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Absorption-Edge-Modulated Transmission Spectra for Water Contaminant Monitoring

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14. ABSTRACT Monitoring of contaminants associated with specific water resources using transmission spectra, with respect to types and relative concentrations, requires tracking statistical profiles of water contaminants in terms of spatial-temporal distributions of electromagnetic absorption spectra ranging from the ultraviolet to infrared. For this purpose, correlation between spectral signatures and types of contaminants within specific water resources must be made, as well as correlation of spectral signatures with results of processes for removal of contaminants, such as ozonation. Correlation between absorption spectra and changes in chemical and physical characteristics of contaminants, within a volume of sampled solution, requires sufficient sensitivity. The present study examines the sensitivity of absorption-edge-modulated transmission spectra with respect to general characteristics of water contaminants for spectral analysis of water samples.								
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Table of Contents

Introduction	1
Sensitivity Analysis of Transmission Spectra	2
Prototype Modulated-Absorption-Edge Spectral Analysis	4
Parametric Modeling of Transmission Spectra	4
Conclusion.....	5
Acknowledgement.....	6
References	6

Introduction

Multispectral analysis of water samples taken from public water resources in the New York City metro area has demonstrated the potential application of this type of analysis for water monitoring, treatment and evaluation prior to filtration (1, 2, 3, 4). Spectral monitoring of contaminants with respect to types and relative concentrations requires tracking statistical profiles of water contaminants in terms of spatial-temporal distributions of electromagnetic absorption spectra ranging from the ultraviolet to infrared, which are associated with specific water resources. To achieve this, it is necessary to establish correlation between spectral signatures and types of contaminants to be found within specific water resources. Correlation between absorption spectra and changes in chemical and physical characteristics of contaminants requires sufficient sensitivity. The present study examines the sensitivity of spectral features that are within the neighborhood of strong absorption for water, which are associated with water contaminants. That is to say, the sensitivity of absorption-edge-modulated transmission spectra is examined with respect to general characteristics of water contaminants for spectral analysis of water samples.

In what follows, results of experimental measurements are presented. A discussion of these results examines their relevance for monitoring water contaminants using absorption-edge-modulated transmission spectra, which are within the UV range and having tails extending into the IR range. In particular, our goal is to examine the problem of assessing to what extent spectral measurements can be used for quantitative water monitoring, and thus no specific procedure for “solution” of this problem is considered. Our purpose at this stage is to describe conceptually a general water monitoring methodology for potential application. Accordingly, the analysis that follows is prototypical and only for proof-of-concept.

The theoretical foundation of our approach is similar to that of hyperspectral imaging using remote sensors. Accordingly, hyperspectral imaging represents the motivation of our approach in terms of formal structure (5-11). Reference 8 presents a comprehensive review of hyperspectral remote sensing. Our spectral analysis approach is significantly different both in terms of type of measurements and analysis procedure. In contrast to hyperspectral imaging, which uses remote sensor reflectivity measurements to construct a spatial distribution of intensities (i.e., an image), our approach uses transmission measurements for parametric modeling of spectra, where issues of spatial resolution are not relevant. The general spectral analysis methodology is that of inverse analysis, which entails parameter estimation for parametric model representations of transmission spectra (12, 13, 14). These model parameters, which provide an optimal encoding of spectral signatures, can in principle comprise the contents of databases for characterization of water systems. Spectral analysis considers the spectrum extending from ultraviolet to infrared. Our proposed spectral analysis of water samples seeks to achieve a result similar to fingerprinting, where a number of points are matched resulting in statistical certainty. In our analysis, we expect to have a number of match points or readings from the ultraviolet through visible to the infrared spectrum that would allow us to achieve statistically accurate determination of particular water quality parameters, by comparing those readings to a database of similar spectral measurements of samples, which is in terms of their parameterization, from a collection of water resources. The problem of assessing to what extent spectral measurements can be used for quantitative water monitoring implies consideration of not only issues related to feasibility, but also sensitivity concerning correlation of spectral signatures with types and relative levels of water contaminants.

