



Research Article

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3D Fluorescence Spectroscopy for characterization of CDOM Components in the Qijiang River, China

Xiaonian Deng*, Yingli Chen and Wenke Sun

Chongqing Qijiang Nanzhou Middle School, Qijiang 401420, China

*Corresponding author: Xiaonian Deng, Chongqing Qijiang Nanzhou Middle School, Qijiang 401420, China Email: 15823853610@163.com

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Abstract

In this study, three-dimensional excitation-emission matrix fluorescence spectroscopy (EEMs), combined with fluorescence regional integration (FRI), fluorescence index analysis, and parallel factor analysis (PARAFAC), was employed to systematically characterize the spectral features, sources, and degradation status of chromophore dissolved organic matter (CDOM) in the Qijiang River. The results indicate that CDOM in the Qijiang River is predominantly characterized by fresh autochthonous sources, low humification, and limited allochthonous input. FRI analysis showed that protein-like substances (Regions I+II) dominated the CDOM pool, accounting for an average of 62.89%. Fluorescence index analysis revealed a mean fluorescence index (FI) of 1.66 (mixed sources), a mean biological index (BIX) of 0.86 (indicating a predominance of newly produced autochthonous components), a mean humification index (HIX) of 0.45 (low humification degree), and a mean freshness index ($\beta:\alpha$) of 0.81 (high proportion of newly produced components). Correlation analysis demonstrated a strong positive correlation between BIX and freshness ($R^2 = 0.89$) and a moderate positive correlation between the proportion of region V (V%) and HIX ($R^2 = 0.57$). PARAFAC identified three fluorescent components, attributed to tyrosine-like (Ex/Em = 200/300 nm), tryptophan-like (Ex/Em = 200–225/300 nm), and fulvic acid-like (Ex/Em = 225–250/350–450 nm) substances, further corroborating the dominance of protein-like materials. These mutually reinforcing findings from multiple analytical approaches provide a scientific basis for water quality management and pollution source tracking in the Qijiang River.

Keywords: Chromophore dissolved organic matter, Three-dimensional excitation-emission matrix fluorescence spectroscopy, Fluorescence regional integration, Parallel factor analysis, Qijiang River

Introduction

The composition of dissolved organic matter (DOM) in natural water bodies is complex and exhibits significant spatial heterogeneity. Its content, sources, and molecular characteristics are governed by multiple factors, including watershed geography, climate, vegetation, and human activities. Developing rapid, efficient, and information-rich characterization methods is of great scientific significance for revealing the mechanisms of regional water environment evolution, carbon cycling processes, and the maintenance of ecosystem functions [1–4]. Three-dimensional excitation-emission matrix fluorescence spectroscopy (EEMs), with its advantages of high sensitivity, non-destructive measurement, and rich information content, combined with methods such as parallel factor analysis (PARAFAC), has become a key tool for elucidating the sources, composition, and migration-transformation patterns of organic matter, enabling the effective identification and semi-quantitative assessment of humic-like and protein-like components [5–6].

Chromophore dissolved organic matter (CDOM), as the light-absorbing and fluorescent fraction of DOM, originates from autochthonous inputs by aquatic microorganisms and allochthonous inputs from terrestrial plants and soil organic matter [7–10]. Its composition and degradation status can effectively indicate the biological activity and pollution status of water bodies [11–15]. The Qijiang River in China, as a first-order tributary of the upper Yangtze River, directly influences the water quality and safety of the main stream through its aquatic ecological environment. However, systematic studies focusing on the spectral characteristics and compositional analysis of DOM in this river section remain scarce.

Therefore, this study takes water samples from the Qijiang River as the research object. Using three-dimensional fluorescence spectroscopy combined with parallel factor analysis (PARAFAC) and fluorescence regional integration (FRI), we systematically analyze the spectral characteristics, sources, composition, and degradation patterns of CDOM. Fluorescence indices (FI, BIX, HIX, Freshness) are employed to reveal its main environmental controlling factors.

