HOW MUCH DATA IS REQUIRED FOR A ROBUST AND RELIABLE WASTEWATER CHARACTERIZATION

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ABSTRACT

Water resource recovery facility modeling requires a robust and reliable characterization of the wastewater to be treated. Current wastewater characterization practice often involves a limited number of relatively short-duration but intensive campaigns, where few studies have been conducted over characterization representativeness. With the one-year detailed wastewater characterization campaign conducted weekly in the Great Lakes Water Authority (GLWA) Water Resource Recovery Facility (WRRF) and a simplified standard Activated Sludge Model Number 1 (ASM1) model, this paper provided an overview of fractionation variety throughout the whole year, evaluated consequences of different campaign strategies to identify reasonable sample size and campaign periods. Finally, it proposed an adaptive approach for wastewater characterization. Results showed that characteristics of wastewater varies significantly throughout the year and a campaign size around 20 is suggested to ensure robustness. Characterization should be conducted during periods of normal and stable plant operation, which could be identified with suggested indicators.

KEYWORDS

Activated Sludge, Wastewater, Characterization, Models, Campaigns, Reliable, Robust

INTRODUCTION & BACKGROUND

Process modeling based on the International Water Association (IWA) Activated Sludge Models (ASM's) has become the standard technique for the design of Water Resource Recovery Facilities (WRRF's)(Hauduc et al. 2013; Phillips et al. 2009; Henze et al. 2000). These models depend on a detailed characterization of the influent wastewater which goes beyond the general simple lumped parameters, such as total five-day biochemical oxygen demand (BOD_5) and chemical oxygen demand (COD) typically collected for plant operation. Robust and valid characterization is essential for process modeling, as inaccurate wastewater composition inputs can lead to significant modeling error(Rieger 2012). The profound effect of wastewater characterization on modeling outputs has been demonstrated many times(Choubert et al. 2013; Petersen et al. 2002; Phillips et al. 2009), and include:

- Sludge production is influenced by the estimated inert particulate COD.
- Oxygen demand is influenced by the estimated total bio-degradable COD.
- Anoxic denitrification rate and anaerobic phosphorus release are influenced by the estimated readily biodegradable COD.
- Effluent COD is influenced by the estimated inert soluble COD.

In practice, wastewater characterization is conducted mainly via two methods: (1) physical-chemical and (2) respirometric. STOWA(Roeleveld and van Loosdrecht 2002) proposed simple and easy to implement guidelines based on physical-chemical methods. WERF(Melcer et al. 2003) provided a state-of-the-art and frequently used method for measuring key influent wastewater characteristics and kinetic/stoichiometric parameters covering both methods. BIOMATH(Vanrolleghem et al. 2003) developed a protocol for activated sludge model calibration, with influent wastewater characterized by the respirometric method. Recent attempts at integrated characterization suggested a combination of both methods (Lu, Zhang, and Zhang 2010). These various methods were compared by (Gillot and Choubert 2010) and Fall(Fall et al. 2011), where significant gaps were found in results.

Despite lack of agreement on the best characterization method, the choice should fit the purpose for which the model is being developed. Due to its time-consuming and labor-intensive nature, wastewater characterization is often conducted intensively within one or a limited number of short duration campaigns. While these data allow a simulation model to be set-up, concerns exist when the model is to be used to simulate future performance. For example, "Are sufficient data collected to robustly characterize the wastewater on a long-term basis?" and "Do wastewater characteristics vary on a seasonal or more random basis?". Non-representative wastewater characterizations can lead to significant cost implications when model results are used to make decisions on facility upgrades/expansions and operation.

On-going work at the Great Lakes Water Authority (GLWA) Water Resource Recovery Facility (WRRF) in Southeast Michigan provided an opportunity to conduct detailed wastewater characterization over an annual cycle. Building on this long-term data set, an assessment of

variations in wastewater characteristics and impacts of different strategies for wastewater characterization campaigns was conducted.

This paper evaluates alternative wastewater characterization campaign designs, mainly focusing on campaign size and timing. Following physical-chemical guidelines provided by WERF(Melcer et al. 2003), detailed wastewater fractionation and characterization was conducted every week for a one-year period. Characterization results were fed into a standard ASM1 model, and different practical campaign strategies were evaluated. Based on these investigations, suggestions about obtaining robust and reliable wastewater characterization estimates by campaign design are proposed. Bioreactor mixed liquor volatile suspended solids (MLVSS) concentration, which responds in a straightforward fashion to process operating conditions and the relative fractions of biodegradable and non-biodegradable particulate matter in the influent wastewater, was used as the modeled response variable, compared to actual daily values. GLWA uses the high purity oxygen (HPO) activated sludge process operated with an average 2.3-day solids resident time (SRT), making MLVSS concentration responsive to variations in wastewater characteristics.

METHODOLOGY

Description of the Plant

The GLWA WRRF is a 3,560,000 m^3/d (940 MGD) peak flow (secondary treatment) facility serving 3.1 million residents in Southeast Michigan. The liquid process treatment train consists of influent pumping and preliminary treatment (screening and grit removal), conventional primary treatment with ferric chloride addition for phosphorus removal, HPO activated sludge, and effluent disinfection. Flows above 3,560,000 m^3/day and up to 4,500,000 m^3/day, receive primary treatment with ferric chloride addition. Secondary treatment requirements apply, along with seasonally varied monthly effluent total phosphorus (TP) limits of 0.7 mg-P/L (October to March) and 0.6 mg-P/L (April to September). The plant routinely meets all discharge standards. Solids are thickened, dewatered, and either subject to drying or incineration and landfill.