A previous study (15) examined water samples obtained from various water resources in the New York City metropolitan area at different times. These water sample sources varied from NYC's chemically treated tap water, to lakes NY and Orange, to the East and Hudson Rivers, and thus varied with respect to concentration and types of water quality parameters contained therein. For instance, it was shown in reference 15 that NYC's tap water is comparative to the quality of the lake water, with primarily soluble compounds and colloids, but with fewer pollutants and bacteria/algae concentrations, owing to originating from a much less developed watershed in upstate New York. In contrast, both the East and Hudson Rivers are highly polluted. The East River, however, has relatively lower concentrations of various water quality parameters and carries much fewer toxic industrial discharges than the Hudson River, which transverses many 100s of miles from upstate New York. Finally, it should be expected that compared with the other resources subject to water sampling (see 15), the East and Hudson Rivers would have the most temporal variations in levels and maybe even types of water quality parameters encountered.

This study considers a general approach for spectral analysis of water samples that is based on comparison of near-absorption-edge spectral features, which is in contrast to analysis based on comparison of spectral features associated with windows of transmission for water. This type of analysis has potential for increased sensitivity with respect to detection, in contrast to analysis based on windows of transmission.

The organization of the subject areas presented here are as follows. First, a general discussion is presented concerning aspects of the spectral analysis of water samples and of near-absorption-edge sensitivity of transmission spectra. Second, a prototype spectral analysis is presented showing various aspects of water monitoring using comparisons of near-absorption-edge spectral features. Third, a general discussion is presented concerning parametric modeling of near-absorption-edge spectral features. Finally, a conclusion is given.

Sensitivity Analysis of Transmission Spectra

Spectral analysis and ozonation of water contaminants [1, 2, 3, 4] represent mature capabilities for water monitoring and decontamination. As proposed previously [15], these capabilities can be enhanced for the purposes of water monitoring and decontamination using parametric model representations, in conjunction with their spectral signature interpretation, before and after water treatment processes that deactivate contaminant toxicity, such as ozonation. The water treatment process of ozonation results in the formation of sediments that fall out of solution. In practice, these sediments are filtered from the water as part of a pre-ozonation-filtration procedure [1, 2]. Parametric modeling of spectral signatures for water and contaminants will allow better interpretation of spectral features, which can optimize both water monitoring algorithms and treatment processes.

Water monitoring based on analysis of spectral signatures poses a significant problem owing to the wide variability of ambient environments associated with waterways, i.e., ground water environments and reservoirs [4]. This follows in that the problem to be posed for quantitative monitoring of water and contaminants via spectra requires the construction of water-system-specific databases of spectra [15]. These databases are constructed by sampling over time, for specified locations within specific water environments, e.g., rivers and various types of ground water environments and spectral measurements associated with this sampling, i.e., absorption spectra. The utility of a given database will depend upon its adaptability for spectral signature

isolation and correlation with various types of water contaminants. The correlation of spectral signatures with various types of water contaminants defines an inverse problem. This inverse problem must address two major aspects of water contamination: the statistical variability of spectra that are measured for sampling within specific water environments, containing both contaminants and nontoxic materials, extending over long time periods; and the inherent complexity of the absorption spectra of chemicals and materials dissolved in water.

Inverse analysis of spectra having variability with time requires isolation of statistically significant features of the spectra that can be correlated with a specific water environment [12, 13]. This problem can be addressed by noting that, although the relative percentages and types of materials within a given water environment can vary nondeterministically, a given water environment can be associated with a well-defined statistical ensemble of spectral signatures. This follows from the fact that, although the relative percentages and types of materials will vary, this variation will occur within limits. In principle, for a given water environment, its associated ensemble of spectral signatures should be well defined. Accordingly, databases for spectra must be structured to include not only spectral signatures, and their correlation with various types of additives, but also ensembles of spectral signatures corresponding to specific water environments.

