0.8	24.6	7.1	3	2	0.4	5.6
8/30/13	10.058	23.3	7.1				1.6	25.0	7.0				5.9
8/31/13	10.119	23.8	7.3				1.3	24.6	7.0				5.8
9/1/13	9.622	23.7	7.3	140	341	27.3	1.3	24.5	7.0	2	2	0.1	5.9
9/2/13	10.596	23.8	7.2	144	218		1.2	24.3	7.0	3	2		5.8
9/3/13	9.970	23.1	7.2	140	235		1.2	24.2	6.9	2	3	0.5	5.2
9/4/13	9.760	23.5	7.1	128	258		0.7	24.7	7.0	3	2		5.1
9/5/13	9.710	23.2	7.2	152	261	14.4	1.0	24.6	6.9	2	2	0.3	5.6
9/6/13	9.627	23.4	7.2				0.9	24.9	7.0				5.6
9/7/13	9.513	23.0	7.1				1.3	25.0	6.8				6.2
9/8/13	10.382	24.0	7.2	128	213	27.0	1.1	25.4	6.9	4	4	0.8	5.9
9/9/13	9.670	23.5	7.1	128	232		0.9	24.9	6.9	5	3		5.8
9/10/13	9.692	23.3	7.2	156	230		0.9	24.8	7.0	4	3	0.3	5.6
9/11/13	9.681	23.5	7.2	136	218		0.9	25.0	6.9	4	4		5.9
9/12/13	9.853	23.4	7.2	180	244	11.8	0.9	25.1	6.9	4	3	0.2	5.5
9/13/13	9.845	23.6	7.2				0.8	24.8	6.9				5.5
9/14/13	9.551	25.5	7.2				1.1	26.3	6.8				5.7
9/15/13	9.653	23.0	7.2	144	245	28.7	0.7	24.0	6.9	3	3	0.1	5.6
9/16/13	9.609	23.2	7.2	148	251		1.1	24.2	6.7	2	2		6.6
9/17/13	9.767	23.0	7.2	136	186		1.2	24.5	6.7	3	2	0.2	6.1
9/18/13	9.642	23.4	7.2	160	249		0.8	24.7	7.0	3	2		5.7
9/19/13	10.796	23.2	7.2	260	249	25.4	1.1	24.5	7.0	3	2	0.4	5.6
9/20/13	9.885	22.8	7.3				0.9	23.2	6.8				5.6
9/21/13	9.114	24.5	7.2				1.1	26.2	6.9				5.9
9/22/13	9.246	24.5	7.2	132	216	26.8	1.0	25.0	6.9	4	3	0.2	5.8
9/23/13	9.606	22.4	7.2	144	274		1.1	23.2	7.0	3	2		5.7
9/24/13	9.276	22.8	7.1	176	221		1.0	23.3	7.0	2	2	0.1	5.7
9/25/13	9.162	22.6	7.3	128	226		0.7	23.5	7.0	3	3		5.4

