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Title

Chemical Dosage Prediction for Drinking Water Treatment Using Random Forest and Polynomial Regression

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Coversheet Statement

This manuscript is a non-peer-reviewed preprint submitted to EarthArXiv. The manuscript is currently under peer review at Drinking Water Engineering and Science.

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Abstract

Predictive modeling of chemical dosage based on raw water quality can be useful in decision-making in operating a water treatment plant. In this study, two statistical methods, i.e., random forest and polynomial regression, are used for modeling the chemical usages in drinking water treatment based on the measured water quality parameters in source water. The daily chemical dosages and eight water quality parameters were recorded from 2014 to 2021. The dataset is split into training (80%) and testing (20%) sets. For the training set, random forest has better performance than polynomial regression for all three chemical usages. However, random forest and polynomial regression have comparable performance for the testing set; particularly, the performance of polynomial regression on modelling sulfuric acid is slightly better than that of random forest, but random forest has a slightly better performance on modelling ferric sulfate and Actiflo polymer. The polynomial regression model is robust due to its explicit polynomial equation and its interaction terms capturing the impact of the interdependency of water quality parameters. It is found that both random forest and polynomial regression are able to model the dosages of sulfuric acid and ferric sulfate effectively, and the dosage of Actiflo polymer acceptably.

Keywords: Chemical dosage, water quality, machine learning, random forest, polynomial regression, water treatment

1. Introduction

Chemicals are usually used in drinking water treatment processes to meet the federal and local standard levels of potable water quality (Rotton et al., 1982; Gitis and Hankins, 2018). Different types of chemicals are used in practices such as alum, ferric sulfate, lime, micro-sand, sodium hypochlorite, and others. For example, ferric sulfate, as a coagulant, is added at a certain pH so that flocs are formed for aiding the removal of suspended particles during sedimentation (Sulistyo et al, 2012). (Le et al., 2021) showed that more than 96% of cyanobacterial cells and 97% of intracellular microcystins could be removed in river water when ferric sulfate was used. Lime was used to normalize pH by increasing alkalinity (Evuti et al., 2012); and Gregor et al. (1997) applied alum and lime to remove turbidity using a pH-controlled system. The removal rate of turbidity, chemical oxygen demand, and total phosphorus by micro-sand and magnetic powder is 96%, 57%, and 55%, respectively (Su et al., 2013). Sodium hypochlorite with the combination of potassium permanganate has been used for removing manganese in organic-rich surface waters (Yu, et al., 2015).

The chemical dosages for potable water treatment need to be determined accurately to achieve acceptable water quality (Zhao et al., 2006). The dosages for the chemicals used in drinking water treatment depend on the water quality parameters of source water such as alkalinity, chloride, color, conductivity, pH, temperature, and turbidity (Piri et al., 2010). (Santana et al., 2014) reported that the dosage concentration of ferric sulfate needs to be accurate and more ferric sulfate can lead to increased floc formation but also more sludge (Santana et al., 2014). Yonge (2012) reported that the lowest dosage concentration is 120 mg/L for ferric chloride and 100 mg/L for aluminum chlorohydrate to achieve the highest removals of dissolved organic carbon and color in Florida. (Al-Baidhani and Alameedee, 2017) documented that 5 ~ 50 mg/L of aluminum dosage was applied to achieve the

acceptable level of turbidity in the lab experiments. Therefore, water quality parameters need to be monitored to determine the dosages of chemicals.

Meanwhile, over-dosage applications of chemicals may result in significant risk to the environment and the health of consumers (van Leeuwen, 2000). For example, water bodies containing high concentrations of sulfates may negatively impact erosion processes, carbon cycles, and aquatic plants, and cause health problems such as diarrhea, dehydration, and gastrointestinal disorder (Wang and Zhang, 2019). As a result, water quality parameters need to be monitored for changes caused by the applied chemicals to avoid any toxic effects on consumers and environment (Mwitirehe et al., 2022; Kazi et al., 2009).

Accurate prediction of chemical dosages enhances drinking water quality and eliminates the risk of health hazards. Jar tests are usually conducted for determining the chemical dosages; however, this process is time consuming and expensive. Given the recent development and increasing application of machine learning models in real-time decision-making, different methods have been used to provide predictions of chemical dosages. Maier (2004) used artificial neural networks to determine the precise concentrations of aluminum and pH in treated water. Sikder et al. (2023) utilized machine learning models (e.g., least squares boosting, extreme gradient boosting, artificial neural network, principal component analysis, support vector machines, and random forest) to predict the formation of trihalomethanes, which consist of chlorine and organic matter, based on water quality parameters including chlorine, pH, and dissolved organic carbon. Huan et al. (2021) utilized random forest to determine the key factors that influence dissolved oxygen in rivers. Random forest has been used for estimating Coliform bacteria and E. coli. (Mohammed et al., 2017) and nitrate concentration (Regier et al., 2023) based on measured water quality parameters such as conductivity, pH, color, and turbidity.

Machine learning models have also been used for predicting chemical dosages by taking the measured water quality parameters as inputs. Zhang et al. (2013) reported that support vector machine and K-nearest neighbor method have competing abilities for predicting coagulant dosage based on turbidity, pH, and temperature. Wang et al. (2022) deployed principal component regression, support vector regression and long short-term memory neural network to build models for predicting chemical dosage based on raw water quality for drinking water treatment plants. In this paper, two machine learning algorithms, including random forest and polynomial regression, are used to determine the required chemical usages in drinking water treatment processes.

For the remaining of the paper, Section 2 introduces the random forest and polynomial regression models as well as the metrics for evaluating the performance of the models. Section 3 describes the study site, data availability, and the exploratory data analysis. Section 4 presents and discusses the results of random forest and polynomial regression. Section 5 summarizes the findings.

2. Methodology

Random forest and polynomial regression, which are used for predicting chemical dosages, are briefly introduced in this section. The random forest algorithm and the polynomial regression model in scikit-learn, which is an open-source Python library, are used in this study. Scikit-learn implements a range of machine learning algorithms using a unified interface. The metrics for model performance evaluation for training and test datasets are presented following the machine learning algorithms.