Wastewater Fractionation

Flow-proportioned 24-hour composite samples are collected daily for influent wastewater, secondary influent (primary effluent) and secondary effluent by GLWA WRRF staff. There are actually three separate influent streams to the GLWA facility, and each is sampled separately. While a combined primary effluent stream is conveyed to secondary treatment, it passes through two different pumping stations to secondary treatment, and each secondary influent stream is sampled separately. Return activated sludge (RAS) is combined and conveyed to the HPO bioreactors, resulting in a "single" biological population, but two separate sets of secondary clarifiers exist and each set is sampled separately. Detailed wastewater fractionation was conducted weekly on all seven streams on samples collected on random weekdays over the period from October 19, 2017 to October 17, 2018. Wastewater fractionation generally followed the physical-chemical guidelines provided by WERF(Melcer et al. 2003) ,and consisted of stepwise filtration through the standard glass fiber filter (1.2 μm nominal pore size) and an 0.45 μm membrane filter. Filtrate through the glass fiber filter (1.2 μm) was defined as the sum of

soluble and colloidal COD (SCCOD). Filtrate through the 0.45 μm membrane filter was defined as soluble COD (SCOD). The difference between these two filtrates was defined as colloidal COD (CCOD). Particulate COD (PCOD) was defined as the difference between the total COD and SCCOD. COD and BOD$_5$ analyses were conducted by GLWA staff according to Standard Methods(American Public Health Association - APHA 2005).

Flocculation and filtration (Mamais, Jenkins, and Prrr 1993; Roeleveld and van Loosdrecht 2002)is more generally applied to determine the soluble fraction of wastewater. Previous work(Yan et al. 2018) had indicated that, for this wastewater, there was no significant difference for COD and BOD$_5$ between 0.45 μm membrane filtrate and the results when flocculation and filtration per the WERF protocol. Note that ferric chloride is added prior to the primary clarifiers for phosphate removal, and this may function, to a certain extent, to achieve the flocculation of colloidal organic matter present in the influent wastewater. An independent wastewater characterization effort was conducted during this period in connection with an on-going master planning effort(Mehrotra 2018) which reached similar conclusions. In this study they performed six days of COD characterization at the GLWA WRRF following standard physical-chemical guidelines(American Public Health Association - APHA 2005) ,and these results generally support that use of simple membrane filtration, rather than the more complicated flocculation and filtration procedure, is reasonable to characterize soluble organic constituents for this wastewater. Secondary influent (primary effluent) data were used in this study for modeling purposes. Not including flocculation and filtration of the samples collected from the several locations each week also facilitated the significant duration of the sampling program and became a practical consideration in proceeding with the characterization campaign.

Mapping Measured Wastewater Fractions into Model Inputs

Required IWA ASM inputs include readily biodegradable COD (S_s), slowly biodegradable COD (X_s), soluble inert COD (S_I) and particulate inert COD (X_I)(Henze et al. 2000), which were calculated as fractions of total COD. As discussed below, colloidal COD was found to be insignificant for this wastewater and, therefore, was incorporated into the particulate COD fraction. The soluble inert COD (S_I) was determined directly as the measured second effluent membrane filtrated COD (SCOD$_{nb}$). The readily biodegradable COD (S_s or SCOD$_{bio}$) was calculated as the difference between the total soluble COD (SCOD) and SCOD$_{nb}$. The total biodegradable COD (SCOD$_{bio}$ + PCOD$_{bio}$) was determined using the measured BOD$_5$ following STOWA guidelines(Roeleveld and van Loosdrecht 2002) and using a biodegradable COD/BOD$_5$ ratio of 1.73 mg COD/mg BOD$_5$. The slowly biodegradable COD (X_s or PCOD$_{bio}$) was determined as the difference between the total biodegradable COD and SCOD$_{bio}$. The final remaining COD (PCOD$_{nb}$) was then the particulate inert COD (X_I). A manual reconciliation process, including mass balance check, specific ratio check, non-negativeness check etc.(Belia et al. 2009) was applied to the four wastewater component data, and records with apparent abnormalities were omitted. The reconciled COD concentrations were converted into fractions and then fed into the model.

Biological Process Modeling

The HPO process was modeled in MATLAB® using a standard IWA ASM1(Henze et al. 2000) ,modified as described below, with measured secondary influent total COD and fractions determined as above as input. Secondary influent was used in the model for two reasons. One is that it represents the direct input to the secondary treatment process and, consequently, the impacts of upstream treatment on wastewater constituents need not be included in the model. Secondly, GLWA measures secondary influent total COD daily, so a several-year-database was available for extensive evaluation of model performance based on various approaches for analyzing the fractionation results, as described below. Two long-term data sets were used for modeling and model evaluation. Daily data for the period of October 19, 2017 to October 17, 2018, corresponding to the year over which detailed wastewater fractionation occurred, were used as the model training set. Daily data from October 18, 2013 to October 17, 2017 were used for model evaluation and verification.

A simplified model based on a single completely-mixed bioreactor was used to compute the MLVSS, the response model variable which was compared to the measured MLVSS concentration. This simplified model facilitated process modeling and data analysis (around 50 times reduction on run-time). A more complete model of the entire liquid treatment process had previously been developed in SUMO (Dynamita). Comparison of the results from the two models demonstrated that use of the simplified bioreactor configuration did not materially affect MLVSS predictions. Further details of the model used include:

- Biochemical processes included growth, decay and hydrolysis. Because biomass prediction was the main objective of this study, only these highly biomass-related reactions were considered.
- Heterotrophic biomass was used to estimate the overall biomass. As is typical for HPO processes used for secondary treatment due to the relatively low SRT (average= 2.3 days) and the reduced bioreactor pH due to the retention of CO2 in solution, nitrification does not occur in the full-scale system.
- Since it is an HPO process, where oxygen is not limiting, oxygen limiting terms in reaction rate expressions were not included.
- Standard stoichiometric and kinetic parameters and temperature correction factors from the literature(Alikhani et al. 2017; Grady et al. 2011; Hauduc et al. 2011) were used, as summarized in **Table 1**.