9/26/13	9.500	22.8	7.2	188	257	24.5	0.8	23.9	7.0	3	2	0.3	5.8
9/27/13	9.119	23.2	7.3				0.6	23.8	7.0				5.8
9/28/13	12.131	23.2	6.5				0.9	24.5	6.8				5.8
9/29/13	9.597	21.5	7.3	128	217	24.9	1.2	22.2	6.7	3	3	0.3	6.1
9/30/13	9.492	22.2	7.2	132	239		1.0	22.8	6.9	3	2		5.8
10/1/13	9.451	22.5	7.3	124	244		1.0	23.3	6.9	2	2	0.4	6.0
10/2/13	9.863	22.7	7.1	152	232		0.8	23.4	6.9	3	2		6.0
10/3/13	9.639	22.4	7.2	136	229	17.6	1.2	23.7	6.8	2	2	0.1	6.0
10/4/13	9.625	22.7	7.1				1.0	23.8	6.9				5.8
10/5/13	10.599	20.4	7.2				1.1	21.5	6.8				5.1
10/6/13	9.630	21.2	7.1	148	241	29.0	0.7	21.1	6.9	2	2	0.1	6.2
10/7/13	9.312	21.6	7.3	196	254		1.0	21.9	6.9	3	3		5.7
10/8/13	9.202	21.8	7.2	144	250		0.9	22.0	6.8	2	2	0.3	5.7
10/9/13	9.490	20.5	7.2	140	250		1.0	21.0	6.9	2	2		6.0
10/10/13	9.172	20.9	7.1	136	248	27.2	1.0	21.3	6.9	3	3	0.2	5.8
10/11/13	8.619	20.9	7.2				1.0	21.4	7.0				5.8
10/12/13	8.254	20.1	7.2				1.1	21.2	6.9				5.9
10/13/13	8.836	20.4	7.2	128	254	28.1	1.1	21.0	6.9	1	2	0.1	5.9
10/14/13	11.234	20.0	7.2	152	222		1.1	20.5	6.9	10	2		5.9
10/15/13	12.190	19.0	7.4	124	290		1.3	19.0	6.9	2	7	0.1	6.3
10/16/13	9.700	19.3	7.4	156	286		0.9	18.8	6.9	2	4		6.0
10/17/13	9.375	19.2	7.4	124	303	22.2	1.0	19.0	6.9	2	6	0.2	6.2
10/18/13	9.340	18.9	7.2				1.2	19.1	6.9				6.0
10/19/13	9.030	18.5	7.3				1.3	19.2	6.9				6.2
10/20/13	9.375	20.2	7.2	132	221	29.0	0.9	22.3	6.9	2	2	0.4	5.7
10/21/13	11.442	18.0	7.2	144	212		1.2	18.5	7.0	2	2		6.1
10/22/13	9.615	19.1	7.3	136	264		1.1	18.8	7.0	2	2	0.4	6.2
10/23/13	9.304	19.0	7.3	140	267		1.0	18.9	7.0	3	2		6.0
10/24/13	9.246	18.9	7.3	140	284	34.3	0.9	18.8	7.0	2	4	0.6	6.0
10/25/13	9.076	18.7	7.2				1.1	18.1	6.9				6.0
10/26/13	9.966	17.3	7.1				1.3	18.0	6.9				6.1
10/27/13	9.627	19.3	7.2	124	246	26.9	1.0	22.0	7.0	2	3	0.1	5.3
10/28/13	9.595	18.6	7.3	132	248		1.2	18.8	6.9	2	3		5.8
10/29/13	9.550	18.9	7.2	144	241		1.1	19.3	6.9	2	2	0.4	5.9
10/30/13	10.627	18.9	7.1	164	236		0.7	19.4	7.0	2	2		5.7
10/31/13	10.842	18.0	7.3	120	185	35.4	1.2	18.2	6.8	6	8	0.2	5.9
11/1/13	9.589	18.3	7.3				1.0	18.1	7.0				6.1
11/2/13	9.180	17.6	7.3				1.0	18.0	6.9				6.1
11/3/13	9.646	17.4	7.2	160	219	28.4	1.0	18.1	6.9	2	2	0.7	5.9
11/4/13	9.646	17.9	7.3	152	249		1.0	17.7	6.9	3	2		6.0