2.1. Random Forest

The random forest (RF) algorithm uses multiple decision trees to create a robust model by averaging the predictions from each tree individually. Therefore, RF is an ensemble method, which reduces the over-fitting of a single decision tree by averaging the result (Sarica et al., 2017). Within each tree, the target variable or parent node is split into two nodes; and the nodes are split iteratively

until minimum variance is achieved, improving the accuracy of the chemical prediction to match the trained values. Each generation of child nodes is purer than their parent nodes. The dataset for prediction is divided into multiple subdivisions by each tree based on a random sample of dataset using the bootstrap method, where data is repeatedly sampled with random replacement to maintain accurate and unbiased performance. The model inputs can occur in multiple decision paths based on each tree's structure and properties (Zhao et al., 2019). The optimal split is determined by minimizing the impurity (or maximizing the purity) of the decision tree (Tahsin et al., 2017). The impurity is typically quantified using metrics such as the Gini index or entropy (Breiman, 2001; Disha and Waheed, 2022) and assessed within the model using feature importance. Feature importance measures how effectively each feature reduces impurity and enhances prediction accuracy during the data splitting. This methodology aims to construct tree splits that minimize prediction variance while maintaining low bias (Vens and Costa, 2011). The parameters for the random forest regression (RFR) model should be adjusted appropriately to decrease memory usage and model complexity. The most suitable split is determined through majority voting based on mean squared error. The model is fitted using the training set and applied for prediction.

2.2. Polynomial Regression

Polynomial regression (PR), as a machine learning model, can capture the non-linear relationships between variables by fitting a non-linear regression line, which may not be possible with simple linear regression. Therefore, PR is able to capture the complexity of the relationship between chemical dosages and water quality parameters. If the inputs only include one independent variable, a first-degree (k = 1) polynomial forms a linear regression; a second-degree (k = 2) polynomial forms a quadratic expression; and a third-degree (k = 3) polynomial forms a cubic expression. If the

independent variables are a vector, PR is in matrix form. As an example, Equation (1) shows the polynomial equation for a second-degree polynomial regression:

$$y = C_0 + C_i \sum_i^N x_i + C_{ii} \sum_i^N {x_i}^2 + C_{ij} \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} x_i x_j \quad (1)$$

where x is the independent variables; N is the number of independent variables; and C_0, C_i, C_{ii}, and C_{ij} are coefficients. C_0 is the constant term; C_i are the coefficients for the linear terms; C_{ii} are the coefficients for the squared terms; and C_{ij} are the coefficients for the interaction terms. The interaction terms capture the impact of interdependency of input variables (e.g., water quality parameters). The number of coefficients is dependent on the value of N. For example, the number of coefficients is 6 when N = 2 but 36 when N = 7 for a second-degree polynomial shown in Equation (1). The number of coefficients is also dependent on the degree of polynomial (k). Higher degree of polynomial has a larger number of coefficients, capturing the more complex relationship. For example, when N = 8, the number of coefficients is 165 for the third-degree polynomial. As a result, there is a trade-off between the performance of polynomial model and its number of coefficients. The degree of polynomial, that best describes the relationship in the data, needs to be identified.

In the PR algorithm of the scikit-learn library, the original dataset is transformed to the polynomial terms for a selected degree of polynomial. A linear regression model is conducted for the transformed polynomial components. The coefficients of the polynomial are estimated based on the training dataset. The polynomial model and its coefficients are used for prediction of dependent variables (e.g., chemical dosages).

2.3. Model Performance Metrics

Three statistical metrics, including the relative root mean square error (*RRMSE*), the Nash-Sutcliffe efficiency (*NSE*, Nash and Sutcliffe, 1970), and the Kling-Gupta Efficiency (*KGE*, Gupta et

al., 2009), employed to evaluate the performance of RF and PR algorithms on predicting the daily chemical quantities. The calculation of *RRMSE* is shown in in Equations (2):

$$RRMSE = \frac{\sqrt{\frac{\sum_{t=1}^{n}\left(D_{mod,t}-D_{obs,t}\right)^2}{n}}}{\bar{D}_{obs}} \quad (2)$$

where $D_{mod,t}$ and $D_{obs,t}$ are modelled and observed chemical dosage at the tth day; $\bar{D}_{obs}$ is the mean value of the observed daily chemical dosage; and n is the total number of observations for a chemical. *RRMSE* is the ratio of root mean square error (*RMSE)* to observed mean value; and *RRMSE* can be compared among different chemicals.

The coefficient of determination (R^2) is square of the Pearson's linear correlation coefficient (r) and is calculated by:

$$R^2 = \frac{\left[\sum_{t=1}^{n}\left(D_{obs,t}-\bar{D}_{obs}\right)\left(D_{mod,t}-\bar{D}_{mod}\right)\right]^2}{\sum_{t=1}^{n}\left(D_{obs,t}-\bar{D}_{obs}\right)^2 \sum_{t=1}^{n}\left(D_{mod,t}-\bar{D}_{mod}\right)^2} \quad (3)$$

The correlation coefficient is the most common way of measuring a linear correlation, and it ranges between –1 and 1 that measures the strength and direction of the relationship between two variables. Therefore, R^2 ranges between 0 and 1, and it provides a measure of how well observations are replicated by the model, based on the proportion of total variation of observations explained by the model.

The *NSE* has been widely used for evaluating the goodness-of-fit for hydrological modelling. *NSE* is calculated by the following equation:

$$NSE = 1 - \frac{\sum_{t=1}^{n}\left(D_{mod,t}-D_{obs,t}\right)^2}{\sum_{t=1}^{n}\left(D_{obs,t}-\bar{D}_{obs}\right)^2} \quad (4)$$

The mean square error is normalized by the variance of observation in Equation (3); whereas the root mean square error is normalized by the mean of observation in Equation (2). *NSE* ranges from $-\infty$ to

1, and a value of one means a perfect match between observation and estimation. If the mean value of observed chemical dosage is used for prediction, the value of *NSE* is zero.

The *KGE* metric incorporates the correlation coefficient, the ratio of standard deviations of modelled and observed daily chemical dosage (α), and the ratio of mean values of modelled and observed daily chemical dosage (β):

$$KGE = 1 - \sqrt{(r-1)^2 + (\alpha-1)^2 + (\beta-1)^2} \quad (5)$$

KGE is the Euclidean distance computed using the coordinates of bias, standard deviation, and correlation (Gupta et al., 2009). The *KGE* is sensitive to variance and high values, with its values varying from $-\infty$ (poor fit) to 1 (perfect fit). There is no specific meaning attached to the KGE value when it equals zero. By comparing the *KGE* with the *NSE*, Knoben et al. (2019) reported that *KGE* values above −0.41 represented a reasonable performance.