The absorption coefficient α as a function of wavelength provides a method for understanding the relationship between spectral features and specific molecules in solution (see reference 16). To a first order approximation, measurement of α is via the relationship for transmission

$$T(\lambda) = I / I_0 = \exp(-\alpha d) \quad (\text{Eq 1})$$

where I and I_0 are the transmitted and incident intensity, respectively, and d is the thickness of the sample. In that all spectral analysis for water monitoring is with respect to an ambient water environment, a primary reference component should be the absorption coefficient of chemically pure water. For any spectral analysis of water contaminants, this quantity establishes the range of frequencies corresponding to windows of transmission, as well as windows associated with partial transmission, through an ambient water background. Another quantity that provides for understanding the relationship between spectral features and specific molecules in solution is the transmission spectrum of a given sample with respect to a reference sample defined by the relation

$$T(\lambda) = \frac{T_s(\lambda)}{T_R(\lambda)} \quad (\text{Eq. 2})$$

where T_R and T_s are the measured transmittance of the reference sample, e.g, Type IV purified water (ASTM D1193-06), and transmittance of sample for analysis, respectively. Interpretation of spectra with respect to Eq.(2) must be for wavelength ranges corresponding to windows of transmission through an ambient water background (see reference 15).

Spectral analysis of water samples based on comparison of near-absorption-edge spectral features has potential for increased sensitivity with respect to detection, in contrast to analysis based on comparison of spectral features associated with windows of transmission for water. The general approach based on analysis of near-absorption-edge spectral features follows from the characteristically strong absorption of water for wavelengths within the range 0.1 to 185 nm (see reference 17). This approach has certain aspects that must be considered for its potential

application in practice. First, analysis of spectral features within the range of wavelengths for strong absorption cannot adopt pure water as a reference system for the purpose of background subtraction. This follows in that the spectrum calculated using Eq.(2) will be characteristically singular for strong resonance minima in the denominator. Second, the range of wavelengths corresponding to strong absorption for water can overlap, as well as exceed, that range corresponding to absorption by the quartz cuvette containing the water sample. In addition, the transmission spectrum of quartz tends to vary with wavelength for the range 0.1 to 185 nm, which is within the region of interest for the general analysis approach. The following prototype spectral analyses show characteristics of near-absorption-edge spectral features that can be adopted potentially for water contaminant monitoring, as well as for proof-of-concept for such monitoring.

Prototype Modulated-Absorption-Edge Spectral Analysis

In this section a prototype analysis is presented for the purpose of showing various aspects of spectral analysis of water samples using comparisons of near-absorption-edge spectral features. For this prototype study, the Cooper Union Environmental Research Laboratory (NYC) prepared water samples consisting of various concentrations of As_2O_3 , Mn and Fe in solution, with and without ozonation, for spectral analysis by the Naval Research Laboratory. These spectra are shown in Figure 1. Descriptions of the different water samples are given in Tables 1 and 2. Transmission spectra for the water samples were measured using a Perkin-ElmerTM Lambda 900 UV/Vis/IR spectrometer (Shelton, CT) in transmission mode.

Shown in Figure 1 are transmission spectra of water samples consisting of various concentrations of As_2O_3 , Mn and Fe in solution, with and without ozonation, and ionized water samples (PW-A in Figure 1) calculated using an empty cuvette as a reference sample according to Eq. (2) and normalized with respect to the maximum transmission of ionized water. Also shown in Figure 1 is a transmission spectrum calculated using the permittivity function given in reference 14 (PW-B in Figure 1). The changes in spectral features shown in Figure 1 are associated with different concentrations of the simulated contaminants and influence of the ozonation processes, which modulate absorption-edge features, as compared with pure water. A quantitative calibration of the influence of these processes is beyond the scope of the present study, whose goal is only that of proof-of-concept. The changes in spectral features shown in Figure 1, however, are sufficient for demonstrating the sensitivity of spectral features with respect to these processes. In particular, that variation of features within the neighborhood of water's large absorption minimum, within the wavelength range 0.1 to 185 nm, demonstrate higher sensitivity relative to wavelength regions of low absorption.