11/5/13	10.019	18.0	7.1	144	222		1.0	17.8	6.9	5	5	0.3	6.0
11/6/13	15.271	16.5	7.4	112	205		1.2	16.0	6.8	4	3		6.2
11/7/13	10.061	17.8	7.5	148	262	27.6	1.5	16.8	6.8	3	2	0.3	6.3
11/8/13	9.740	17.2	7.4				1.7	16.7	6.9				6.4
11/9/13	9.457	16.8	7.3				1.1	17.5	6.9				6.1
11/10/13	9.597	17.8	7.2	136	249	27.4	1.2	18.8	7.0	3	2	0.1	6.0
11/11/13	9.456	17.2	7.3	120	219		1.2	18.0	6.9	3	3		6.1
11/12/13	9.396	16.9	7.3	112	232		1.6	15.9	7.0	6	17	0.6	6.4
11/13/13	9.633	16.8	7.3	128	240		1.1	16.0	7.0	4	3		6.3
11/14/13	9.668	16.9	7.3	188	289	22.3	1.1	15.9	7.0	4	2	0.8	6.4
11/15/13	9.204	17.1	7.2				1.3	16.8	7.0				6.4
11/16/13	9.780	17.6	7.3				1.1	18.2	7.0				6.3
11/17/13	9.487	21.3	7.3	148	261	31.8	1.0	21.5	6.9	3	3	2.5	6.0
11/18/13	9.147	21.3	7.3	160	234		1.3	20.9	7.0	3	2		6.1
11/19/13	9.137	21.0	7.2	152	257		1.0	20.7	7.0	4	3	0.9	6.2
11/20/13	9.245	20.8	7.0	148	267		1.1	20.3	7.0	5	4		6.1
11/21/13	9.231	21.1	7.3	160	238	30.5	0.9	21.2	6.9	5	2	0.7	5.3
11/22/13	9.105	19.6	7.4				1.1	18.1	7.0				6.3
11/23/13	9.699	18.2	7.3				1.0	18.6	7.0				6.4
11/24/13	9.752	17.0	7.4	124	256	26.9	1.0	17.9	6.9	5	2	1.3	6.4
11/25/13	9.957	19.4	7.3	148	246		1.1	18.3	6.9	3	4		6.2
11/26/13	9.500	19.4	7.3	112	233		1.2	18.4	7.0	4	2	1.4	6.4
11/27/13	9.005	19.0	7.3	136	259		1.3	18.3	6.9	4	2		6.3
11/28/13	8.221	19.0	7.3	116	239	25.6	1.1	18.5	6.9	3	2	0.4	6.3
11/29/13	7.971	18.7	7.3				1.5	18.2	6.8				6.6
11/30/13	8.566	19.0	7.2				1.1	18.5	6.8				6.4
12/1/13	8.917	18.0	7.2	136	264	29.1	1.2	18.3	6.8	4	2	0.7	6.4
12/2/13	9.277	19.3	7.3	164	293		1.4	19.0	6.8	4	2		6.2
12/3/13	9.196	19.0	7.2	184	268		1.1	19.2	6.9	4	3	0.6	6.3
12/4/13	9.101	19.4	7.3	188	273		1.5	18.4	7.0	4	2		6.3
12/5/13	9.407	18.1	7.3	156	272	27.5	1.2	16.3	6.9	4	2	0.6	6.6
12/6/13	9.555	17.4	7.3				1.4	15.7	7.0				6.5
12/7/13	9.835	17.4	7.4				1.3	15.9	6.9				6.5
12/8/13	10.236	17.0	7.3	144	263	31.2	1.3	16.2	6.9	4	3	0.5	6.5
12/9/13	9.894	17.6	7.2	152	278		1.2	16.0	6.9	4	2		6.5
12/10/13	9.905	18.1	7.3	156	261		1.5	15.9	7.0	5	5	0.5	6.6
12/11/13	9.662	17.3	7.3	132	269		1.3	17.0	6.9	4	2		6.6
12/12/13	9.702	18.0	7.3	140	283	23.0	1.2	16.9	7.0	4	2	0.4	6.8
12/13/13	9.697	18.2	7.2				1.0	17.3	7.0				6.2
12/14/13	9.432	17.3	7.2				1.2	16.8	7.0				6.6