3. Study Site and Exploratory Data Analysis

The surface water sources for the drinking water treatment in Tampa Bay Water are from Alafia River, Tampa Bypass Canal with Hillsborough River, and C. W. Bill Young Regional Reservoir, as outlined in Figure 1. This figure provides the specific locations of these surface water withdrawals. Sufficient chemical quantities of diverse types need to be added to the source water for water treatment purposes. The following 7 chemicals are used for water treatment: Actiflo polymer, ferric sulfate, lime, liquid oxygen, micro-sand, sodium hypochlorite, and sulfuric acid. The daily chemical usages were recorded from 2014 to 2021. Meanwhile, 8 water quality parameters (i.e., alkalinity, chloride, color, conductivity, pH, sulfate, temperature, and turbidity) during this period were also measured for the mixed source water.

Figure 1. Map for the study area with Tampa Bypass Canal, Alafia River, and Hillsborough River.

The total number of days with available data is 2876 days. Individual water quality parameter or chemical usage data is missing on some days. The number of days with missing water quality data is 30 for chloride, 30 for sulfate, 1 for turbidity, and 1 for temperature. For chemical usage data, the number of days with missing data is 12 for Actiflo polymer, 104 for lime, and 1112 for micro-sand (38.66%). As discussed later in Section 3.2, lime and micro-sand will be removed from analysis since their usages are quite uniform temporally.

The dataset is split into training and testing sets randomly. The training set, including 80% of the dataset, is used to train the RF and PR algorithms. The rest of the dataset (20%) is used for testing the performance of the machine learning algorithms, and the performance is evaluated by the metrics described in Section 2.3. Once a model reaches a satisfactory level of prediction, it can be used for predictions in practices, reducing the cost of experiments to determine the optimal chemical dosage for water treatment.

Exploratory data analysis (EDA) is employed to select data for both water quality and chemicals before applying RF and PR algorithms to the dataset. For water quality parameters, EDA

provides an initial understanding of how chemical usage depends on these parameters by examining their correlations. Input features with low correlations with all chemicals are excluded from the model, resulting in the inclusion of 8 water quality parameters. Initially, the dataset is examined for 7 chemicals. Chemical usages that exhibit seasonal uniformity are eliminated from further analysis. Ultimately, a prediction model necessitates the inclusion of 3 chemicals. The correlations between water quality parameters, between chemical dosages, and between water quality parameter and chemical dosage are evaluated as a preliminary understanding on the dataset.

3.1. Water Quality Parameters

3.1.1. Seasonal Variations

Figure 2 shows the seasonal variations for alkalinity, chloride, color, conductivity, pH, sulfate, temperature, and turbidity. Alkalinity, pH, conductivity, chloride, and sulfate have similar seasonal variations. Their minimum mean monthly values occur in August or September and the maximum mean monthly values occur in the winter season. For color, the minimum mean monthly value is in April and the maximum mean monthly value is in September. For temperature, the minimum mean monthly value is in January and the maximum is in July. For turbidity, the minimum mean monthly value is in November and the maximum is in July. For the box plots in Figure 2, the concentrations of water quality parameters have a large variation within a month. Using various statistical tests, including the Kolmogorov-Smirnov test, Shapiro-Wilk test, and Anderson-Darling statistics, significant deviations from the normal distribution are identified. These findings induce the utilization of RF and PR algorithms to effectively capture complex relationships.