Model Performance Evaluation

Mean and standard deviation values were calculated for model predictions and actual MLVSS data, and the root mean square error (RMSE) between model predictions and actual MLVSS concentrations was calculated to evaluate model performance. Our evaluation focused particularly on instances where model predictions appeared to differ noticeably from measured values, as they suggested periods of lack of fit for the model. We defined two types of deviations, namely outliers and spikes. Outliers were defined by comparison of individual model predictions to individual actual values where the deviation exceeded +/- three standard deviation from the actual MLVSS (corresponding to a probability of occurrence 0.3 % based on the

assumption of a normal distribution). Spikes were defined by deviations exceeding +/- two standard deviation of actual MLVSS (corresponding to a probability of 4.6 %)(Taylor 1982).

Table 1 *Stoichiometric and Kinetic Parameter Values and Temperature Correction Factors Used in Model.*

Type	symbol	Parameter	Unit	Value	Factor θ^a
	μ_H	Maximum specific growth rate of Heterotrophs	d^{-1}	6	1.072
	K_s	Substrate half saturation for heterotrophs	mg COD L^{-1}	20	1.03
Kinetics	f_D'	Fraction of biomass contributing to debris	g COD g COD^{-1}	0.08	1
	b_L	Aerobic decay coefficient for heterotrophs	d^{-1}	0.63	1.03
	k_h	Hydrolysis rate coefficient	d^{-1}	2.2	1.03
	K_x	Hydrolysis half saturation coefficient	g COD g VSS^{-1}	0.15	1
Stoichiometries	Y_H	Yield of Heterotrophs on substrate	g COD g VSS^{-1}	0.67	1
	$i_{VSS,B}$	COD/VSS ratio of biomass	g COD g VSS^{-1}	1.42	1
Partitioning Coefficients	$i_{VSS,XI}$	COD/VSS ratio of particulate inert	g COD g VSS^{-1}	1.5	1
	$i_{VSS,Xs}$	COD/VSS ratio of particulate substrate	g COD g VSS^{-1}	1.8	1
	$i_{VSS,XD}$	COD/VSS ratio of biomass debris	g COD g VSS^{-1}	1.3	1

[a] Temperature dependent parameter: $P(T)=P_{20} \theta^{(T-20)}$. The referral temperature is 20 °C.

Table 2 *Comparison of the Results from this Study for Wastewater COD fractions Compared to Literature Values*

Source	Total COD mg/L	COD Fraction in Percentage				
		S_s	S_I	X_s	X_I	Biomass, X_H
Primary Effluent Characteristics						
This study *	159 ± 41	22 ± 9	15 ± 7	28 ± 13	35 ± 15	-
(Fall et al. 2011) *	492	36	5	35	24	-
(Siegrist et al. 1995) [1]	250	10	8	58	24	-
(Henze 1992)		29	3	43	11	14
Raw Influent Characteristics						
This study *	280 ± 85	20 ± 10	9 ± 5	35 ± 15	36 ± 20	-
(Mehrotra 2018) *	290	15	9	24	52	-
(Lu et al. 2010)	540	8 - 10	1 - 4	27 - 40	14 - 36	23 - 46
(Zhou et al. 2008)	176 - 220	19.5 -27.8	8.4 - 12.8	16.1 - 37.3	13.9 - 33.4	14.7 - 18.9
(Roeleveld et al. 2002) *	241 - 827	9 - 42	3 - 10	10 - 48	23 - 50	-
(Kappeler et al. 1992)	250 - 430	7 - 11	12 - 20	53 - 60	8 - 10	7 - 15
(Henze 1992)	400	27	15	40	17	-

*The fractions were measured and calculated purely with physical-chemical method
[1] The Siegrist's fraction was calibrated estimations used in modeling based on literature (not directly measured)

Practical Campaign Strategies Evaluation

Three averaging strategies, yearly-, quarterly- and monthly-, were applied for conversion of the measured fractionation data to determine model inputs, and then fed into the model to predict the bioreactor MLVSS concentration. This approach was used, not only for the period over which detailed wastewater fractionation was conducted (October 19, 2017 to October 17, 2018). To further evaluate the general applicability of the fractionation data and averaging strategies, the results from the three different averaging strategies were applied over the preceding four years of data and the resulting bioreactor MLVSS concentrations were calculated. In addition, each single-monthly-average fraction value was used to represent whole-year values to evaluate the performance of shorter period characterization campaigns.

Potential Indicators of Days Bad for Campaign

Using the yearly-average model for the training data set, individual days were divided into two categories - spikes ($\geq$ 2 STD) and non-spikes. Differences in important plant conventional influent wastewater and operational features for these two data sets were investigated. Unpaired two sample t-tests were conducted over those features to detect statistically significant differences in mean values. Significantly different features can potentially serve as a flag for a bad campaign day.

Campaign Size Evaluation

Random sampling without replacement was conducted for different sample sizes from the year-long campaign data to determine the effect of sample size on wastewater characteristic estimates. Estimates of COD fractions gained from different sample size were averaged and fed into the model for simulation. Fifty iterations were conducted for each sample size. Maximum and mean values for averages of year-long predicted MLVSS, RMSE, number of outliers and number of spikes were calculated for each sample size.