12/15/13	9.192	18.4	7.3	156	272	26.3	1.1	17.5	7.0	3	2	0.4	6.6
12/16/13	8.826	18.5	7.2	123	283		1.4	18.3	6.9	3	2		6.6
12/17/13	8.814	18.6	7.3	124	254		1.5	18.4	7.0	3	3	0.5	6.6
12/18/13	8.780	18.5	7.4	148	250		1.5	18.5	7.0	3	3		6.5
12/19/13	8.743	18.5	7.3	244	284	27.8	1.2	18.3	7.1	3	2	0.3	6.7
12/20/13	8.789	17.7	7.2				1.4	16.9	7.0				6.5
12/21/13	15.215	15.0	7.2				1.7	15.9	7.1				5.8
12/22/13	10.862	15.7	7.2	92	241	18.9	1.6	15.0	7.0	4	2	0.6	5.9
12/23/13	10.010	16.6	7.4	108	213		1.6	15.8	7.0	4	3		6.9
12/24/13	10.027	16.2	7.4	132	225		1.5	15.5	7.1	4	3	0.7	6.4
12/25/13	9.362	16.0	7.5	92	232		1.9	16.5	6.9	4	2		5.4
12/26/13	9.047	16.8	7.4	120	220	17.5	1.6	16.6	7.0	4	2	0.5	6.8
12/27/13	8.980	17.2	7.3				1.4	17.1	7.0				6.9
12/28/13	8.148	17.4	7.4				1.3	17.2	7.0				6.8
12/29/13	8.919	17.2	7.4	132	248	22.7	1.9	16.6	7.1	4	2	0.4	5.4
12/30/13	9.221	15.8	7.4	108	220		1.2	16.2	6.9	5	3		6.0
12/31/13	9.255	16.2	7.3	128	224		1.7	16.4	6.9	4	2	0.4	6.5

Appendix B: CECs (and MRLs) Analyzed

Compound	MRL (ng/L)	Compound	MRL (ng/L)
1,7-Dimethylxanthine	100	**Iohexol**	1000
2,4-D	5	**Iopromide**	5
4-nonylphenol	100	**Isobutylparaben**	5
4-tert-Octylphenol	50	**Isoproturon**	100
Acesulfame-K	200	**Ketoprofen**	5
Acetaminophen	500	**Ketorolac**	5
Albuterol	5	**Lidocaine**	5
Amoxicillin (semi-quantitative)	200	**Lincomycin**	10
Andorostenedione	5	**Linuron**	5
Atenolol	5	**Lopressor**	20
Atrazine	5	**Meclofenamic Acid**	5
Azithromycin	20	**Meprobamate**	5
Bendroflumethiazide	5	**Metazachlor**	5
Bezafibrate	5	**Methylparaben**	20
BPA	10	**Metolachlor**	5
Bromacil	5	**Naproxen**	10
Butalbital	5	**Nifedipine**	20
Butylparaben	5	**Norethisterone**	5
Caffeine	500	**OUST (Sulfameturon,methyl)**	5
Carbadox	5	**Oxolinic acid**	10
Carbamazepine	5	**Pentoxifylline**	5
Carisoprodol	5	**Phenazone**	5
Chloramphenicol	100	**Primidone**	50
Chloridazon	5	**Progesterone**	5
Chlorotoluron	5	**Propazine**	5
Cimetidine	5	**Propylparaben**	5
Clofibric Acid	5	**Quinoline**	5
Cotinine	10	**Salicylic Acid**	100
Cyanazine	5	**Simazine**	5
DACT	5	**Sucralose**	1000
DEA	5	**Sulfachloropyridazine**	5
DEET	100	**Sulfadiazine**	5
Dehydronifedipine	5	**Sulfadimethoxine**	5
DIA	5	**Sulfamerazine**	5
Diazepam	5	**Sulfamethazine**	5
Diclofenac	5	**Sulfamethizole**	5
Dilantin	20	**Sulfamethoxazole**	50
Diltiazem	5	**Sulfathiazole**	5

Diuron	5	**TCEP**	10
Erythromycin	10	**TCPP**	100
Estradiol	5	**TDCPP**	100
Estriol	5	**Testosterone**	5
Estrone (E1)	5	**Theobromine**	100
17β-Estradiol (E2)	5	**Theophylline**	200
Ethylparaben	20	**Thiabendazole**	5
Flumeqine	10	**Triclocarban**	5
Fluoxetine	10	**Triclosan**	10
Gemfibrozil	50	**Trimethoprim**	50
Ibuprofen	10	**Warfarin**	5