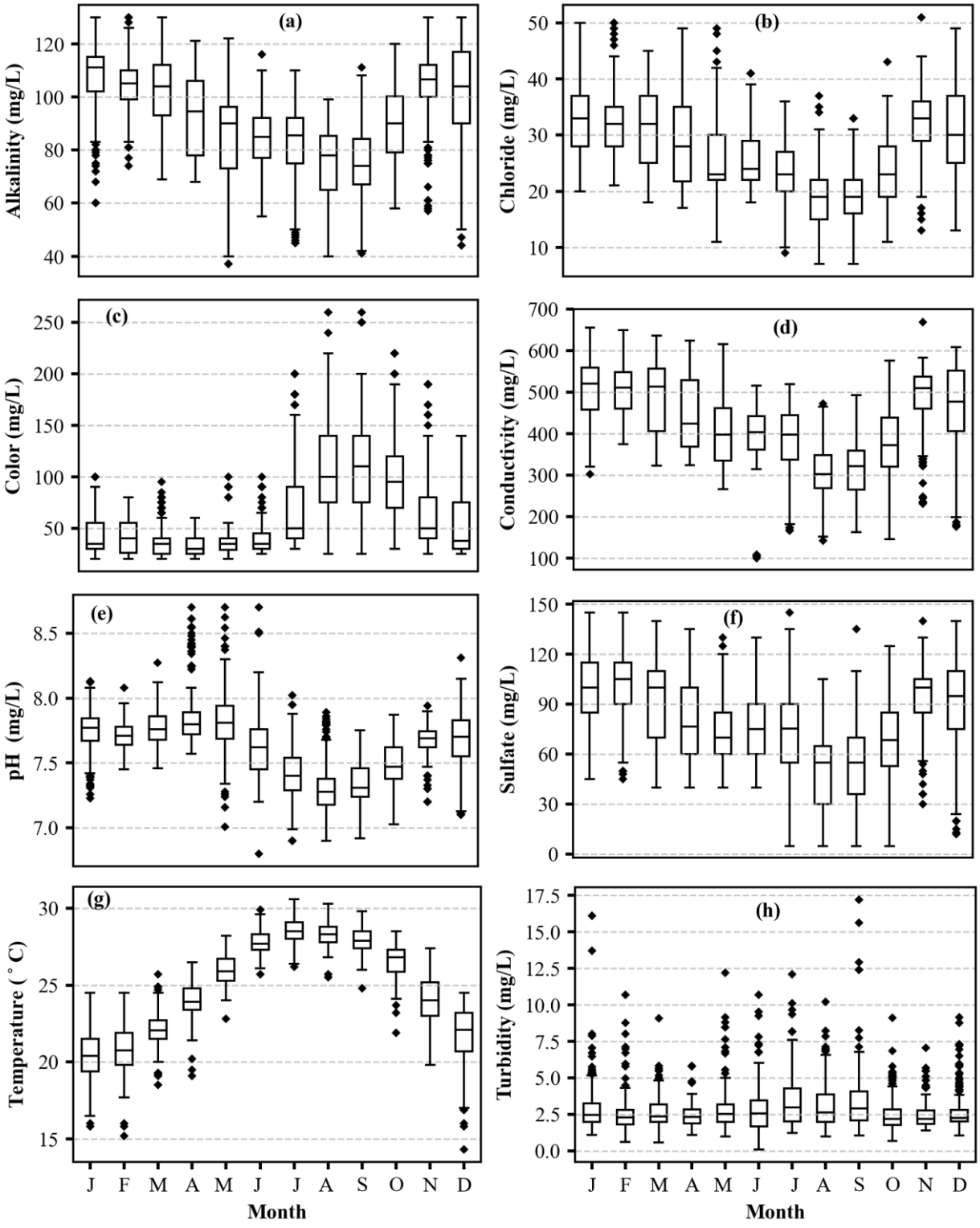

Figure 2. The seasonal variations of eight water quality parameters: (a) alkalinity; (b) chloride; (c) color; (d) conductivity; (e) pH; (f) sulfate; (g) temperature; and (h) turbidity.

3.1.2. Correlations

Further EDA is conducted to assess the correlations between water quality parameters. The correlations between any two of eight water quality parameters are calculated using Spearman correlation (r), which is suitable for non-normally distributed data. These correlations can be presented in a correlation heatmap, a graphical representation of a correlation matrix. The correlation ranges from -1 to +1, with larger absolute values indicating a higher correlation, representing the strength and direction of the relationship (Schober et al., 2018).

Figure 3 plots the correlation heatmap for the water quality parameters. As shown in Figure 3, conductivity has a strong positive correlation with chloride (r = 0.91), alkalinity (r = 0.90), and sulfate (r = 0.86); chloride also has a strong positive correlation with alkalinity (r = 0.80) and sulfate (r = 0.79); and alkalinity has a strong positive correlation with sulfate (r = 0.73). Therefore, any two among these four water quality parameters (conductivity, chloride, alkalinity, and sulfate) have highly positive correlations. Moreover, these four water quality parameters have moderately positive correlation with pH, i.e., r = 0.54 for conductivity, r = 0.54 for alkalinity, r = 0.48 for chloride, and r = 0.44 for sulfate. On the other hand, color has highly negative correlations with pH (r = -0.73) and conductivity (r = -0.63); and color also has moderately negative correlations with sulfate (r = -0.57), alkalinity (r = -0.56), and chloride (r = -0.53). Temperature has moderately negative correlations with conductivity (r = -0.52), chloride (r = -0.48), alkalinity (r = -0.47), and sulfate (r = -0.45). One water quality parameter has high or moderate correlations with multiple water quality parameters. For example, Figure 4 shows the correlations of alkalinity with conductivity, chloride, and temperature. The scatter plot of alkalinity versus conductivity in Figure 4 shows their positive correlation (r = 0.90). Higher chloride is associated with higher alkalinity and conductivity; but lower temperature is associated with higher alkalinity and conductivity.

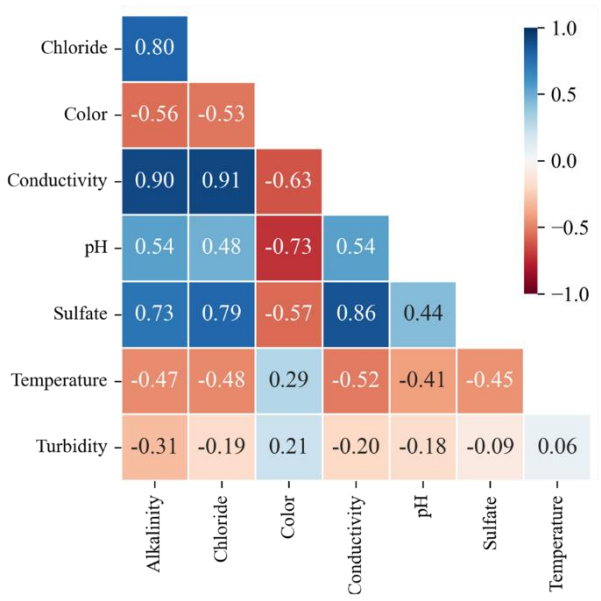

Figure 3. The correlation heatmap for eight water quality parameters.

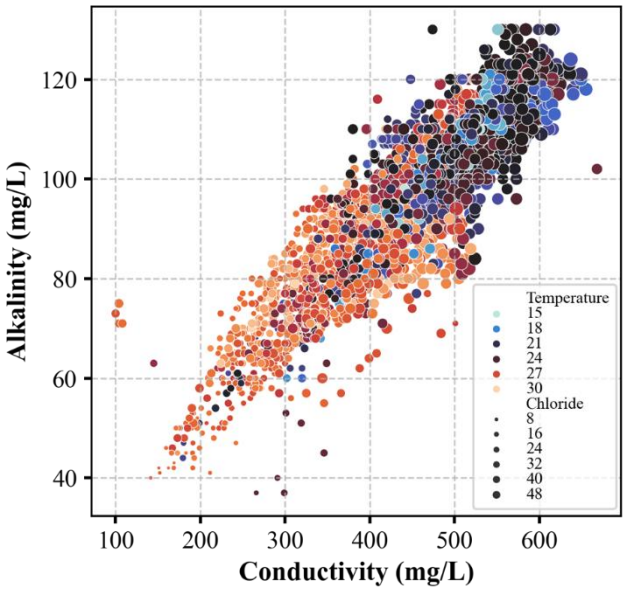

Figure 4. The correlations of alkalinity with conductivity, temperature, and chloride.