RESULTS AND DISCUSSION

Determination of Model Input Values Based on Measured Fractionation Data

Raw secondary influent total COD and concentration fraction data for the year over which these data were collected are presented in **Figure** 1. The total COD concentration varied significantly (158 $\pm$ 40 mg/L, ranging from87.5 to 259 mg/L) throughout the year, primarily as a result of dilution during wet weather periods considering the GLWA WRRF is a combined sewage system. Particulate components appeared to be the most varied, covering a range of 27 - 217 mg/L, while the soluble component fluctuated with a range of 21 – 104 mg/L. The colloidal component was generally smaller than the particulate and soluble components, and some negative values were recorded. This can arise because the colloidal component is calculated by difference between the measured glass fiber and 0.45 μm filter filtrates. Since any measurement is subject to random errors, a measured value for the 0.45 μm filtrate that is randomly higher than the true value and the measured value for glass fiber filtrate that is randomly lower than the true value can result in the calculation of a negative value. The uncertainties (standard deviations) for total COD and glass fiber filtered COD were 40 and 27 mg COD /L respectively, and the

maximum absolute value of colloidal component was 56 mg/L, mathematically supporting that the colloidal concentration was subject to measurement error. Analysis of the secondary influent wastewater characterization data collected by (Mehrotra 2018) during this same period suggested that the colloidal fraction is not statistically significant. Thus, it appears likely that the concentration of colloidal COD in the secondary influent (primary effluent) may be small enough that it cannot be accurately measured for this wastewater. Inspection of the data presented in Figure 1 also suggests that colloidal COD is a small fraction of the total COD and that it can, perhaps, be neglected as long as it is incorporated into another COD fraction.
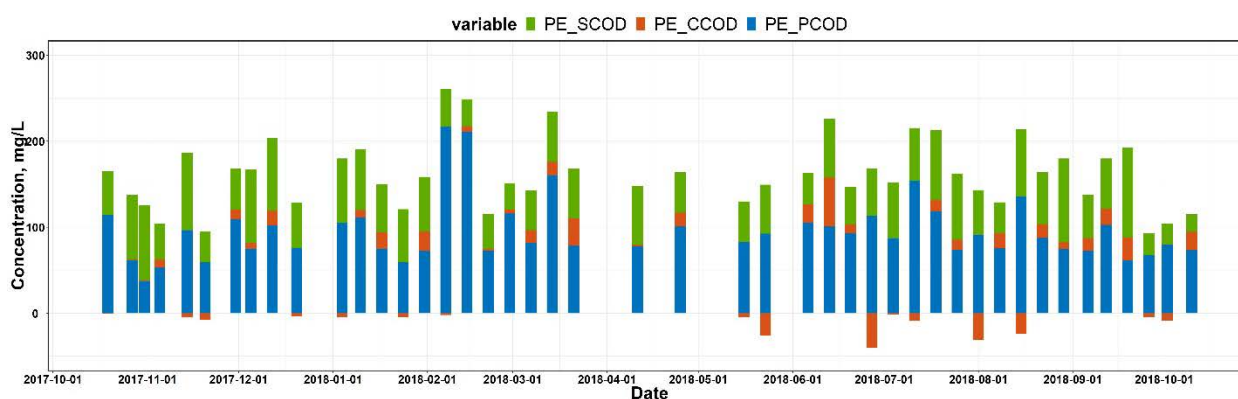
Figure 1 Variation of Secondary Influent (Primary Effluent) COD Concentration Fractions Based on Filtration Procedure Applied Throughout the Campaign Year.
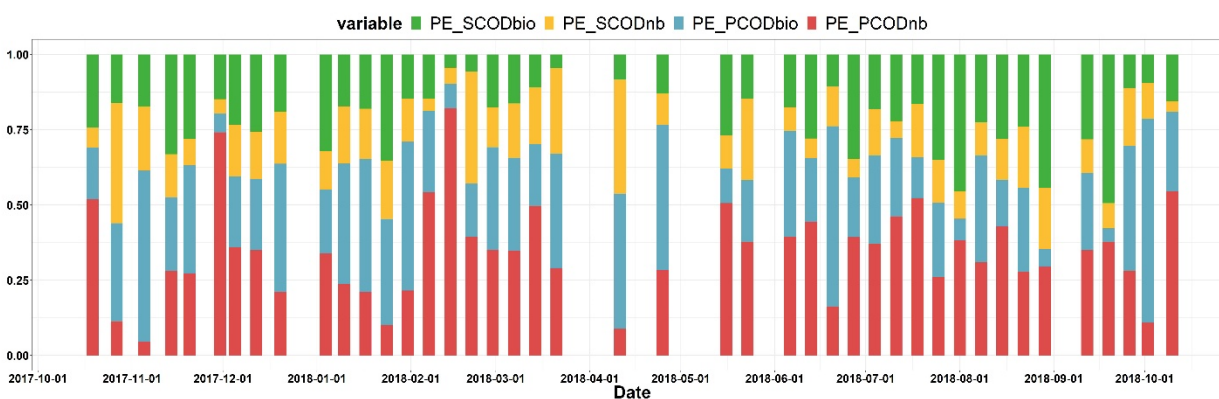
Figure 2 COD Model Input Values as a Fraction of Total COD for the Campaign Year. Components: Biodegradable COD (S_s), slowly biodegradable COD (X_s), soluble inert COD (S_I) and particulate inert COD (X_I)

Based on the observations above, a one-sample-t-test was conducted with a null hypothesis that the mean value of the colloidal COD is not equal to zero. With 95% confidence, the analysis failed to reject the null hypothesis (p-value = 0.13). In addition, ordinary least square linear regression analysis was conducted for the relationship between colloidal COD and total COD. Results showed that: (1) both slope and intercept were not significant; (2) The goodness of fit, R square, was 0.022 (3) the p-value of the ANOVA test comparing this linear fitting with no fitting was 0.32. These results all indicate that the colloidal component is sufficiently small that it cannot be measured for this wastewater with this technique. Consequently, this fraction was incorporate into particulate components as is the typical approach when ASM1 is applied.

Figure 2 summaries the reconciled input fractions for each day of the campaign year. There was no obvious pattern throughout the campaign year, and particulate COD (both biodegradable and non-biodegradable) varied more than soluble COD components**. Table 1** provides both raw influent wastewater and primary effluent characteristics, as determined in this study, compared to recent literature values. The results for this wastewater are within the range of those obtained with other wastewaters, suggesting that it may be generally representative of domestic wastewater from a large metropolitan area.