This research aims to elucidate the fluorescence fingerprint characteristics of DOM in the Qijiang River, providing fundamental data and a scientific reference for regional water environment quality assessment and watershed aquatic ecological management.

Sampling and Analysis

This study investigated CDOM in the Qijiang River in Qijiang District, Chongqing Municipality, China. Pre-cleaned glass bottles were used to collect surface water samples. Immediately after collection, the samples were stored in a refrigerated container (4°C) in the dark and transported back to the laboratory for processing within 24 hours. Water samples were first filtered through 0.45 µm glass fiber membranes to remove suspended particulate matter. Subsequently, three-dimensional excitation-emission matrix fluorescence spectroscopy (3D-EEM) was performed using a spectrofluorometer (RF-6000, Shimadzu, Japan). The excitation wavelength ranged from 200 to 550 nm with a step size of 2 nm; the emission wavelength ranged from 200 to 550 nm with a step size of 2 nm; the scanning speed was 12,000 nm/min; both excitation and emission slit widths were set to 5 nm; the response time was 0.5 s; the photomultiplier tube voltage was 700 V; and the excitation source was a 150 W xenon arc lamp. Spectral measurements were conducted for each water sample. In this study, 3DFluo Core Pro software was used to analyze the three-dimensional fluorescence spectra. Parallel factor analysis (PARAFAC) was employed to characterize and resolve the fluorescence components of dissolved organic matter (DOM) in the water samples. By establishing the PARAFAC model, qualitative identification of different types of fluorescent components in DOM was achieved, providing a reliable technical means for source apportionment and dynamic monitoring of organic matter in water bodies. To assist in analyzing the sources, composition, and humification degree of DOM, three commonly used fluorescence indices—Fluorescence Index (FI), Humification Index (HIX), and Biological Index (BIX)—along with regional integration, were calculated.

Results and Discussion

Fluorescence characteristics of the Qijiang River

Through the measurement of fluorescence indices in the Qijiang River, the sources, degradation degree, and biological activity characteristics of chromophore dissolved organic matter (CDOM) can be systematically evaluated. Relevant analytical indicators include the Fluorescence Index (FI), Biological Index (BIX), Humification Index (HIX), Freshness index ($\beta:\alpha$), and five-region fluorescence regional integration (FRI) [13]. These indices serve as important scientific bases for indicating CDOM characteristics [17]. The results are shown in Tables 1 and 2.

The CDOM in the Qijiang River originates from both autochthonous and allochthonous sources. FI reflects the relative contribution of aromatic vs. non-aromatic amino acids to CDOM fluorescence intensity and is closely related to the aromaticity and molecular conjugation degree of CDOM, making it an important parameter for determining its source and degradation status. Analysis shows that the mean FI value of the Qijiang River is 1.64. According to the discrimination criteria [17]: FI > 1.9 indicates that CDOM is primarily autochthonous, mainly derived from

extracellular release by bacteria and algae; FI < 1.4 indicates allochthonous dominance, mainly derived from terrestrial plants and soil organic matter. Based on this, the CDOM in the Qijiang River exhibits characteristics of both autochthonous and allochthonous sources.

Newly produced autochthonous CDOM is significant in the Qijiang River. BIX is used to measure the proportion of newly produced autochthonous CDOM in the total CDOM pool. It is generally considered that BIX values between 0.8 and 1.0 indicate an abundance of newly produced autochthonous components, a high degree of CDOM degradation, which favors the generation of autochthonous carbon products; BIX values between 0.6 and 0.8 indicate fewer newly produced autochthonous components. All BIX values in the Qijiang River fall within the range of 0.8–1.0 (mean 0.86), exhibiting typical characteristics of newly produced autochthonous sources, indicating active biological activity in the water column and a significant contribution from autochthonous organic matter.

