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DEVELOPMENT OF REMOVAL EFFICIENCY-DRIVEN MULTIPLE REGRESSION MODELS FOR 2-MIB AND GEOSMIN PREDICTION

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Highlights

- Sulfonic acid-modified carbon outperformed unmodified activated carbon.
- Removal reached 91% for 2-MIB and 83% for geosmin.
- Log-log models generally outperformed classical linear regression.
- TOC was a key predictor; chlorophyll-a was more influential for 2-MIB.
- Regression models enable early warning and process optimization.

Graphical Abstract

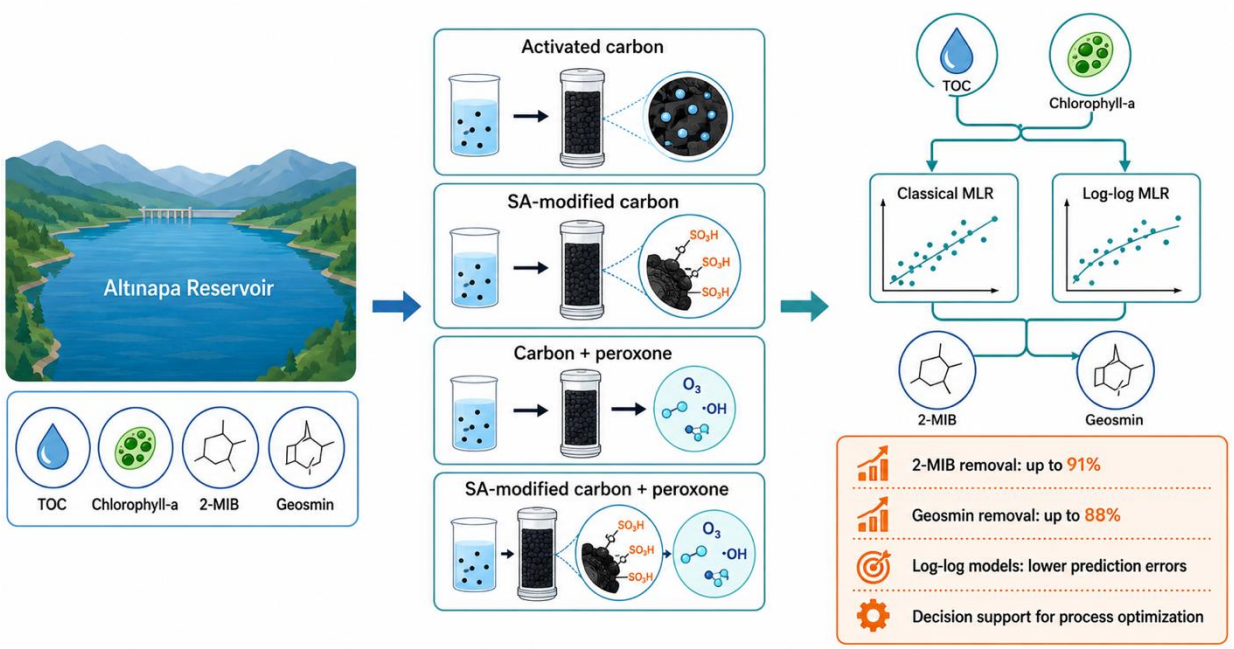


Figure *Schematic overview of the experimental and modeling framework for 2-MIB and geosmin removal from Altınapa Reservoir water using activated carbon, SA-modified carbon, peroxone-assisted adsorption, and SA-modified carbon–peroxone treatment, with TOC- and chlorophyll-a-based classical and log–log multiple linear regression models for process prediction and optimization.*

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ABSTRACT: 2-Methylisoborneol (2-MIB) and geosmin, two primary taste and odor compounds in drinking water, cause significant quality concerns due to their algal origin and extremely low odor thresholds. This study aims to develop multiple linear regression (MLR) models to estimate 2-MIB and geosmin concentrations using total organic carbon (TOC) and chlorophyll-a as explanatory variables. Experimental data were obtained from water samples collected from Altınapa Dam and treated through various processes, including activated carbon adsorption, sulfonic acid-modified activated carbon adsorption, integrated activated carbon and peroxone process, and integrated sulfonic acid-modified activated carbon and peroxone process. Both classical linear regression and log-log models based on natural logarithmic transformations were constructed and comparatively evaluated. The results showed that sulfonic acid-modified activated carbon exhibited higher removal efficiencies for TOC, chlorophyll-a, 2-MIB, and geosmin compared to unmodified activated carbon. Maximum removal efficiencies of 91% for 2-MIB and 83% for geosmin were achieved using 8 mg/L of sulfonic acid-modified activated carbon combined with a 0.3 peroxone ratio. The log-log regression models yielded lower root mean square error (RMSE) and mean absolute percentage error (MAPE) values compared to classical linear models, indicating improved predictive capability. TOC was identified as a consistently significant predictor, while chlorophyll-a had a stronger influence on 2-MIB prediction and a more limited effect on geosmin. The findings suggest that statistical regression modeling—particularly log-log approaches—can serve as effective decision-support tools for optimizing treatment strategies to control taste and odor events in drinking water systems.

Keywords: *2-MIB, Activated carbon, Drinking water quality, Geosmin, Multilinear regression, Peroxone.*

1. INTRODUCTION

Taste and odor compounds such as 2-methylisoborneol (2-MIB) and geosmin are organic substances produced primarily by algae and actinobacteria in drinking water sources and are known for their extremely low sensory thresholds [1]. Although these compounds are non-toxic, they are detectable by the human senses, even at very low concentrations, often leading to consumer dissatisfaction [2]. Taste and odor issues are therefore considered critical aesthetic parameters that threaten not only the perceived quality of drinking water but also the public trust in water treatment facilities [3]. As the removal of these compounds from source waters is often not achievable by conventional treatment methods, advanced treatment and monitoring strategies are required [4].