Comparison of Model Results with Actual Data

The three different methods for averaging the fractionation data were evaluated using the campaign year as the training set, and the preceding four years as the validation set, as described above. **Figure 3** compares predicted and measured MLVSS concentrations for the three methods for the training set, while **Table 3** summarizes performance statistics for the training and validation data sets. While variations occur between model-predicted and actual MLVSS values, the model-predicted and measured MLVSS concentrations are generally of the same order of magnitude for all three averaging methods. This is significant as the modeling approach does not include a mechanism to directly calibrate the model results to measured values. Model stoichiometric and kinetic parameters are standard values taken from the literature, as discussed above and summarized in Table 1, and wastewater influent values are based on measured influent values, as described previously. As noted in **Table 3**, actual average MLVSS concentrations compare quite well with model values, irrespective of the averaging method used. Importantly, this suggests that the wastewater characterization method used, along with the use of relatively standard stoichiometric and kinetic coefficients, can lead to a reasonable model to begin with.

Table 3 *Simulation Results for the Three Different Fractionation Averaging Methods for the Training and Testing Data Sets.*

Set	Average Method	Mean mg VSS/L	STD mg VSS/L	RMSE mg VSS/L	> 1 STD	> 2 STD	>3 STD
Training (2017/10/18-2018/10/17) Size: 365	Actual	1311.6	170.9				
	Yearly	1419.3	216.5	229.4	38.9%	14.0%	4.4%
	Quarterly	1411.2	213.7	243.2	45.4%	15.6%	4.9%
	Monthly	1413.5	361.7	343.5	55.6%	27.4%	10.7%
Testing (2013/10/18-2017/10/17) Size: 1461	Actual	1165.9	185.9				
	Yearly	1119.7	281.0	256.3	44.0%	16.2%	3.0%
	Quarterly	1112.8	288.1	185.9	47.8%	17.2%	3.8%
	Monthly	1106.9	332.5	312.2	56.0%	24.4%	6.0%

Visual inspection of the data presented in **Figure 3** indicates a noticeable lack of fit from early February to late March. Model predictions consistently exceed actual values, and the deviations exceed the 10 % criteria often applied to indicate model lack of fit (Rieger 2013). Inspection of the individual data during this period indicated that this arose because of the nature of the model used. As indicated in **Table 1,** values for the COD/VSS for influent particulate inert material ($iVSS,X_I$) and influent particulate substrate ($iVSS,X_s$) of 1.5 and 1.8 g COD g VSS^{-1} are used,

while the actual measured value for the influent particulate matter throughout the year was 1.9 ± 0.7, ranging from 0.7- 4.1g COD g VSS^{-1}. The ratio for February to April was 2.5 ± 1.0. In fact, use of higher values in the model for this period resulted in near elimination of this lack of fit. By adjusting iVSS,Xs from 1.8 to 2.3 and iVSS,XI from 1.5 to 2.0, the February spike was eliminated, but the resulting model underestimated the actual MLVSS for March. Overall, the mean predicted MLVSS was improved to 1361.4 mg/L, along with small improvements of RMSE and standard deviation (221.3 and 204.5 mg/L, less than 8 %). From a modeling perspective, the lack of fit during the February to March period did not occur due to variations in wastewater characteristics, but rather because of poor model structure as the COD to VSS ratio for these individual model components was not formulated as a wastewater characteristic but as a model parameter. Interestingly, the months of February and March represent a distinct operating period when influent flows tend to be somewhat higher and periods of precipitation occur (this is a combined system, as described above). This unusual operating period may explain why the COD to VSS ratio is higher during this period. The impact of unusual operating conditions is addressed in additional detail below. From a modeling perspective, a-priori knowledge concerning this failure of model structure would be required if the model is to be used to predict future performance.

Table 4 *Simulation Results Using Fractionation Data from an Individual Month to Represent the Whole Year.*