Appendix C: Stoichiometry Matrix

	Description	Units
r1	aerobic growth of heterotrophs on soluble substrate with ammonia as N source	gCOD/m3/d
r2	anoxic growth of heterotrophs on soluble substrate with ammonia as N source	gCOD/m3/d
r3	aerobic growth of heterotrophs on soluble substrate with nitrate as N source	gCOD/m3/d
r4	anoxic growth of heterotrophs soluble substrate with nitrate as N source	gCOD/m3/d
r5	decay of heterotrophs	gCOD/m3/d
r6	hydrolysis of entrapped organics	gCOD/m3/d
r7	hydrolysis of entrapped organic nitrogen	gCOD/m3/d
r8	ammonification of soluble organic nitrogen	gN/m3/d
r9	growth of autotrophs	gCOD/m3/d
r10	decay of autotrophs	gCOD/m3/d
r11	biodegradation of E1	g/m3/d
r12	adsorption of E1	g/m3
r13	desorption of E1	g/m3/d
r14	biodegradation of atenolol	g/m3/d
r15	adsorption of atenolol	g/m3
r16	desorption of atenolol	g/m3/d
r17	biodegradation of lopressor	g/m3/d
r18	adsorption of lopressor	g/m3
r19	desorption of lopressor	g/m3/d
r20	biodegradation of meprobamate	g/m3/d
r21	adsorption of meprobamate	g/m3
r22	desorption of meprobamate	g/m3/d
r23	biodegradation of triclosan	g/m3/d
r24	adsorption of triclosan	g/m3
r25	desorption of triclosan	g/m3/d
r26	biodegradation of gemfibrozil	g/m3/d
r27	adsorption of gemfibrozil	g/m3
r28	desorption of gemfibrozil	g/m3/d
r29	biodegradation of DEET	g/m3/d
r30	adsorption of DEET	g/m3
r31	desorption of DEET	g/m3/d
r32	biodegradation of caffeine	g/m3/d
r33	adsorption of caffeine	g/m3
r34	desorption of caffeine	g/m3/d
r35	biodegradation of theobromine	g/m3/d
r36	adsorption of theobromine	g/m3
r37	desorption of theobromine	g/m3/d
r38	biodegradation of sucralose	g/m3/d
r39	adsorption of sucralose	g/m3
r40	desorption of sucralose	g/m3/d
r41	biodegradation of acesulfame-K	g/m3/d
r42	adsorption of acesulfame-K	g/m3
r43	desorption of acesulfame-K	g/m3/d
r44	biodegradation of iopromide	g/m3/d
r45	adsorption of iopromide	g/m3
r46	desorption of iopromide	g/m3/d
r47	biodegradation of iohexol	g/m3/d
r48	adsorption of iohexol	g/m3
r49	desorption of iohexol	g/m3/d

	xii	si	ss	xi	xs	xbh	xba	xu
r1			- 1/yh			1		
r2			- 1/yh			1		
r3			- 1/yh			1		
r4			- 1/yh			1		
r5					1-fuh	-1		fuh
r6			1		-1			
r7								
r8								
r9							1	
r10					1-fua		-1	fua
r11						1		
r12								
r13								
r14						1		
r15								
r16								
r17						1		
r18								
r19								
r20						1		
r21								
r22								
r23						1		
r24								
r25								
r26						1		
r27								
r28								
r29						1		
r30								
r31								
r32						1		
r33								
r34								
r35						1		
r36								
r37								
r38						1		
r39								
r40								
r41						1		
r42								
r43								
r44						1		
r45								
r46								
r47						1		
r48								
r49								