3.2. Chemical Dosages

3.2.1. Seasonal Variations

The seasonal variations of chemical usages are explored for selecting the chemicals for modelling using machine learning algorithms. The usages for Actiflo polymer, ferric sulfate, and sulfuric acid present apparent seasonal variations as shown in Figure 5. The seasonal variations for these three chemicals are distinct even though Actiflo polymer and ferric sulfate have similar seasonality. The mean monthly value for Actiflo polymer and ferric sulfate is highest in August; but the mean monthly value for sulfuric acid is highest in November. The lowest mean monthly value is in June for Actiflo polymer, February for ferric sulfate, and September for sulfuric acid. Actiflo polymer and ferric sulfate usages increase from June to August, while sulfuric acid usage increases from September to November. The dosages for lime, liquid oxygen, micro-sand, and sodium hypochlorite are stable temporally, and they are not plotted in the figure. As a result, lime, liquid oxygen, micro-sand, and sodium hypochlorite are excluded from further analysis; and the RF and PR algorithms are tested for modelling the dosages for Actiflo polymer, ferric sulfate, and sulfuric acid.

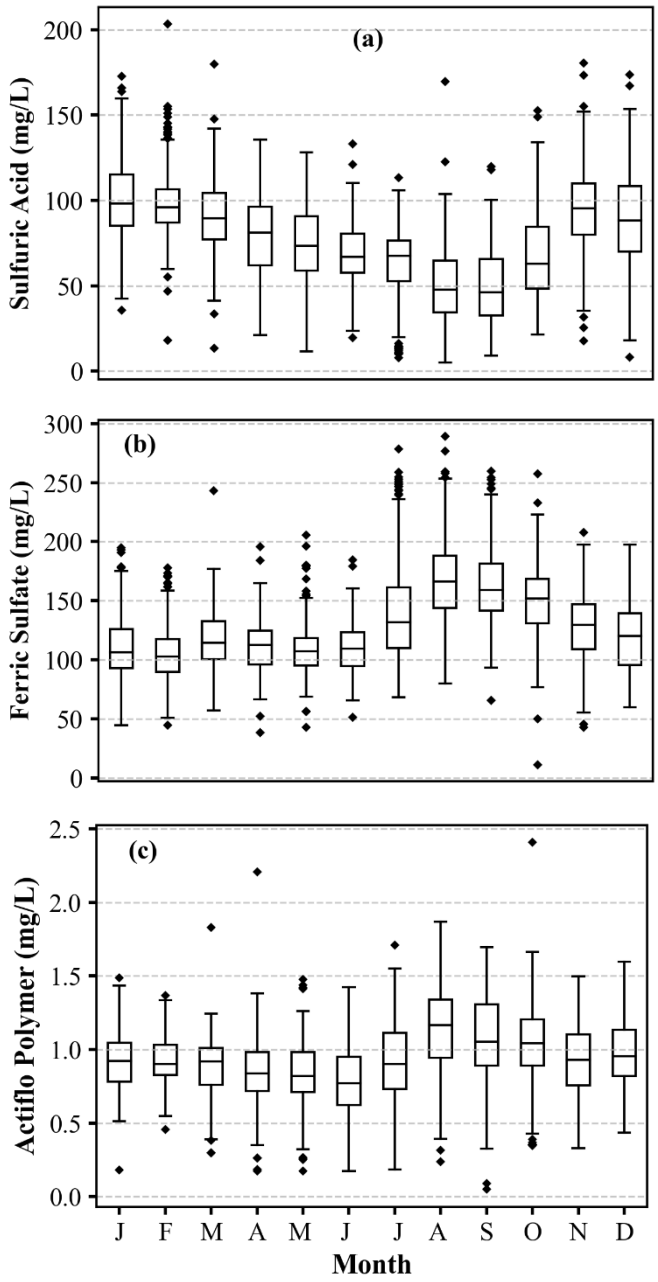

Figure 5. The seasonal variations of chemical usages: (a) sulfuric acid; (b) ferric sulfate; and (c) Actiflo polymer.

3.2.2. Correlations

The correlations between the three selected chemicals (Actiflo polymer, ferric sulfate, and sulfuric acid) are analyzed. Figure 6a shows the scatter plot for Actiflo polymer versus ferric sulfate. As expected, Actiflo polymer and ferric sulfate have a positive correlation since they have similar seasonal variations shown in Figure 5. The correlation between Actiflo polymer and ferric sulfate is 0.46 which is moderately positive. Figure 6b shows a negative correlation between Actiflo polymer and sulfuric acid as expected from Figure 5, and the correlation between sulfuric acid and Actiflo polymer is -0.27. The correlation between sulfuric acid and ferric sulfate is moderately negative as shown in Figure 6c, and correlation between them is -0.55. Therefore, sulfuric acid was used in less amounts when ferric sulfate was used in high dosages.