Month	Mean mg VSS/L	STD mg VSS/L	RMSE mg VSS/L	> 1 STD	> 2 STD	>3 STD	Size
January	947.9	145.7	400.4	86.6%	60.3%	16.7%	5
February	1915.9	292.2	656.2	96.2%	8.8%	58.6%	4
March	1424.2	217.2	230.0	40.4%	12.9%	4.4%	3
April	1068.5	163.2	297.8	72.3%	28.5%	4.7%	2
May	1525.5	232.7	302.2	57.5%	24.1%	8.2%	2
June	1441.8	219.9	242.7	40.8%	15.9%	5.8%	4
July	1512.2	230.7	292.4	54.2%	22.5%	7.4%	4
August	1651.8	251.9	409.7	81.1%	43.0%	20.0%	5
September	1494.5	228.0	279.1	51.0%	20.5%	6.3%	3
October	1337.4	204.0	195.8	34.2%	8.2%	2.5%	4
November	1342.8	205.1	198.8	32.6%	8.2%	2.2%	4
December	1304.2	199.5	194.1	35.6%	8.8%	1.6%	3
Actual	1311.6	170.9					43
Yearly Average	1361.3	326.0	294.4	53%	23%	8%	43
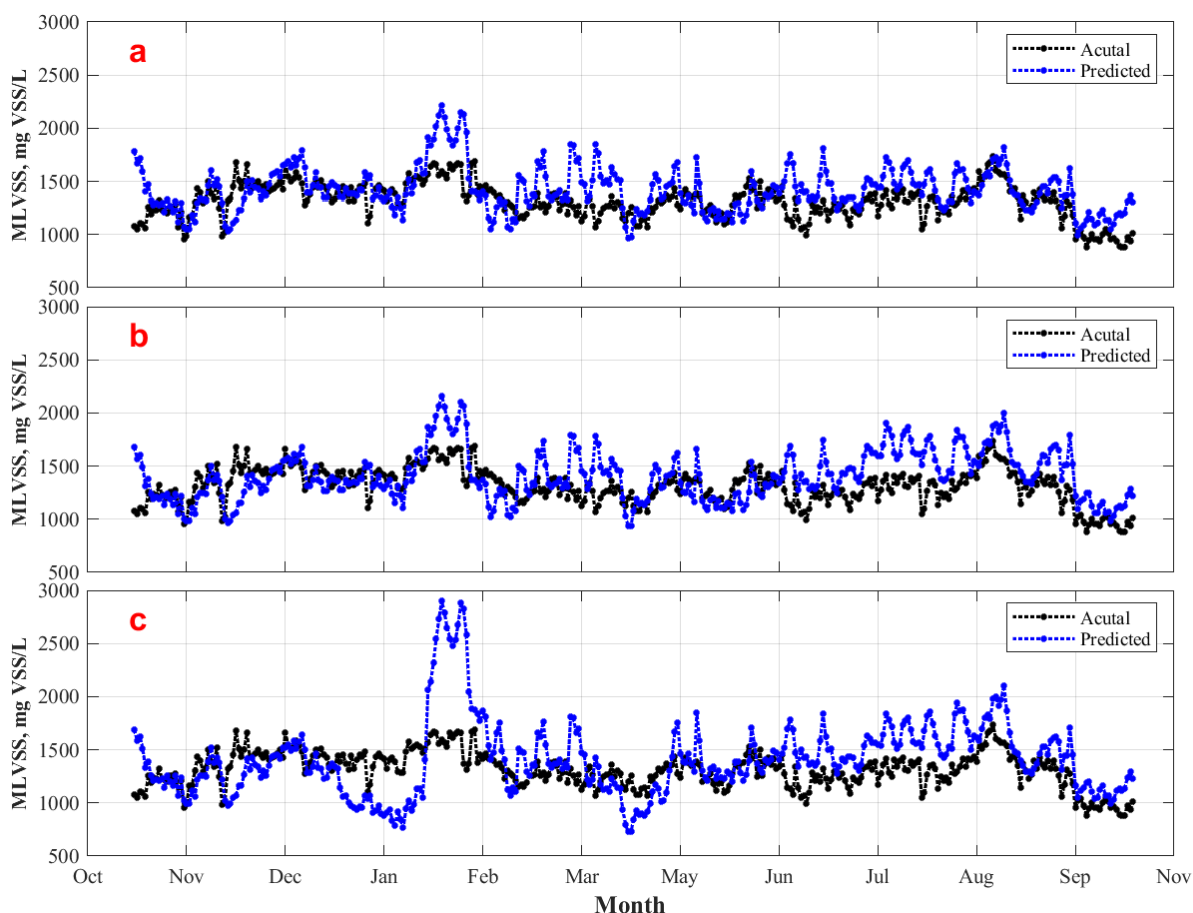
Figure 3 *Simulation Results for the Three Different Fractionation Averaging Methods for the Training Data Set. (a) Yearly-average; (b) Quarterly-average; (c) Monthly average.*

The results summarized in **Table 4** address a different question, that is whether there were better and worse times to conduct fractionation studies. It differs from the monthly analysis summarized in **Table 3** and illustrated in **Figure 3** in that the fractionation results for a single month are used to model the entire year. The results indicate that some time periods are better than others.

The poorest results occur when characterization data from February is used, as might be expected from the results presented immediately above. The difference between the mean predicted and actual MLVSS increases to 46 % of the actual value, the RMSE is more than triple the value for yearly average results presented in **Table 3**, the percentage of predictions exceeding one STD increased to 96.2 %, and 58.6 % exceeded three STD. On the other hand, the fractionation data from certain months, such as March and October to December, generally performed better in terms of mean values, RMSE, and the percentage exceeding two and three STD (spikes and outliers) as summarized in **Table 3**. Note that the number of fractionation measurements was not the main contributor to improved performance, as larger sample size did not guarantee good performance (August and February) and smaller sample size did not diminish performance (April). It is noted that the period of October to December generally represents a period of lower plant influent flow.