Taste and odor problems in water bodies are not only technical issues of treatment performance but also constitute social risk factors that directly affect public perceptions of water safety [5]. The detectable presence of 2-MIB and geosmin in tap water can lead to suspicions regarding water safety and erode public confidence in water utilities [6]. Even without observable health risks, the sensory disturbances caused by these compounds may result in increased complaints to local authorities and a tendency among consumers to seek alternative water sources [7]. Therefore, the management of taste and odor

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problems in drinking water supplies should be addressed not only from a technical but also from a perception-based water safety framework [8].

Reservoirs, which are frequently affected by taste and odor events, represent complex aquatic systems exposed to both point and non-point pollution sources [9]. In such surface waters, factors like organic matter load, phytoplankton abundance, and nutrient levels directly contribute to the formation of taste and odor compounds [10]. Understanding the causal relationships between water quality parameters and these odorants is essential for early detection and management.

In recent years, scientific interest has grown in using remote sensing data and statistical modeling techniques to estimate taste and odor compound concentrations, rather than relying solely on direct chemical analyses [11]. The high cost and time demand of conventional analyses have led researchers to develop indirect models based on indicators such as chlorophyll-a, dissolved organic carbon, and trophic status [12]. In this context, regression analyses [13], artificial neural networks [14], machine learning-based models [15], and multivariate statistical approaches [16] have become increasingly popular tools.

The multiple linear regression (MLR) method employed in this study is a widely used statistical tool in environmental modeling and provides a robust framework for evaluating relationships between dependent and independent variables [17]. MLR is particularly effective in predicting target variables influenced by multiple environmental parameters [18]. Such models are not only useful for statistical interpretation but also serve as a foundation for process optimization, early warning, and decision support systems in water quality management [19].

Although academic interest in modeling taste and odor compounds has grown substantially in recent years, the application of these models in operational water treatment systems remains limited. Predictive models for compounds such as 2-MIB and geosmin hold great potential for optimizing treatment strategies, reducing operational costs, and improving chemical dosing efficiency [2]. Therefore, it is essential that such models be not only academically sound but also practically applicable as decision-support tools in real-world engineering settings. The modeling approach proposed in this study is developed using field-based data and is designed to be directly transferable to monitoring and optimization systems at the operational scale.

This study aims to develop multiple linear regression models to estimate 2-MIB and geosmin concentrations based on total organic carbon (TOC) and chlorophyll-a values in water samples collected from the Altınapa Reservoir. For this purpose, both classical linear regression and log-log models based on natural logarithmic transformations were constructed and compared regarding model fit (R^2) and error metrics (RMSE and MAPE). The results aim to provide a scientific and practical approach to predicting and managing taste and odor risks in drinking water sources.

2. MATERIAL AND METHODS

2.1. Water Quality Tests

2.1.1. Total organic carbon analysis

The total organic carbon (TOC) content of the samples was determined using the high-temperature combustion method (Standard Method 5310B) with a TOC-L CPH analyzer (Shimadzu). Six calibration standards ranging from 0.2 to 8 mg/L were prepared using potassium hydrogen phthalate (EM-PX1476-3, EMD).

2.1.2. Chlorophyll-a analysis

The chlorophyll-a concentration was determined using a spectrophotometric method. Reservoir water samples were filtered through cellulose acetate filter paper placed on a vacuum filtration system. The filter paper was folded and placed into a chemical oxygen demand (COD) vial containing 10 mL of

acetone. The vial was shaken thoroughly to ensure complete dissolution of the filter in acetone. It was then wrapped with aluminum foil to prevent light exposure and stored in a refrigerator at +4 °C for 2 hours. After reaching 3000 rpm within 1–2 minutes, the sample was centrifuged for 15 minutes. The clear supernatant was collected and analyzed at 630, 647, 664, and 750 nm wavelengths using a UV-visible spectrophotometer. Acetone was used as the blank.

2.1.3. 2-MIB and geosmin analysis

The analysis of 2-methylisoborneol (2-MIB) and geosmin was conducted using gas chromatography-mass spectrometry (GC–MS) in accordance with Standard Method 6040B. A GC (Perkin Elmer Clarus 680) equipped with an MS (Clarus SQ 8T) and an Elite-5ms column was used for the measurements. The GC oven temperature was initially set at 60 °C and then increased to 260 °C at a rate of 15 °C/min. Helium was used as the carrier gas at a 1 mL/min flow rate. Quantification of 2-MIB and geosmin was performed in selected ion monitoring (SIM) mode targeting specific ions.

2.2. Activated Carbon Experiments

In this study, AC Puriss was used as the activated carbon. AC Puriss has a surface area of 300 m^2/g, a density of 1.8–2.1 g/cm^3, and a point of zero charge (pH_{pzc}) of 7.1.

2.2.1. Functionalization of activated carbon with sulfonic acid

The modification of AC Puriss activated carbon with sulfonic acid was carried out using a modified version of the method proposed by Goswami and Phukan [20]. Prior to modification, the activated carbon was washed with distilled and deionized water and dried in an oven at 105 °C. A total of 30 g of activated carbon was weighed, and 900 mL of dichloromethane (CH_2Cl_2) was added. The solution was subjected to ultrasonic agitation for 45 minutes. After sonication, the mixture was cooled using ice blocks. Then, 30 mL of chlorosulfonic acid was added dropwise at room temperature over a 30-minute period to the cooled solution. Following the addition, the mixture was stirred for an additional 3 hours to ensure complete dispersion of the chlorosulfonic acid. The final product was then filtered and washed with ethanol and water, followed by drying at 80 °C to obtain sulfonic acid-functionalized activated carbon. The carbon samples were periodically weighed until a constant mass was achieved, after which they were stored in a desiccator. The modification of the activated carbon was performed in five stages, as illustrated in Figure 1.