The organic matter content in the Qijiang River is low, and the water is fresh. HIX is used to evaluate the degree of CDOM humification, reflecting the degradation and accumulation status of organic matter. The HIX in the Qijiang River is at a low level (mean 0.45, < 0.5), indicating that the organic matter content in the water is low, the degree of humification is light, and the water body maintains a relatively high level of freshness overall.

The biological activity in the Qijiang River is high, with a high proportion of newly produced components. The Freshness index ($\beta:\alpha$) is used to quantitatively assess the proportion of newly produced CDOM and is an important indicator reflecting the biological activity of water. The mean Freshness value of the Qijiang River water samples is approximately 0.81, further supporting the active generation state of biogenic organic matter in the water.

Protein-like substances dominate the fluorescence components of the Qijiang River. Based on five-region fluorescence regional integration (FRI) analysis, the fluorescence components of CDOM in the Qijiang River exhibit a clear “protein-dominated” characteristic. Region I (tyrosine-like proteins) accounts for an average of 46.21%, Region II (tryptophan-like proteins) accounts for an average of 16.68%, and together they account for as much as 62.89%, constituting the absolute majority of CDOM. Region III (fulvic acid-like) accounts for an average of 17.27%, Region V (humic acid-like) accounts for an average of 10.43%, and together they account for only 27.70%. Region IV (microbial metabolites) has the lowest proportion, averaging 9.41%. Among all regions, Region V has the largest coefficient of variation (12.5%), while Region II is the most stable (5.5%), with overall low spatial heterogeneity. This compositional pattern is highly consistent with the FI, BIX, HIX, Freshness and other indices, further confirming the conclusion that CDOM in the Qijiang River is dominated by fresh, autochthonous biogenic sources with limited allochthonous terrestrial humic input.

Overall, CDOM in the Qijiang River water body exhibits mixed autochthonous and allochthonous sources, dominated by newly produced autochthonous components, with a low degree

of humification and high biological activity. The fluorescence components are overwhelmingly dominated by protein-like substances (especially tyrosine-like). Overall, the water body presents a state characterized by autochthonous dominance, high

freshness, and low humification.

Table 1

Table 2

Table 1: Florescence index

Number	FIR (%)					FI	HIX	BIX	Freshness
	I%	II%	III%	IV%	V%				
1	46.28	16.18	16.79	10.34	10.41	1.64	0.42	0.87	0.81
10	44.87	16.71	18.4	8.91	11.11	1.65	0.47	0.88	0.82
11	49.77	16.58	15.9	8.61	9.14	1.66	0.42	0.86	0.8
12	49.09	17.24	15.07	9.48	9.12	1.65	0.41	0.87	0.81
13	46.66	16.91	17.59	7.63	11.2	1.67	0.52	0.85	0.8
14	41.36	18.1	18.2	9.66	12.68	1.66	0.48	0.88	0.82
15	46.37	18.11	15.59	9.29	10.64	1.66	0.45	0.88	0.82
2	38.05	16.27	21.01	11.19	13.48	1.68	0.48	0.86	0.81
3	42.42	18.66	17.97	9.82	11.13	1.66	0.44	0.87	0.82
4	47.93	16.48	16.68	8.68	10.23	1.65	0.46	0.87	0.82
5	46.64	15.71	16.72	9.92	11.01	1.66	0.46	0.87	0.81
6	47.29	15.85	17.46	9.54	9.86	1.65	0.43	0.86	0.8
7	49.15	15.56	16.43	9.28	9.58	1.66	0.44	0.86	0.81
8	46.72	16.58	17.41	9.35	9.94	1.65	0.44	0.86	0.8
9	49.29	16.24	16.08	9.57	8.83	1.64	0.4	0.85	0.8

Table 2: Statistical results of five-region fluorescence regional integration (FRI) for CDOM in the Qijiang River (n = 15)