Parametric Modeling of Transmission Spectra

Parametric modeling of spectra must be well posed for spectral analysis of water samples where the relative percentages and types of materials dissolved can vary nondeterministically. For such water samples, it is appropriate to model spectra using parameterizations that are both phenomenological and optimal in terms of representing trend features of spectra [12]. A general approach for parametric modeling of spectra is the fitting of absorption spectra to a linear combination of Gaussian and Lorentian functions. This type of inverse analysis provides convenient representation of absorption bands for statistical analysis of signatures that are associated with an ensemble of spectral measurements, where there exists variability of

contaminants within a restricted range of values, and enables the identification of materials that are present by comparison with reference or database spectra [12, 13, 14]. With respect to this type of inverse analysis, near-absorption-edge spectral features associated with water samples suggest an optimal parametric model of the transmission spectrum $T(\lambda)$ given by

$$T(\lambda) = \left(1 - \sum_{j=1}^{N_j} w_j \exp \left[-\frac{(\lambda - \lambda_0)^2}{2\sigma_j^2} \right] \right) H(\lambda - \lambda_0) \quad \text{Eq.(3)}$$

where

$$\sum_{j=1}^{N_j} w_j = 1 \quad \text{Eq.(4)}$$

$H(x)$ is the unit step function, whose value is 1 for x greater than or equal to 0, and 0 otherwise.

The fitting of absorption spectra to the parametric model Eqs.(3)-(4) represents a parametric fit to a specific spectral measurement. It follows that for ensembles of spectral measurements, which would be associated with a given water environment, the parameters defined with respect to Eqs. (3)-(4) must be generalized to represent statistical quantities. Accordingly, the sets of parameters $(w_j, \lambda_0, \sigma_j)$ defined by Eqs. (3)-(4) can represent statistical distributions, and thus provide an encoding of statistical characteristics of spectral signatures associated with water systems, which can be used for monitoring contaminant levels. In particular, with respect to inverse analysis based on constrained least-squares parameter optimization, i.e., parameter optimization according to minimization of the objective function

$$Z_T = \sum_{n=1}^N w_n (T(\lambda_n) - T_m(\lambda_n))^2, \quad \text{(Eq 5)}$$

where $T_m(\lambda_n)$ is the measured or target transmission for wavelength λ_n , Eq. (3) represent optimal basis functions for parametric representation of transmission spectra of water samples. Finally, application of the parametric model Eqs. (3)-(4) for analysis of statistical characteristics of spectral signatures suggests insensitivity with respect to relatively large numbers of parameters. Accordingly, the parametric model given by

$$T(\lambda) = \left(1 - \exp \left[-\frac{(\lambda - \lambda_0)^2}{2\sigma_0^2} \right] \right) H(\lambda - \lambda_0) \quad \text{(Eq. 6)}$$

should be appropriate for representation of statistical characteristics, where there are only two adjustable parameters.

Conclusion

In practice, no natural water system can be characterized by water containing specific contaminants of known concentrations. It is expected, however, that specific water systems can be characterized by finite ranges of contaminants, and by associated distributions of relative concentrations of these contaminants. In principle, classification can be based on minimizing the

difference between estimates of model parameters obtained from specific measurements and those of a database. Error tolerances associated with parameter estimation remains an open question for future investigation. In general, near-absorption-edge spectral features are relatively more sensitive to changes in solvent characteristics. Accordingly, parametric modeling of near-absorption-edge features should be optimal, in terms of formulation with respect to this increased sensitivity, e.g., Eq.(6).

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Table 1. Water sample sets WS1 and WS2 for different concentrations of As and Fe in solution, respectively, with and without Ozonation.

Sample (#)	Solvent Vol. (mL)	Element	Solute Conc. (mg/L)	Cum. Conc. of Solute (mL)	Time (min)	Notes
WS1-A	1020	As	30.4	0	0	No Ozone
WS1-B	1020	As	30.4	0.72	2.5	Ozone-800 mg/hr
WS1-C	1020	As	30.4	1.43	6	Ozone-800 mg/hr
WS1-D	1020	As	30.4	2.15	9.5	Ozone-800 mg/hr
WS1-E	1020	As	30.4	2.86	13.5	Ozone-800 mg/hr
WS2-A	1050	Fe	7500	0	0	No Ozone
WS2-B	1050	Fe	7500	1.7	5	Ozone-800 mg/hr
WS2-C	1050	Fe	7500	3.4	10.5	Ozone-800 mg/hr
WS2-D	1050	Fe	7500	5.1	15.5	Ozone-800 mg/hr
WS2-E	1050	Fe	7500	6.7	21	Ozone-800 mg/hr

Table 2. Water sample sets WS3, WS4, WS5, WS6, WS7 and WS8 for different concentrations of As, Mn and Fe in solution, respectively, with and without Ozonation.