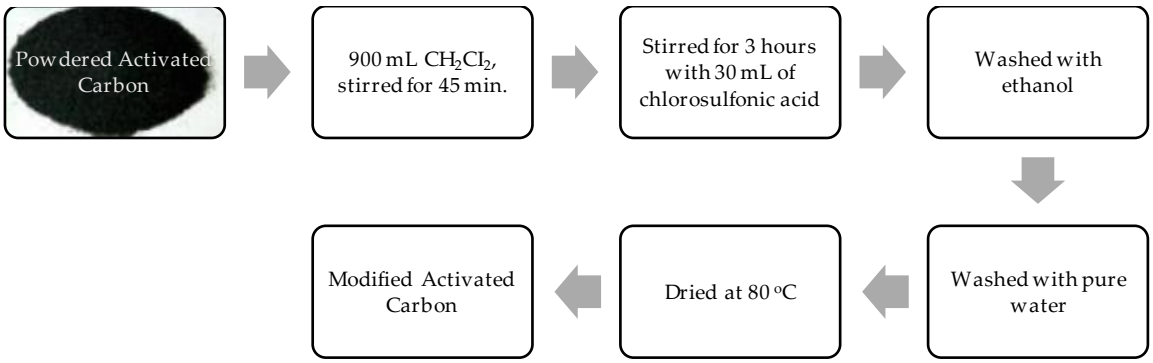


Figure 1. Modification steps of activated carbon with chlorosulfonic acid

2.2.2. Adsorption + peroxone tests

The peroxone process is an advanced oxidation process that involves the combined use of hydrogen peroxide and ozone. For the ozonation experiments, the ozone dose was determined based on a

commonly used 1.5:1 (ozone/TOC) ratio in water treatment, meaning that the ozone was applied at a dose 1.5 times higher than the TOC concentration of the samples. The ozone stock solution was prepared using ultra-high purity oxygen gas (99.998%). Following the 1.5:1 ozone/TOC dosing, the samples were stirred for 5 minutes. After each dosing, the bottles were sealed and stirred for 5 minutes, then allowed to stand for a reaction period of 30 minutes.

2.3. Multiple Linear Regression Analysis

The multiple linear regression (MLR) analysis examined correlations between water quality parameters and the concentrations of 2-MIB and geosmin. The MLR analysis was performed using the regression analysis tool available in Microsoft Excel. The model is based on the data obtained from water samples collected from the Altınapa Dam and aims to predict the concentrations of 2-MIB and geosmin. In this analysis, total organic carbon (TOC) and chlorophyll-a were selected as independent variables, while 2-MIB and geosmin concentrations were treated as the dependent variables.

The performance of the MLR models was evaluated based on the coefficient of determination (R^2) and the significance level (p-value) [21]. In order to obtain the relationship expressed in Equation 1, the natural logarithmic transformations of the independent variables were first applied. Subsequently, the regression coefficients obtained from the MLR analysis were exponentiated, and the transformed variables were multiplied to construct the predictive equations.

Furthermore, the difference between the measured and predicted values of the target variable was calculated using the root mean square error (RMSE), which was employed to evaluate the predictive performance of the model (Equation 2). The mean absolute percentage error (MAPE) was also used to define the relative accuracy between observed and predicted values (Equation 3). RMSE was chosen because it expresses the error magnitude in the same unit as the predicted parameter (in this case, ng/L) [22].

$$y = a * x^b \Longrightarrow \ln(y) = \ln(a) + b * \ln(x) \quad (1)$$

y: *Dependent variable*
x: *Independent variable*
a: *Constant coefficient (the predicted value of y when x = 1)*
b: *Exponent that defines the relationship between x and y*
$ln(y)$:*Natural logarithm of the dependent variable*
$ln(x)$:*Natural logarithm of the independent variable*

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - y'_i)^2} \quad (2)$$

y_i:*Observed (measured) value*
y'_i:*Predicted value from the model*
n:*Number of observations*
$(y_i - y'_i)^2$:*Squared error for each observation*
$\sum$: *Sum of all squared errors*
$\sqrt{}$:*Square root of the mean squared error*

$$\mathrm{MAPE} = \frac{100}{n}\sum_{i=1}^{n}\left|\frac{y_i - y'_i}{y_i}\right| \quad (3)$$

y_i:*Observed (measured) value*
y'_i:*Predicted value from the model*
n:*Number of observations*
$\left|\frac{y_i - y'_i}{y_i}\right|$:*Absolute percentage error of each prediction*
$\sum$: *Sum of all percentage errors*
$\frac{100}{n}$:*Mean of the percentage errors expressed as a percentage*

MAPE (%)	*Model Accuracy*
0-10%	*Very Good*

10-20%	*Good*
20-50%	*Acceptable*
>50%	*Poor*

3. RESULTS AND DISCUSSION

3.1. Water Quality Parameters

3.1.1. Total organic carbon

The total organic carbon (TOC) concentration in Altınapa Dam was determined to be 5.52 mg/L. According to the "Regulation on the Quality and Treatment of Water Intended for Human Consumption," the TOC concentration should be below 4 mg/L for Class A1 waters, below 4.7 mg/L for Class A2 waters, and below 10 mg/L for Class A3 waters. Based on the measured value, the TOC level of Altınapa Reservoir corresponds to the Class A3 water quality category.

3.1.2. Chlorophyll-a

Chlorophyll-a analysis of the reservoir water revealed a concentration of 10.22 mg/m^3. Chlorophyll-a is a key parameter that provides important information about phytoplankton density and the trophic status of the water body.

3.1.3. 2-MIB

The concentration of 2-MIB in the reservoir water was calculated to be 11.61 ng/L. 2-MIB is an organic compound that can contribute to taste and odor problems in water.

3.1.4. Geosmin

Based on the analyses, the geosmin concentration in the water sample taken from Altınapa Reservoir was determined to be 11.96 ng/L. Geosmin is a naturally occurring compound known to be produced by algae and actinobacteria in water sources, and it is recognized for causing taste and odor problems.

3.2. Multiple Linear Regression Models

Using TOC and chlorophyll-a measurements, the influence of these variables on the formation of 2-MIB and geosmin was determined through multiple linear regression (MLR) analysis. MLR is a statistical method used to predict a dependent variable (target parameter) based on multiple input (independent) variables. In contrast to simple linear regression, which uses only a single predictor variable, MLR identifies the linear relationship between multiple independent variables (x_1, x_2, …, x_n) and the dependent variable (y). Moreover, MLR also evaluates the statistical significance of the relationships between the independent and dependent variables. In this method, the correlations among the independent variables and between the independent and dependent variables can be expressed as either positive or negative.