Parameter	Region I (%)	Region II (%)	Region III (%)	Region IV (%)	Region V (%)
Mean	46.21	16.68	17.27	9.41	10.43
Standard deviation	3.13	0.92	1.35	0.81	1.3
Minimum	38.05	15.56	15.07	7.63	8.83
Maximum	49.77	18.66	21.01	11.19	13.48
Coefficient of variation (%)	6.8	5.5	7.8	8.6	12.5

Correlation Analysis of CDOM Fluorescence Characteristics

Pearson correlation analysis was conducted on various fluorescence indices, and the results are shown in Table 3 and Fig. 1. Strong correlation between BIX and Freshness ($R^2 = 0.89$): The two exhibited an extremely strong positive correlation, indicating that CDOM in the Qijiang River is dominated by “fresh autochthonous sources”, and endogenous biological activity is the key factor controlling the dynamics of organic matter in the water. High BIX values indicate vigorous microbial/algal metabolism, while high Freshness values indicate that the organic matter is primarily newly produced. Their synchronous changes collectively reveal a “production-freshness” coupling mechanism. Moderate correlation between V% and HIX ($R^2 = 0.57$): V% (proportion of humic acid-like substances) showed a moderate positive correlation with HIX, indicating that humic acid-like substances are an important component of the humification characteristics of CDOM, but not

the sole factor. HIX is also influenced by Region III (fulvic acid-like substances). Moreover, the overall HIX level in the Qijiang River is low (<0.5), with a narrow data range, making it statistically difficult to achieve an extremely high correlation coefficient. This moderate correlation strength precisely corroborates the CDOM characteristics of the Qijiang River, characterized by “low humification degree and fresh water”.

Table 3

Table 3: Correlation matrix (R^2) of fluorescence indices for the Qijiang River

Index	FI	HIX	BIX	Freshness
FI	1	—	—	—
HIX	-0.23	1	—	—
BIX	0.31	-0.35	1	—
Freshness	0.28	-0.38	0.89	1

Figure 1

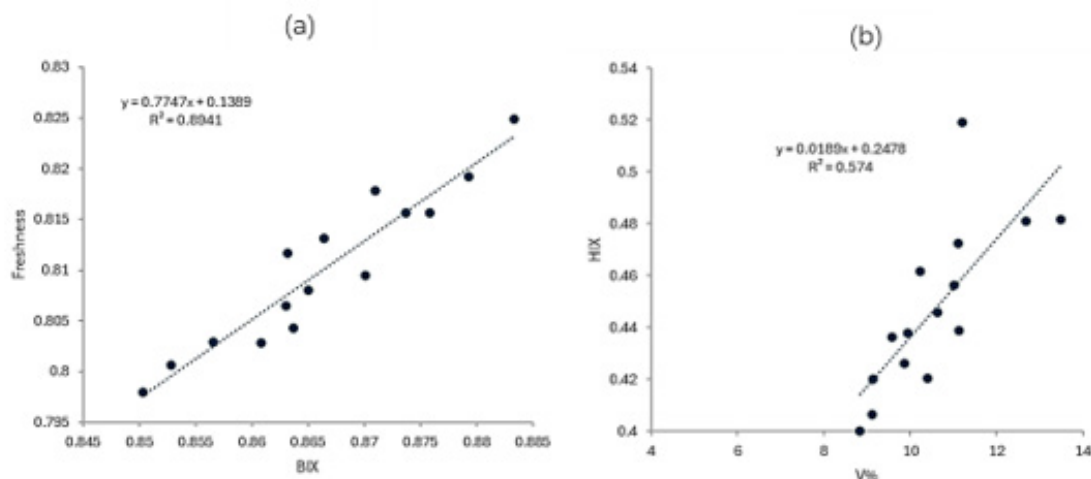


Figure 1: Correlation analysis of components: (a) BIX vs. Freshness, (b) V% vs. HIX

