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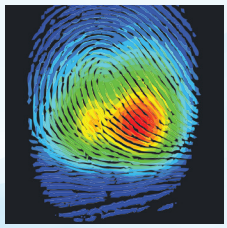
Fluorescence

Detecting Biochemical Oxygen Demand (BOD) Using A-TEEM Fluorescence Spectroscopy



Application Note
A-TEEM
FL-2024-8-22

Introduction

Biochemical Oxygen Demand (BOD) is a crucial parameter in assessing water quality, representing the amount of oxygen consumed by microorganisms in decomposing organic matter. Traditional BOD measurement methods are time-consuming and labor-intensive. Recently, A-TEEM (Absorbance–Transmittance Excitation–Emission Matrix) fluorescence spectroscopy has emerged as a rapid and effective alternative for BOD detection. This application note outlines a study by T. Ingwani et al., demonstrating the use of A-TEEM fluorescence spectroscopy combined with chemometric modeling for accurate BOD prediction in surface water.

Study Overview

The study aimed to develop a robust model for predicting BOD concentrations using A-TEEM fluorescence spectroscopy. Surface water samples spiked with tyr–tryptophan (tyr–trypt) mix standards were analyzed to create a data set of Excitation-Emission Matrices (EEMs). The data set comprised 120 EEMs, which were divided into a 100-member calibration set and a 20-member validation set.

Experimental Design

Surface water samples were spiked with tyr–trypt mix standards at various concentrations. A-TEEM fluorescence spectroscopy was employed to generate EEMs, capturing the fluorescence response of the samples. The data was then split into calibration and validation sets to develop and test the predictive model.

Chemometric Modeling

Partial Least Squares (PLS) regression was used to create a predictive model for BOD concentrations. The calibration and validation curves (predicted vs. measured concentrations) demonstrated the model's performance. Key parameters and metrics for the PLS model included:

Number of Latent Variables (LVs): 19

Root Mean Square Error of Calibration (RMSEC): 3.789 × 10^(-8) M

Root Mean Square Error of Cross-Validation (RMSECV): 8.372 × 10^(-8) M

Calibration Bias: -1.351

Cross-Validation Bias: -1.290

R^2 Calibration (R^2 Cal): 0.972

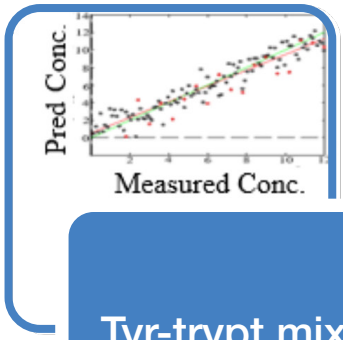
R^2 Cross-Validation (R^2 CV): 0.839

Results

The PLS model displayed high accuracy and robustness, as indicated by the performance metrics. The calibration and validation curves showed strong agreement between predicted and measured tyr–trypt mix concentrations, with an R^2 Cal value of 0.917 and an R^2 CV value of 0.569. Although the R^2 CV was lower, the model's overall prediction ability was validated with a high R^2 Pred value of 0.69.

Surface water containing try-trypt mix

Aqualog Spectrometer



Tyr-trypt mix quantification

Statistical Evaluation

The model's performance was further validated using spiked surface water samples with tyr–trypt mix concentrations ranging from 2.500 × 10^(-7) to 6.000 × 10^(-7) M. The linear correlation between predicted and measured concentrations confirmed the model's reliability, with R^2 and Pearson r values of 0.991 and 0.995, respectively. The residual plot indicated consistent and random distribution of residuals, reinforcing the model's accuracy.

Practical Applications

The study demonstrates that A-TEEM fluorescence spectroscopy, combined with PLS regression modeling, offers a rapid and reliable method for BOD detection in surface water. This approach significantly reduces the time and effort required for traditional BOD measurements, providing a valuable tool for water quality monitoring and environmental assessment.

Conclusion

A-TEEM fluorescence spectroscopy, integrated with chemometric analysis, proves to be an effective method for detecting BOD in surface water. The robust PLS model developed in this study ensures accurate and reliable BOD predictions, facilitating efficient water quality monitoring. This technique can be adopted for routine laboratory analysis, supporting environmental and public health initiatives.

References

T. Ingwani, Nhamo Chaukura, Bhekie B Mamba, Thabo T I Nkambule, Adam M Gilmore, *Study on BOD Detection and quantification in surface water Using A-TEEM Fluorescence Spectroscopy and Chemometric Modeling*.

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