All statistical models in this study were based on the MLR structure proposed by Song et al. [23]. Unlike traditional linear regression models expressed as $y = ax_1 + bx_2 + cx_3 + d$, this approach represents the model as $y = 10^d \times [x_1]^a \times [x_2]^b \times [x_3]^c$. Therefore, instead of a linear function, the variables are expressed in the form of a power function. The main advantage of this method is the ability to normalize variables with different units by converting them into logarithmic form, thereby resulting in regression equations that are more realistic and statistically valid [23]. Additionally, the standardized exponential regression coefficients allow for direct identification of the predictive capacity or contribution of each independent variable to the equation. As a result, a separate sensitivity analysis becomes unnecessary.

Prior to model development, all variables were transformed using natural logarithms. The MLR analyses were performed at a 95% confidence level. Accordingly, the significance level (p-value) for the variables in the model was set at 0.05.

3.2.1. Activated carbon and sulfonic acid-modified activated carbon

The TOC removal efficiency using original activated carbon was found to be 24% at a dose of 1 mg/L, increasing to 33% at 8 mg/L. While TOC removal improved with increasing dosage, the rate of improvement was relatively low [24]. In contrast, sulfonic acid-modified activated carbon yielded a removal efficiency of 72% at 1 mg/L and 76% at 8 mg/L. The modified carbon exhibited a higher initial removal rate and a steeper increase with dose. Especially at lower doses, sulfonic acid-modified activated carbon proved significantly more effective [25]. Jeirani et al. [26] confirmed that the increase in surface area and adsorption capacity of activated carbon enhances its potential to remove pollutants as the dose increases.

The efficiency of TOC removal using sulfonic acid-modified activated carbon reached 66% at a 10 mg/L dose. This modification demonstrated both higher effectiveness and faster improvement with dose. Cheng et al. [27] found that improved surface area, enhanced pore structure, and the addition of functional groups during modification increased adsorption capacity and selectivity for specific contaminants. These findings suggest that sulfonic acid-modified activated carbon is a cost-effective and efficient alternative for water and wastewater treatment applications.

Chlorophyll-a removal with original activated carbon was 23% at 1 mg/L and increased to 69% at 10 mg/L. The increase in chlorophyll-a removal was significant with dose. Using sulfonic acid-modified activated carbon, removal efficiencies reached 59% at 1 mg/L and 85% at 10 mg/L. The modified carbon showed a very high initial removal rate and a sharper increase curve. In both TOC and chlorophyll-a removal, sulfonic acid-modified activated carbon was highly effective, achieving up to 76% and 85% removal, respectively. Although original activated carbon also showed increased efficiency with dose, the performance gain was limited. Sun and Webley [28] attributed this to the saturation of surface area and adsorption capacity of activated carbon.

Sulfonic acid-modified activated carbon showed greater removal efficiency and faster improvement with increasing doses. Hokkanen et al. [29] emphasized that modification significantly enhances performance, especially at low doses, by increasing adsorption capacity.

Geosmin removal with original activated carbon achieved 66% at 1 mg/L and increased slightly to 68% at 8 mg/L. The efficiency reached a plateau at lower doses. Matsui et al. [30] explained that minor improvements at higher doses may result from additional adsorption sites or improved dispersion of geosmin molecules at higher carbon concentrations. Although effective at low doses, original activated carbon showed limited potential for improvement with higher doses, underscoring the need for optimization or the use of modified activated carbon.

With sulfonic acid-modified activated carbon, geosmin removal was 77% at 1 mg/L and 83% at 8 mg/L. The modified carbon was more effective and more responsive to dose increases. For 2-MIB, original activated carbon provided 75% removal at 1 mg/L, which increased to 78% at 8 mg/L, again indicating limited performance gains. In contrast, sulfonic acid-modified activated carbon achieved 81% removal at 1 mg/L and 91% at 8 mg/L. Especially at higher doses, it proved to be much more effective in removing 2-MIB.

Overall, sulfonic acid-modified activated carbon achieved higher removal efficiencies than unmodified carbon for both compounds. Geosmin removal ranged between 77–83% with modified carbon, compared to 66–68% with unmodified carbon. The improvement was more pronounced with the dose increase for the modified carbon. Mustapha et al. [2] attributed this enhancement to the increased surface area and functional groups introduced during the modification process.

In the case of 2-MIB, even at low doses, modified carbon provided high removal efficiency (81%), which reached up to 91% at higher doses. In contrast, original activated carbon remained between 75–78%, showing limited performance. The apparent increase in removal efficiency with dose in the

modified carbon indicates that the modification significantly improved its adsorption capacity. The increase observed with unmodified carbon was comparatively limited. Literature studies have also emphasized that modified activated carbon is particularly effective in removing taste and odor compounds, offering high efficiency even at low doses [31]. The removal of 2-MIB and geosmin using sulfonic acid-modified activated carbon has been especially highlighted for its effectiveness [32].

Table 1 presents the TOC, chlorophyll-a, 2-MIB, and geosmin concentrations obtained under 0–10 mg/L doses of both original and modified activated carbon. These results are provided to compare the performance of adsorption processes in removing taste and odor compounds.