PARAFAC Fluorescent Components

The PARAFAC model was applied to decompose the EEMs dataset. The optimal number of components was determined through split-half analysis and residual analysis, and the spectral characteristics and material assignments of each component were identified. A total of three fluorescent components were identified (Fig. 2a-c). Component 1 (Ex/Em = 200/302 nm) was assigned to tyrosine-like proteins, representing highly labile organic matter produced by fresh biological activity. Component 2 (peak: Ex/Em = 222/304 nm) was assigned to tryptophan-like proteins,

indicating microbial metabolic products and potential exogenous sewage input. Component 3 (peak: Ex/Em = 240/424 nm) was assigned to fulvic acid-like substances, reflecting the contribution of microbially transformed humic substances. This compositional pattern is highly consistent with multiple indices, including FI (1.66), BIX (0.86), Freshness (0.81), HIX (<0.5), and FRI regional integration (Region I+II proportion = 62.89%). Together, these results reveal the overall characteristics of CDOM in the Qijiang River as "dominated by fresh autochthonous sources, with limited humification and minor terrigenous input.

Figure. 2

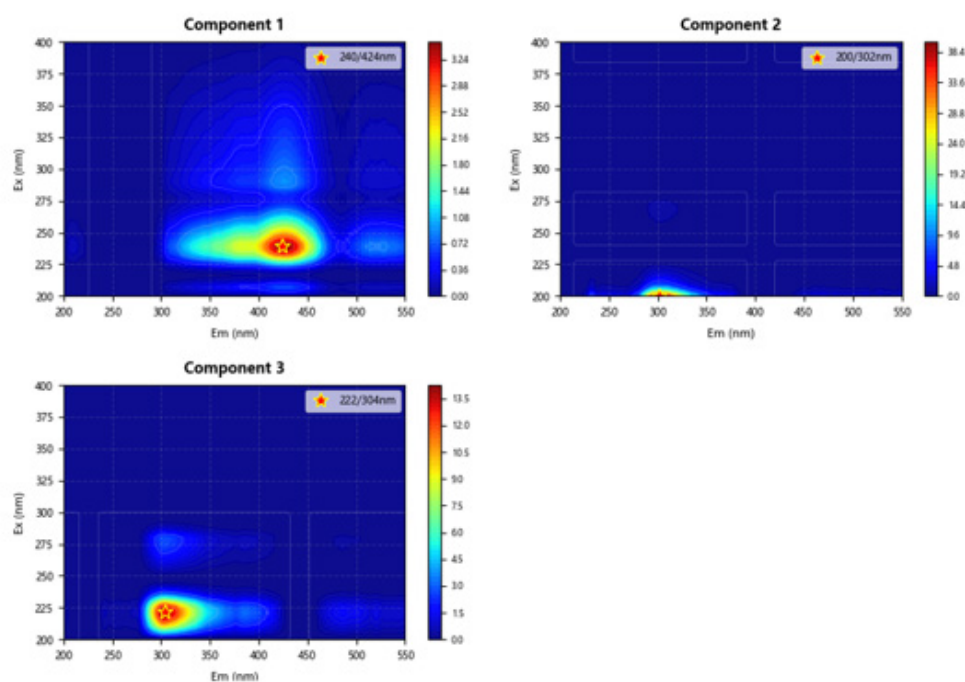


Figure 2: Fluorescent components of CDOM in the Lijiang River

Conclusion

This study explored the fluorescence characteristics of the Qijiang River water and revealed the source characteristics of CDOM as well as the water quality status of the Qijiang River. The CDOM in the Qijiang River is generally characterized as “dominated by fresh autochthonous protein-like substances, with limited humification and minor terrigenous input.” Among the PARAFAC components, the high proportions of Component 1 and Component 2 indicate intense microbial activity (e.g., phytoplankton and bacteria) in the water, with the organic matter remaining in a “fresh” state. The presence of Component 3 suggests a certain degree of microbial transformation; however, its relatively low proportion further confirms the low humification degree and high overall freshness of the water. These findings provide a scientific basis for water environment management and pollution source tracking in the Qijiang River.

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