	so	snh	snd	xnd	sno	snn
r1	-(1-yh)/yh	-ibhn				
r2		-ibhn			-(1-yh)/(2.86*yh)	(1 - yh)/(2.86*yh)
r3	-(1-yh)/yh				-ibhn	
r4					-ibhn -(1-yh)/(2.86*yh)	(1 - yh)/(2.86*yh)
r5				ibhn - fuh*iuhn		
r6						
r7			1	-1		
r8		1	-1			
r9	-(4.57-ya)/ya	-ibhn-1/ya			1/ya	
r10				ibhn - fua*iuhn		
r11						
r12						
r13						
r14						
r15						
r16						
r17						
r18						
r19						
r20						
r21						
r22						
r23						
r24						
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r36						
r37						
r38						
r39						
r40						
r41						
r42						
r43						
r44						
r45						
r46						
r47						
r48						
r49						

	salk	sza	xza	szb	xzb	szc	xzc	szd	xzd
r1	- ibhn/14.								
r2	(- ibhn/14.) + ((1 - yh)/(14*2.86*yh))								
r3	- ibhn/14.								
r4	(- ibhn/14.) + ((1 - yh)/(14*2.86*yh))								
r5									
r6									
r7									
r8	1/14.								
r9	(- ibhn/14.) - 1./(ya*7)								
r10									
r11		-1							
r12		-1	1						
r13		1	-1						
r14				-1					
r15				-1	1				
r16				1	-1				
r17						-1			
r18						-1	1		
r19						1	-1		
r20								-1	
r21								-1	1
r22								1	-1
r23									
r24									
r25									
r26									
r27									
r28									
r29									
r30									
r31									
r32									
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r40									
r41									
r42									
r43									
r44									
r45									
r46									
r47									
r48									
r49									

	sze	xze	szf	xzf	szg	xzg	szh	xzh	szi	xzi
r1										
r2										
r3										
r4										
r5										
r6										
r7										
r8										
r9										
r10										
r11										
r12										
r13										
r14										
r15										
r16										
r17										
r18										
r19										
r20										
r21										
r22										
r23	-1									
r24	-1	1								
r25	1	-1								
r26			-1							
r27			-1	1						
r28			1	-1						
r29					-1					
r30					-1	1				
r31					1	-1				
r32							-1			
r33							-1	1		
r34							1	-1		
r35									-1	
r36									-1	1
r37									1	-1
r38										
r39										
r40										
r41										
r42										
r43										
r44										
r45										
r46										
r47										
r48										
r49										

	szj	xzj	szk	xzk	szl	xzl	szm	xzm
r1								
r2								
r3								
r4								
r5								
r6								
r7								
r8								
r9								
r10								
r11								
r12								
r13								
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r26								
r27								
r28								
r29								
r30								
r31								
r32								
r33								
r34								
r35								
r36								
r37								
r38	-1							
r39	-1	1						
r40	1	-1						
r41			-1					
r42			-1	1				
r43			1	-1				
r44					-1			
r45					-1	1		
r46					1	-1		
r47							-1	
r48							-1	1
r49							1	-1