Table 1. TOC, chlorophyll-a, 2-MIB, and geosmin removal results for activated carbon and sulfonic acid-modified activated carbon adsorption

	Activated Carbon Dosage (mg/L)	Activated Carbon Adsorption Results	Sulfonic Acid-Modified Activated Carbon Adsorption Results
TOC (mg/L)	0	5.52	5.52
	1	4.20	1.52
	2	4.14	1.49
	4	4.03	1.38
	6	3.85	1.34
	8	3.70	1.32
	10	3.68	1.30
Chlorophyll-a (mg/m^3)	0	10.22	10.22
	1	7.92	4.14
	2	7.85	4.10
	4	5.43	2.75
	6	4.50	2.34
	8	3.82	1.80
	10	3.12	1.50
2-MIB (ng/L)	0	11.61	11.61
	1	2.88	2.23
	2	2.90	2.22
	4	2.59	1.29
	6	2.59	1.19
	8	2.59	1.10
Geosmin (ng/L)	0	11.96	11.96
	1	4.06	2.77
	2	4.04	2.78
	4	4.03	2.47
	6	3.99	2.41
	8	3.83	2.00

In the activated carbon adsorption process, two different multiple regression models were developed to predict the concentrations of 2-MIB and geosmin—compounds responsible for taste and odor—based on TOC and chlorophyll-a parameters: a classical linear model and a log-log model using natural logarithmic transformations. The model fits, error metrics, and statistical significance of the variables were comparatively evaluated. The model developed for the prediction of 2-MIB using the classical linear regression approach is presented in Equation 4.

$$2 - MIB = -2.0370 + 1.7737 * TOC + 0.3774 * (Chlorophyll - a) \quad (4)$$

According to Equation 4, the coefficient of determination was calculated as $R^2 = 0.999$, while the

error metrics were RMSE = 0.0859 ng/L and MAPE = 4.84%. Both TOC (p = 0.00075) and chlorophyll-a (p = 0.0114) were found to be statistically significant predictors. Our findings are in agreement with Chong et al. [33], who demonstrated that chlorophyll-a levels were strongly correlated with 2-MIB and geosmin concentrations in a shallow reservoir system. The log-log model developed through natural logarithmic transformation is presented in Equation 5.

$$\ln(2-MIB) = -0.6663 + 0.7556 * \ln(TOC) + 0.7876 * \ln(Chlorophyll-a) \quad (5)$$

According to Equation 5, the coefficient of determination was R^2 = 0.993, with RMSE = 0.0688 (in natural logarithmic units) and MAPE = 5.82%. Both independent variables were statistically significant: TOC (p = 0.0228) and chlorophyll-a (p = 0.0162). The classical linear regression model developed for geosmin prediction is presented in Equation 6.

$$Geosmin = -0.8268 + 2.1051 * TOC + 0.1140 * (Chlorophyll-a) \quad (6)$$

According to Equation 6, the model's coefficient of determination was R^2 = 0.999, with RMSE = 0.0989 ng/L and MAPE = 3.34%. The TOC parameter was found to be statistically significant (p = 0.00068); however, the contribution of chlorophyll-a did not reach the significance threshold (p = 0.2397). This finding is consistent with the literature, which suggests that chlorophyll-a is not always a significant predictor of geosmin and may sometimes introduce background noise [34]. The geosmin model developed within the framework of the log-log transformation is presented in Equation 7.

$$\ln(Geosmin) = 0.3628 + 0.9681 * \ln(TOC) + 0.1991 * \ln(Chlorophyll-a) \quad (7)$$

According to Equation 7, the model exhibited a high level of fit with R^2 = 0.996, and the error metrics were determined as RMSE = 0.0389 and MAPE = 3.15%. While the TOC variable provided a statistically significant contribution (p = 0.0023), chlorophyll-a did not reach the significance threshold in this model either (p = 0.1161).

The findings indicate that the adsorption process using sulfonic acid-modified activated carbon can successfully predict the removal of 2-MIB and geosmin through both linear and multiplicative regression models. For 2-MIB, the classical linear model outperformed with lower error values and stronger statistical significance. In contrast, for geosmin, the log-log model with natural logarithmic transformation yielded more robust results with lower RMSE and MAPE values. In all models, TOC emerged as the most influential predictor directly affecting estimation performance. In contrast, chlorophyll-a made a statistically significant contribution only to the prediction of 2-MIB, and its effect on geosmin modeling remained weaker.

These results demonstrate that both classical linear and log-log regression models can be effectively used in drinking water quality applications and highlight the importance of selecting a model appropriate to the nature of the relationships among parameters. The model obtained for 2-MIB prediction in the sulfonic acid-modified activated carbon process is presented in Equation 8.

$$2-MIB = -2.0370 + 1.7737 * TOC + 0.3774 * (Chlorophyll-a) \quad (8)$$

According to Equation 8, the model exhibited a coefficient of determination of R^2 = 0.999, with RMSE = 0.086 ng/L and MAPE = 4.84%. Both TOC (p = 0.00075) and chlorophyll-a (p = 0.0114) were found to be statistically significant predictors. The model developed for the prediction of geosmin is presented in Equation 9.

$$Geosmin = -0.8268 + 2.1051 * TOC + 0.1140 * (Chlorophyll-a) \quad (9)$$

According to Equation 9, the model exhibited a coefficient of determination of $R^2 = 0.999$, with RMSE = 0.099 ng/L and MAPE = 3.34%. The TOC parameter was found to be statistically significant (p = 0.00068), whereas chlorophyll-a did not reach the significance threshold (p = 0.2397). The model developed for the prediction of 2-MIB is presented in Equation 10.

$$\ln(2 * MIB) = -0.6663 + 0.7556 * \ln(TOC) + 0.7876 * \ln(Chlorophyll - a) \quad (10)$$

According to Equation 10, the model's coefficient of determination was $R^2 = 0.993$, with RMSE = 0.069 (in natural logarithmic units) and MAPE = 5.82%. Both TOC (p = 0.0228) and chlorophyll-a (p = 0.0162) provided statistically significant contributions. The log-log model developed for geosmin prediction is presented in Equation 11.

$$\ln(Geosmin) = 0.3628 + 0.9681 * \ln(TOC) + 0.1991 * \ln(Chlorophyll - a) \quad (11)$$

According to Equation 11, the model exhibited a coefficient of determination of $R^2 = 0.996$, with RMSE = 0.039 and MAPE = 3.15%. TOC was found to be statistically significant (p = 0.0023), whereas chlorophyll-a did not reach the significance threshold (p = 0.1161).