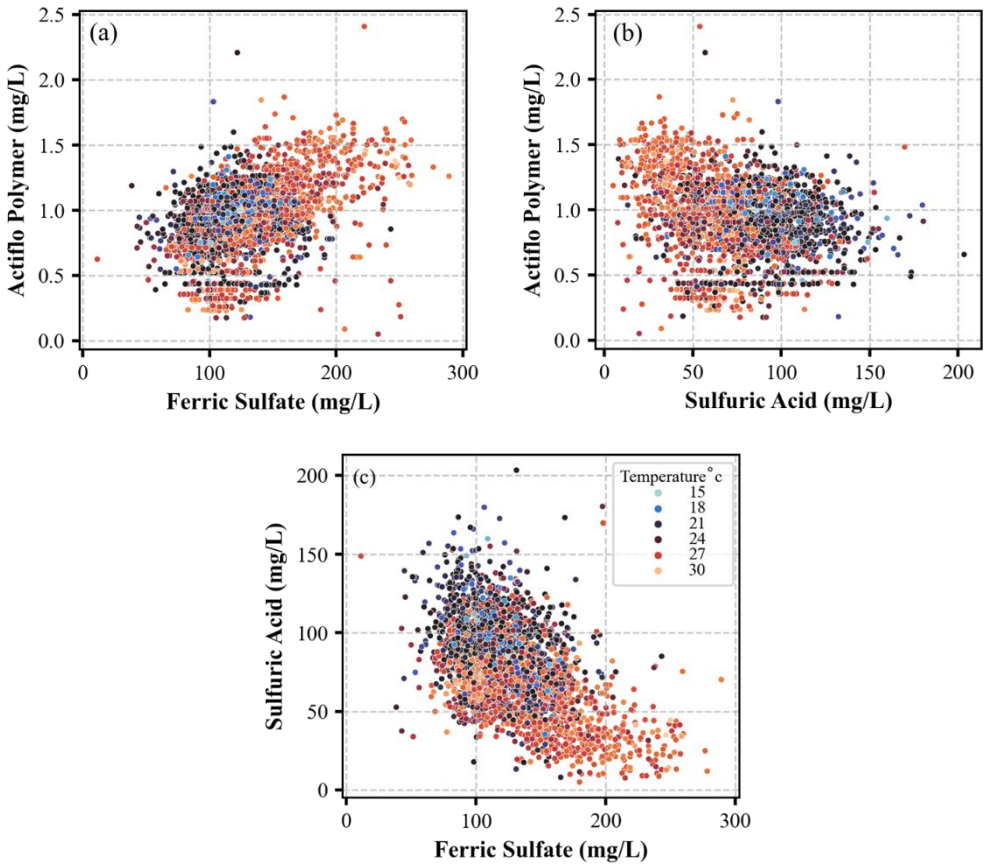

Figure 6. Scatter plots between Actiflo polymer and ferric sulfate (a), between Actiflo polymer and sulfuric acid (b), and between sulfuric acid and ferric sulfate (c).

3.3. Correlations between Chemical Dosages and Water Quality Parameters

The correlations between chemical dosages and water quality parameters are further evaluated since the objective is to model chemical dosages based on water quality parameters. Figure 7 shows the correlation heatmap between chemical dosages and water quality parameters. The vertical axis is for chemical dosages (Actiflo polymer, ferric sulfate, and sulfuric acid); and the horizontal axis is for water quality parameters in descending order of correlations for sulfuric acid. As shown in Figure 7, sulfuric acid has highly positive correlations with alkalinity (r = 0.82), conductivity (r = 0.79), chloride (r = 0.68), and sulfate (r = 0.66); moderately positive correlation with pH (r = 0.53); and moderately negative correlations with color (r = -0.59) and temperature (r = -0.47). Ferric sulfate has a high correlation with color (r = 0.77) and pH (r = -0.63); and moderate correlations with conductivity (r = -0.55), alkalinity (r = -0.50), sulfate (r = -0.48), and chloride (r = -0.46). Actiflo polymer has a moderate correlation with color (r = 0.46) and pH (r = -0.44). The correlations of sulfuric acid with alkalinity, conductivity, chloride, sulfate, turbidity, and temperature are higher than those of ferric sulfate; and the correlations of ferric sulfate with all the water quality parameters are higher than those of Actiflo polymer.

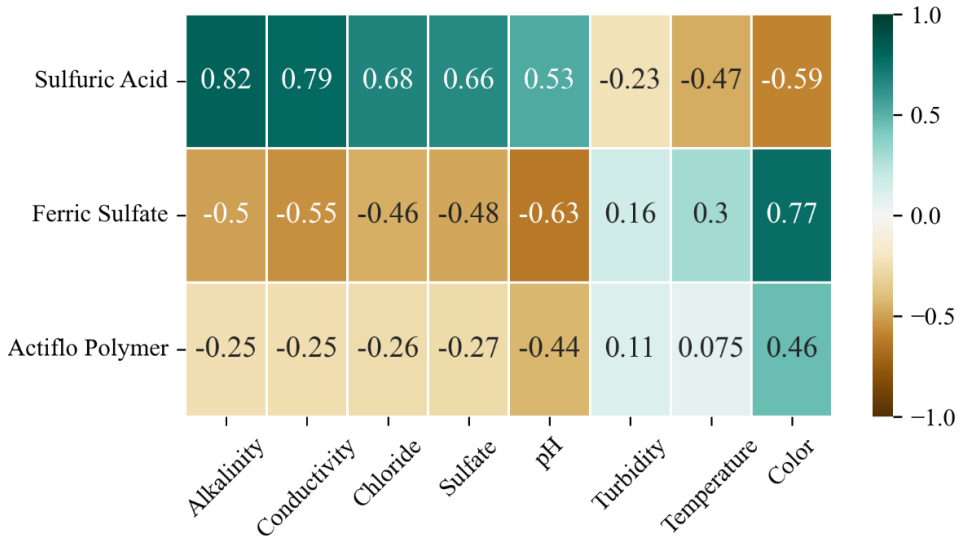

Figure 7. Correlation heatmap between chemical dosages and individual water quality parameters.

4. Results and Discussion

Having the proper dose regarding the interactions of the overall processes is important. An over-feed or under-feed of chemicals in one process will adversely affect downstream processes. It is important, for instance, not to overfeed ferric sulfate in the Actiflo because, it will leave some ferric in a dissolved state to go downstream to the ozone process, where it is oxidized into a precipitate that goes further downstream to the filters to provided additional loading.

4.1. Results by Random Forest

The modelled chemical dosages are compared with the observed ones and the model performance is evaluated based on the evaluation metrics. Figures 8a, 8b and 8c show the scatter plots between the modelled and observed chemical dosages by RF. The black dots represent the training set, and the red circles represent the testing set. Most of the points are close to the 1:1 line, indicating good matches between modelled and observed chemical dosages. Table 1 shows the model performance metrics of RF for both training and testing sets. As shown in Table 1, the performance of the training set is better than that of the testing set. The values of NSE and R^2 are the same for a given chemical dosage and training (or testing) set. For the testing set, the lowest RRMSE is 0.15 for ferric sulfate, and the RRMSE is 0.19 for sulfuric acid and 0.20 for Actiflo polymer; sulfuric acid and ferric sulfate have the same NSE (0.75) which is higher than that of Actiflo polymer (0.53); and the highest KGE is 0.81 for sulfuric acid, and the KGE is 0.76 for ferric sulfate and 0.57 for Actiflo polymer. As discussed in Section 3.3, the overall correlation with water quality parameters decreases from sulfuric acid to ferric sulfate and to Actiflo polymer. The performance based on KGE is consistent with the correlation heatmap shown in Figure 7. Therefore, KGE might be a better performance metric since it combines correlation coefficient, mean, and standard deviation.