Sample (#)	Solvent Vol. (mL)	Element	Solute Conc. (mg/L)	Cum. Conc. of Solute (mL)	Ozone (5 min)
WS3-A1	1030	As	1000	0.1	No
WS3-A2	1030	As	1000	0.1	No
WS3-B1	1030	As	1000	0.2	No
WS3-B2	1030	As	1000	0.2	No
WS3-C1	1030	As	1000	0.5	No
WS3-C2	1030	As	1000	0.5	No
WS3-D1	1030	As	1000	0.7	No
WS3-D2	1030	As	1000	0.7	No
WS3-E1	1030	As	1000	1	No
WS3-E2	1030	As	1000	1	No

WS4-A1	1030	As	1000	0.1	Yes
WS4-A2	1030	As	1000	0.1	Yes
WS4-B1	1030	As	1000	0.25	Yes
WS4-B2	1030	As	1000	0.25	Yes
WS4-C1	1030	As	1000	0.58	Yes
WS4-C2	1030	As	1000	0.58	Yes
WS4-D1	1030	As	1000	0.71	Yes
WS4-D2	1030	As	1000	0.71	Yes
WS4-E1	1030	As	1000	1	Yes
WS4-E2	1030	As	1000	1	Yes

WS5-A1	1030	Mn	1000	0.53	No
WS5-A2	1030	Mn	1000	0.53	No
WS5-B1	1030	Mn	1000	1.03	No
WS5-B2	1030	Mn	1000	1.03	No
WS5-C1	1030	Mn	1000	1.53	No
WS5-C2	1030	Mn	1000	1.53	No
WS5-D1	1030	Mn	1000	2.04	No
WS5-D2	1030	Mn	1000	2.04	No
WS5-E1	1030	Mn	1000	2.53	No
WS5-E2	1030	Mn	1000	2.53	No

WS6-A1	1020	Mn	1000	0.51	Yes
WS6-A2	1020	Mn	1000	0.51	Yes
WS6-B1	1020	Mn	1000	1	Yes
WS6-B2	1020	Mn	1000	1	Yes
WS6-C1	1020	Mn	1000	1.5	Yes
WS6-C2	1020	Mn	1000	1.5	Yes
WS6-D1	1020	Mn	1000	2	Yes
WS6-D2	1020	Mn	1000	2	Yes
WS6-E1	1020	Mn	1000	2.5	Yes
WS6-E2	1020	Mn	1000	2.5	Yes

WS7-A1	1020	Fe	1000	0.5	No
WS7-A2	1020	Fe	1000	0.5	No
WS7-B1	1020	Fe	1000	1.5	No
WS7-B2	1020	Fe	1000	1.5	No
WS7-C1	1020	Fe	1000	2.1	No
WS7-C2	1020	Fe	1000	2.1	No
WS7-D1	1020	Fe	1000	3.1	No
WS7-D2	1020	Fe	1000	3.1	No
WS7-E1	1020	Fe	1000	4	No
WS7-E2	1020	Fe	1000	4	No

WS8-A1	1030	Fe	1000	0.6	Yes
WS8-A2	1030	Fe	1000	0.6	Yes
WS8-B1	1030	Fe	1000	1.1	Yes
WS8-B2	1030	Fe	1000	1.1	Yes
WS8-C1	1030	Fe	1000	2	Yes
WS8-C2	1030	Fe	1000	2	Yes
WS8-D1	1030	Fe	1000	3	Yes
WS8-D2	1030	Fe	1000	3	Yes
WS8-E1	1030	Fe	1000	4	Yes
WS8-E2	1030	Fe	1000	4	Yes















