The findings indicate that sulfonic acid-modified activated carbon offers high-performance and reliable predictive results for estimating 2-MIB and geosmin concentrations—two compounds responsible for taste and odor in water. While the classical linear model appears slightly more successful for predicting 2-MIB, the log-log model with natural logarithmic transformation achieved lower error rates in the prediction of geosmin. In both models, TOC consistently emerged as the dominant predictor. On the other hand, Chlorophyll-a provided a statistically significant contribution only in the prediction of 2-MIB.

These results underscore the need for different model structures in environmental systems and highlight the potential of log-log models with natural logarithmic transformations as viable alternatives.

3.2.2. Combined activated carbon adsorption and peroxone process experiments

A significant improvement in TOC removal efficiency was observed by increasing both the peroxone ratio and the activated carbon dose. The highest TOC removal efficiency (55%) was achieved at an 8 mg/L activated carbon dose with a peroxone ratio of 0.3. However, removal efficiencies remained limited at a low dose of 1 mg/L activated carbon (24–25%), indicating that the oxidation effect alone was insufficient due to the lack of adequate adsorption capacity. Although oxidation reactions degrade the chemical structure of organic compounds, the inability to retain target compounds in the system due to low adsorption capacity limits overall effectiveness [35]. The combined use of activated carbon and the peroxone process demonstrated a synergistic effect in TOC removal. Especially at high doses of activated carbon (43–55%), TOC removal efficiencies exceeded those of oxidation alone. Literature also supports that integrating adsorption and oxidation processes allows for more effective removal of complex organic compounds [36].

In contrast, the removal efficiency of chlorophyll-a was relatively low, suggesting that pigment structures may be more resistant to oxidation. The initial chlorophyll-a concentration was 10.22 mg/m³, and the maximum removal efficiency reached was only 24% (achieved at 8 mg/L activated carbon and 0.3 peroxone ratio). This result suggests that complex molecules like chlorophyll-a are more resistant to both oxidation and adsorption. The low removal efficiencies reveal that adsorption on the activated carbon surface and oxidation via the peroxone process had limited effects on macromolecular structures like chlorophyll-a. Studies have shown that advanced oxidation processes (AOPs) often require high oxidant doses and prolonged contact times for the effective removal of pigments such as chlorophyll [37].

In the reservoir water, the initial geosmin concentration was 11.96 ng/L. Removal efficiencies increased with both the activated carbon dose and the peroxone ratio. The highest geosmin removal

(80%) was achieved at 8 mg/L activated carbon and 0.3 peroxone ratio. At lower carbon doses (1–2 mg/L), the removal efficiencies ranged between 74–76%, with little observable impact from changes in the peroxone ratio.

Similarly, the initial concentration of 2-MIB was 11.61 ng/L. The trend in 2-MIB removal was comparable to that of geosmin. At 1–2 mg/L activated carbon, removal efficiencies were about 76%, increasing to 78% at 4 mg/L and 80% at 8 mg/L. The effect of increasing the peroxone ratio on 2-MIB removal was limited, although the combination of higher carbon doses (4–8 mg/L) with peroxone did enhance overall performance.

Activated carbon dose was found to be a significant factor in the removal of both geosmin and 2-MIB. At low doses, removal efficiencies remained limited (74–76%). In contrast, higher doses yielded significant improvements (up to 80%), indicating increased adsorption capacity and more efficient binding of taste and odor compounds to the carbon surface. The peroxone ratio contributed little to removal performance at lower carbon doses, but at 8 mg/L, increasing the peroxone ratio from 0.1 to 0.3 led to a notable improvement (from 79% to 80%), suggesting a potential synergistic effect at higher carbon doses [38].

The removal patterns of 2-MIB and geosmin were remarkably similar. Both compounds were susceptible to oxidation and adsorption, resulting in closely matched removal efficiencies. This similarity may be attributed to the comparable physicochemical properties of 2-MIB and geosmin, which influence their interactions in similar ways [2]. Many studies emphasize the importance of enhancing activated carbon adsorption capacity and combining it with oxidation processes to remove these compounds efficiently. This study demonstrates that high doses of activated carbon optimize the synergistic effect. The limited effectiveness of peroxone at low carbon doses aligns with findings that AOPs are less effective under low organic load conditions [39].

Overall, the results indicate that effective removal of 2-MIB and geosmin can be achieved through the optimized use of high doses of activated carbon and appropriate oxidant levels. This provides a valuable approach for water treatment plant applications. A comparison of TOC, chlorophyll-a, 2-MIB, and geosmin removal efficiencies at different activated carbon and peroxone doses is presented in Table 3.

Table 3. Comparison of TOC, chlorophyll-a, 2-MIB, and geosmin removal efficiencies at different activated carbon and peroxone doses

	Activated Carbon Dosage (mg/L)	Peroxone Process	Combined Activated Carbon Adsorption and Peroxone Process Results
TOC (mg/L)	0	0	5.52
	1	0.1	4.18
	1	0.3	4.16
	2	0.1	3.78
	2	0.3	3.86
	4	0.1	3.16
	4	0.3	3.11
	6	0.1	3.04
	6	0.3	3.01
	8	0.1	2.59
	8	0.3	2.51
	10	0.1	2.57
	10	0.3	2.50
Chlorophyll-a (mg/m^3)	0	0	10.22
	1	0.1	8.99
	1	0.3	8.91
	2	0.1	8.38

	2	0.3	8.32
	4	0.1	8.07
	4	0.3	8.01
	6	0.1	8.01
	6	0.3	7.97
	8	0.1	7.77
	8	0.3	7.73
	10	0.1	7.75
	10	0.3	7.71
2-MIB (ng/L)	0	0	11.61
	1	0.1	2.80
	1	0.3	2.78
	2	0.1	2.78
	2	0.3	2.77
	4	0.1	2.52
	4	0.3	2.50
	6	0.1	2.48
	6	0.3	2.46
	8	0.1	2.34
	8	0.3	2.31
Geosmin (ng/L)	0	0	11.96
	1	0.1	3.06
	1	0.3	3.04
	2	0.1	3.04
	2	0.3	3.01
	4	0.1	2.54
	4	0.3	2.51
	6	0.1	2.50
	6	0.3	2.47
	8	0.1	2.47
	8	0.3	2.42