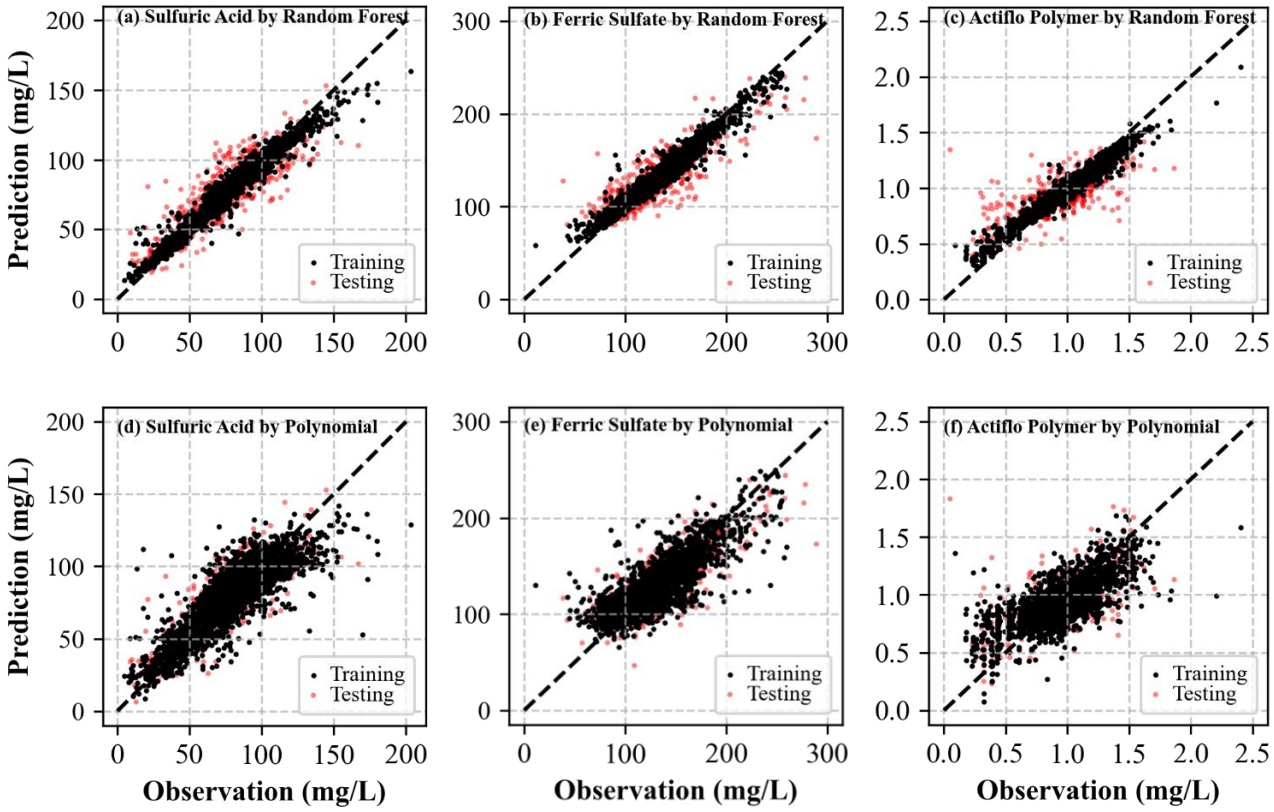

Figure 8. Comparisons of observed and modelled chemical dosages: sulfuric acid (a), ferric sulfate (b), and Actiflo polymer (c) modelled by random forest; and sulfuric acid (d), ferric sulfate (e), and Actiflo polymer (f) modelled by polynomial regression.

Table 1. The performance of random forest and polynomial regression for training and testing sets evaluated by RMSE, RRMSE, NSE, R^2, and KGE.

Algorithm		**Chemical Dosage**	**Model Performance Metric**				
			RMSE	RRMSE	R^2	NSE	KGE
Random Forest	Training	Sulfuric acid	0.003	0.08	0.96	0.95	0.90
		Ferric sulfate	0.003	0.06	0.95	0.95	0.89
		Actiflo polymer	0.004	0.08	0.95	0.93	0.81
	Testing	Sulfuric acid	0.007	0.19	0.75	0.75	0.81
		Ferric sulfate	0.008	0.15	0.75	0.75	0.76
		Actiflo polymer	0.01	0.20	0.53	0.53	0.57
Polynomial Regression	Training	Sulfuric acid	0.007	0.19	0.73	0.73	0.79
		Ferric sulfate	0.008	0.16	0.68	0.68	0.75
		Actiflo polymer	0.01	0.21	0.49	0.49	0.57
	Testing	Sulfuric acid	0.008	0.20	0.73	0.73	0.82
		Ferric sulfate	0.009	0.17	0.68	0.68	0.74
		Actiflo polymer	0.012	0.23	0.38	0.37	0.54

4.2. Results by Polynomial Regression

The second, third- and fourth-degree polynomial regressions are applied to the training and testing sets. It is found that sulfuric acid and ferric sulfate can be modelled well by the second-degree (k = 2) polynomial regression, and but the third-degree (k = 3) polynomial regression provides best performance for the testing sets of all the three chemicals. Figures 8d, 8e and 8f show the scatter plots between the modelled and observed chemical dosages by the third-degree PR. In general, the PR model has good performance since most data points in the figure are around the 1:1 line. For ferric sulfate and Actiflo polymer, the KGE for the testing set is lower than that for the training set; however, for sulfuric acid, the KGE for the testing set (0.82) is higher than that for the training set (0.79). NSE, R^2 and KGE for sulfuric acid are higher than those for ferric sulfate and Actiflo polymer; and NSE, R^2 and KGE for ferric sulfate are higher than those for Actiflo polymer. This is consistent with the correlation heatmap shown in Figure 7.