A further analysis of the potential reasons for deviations was conducted by evaluation of the difference in operating conductions on days where spikes (difference between modeled and actual MLVSS $\geq$ 2 STD) occurred, compared to the operating conditions for days when spikes did not occur. As shown in **Figure 5**, the hypothesis test results indicate that, within a 95% interval, days with spikes tended to occur on days with lower SRT, MLSS, higher secondary influent BOD_5, COD, TSS and VSS concentration, and higher secondary effluent TSS concentration. In short, efforts should be made to conduct fractionation campaigns during periods of relatively normal influent flow, loading, and operation, and results from periods where these factors are somewhat abnormal should be carefully screened and reviewed.
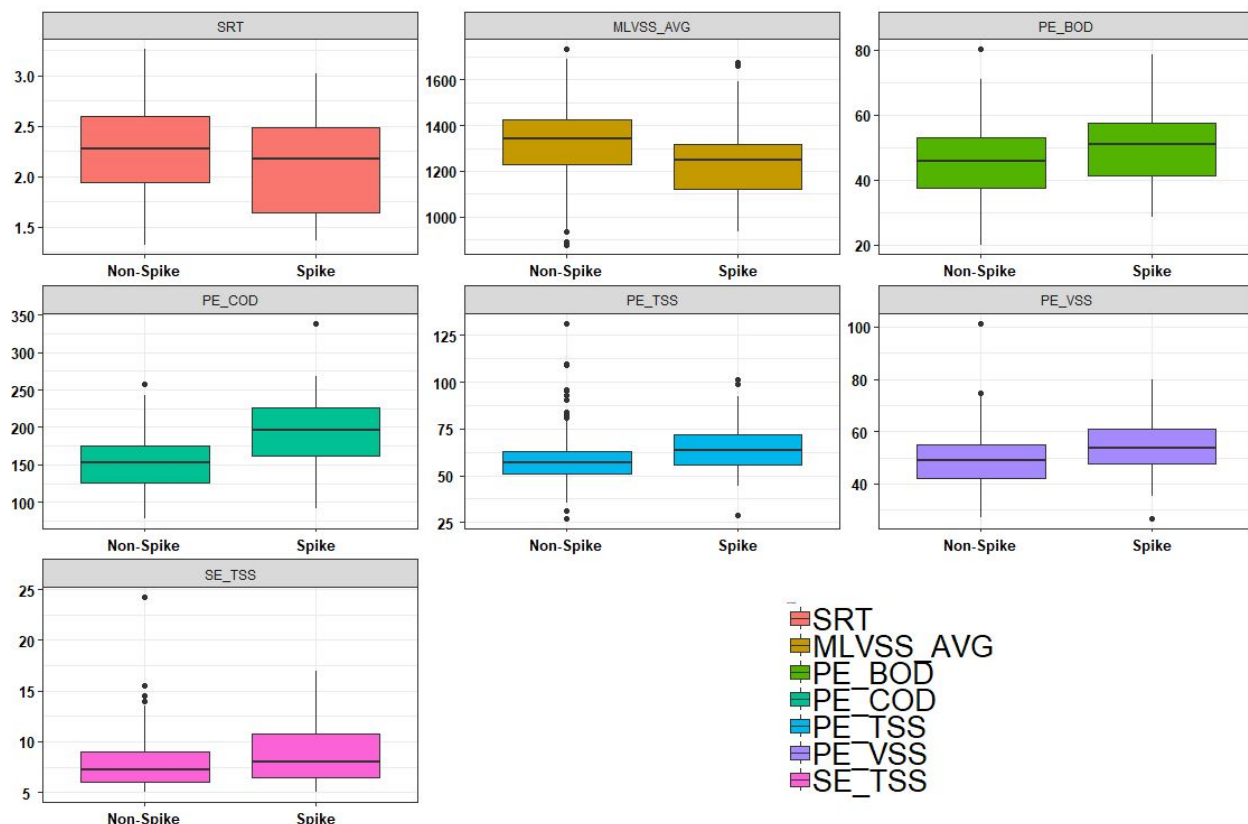

Figure 4 Boxplots of Potential Indicators in Spike Days and Non-Spike Days. These indicators were chosen based on 95% confidence interval of unpaired two sample t-test.

Impacts of Sample Size on Wastewater Characteristic Estimation and Model Performance

Increased sample size can improve estimated fractionation, but with diminished results, as presented in **Figure 4**. Fifty iterations were implemented for each sample size, with the designated characterization records randomly pooled without replacement. Averaged fractions were fed into the model for simulation, and performance was evaluated. To minimize the error introduced by chance in sampling, both the maximum and average values of the model performance statistics among the 50 iterations were calculated. Average values reflect the overall performance of each sample size, while maximum values indicate the robustness, meaning that the result is not significantly influence by individual characterizations. As indicated in **Figure 4**, there is a point of diminishing return. As expected, the desired "elbow point" is controlled by the maximum criteria to achieve robust estimates of wastewater characteristics, making 20 the

desired sample size in this instance. A preliminary analysis regressing the inert particulate fraction on the total COD with bootstrap sampling reached a similar conclusion (data not shown).
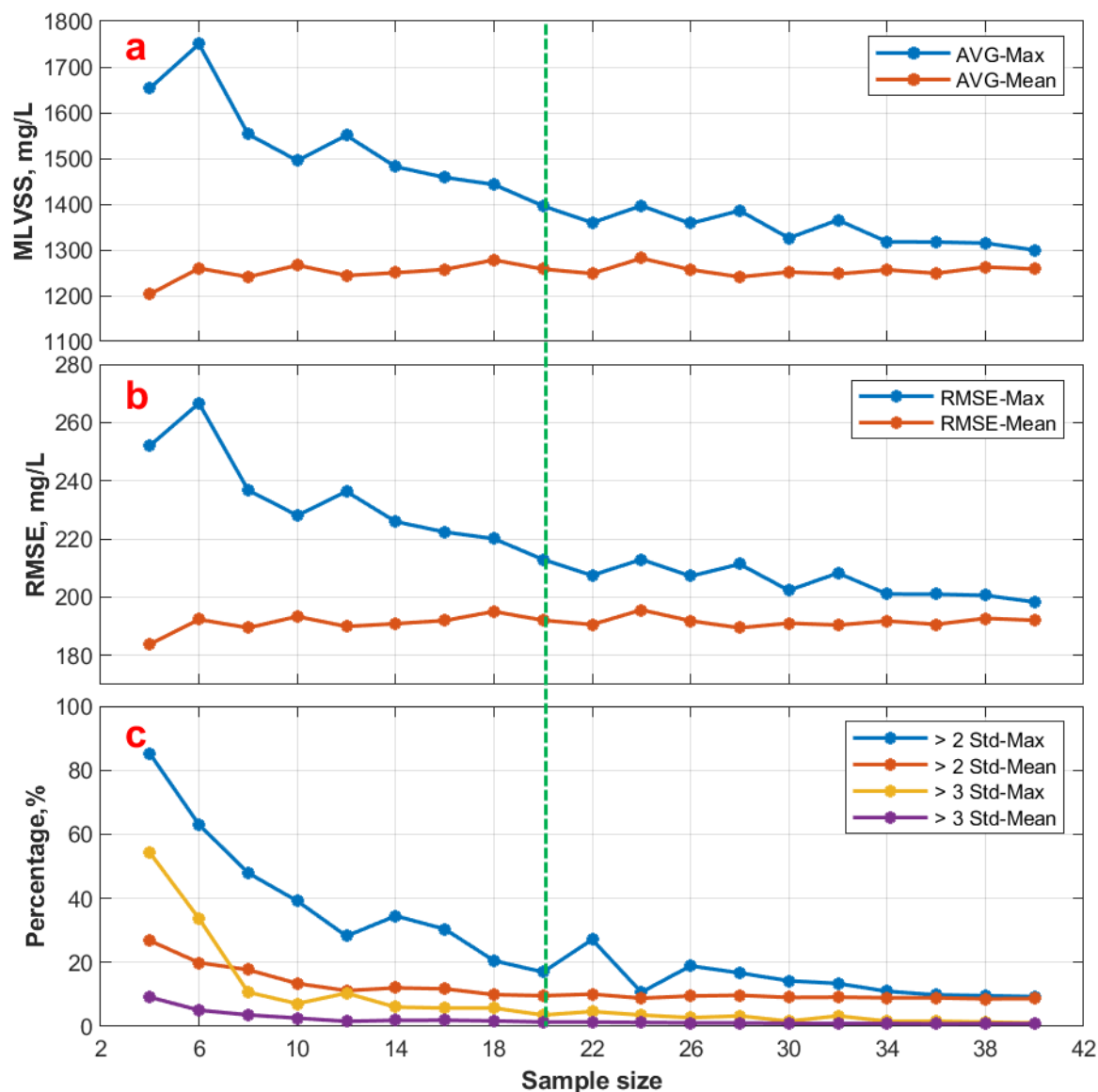
Figure 5 *Elbow plots to Determine Sample Size. Each Sample Size was Iterated 50 Times, and then Maximum and Mean Values for each Model Assessment Parameter were Extracted to Represent each Sample Size. The Model Evaluation Parameters used Include Maximum and Average Values for: (a)Mean of predicted MLVSS; (b) RMSE of predicted MLVSS; (c) Days with different deviations.*