Appendix D: Kinetic Equations

	Description	Kinetic Equation
r1	aerobic growth of heterotrophs on soluble substrate with ammonia as N source	muh*MssHET*MsoHET*MsnhGEN*salksatHET*xbh
r2	anoxic growth of heterotrophs on soluble substrate with ammonia as N source	etag*muh*MssHET*inhibsoaxHET*MsnoHET*MsnhGEN*salksatHET*xbh
r3	aerobic growth of heterotrophs on soluble substrate with nitrate as N source	muh*MssHET*MsoHET*inhibsnhHET*MsnoHET*salksatHET*xbh
r4	anoxic growth of heterotrophs soluble substrate with nitrate as N source	etag*muh*MssHET*inhibsoaxHET*inhibsnhHET*MsnoHET*salksatHET*xbh
r5	decay of heterotrophs	bh*xbh
r6	hydrolysis of entrapped organics	kh* (subsatHET)*(MsoHET + etah*inhibsoo2HET*MsnoHET)*xbh
r7	hydrolysis of entrapped organic nitrogen	r6*(xnd/(xs))
r8	ammonification of soluble organic nitrogen	ka*snd*xbh
r9	growth of autotrophs	mua*MsnhGEN*MsnhNIT*MsoNIT*salksatAUT*xba
r10	decay of autotrophs	ba*xba
r11	biodegradation of E1	kbioE1*sza*xbh
r12	adsorption of E1	kdE1*sza*(xs+xbh+xba+xsto+xbp+xbt+xgly+xi+xu)/icv
r13	desorption of E1	kdes*xza
r14	biodegradation of atenolol	kbioate*szb*xbh
r15	adsorption of atenolol	kdate*szb*(xs+xbh+xba+xsto+xbp+xbt+xgly+xi+xu)/icv
r16	desorption of atenolol	kdes*xzb
r17	biodegradation of lopressor	kbiolop*szc*xbh
r18	adsorption of lopressor	kdlop*szc*(xs+xbh+xba+xsto+xbp+xbt+xgly+xi+xu)/icv
r19	desorption of lopressor	kdes*xzc
r20	biodegradation of meprobamate	kbiomep*szd*xbh
r21	adsorption of meprobamate	kdmep*szd*(xs+xbh+xba+xsto+xbp+xbt+xgly+xi+xu)/icv
r22	desorption of meprobamate	kdes*xzd
r23	biodegradation of triclosan	kbiotri*sze*xbh
r24	adsorption of triclosan	kdtri*sze*(xs+xbh+xba+xsto+xbp+xbt+xgly+xi+xu)/icv
r25	desorption of triclosan	kdes*xze
r26	biodegradation of gemfibrozil	kbiogem*szf*xbh
r27	adsorption of gemfibrozil	kdgem*szf*(xs+xbh+xba+xsto+xbp+xbt+xgly+xi+xu)/icv
r28	desorption of gemfibrozil	kdes*xzf
r29	biodegradation of DEET	kbioDEET*szg*xbh
r30	adsorption of DEET	kdDEET*szg*(xs+xbh+xba+xsto+xbp+xbt+xgly+xi+xu)/icv
r31	desorption of DEET	kdes*xzg
r32	biodegradation of caffeine	kbiocaf*szh*xbh
r33	adsorption of caffeine	kdcaf*szh*(xs+xbh+xba+xsto+xbp+xbt+xgly+xi+xu)/icv
r34	desorption of caffeine	kdes*xzh

	Description	Kinetic Equation
r35	biodegradation of theobromine	kbiothe*szi*xbh
r36	adsorption of theobromine	kdthe*szi*(xs+xbh+xba+xsto+xbp+xbt+xgly+xi+xu)/icv
r37	desorption of theobromine	kdes*xzi
r38	biodegradation of sucralose	kbiosuc*szj*xbh
r39	adsorption of sucralose	kdsuc*szj*(xs+xbh+xba+xsto+xbp+xbt+xgly+xi+xu)/icv
r40	desorption of sucralose	kdes*xzj
r41	biodegradation of acesulfame-K	kbioace*szk*xbh
r42	adsorption of acesulfame-K	kdace*szk*(xs+xbh+xba+xsto+xbp+xbt+xgly+xi+xu)/icv
r43	desorption of acesulfame-K	kdes*xzk
r44	biodegradation of iopromide	kbioiop*szl*xbh
r45	adsorption of iopromide	kdiop*szl*(xs+xbh+xba+xsto+xbp+xbt+xgly+xi+xu)/icv
r46	desorption of iopromide	kdes*xzl
r47	biodegradation of iohexol	kbioioh*szm*xbh
r48	adsorption of iohexol	kdioh*szm*(xs+xbh+xba+xsto+xbp+xbt+xgly+xi+xu)/icv
r49	desorption of iohexol	kdes*xzm