The classical linear model used for predicting 2-MIB concentration is presented in Equation 12.

$$2-MIB = -41.18 - 2.84 * TOC + 6.50 * \ Chlorophyll - a \quad (12)$$

The classical linear regression model in Equation 12 yielded an R^2 value of 0.774, with an RMSE of 1.238 ng/L and a MAPE of 27.29%. An evaluation of the statistical significance of the regression coefficients revealed a p-value of 0.266 for TOC and 0.051 for chlorophyll-a. The log-log model with natural logarithmic transformation is presented in Equation 13.

$$\ln(2-MIB) = -15.82 - 1.45 * \ln(TOC) + 8.80 * \ln(Chlorophyll - a) \quad (13)$$

According to Equation 13, the model yielded an R^2 value of 0.811, with RMSE = 0.191 (in natural logarithmic units) and MAPE = 14.22%. Chlorophyll-a was found to be statistically significant (p = 0.016), whereas TOC did not reach the significance threshold (p = 0.193). The classical linear model developed for geosmin prediction is presented in Equation 14.

$$Geosmin = -41.25 - 2.69 * TOC + 6.47 * \ Chlorophyll - a \quad (14)$$

According to Equation 14, the model yielded an R^2 value of 0.790, with RMSE = 1.224 ng/L and MAPE = 25.05%. Chlorophyll-a was found to be at the threshold of statistical significance (p = 0.050), while TOC did not make a significant contribution (p = 0.284). The log-log model with natural logarithmic transformation developed for geosmin prediction is presented in Equation 15.

$$\ln(Geosmin) = -15.19 - 1.26 * \ln(TOC) + 8.41 * (Chlorophyll - a) \quad (15)$$

According to Equation 15, the model yielded an R^2 value of 0.840, with RMSE = 0.176 and MAPE = 12.78%. Chlorophyll-a was found to be statistically significant (p = 0.014), whereas TOC did not meet the significance threshold (p = 0.217).

The comparative findings indicate that log-log models with natural logarithmic transformations provided lower error rates and higher explanatory power for both 2-MIB and geosmin predictions than classical linear models. While the classical linear model appeared to be slightly more successful in predicting 2-MIB, the log-log transformed model achieved lower error rates in predicting geosmin; similarly, the literature emphasizes that the performance of different regression models can vary depending on the nature of the variable and regional factors [40]. Moreover, in both model types, chlorophyll-a played a more decisive role in predicting the target compounds than TOC. This is particularly noteworthy in integrated treatment processes, where chlorophyll-a indicates algal activity and biological pollution potential.

In conclusion, log-log models offered more reliable predictions, with chlorophyll-a emerging as the dominant predictor variable, while TOC demonstrated a more secondary influence throughout the process.

3.2.3. Combined sulfonic acid-modified activated carbon adsorption and peroxone process experiments

A notable increase in geosmin removal efficiency was observed with increasing doses of sulfonic acid-modified activated carbon and peroxone ratios. The maximum removal efficiency (88%) was achieved at 8 mg/L of modified activated carbon combined with a peroxone ratio of 0.3. These findings suggest that both oxidation and adsorption processes are simultaneously effective in geosmin removal.

Similarly, 2-MIB removal also increased relative to the initial concentration with higher doses of modified activated carbon and increased peroxone ratios. The highest removal efficiency (89%) was achieved at 8 mg/L of sulfonic acid-modified activated carbon and a peroxone ratio of 0.3. Adsorption appeared to be more effective for 2-MIB than for geosmin, indicating that the surface properties of sulfonic acid-modified activated carbon may be more responsive to smaller molecules like 2-MIB. While increasing the peroxone ratio to 0.3 did result in a modest improvement in removal efficiency, the gain was limited compared to that achieved at 0.1, suggesting that the effectiveness of oxidizing agents diminishes beyond a certain threshold, and adsorption capacity becomes more dominant.

This study provides significant insights into the synergistic effect of combining sulfonic acid-modified activated carbon and the peroxone process in removing taste and odor compounds. It is well known in the literature that compounds such as 2-MIB and geosmin, even at very low concentrations, can significantly impair the acceptability of drinking water [41]. The results demonstrate that combining AOPs and adsorption yields higher removal efficiency than either method alone. Particularly, higher peroxone ratios were found to be effective in oxidizing 2-MIB and geosmin, while the high adsorption capacity of activated carbon contributed significantly to the process—findings consistent with the literature [42].

This study offers a new perspective for optimizing treatment processes and reducing operational costs in drinking water treatment facilities to remove 2-MIB and geosmin. The combination of sulfonic acid-modified activated carbon and peroxone presents itself as an environmentally friendly and efficient solution, further strengthening its relevance in the current literature. The removal performances of

selected water quality indicators using the combined sulfonic acid-modified activated carbon and peroxone process are presented in Table 4.

Table 4. Removal performance of selected water quality indicators in sulfonic acid-modified activated carbon and peroxone process applications

	Sulfonic Acid-Modified Activated Carbon	Peroxone Process	Combined Sulfonic Acid-Modified Activated Carbon and Peroxone Process Results
TOC (mg/L)	0	0	5.52
	1	0.1	1.18
	1	0.3	1.16
	2	0.1	1.08
	2	0.3	1.06
	4	0.1	1.06
	4	0.3	1.01
	6	0.1	1.04
	6	0.3	1.01
	8	0.1	1.09
	8	0.3	1.01
	10	0.1	1.09
	10	0.3	1.01
Chlorophyll-a (mg/m^3)	0	0	10.22
	1	0.1	4.99
	1	0.3	4.91
	2	0.1	4.38
	2	0.3	4.32
	4	0.1	4.07
	4	0.3	4.01
	6	0.1	4.02
	6	0.3	3.80
	8	0.1	3.77
	8	0.3	3.73
	10	0.1	3.77
	10	0.3	3.73
2-MIB (ng/L)	0	0	11.61
	1	0.1	1.91
	1	0.3	1.81
	2	0.1	1.78
	2	0.3	1.77
	4	0.1	1.52
	4	0.3	1.50
	6	0.1	1.49
	6	0.3	1.42
	8	0.1	1.34
	8	0.3	1.31
Geosmin (ng/L)	0	0	11.96
	1	0.1	2.05
	1	0.3	2.01
	2	0.1	1.84