Implications for Wastewater Characterization Campaigns

These results provide guidance on the number of individual measurements that can result in a robust assessment of wastewater characteristics. The analysis summarized in **Figure 4** suggests that around 20 measurements represent a reasonable balance between achieving a robust assessment without an excessive number of measurements. The results presented in **Table 3** also support the conclusion that "more is better" (yearly average compared to quarterly and monthly)

when assessing wastewater characteristics and their impact on model performance. This result conflicts, however, with the those presented in **Table 4** which indicated that even a small number of measurements conducted at "the right time" (March and October to December in this case) can result in better characterization of the wastewater relative to model performance. This presents a conundrum for planning wastewater characterization campaigns, as it is not possible to know, a-priori, what the "right time" is. Certainly, periods that are recognized to generally represent unusual conditions can be avoided, but it may not be possible to predict the ideal time. This suggests that an adaptive approach to wastewater characterization may be needed. It may consist of multiple sampling events, each of relatively short duration, with the results carefully evaluated after each event for consistency in model predictions as well as the occurrence of unusual influent or operating conditions. Sampling periods continue until a consistent set of results is achieved. Using this approach, sampling can be terminated when a sufficient number of measurements are obtained during periods of normal operation so that a robust assessment of wastewater characteristics is achieved. Issues related to model structure, as occurred in this instance during February and March of 2018, can also be identified with this approach and addressed appropriately given the objective of the modeling exercise. Use of this approach makes it unnecessary to specify initially the number of measurements required to achieve a robust assessment of wastewater characteristics as the methodology, itself, will determine this. A robust budget is needed to account for unforeseen conditions. Given the significant economic impact of poor wastewater characterization in many instances, unnecessarily limiting the wastewater characterization budget may not be a wise use of funds as the economic impact of poor decisions may be orders of magnitude greater than the cost of additional testing.

The system considered and model application used in this work represents perhaps one of the simplest, but one with potentially significant economic impacts. Accurate prediction of the MLVSS concentration translates directly into the required bioreactor and secondary clarifier sizes, which represents a major capital expense for any suspended growth biological treatment system. The colloidal organic matter fraction of the biological process influent wastewater was found to be negligible in this instance, and the dissolved fraction could be characterized based on membrane filtration rather than flocculation and filtration. Note that GLWA serves a large and diverse metropolitan area, and that a significant portion of the collection system consists of combined sewers, leading to significant variations in influent flows, both seasonal and daily, and significant temperature variations given its location in the Northern U.S. In spite of these factors, it was found that one set of wastewater characteristics applied over the entire year. Thus, while the precise numerical results determined for this application may not generally apply, the adaptive approach to wastewater characterization and model calibration described here may be more generally applicable.

CONCLUSIONS

An extended wastewater fractionation study conducted at the GLWA WRRF provided the basis to evaluate alternative wastewater characterization campaign designs. An ideal campaign results in a robust characterization of the wastewater while managing the time and resources required to achieve this result. Wastewater characterization must, of course, be viewed in the context of the objectives of the modeling exercise and the potential impacts of improper model development. The following conclusions can be offered based on this study:

1. The characteristics of this wastewater originating from a large and diverse metropolitan area, as assessed based on predicted versus actual bioreactor MLVSS concentration, did not vary on a seasonal basis. This occurred in spite of significant daily and seasonal influent wastewater flows and seasonal temperature variations due to the fact that the collection system included a substantial combined sewer component.

2. Sampling during periods of normal and stable plant operation results in the most reliable estimates of wastewater characteristics. Increasing the number of samples can help to partially overcome the adverse impacts on sampling results resulting from occasional periods of unusual plant operation, but the best results will be obtained by avoiding, when possible, sampling during unusual operating periods.

3. For this application, around 20 samples randomly distributed over an annual cycle was found to represents a good trade-off between further increasing the number of samples and the gain in precision in the estimation of wastewater characteristics.

4. An adaptive approach to wastewater characteristics measurement consisting of multiple measurement campaigns, each of limited duration, may provide the best results. Sufficient resources need to be devoted to the campaign to allow for sufficient sampling events to ensure that a reliable and robust assessment of wastewater characteristics is achieved.

5. Attention should be paid to the potential for periods of poor model structure, including numerical values of key parameters, when assessing results. Some redundancy in measured parameters (COD, BOD_5, TSS, VSS) can facilitate identification of such periods.

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