4.3. Discussion

4.3.1. Random Forest versus Polynomial Regression

For the training set, random forest has much better performance than polynomial regression for all three chemical usages (Table 1 and Figure 8). For example, RF's KGE is 0.90 for sulfuric acid, 0.89 for ferric sulfate, and 0.81 for Actiflo polymer; and PR's KGE is 0.79 for sulfuric acid, 0.75 for ferric sulfate, and 0.57 for Actiflo polymer. However, RF's KGE reduces from the training set to the testing set, and the KGE values for RF and PR are comparable for the testing set. For sulfuric acid, KGE for RF is 0.81 which is even lower than the KGE of PR (0.82). The KGE values for ferric sulfate are 0.76 for RF and 0.74 for PR, and the KGE values for Actiflo polymer are 0.57 for RF and 0.54 for PR. Therefore, for the testing set, RF and PR have comparable performance, particularly, the performance of PR on modelling sulfuric acid is slightly better than that of RF, but RF has a little bit

better performance on modelling ferric sulfate and Actiflo polymer. RMSE is also used for interpreting the model performance. In the RF, lower RMSE values indicate better performance on the training set for all three chemicals. The testing set also demonstrates reasonable accuracy as seen in the lower RMSE for sulfuric acid. However, Actiflo polymer has the highest RMSE, indicating least accuracy. In the PR model, sulfuric acid and ferric sulfate show reasonable accuracy in both training and testing sets, while accuracy is lower for Actiflo polymer.

Feature importance is utilized to indicate the contribution of each water quality parameter to the predicted chemical dosage. In the RF model, alkalinity stands out with the highest importance value of 0.63, making it the most influential parameter in predicting sulfuric acid dosage. Following alkalinity, conductivity and turbidity exhibit moderately high importance values of 0.12 and 0.06, respectively. The remaining parameters (color, pH, temperature, chloride, sulfate) have comparatively lower importance values ranging from 0.04 to 0.05. For ferric sulfate predictions, the highest importance value is 0.61, corresponding to the feature 'color'. The feature importance values for predicting Actiflo Polymer dosage indicate that no single water quality parameter exclusively controls the prediction. Instead, all parameters have lower values ranging from 0.06 to 0.11, with Color and pH slightly higher at 0.23 and 0.17, respectively. The model interpretation indicates that for predicting the three chemicals, the water quality parameters with the highest contribution to the model are consistent with those having the strongest correlation with the chemicals in Figure 7. Feature importance cannot be utilized in the PR model due to the complexity of higher-degree polynomial regression.

4.3.2. Interaction of Water Quality Parameters

The PR model is robust due to its explicit polynomial equation and its interaction terms capturing the impact of interdependency of water quality parameters. Beside the terms with individual

water quality parameters, the third-degree polynomial model includes the terms with the product of two water quality parameters as shown in Equation (1). From Figure 7, there is no single water quality parameter dominating the prediction for the chemical dosages, especially for Actiflo polymer and ferric sulfate; and more than one water quality parameters have moderate or high correlations with the chemicals. The correlations between chemical dosages and the products of each combination of two water quality parameters are explored to assess the effect of interactions of water quality parameters on chemical dosages. The correlations could be improved from single water quality parameter to the product of water quality parameters. For sulfuric acid, its correlation is -0.59 with color and -0.47 with temperature; and its correlation with the product of color and temperature is improved to -0.62. The correlation between sulfuric acid and conductivity is 0.79 and its correlation with pH is 0.53; and its correlation with the product of conductivity and pH is improved to 0.80. The correlation between sulfuric acid and chloride is 0.68 and its correlation with sulphate is 0.66; and its correlation with the produce of chloride and sulphate is improved to 0.69.

4.3.3. Other Factors besides Water Quality Parameters

Both random forest and polynomial regression are suitable for predicting sulfuric acid and ferric sulfate usages in practice considering their performance (KGE > 0.7); and the performance of the models for predicting Actiflo polymer usage is acceptable (KGE > 0.5). The lower KGE for Actiflo polymer is due to the lower correlations between Actiflo polymer and water quality parameters (Figure 7). Actiflo polymer could be affected by other factors besides water quality parameters. For example, Actiflo polymer is combined with micro-sand for enhancing floc formation.

5. Conclusion

Chemicals are usually used for drinking water treatment processes. Two machine learning models, random forest, and polynomial regression are used for modeling chemical dosages based on

water quality parameters including alkalinity, chloride, color, conductivity, pH, sulfate, temperature, and turbidity. Exploratory data analysis revealed that alkalinity, pH, conductivity, chloride, and sulfate showed similar seasonal variations, and the minimum mean monthly values occur in August or September. Conductivity, chloride, alkalinity, and sulfate have highly positive correlations, and they have moderately positive correlation with pH. The dosages of sulfuric acid, ferric sulfate, and Actiflo polymer show distinct seasonal variations; but the dosages for lime, liquid oxygen, micro-sand, and sodium hypochlorite are stable seasonally, and therefore they are removed from further analysis. Ferric sulfate and Actiflo polymer are positively correlated with a correlation coefficient of 0.46; and sulfuric acid is negatively correlated with ferric sulfate ($r = -0.55$) and Actiflo polymer ($r = -0.27$).

The random forest and polynomial regression algorithms are applied for modeling sulfuric acid, ferric sulfate, and Actiflo polymer, since they are correlated with the water quality parameters as shown in the correlation heatmap. Specifically, sulfuric acid has higher correlations with water quality parameters (e.g., alkalinity, conductivity, chloride, sulfate, turbidity) than ferric sulfate, and ferric sulfate has higher correlations with water quality parameters than Actiflo polymer. Compared with other three metrics (RRMSE, NSE and R^2), KGE, which combines correlation coefficient, mean, and standard deviation, is a better performance metric since it is consistent with the finding from the correlation analysis, i.e., the KGE value for sulfuric acid is higher than that for ferric sulfate and the KGE value for ferric sulfate is higher than that for Actiflo polymer.

For the training set, random forest has better performance than polynomial regression for all the three chemical usages. However, random forest and polynomial regression have comparable performance for the testing set. The performance of polynomial regression on modelling sulfuric acid is slightly better than that of random forest, but random forest has a little bit better performance on modelling ferric sulfate and Actiflo polymer. The robustness of polynomial regression model is due

to its explicit polynomial equation and its interaction terms capturing the impact of interdependency of water quality parameters.

It is found that both random forest and polynomial regression are able to model the dosages of sulfuric acid and ferric sulfate effectively, and the dosage of Actiflo polymer acceptably. When water quality parameters (e.g., alkalinity, pH, conductivity, chloride, and sulfate) reached their minimum values in August and September, lower sulfuric acid dosages but higher ferric sulfate and Actiflo polymer dosages are required.

Acknowledgements

This research is partially funded by Tampa Bay Water.

Availability of Data and Materials

The raw data is not available publicly due to the restriction of the agency but is available by contacting the corresponding author.

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