	2	0.3	1.81
	4	0.1	1.74
	4	0.3	1.71
	6	0.1	1.67
	6	0.3	1.57
	8	0.1	1.47
	8	0.3	1.42

The classical linear model developed for the prediction of 2-MIB is presented in Equation 16.

$$2-MIB = -41.18 - 2.84 * TOC + 6.50 * Klorofil - a \quad (16)$$

According to Equation 16, the model yielded an R^2 value of 0.999, with RMSE = 0.1006 ng/L and MAPE = 4.98%. Among the independent variables, TOC was found to be highly significant with a p-value of 9.1×10^{-7}, while chlorophyll-a was considered marginally significant with a p-value of 0.0458. The log-log model based on natural logarithmic transformation is presented in Equation 17.

$$\ln(2-MIB) = -15.82 - 1.45 * \ln(TOC) + 8.80 * \ln(Klorofil - a) \quad (17)$$

According to Equation 17, the model yielded an R^2 value of 0.992, with RMSE = 0.0514 and MAPE = 4.20%. Both independent variables were statistically significant: TOC (p = 0.0018) and chlorophyll-a (p = 0.0044). The classical linear model developed for geosmin prediction is presented in Equation 18.

$$Geosmin = -41.25 - 2.69 * TOC + 6.47 * Klorofil - a \quad (18)$$

According to Equation 18, the model yielded an R^2 value of 0.999, with RMSE = 0.0921 ng/L and MAPE = 4.63%. Both TOC ($p = 3.7 \times 10^{-7}$) and chlorophyll-a (p = 0.0364) were found to be statistically significant. The log-log model based on natural logarithmic transformation for geosmin prediction is presented in Equation 19.

$$\ln(Geosmin) = -15.19 - 1.26 * \ln(TOC) + 8.41 * \ln(Klorofil - a) \quad (19)$$

According to Equation 19, the model yielded an R^2 value of 0.994, with RMSE = 0.0455 and MAPE = 4.08%. The p-values for TOC and chlorophyll-a were 0.0006 and 0.0044, respectively, indicating that both variables were statistically significant predictors.

The findings indicate that the combination of sulfonic acid-modified activated carbon and the peroxone process provides high predictive accuracy for removing both 2-MIB and geosmin. In particular, the log-log models based on natural logarithmic transformation demonstrated lower error metrics, thereby enhancing overall model performance. Both TOC and chlorophyll-a were found to contribute significantly to both types of models. These results suggest that the surface properties of sulfonic acid-modified activated carbon, together with the oxidative capacity of the peroxone process, act synergistically on taste and odor compounds.

4. CONCLUSIONS

In this study, multiple linear regression (MLR) models were developed to predict the concentrations of the taste and odor compounds 2-MIB and geosmin under various advanced treatment processes. The processes tested included activated carbon, sulfonic acid-modified activated carbon, activated carbon combined with peroxone, and sulfonic acid-modified activated carbon combined with peroxone. Models were developed using TOC and chlorophyll-a as independent variables and were evaluated in terms of

statistical fit, prediction accuracy, and variable significance.

The main findings of the study are summarized below:

- Sulfonic acid-modified activated carbon demonstrated higher removal efficiencies for TOC, chlorophyll-a, 2-MIB, and geosmin compared to unmodified activated carbon. Removal efficiencies reached up to 91% for 2-MIB and 83% for geosmin.
- The log-log model with natural logarithmic transformation outperformed classical linear models regarding lower RMSE and MAPE values and higher explanatory power.
- TOC consistently emerged as a significant predictor across all models, while chlorophyll-a was particularly influential in the prediction of 2-MIB. Its contribution to geosmin prediction was more limited.
- The combined application of sulfonic acid-modified activated carbon and peroxone provided a synergistic effect, achieving high removal efficiencies at lower chemical doses, thus offering advantages in terms of environmental and operational sustainability.
- The developed models demonstrated the applicability of statistical modeling as a decision-support tool in the treatment of taste and odor compounds.

In conclusion, the log-log model with natural logarithmic transformation was found to be especially effective in predicting biologically derived contaminants. TOC was confirmed as a key indicator, and chlorophyll-a played a critical role, particularly in algal-derived taste and odor compounds. These findings provide important guidance for early warning and process optimization in drinking water treatment.

Declaration of Ethical Standards

The authors declare that this study was conducted in accordance with internationally accepted ethical standards concerning authorship, citation, data reporting, and the publication of original research. The study did not involve human participants or animals; therefore, ethical committee approval and informed consent were not required. All authors have read and approved the final version of the manuscript.

Credit Authorship Contribution Statement

Betül Aykut Şenel: Conceptualization, Investigation, Validation, Writing – original draft. **Şehnaz Şule Kaplan Bekaroğlu:** Conceptualization, Supervision, Writing – review & editing. **Nuray Ateş:** Conceptualization, Supervision, Writing – review & editing. **Cihan Özgür:** Conceptualization, Methodology, Investigation, Project administration, Funding acquisition, Formal analysis, Data curation, Visualization, Writing – original draft.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this manuscript.

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Data Availability

The data supporting the findings of this study are available from the corresponding author upon reasonable request.

Use of Artificial Intelligence

During the preparation of this manuscript, the authors used OpenAI's ChatGPT to improve language quality and readability. An OpenAI image-generation tool was also used to assist in creating the graphical abstract based exclusively on the scientific content, data, and findings provided by the authors. No AI tool was used to generate research data, conduct analyses, or develop scientific interpretations or conclusions. The authors carefully reviewed and verified all AI-assisted content and accept full responsibility for the accuracy, originality, and integrity of the manuscript and graphical abstract.

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