Appendix E: Kinetic Parameters

Cryptic Name	Variable Name	Value at 10ºC	Value at 20ºC	Arrhenius Coefficient	Units
Active Heterotrophic Biomass					
muh	heterotrophic maximum specific growth rate		3.2	1.072	1/d
ksh	readily biodegradable substrate half saturation coefficient		5		gCOD/m3
koh	aerobic oxygen half saturation coefficient		0.2		gO2/m3
kad	anoxic oxygen half saturation coefficient		0.2		gO2/m3
etag	anoxic growth factor		0.5		-
kno	nitrate half saturation coefficient		0.1		gN/m3
knh	ammonia (as nutrient) half saturation coefficient		0.05		gN/m3
bh	heterotrophic decay rate		0.62	1.029	1/d
kalk	alkalinity half saturation coefficient		0.1		mole/m3
Active Autotrophic Biomass					
mua	autotrophic maximum specific growth rate		0.9	1.072	1/d
kna	ammonia (as substrate) half saturation coefficient		0.7		gN/m3
koa	oxygen half saturation coefficient		0.25		gO2/m3
ba	autotrophic decay rate		0.17	1.029	1/d
kalka	alkalinity half saturation coefficient for autotrophic growth		0.5		mole/m3
Hydrolysis					
kh	maximum specific hydrolysis rate		3	1.072	1/d
kx	slowly biodegradable substrate half saturation coefficient		0.1		gCOD/gCOD
etah	anoxic hydrolysis factor		0.6		-
Ammonification					
ka	ammonification rate		0.08	1.072	m3/gCOD/d
High Concentration Inhibition					
kxbh	high concentration inhibition for heterotrophs		30000		gCOD/m3
kxba	high concentration inhibition for autotrophs		5000		gCOD/m3

Cryptic Name	Variable Name	Value at 10ºC	Value at 20ºC	Arrhenius Coefficient	Units
Biodegradation Constants					
kbioE1	biodegradation of E1		0.162	1.072	m3/g/d
kbioate	biodegradation of atenolol		0.0042	1.072	m3/g/d
kbiolop	biodegradation of lopressor			1.072	m3/g/d
kbiomep	biodegradation of meprobamate		0	1.072	m3/g/d
kbiotri	biodegradation of triclosan		0.0012	1.072	m3/g/d
kbiogem	biodegradation of gemfibrozil		0	1.072	m3/g/d
kbioDEET	biodegradation of DEET		0.0015	1.072	m3/g/d
kbiocaf	biodegradation of caffeine		0.04	1.072	m3/g/d
kbiothe	biodegradation of theobromine		0.038	1.072	m3/g/d
kbiosuc	biodegradation of sucralose		0.0000065	1.072	m3/g/d
kbioace	biodegradation of acesulfame-K		0.01	1.072	m3/g/d
kbioiop	biodegradation of iopromide		0.0075	1.072	m3/g/d
kbioioh	biodegradation of iohexol		0.0008	1.072	m3/g/d
Adsorption Constants					
kdE1	adsorption of E1		0.00017	1.072	m3/g
kdate	adsorption of atenolol		0.0003	1.072	m3/g
kdlop	adsorption of lopressor			1.072	m3/g
kdmep	adsorption of meprobamate		0.00079	1.072	m3/g
kdtri	adsorption of triclosan		0.001905	1.072	m3/g
kdgem	adsorption of gemfribrozil		0.0004	1.072	m3/g
kdDEET	adsorption of DEET		0.0001	1.072	m3/g
kdcaf	adsorption of caffeine		0.0002	1.072	m3/g
kdthe	adsorption of theobromine		0.0002	1.072	m3/g
kdsuc	adsorption of sucralose		0.00054	1.072	m3/g
kdace	adsorption of acesulfame-K		0.00017	1.072	m3/g
kdiop	adsorption of iopromide		0.000036	1.072	m3/g
kdioh	adsorption of iohexol		0	1.072	m3/g
kdes	desorption coefficient		0.1	1.072	1/d