
Publications

- Articles in Refereed Scientific Journals:

Report Follows
Title: Monitoring and Modeling Chromophoric Dissolved Organic Matter in Neponset River and Boston Harbor Using GIS and Hyperspectral Remote Sensing

Project Number: S11500000000037

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Research Category: WQL, MOD, HYDGEO

Problem and Research Objectives:

(1) Problems

As one of the major components of DOM, dissolved organic carbon (DOC) is a key factor for water quality. The organic molecules that make up the DOC pool in fresh and coastal waters come from natural sources, mainly from the decay of terrestrial and aquatic plants, algae and bacteria. Meanwhile, anthropogenic activities, such as sewer release and agricultural fertilization, also have strong impact on DOC contents and compositions in watershed regions with high population density. The watershed flux of DOC from terrestrial landscape to rivers has wide-ranging consequences for aquatic chemistry and biology. DOC affects the complexation, solubility, and mobility of metals as well as the adsorption of pesticides to soils, and is therefore a critical water quality parameter important for human health. In addition, DOC also plays an indispensable role in the cycle of terrestrial and atmospheric CO2, and hence implies the climate change. Currently, due to physical and biological complexity, multiple scales of freshwater systems, and biogeochemical reactivity at the land-water interface, changes to DOC fluxes in response to terrestrial sources and climate change are not well-known, and so as to be hard to evaluate their potential impact on water quality. To quantify the seasonal or interannual variation of DOC flux, the first thing is to accurately estimate DOC amount in riverine and estuarine regions. This is not only crucial to analyze their sources and transport mechanisms, but also subsequently helpful for monitoring and controlling water quality and for understanding the regional and global carbon cycle.

Our study site is the Neponset River and Boston Harbor regions. The Neponset River locates in eastern Massachusetts, starting at the Neponset Reservoir and meandering generally northeast for approximately 29 miles to its mouth at Dorchester Bay of Boston Harbor. The Neponset River is fed by a drainage basin or watershed of approximately 130 square miles, including numerous aquifers, wetlands, streams, surrounding upland areas, and about 330,000 populations. The Neponset has been heavily polluted before, but at present it is clearer due to much remediation. Several water quality monitoring programs
are running for this river, for example, the Massachusetts Water Resources Authority's harbor and river monitoring program monitors the impacts of combined sewer overflows (CSOs) on the Harbor and tributary rivers. The sampling crew measures temperature, bacteria, algae, water clarity, nutrients, and suspended solids in Boston Harbor and Neponset rivers. However, there are some shortcomings of current monitoring programs. First, DOM/DOC is not usually directly measured. The conventional water quality parameters, such as ions concentrations, pH values, and dissolved oxygen, are not appropriate to estimate DOC’s concentration. Second, even DOM/DOC are measured sometimes, most of them are only point sampling. Such field survey is insufficient or less reliable for evaluating the distribution and dynamic of organic matters at a large spatial scale. Third, our previous study shows DOC has strong seasonal and even daily variations. Frequent and synoptic DOC measurement is in great need for monitoring DOC flux spatial temporal variation in a large area.

Inversion of DOC concentration from satellite images has great potential to overcome the shortcomings of field survey. The concentrations of in-water components influence water’s absorption and backscattering coefficients and hence change the radiance received by satellite sensors. Therefore, based on satellite images, we can inversely predict those components. Although DOC is unable to be fully estimated from satellite images since part of them are not photoactive substances, the photoactive fraction of DOM, chromophoric dissolved organic matter (CDOM), could be used as the tracer of DOC. Many observations provide the evidence of a good correlation between CDOM and DOM/DOC loading across the different subcatchments, despite the absence of this co-variation in a few cases. CDOM absorbs primarily ultraviolet and blue light, and is fluorescent (350nm – 440nm). Together with the other two ocean-color components, chlorophyll and non-algal particles (NAP), CDOM have a significant contribution to the signals received by satellites and therefore is detectable by remote sensing.

(2) Research objectives

Our study will focus on two aspects: 1) rapidly quantifying CDOM via remote sensing-based inversion and 2) watershed-based modeling to understand CDOM sources and degradation.

Remote sensing-based inversion is to observe CDOM concentrations in freshwater and coastal regions from in situ spectral data measured by ASD FieldSpec® 3 and satellite hyperspectral images EO-1 Hyperion. Hyperion sensor bears relatively high resolutions both in spectral (10nm) and spatial (30m), and hence provides a good platform for optical inversion of CDOM. Specifically, we will improve and calibrate our algorithm, QAA-E (Extended Quasi Analytical Algorithm), to inverse the ag440 (the absorption coefficients of CDOM at 440nm, typically denoting CDOM concentrations in ocean-color science) from satellite images. Our previous study on algorithm development and test shows QAA-E is able to retrieve ag440 with acceptable accuracy in Mississippi River and Atchafalaya River plumes. The implement of this objective is the base for further work of modeling.

Watershed-based modeling is to better understand the DOC sources and its relationship and coupling to a number of environmental factors associated to watershed (vegetation coverage and density, topography, soil type, land cover and land use, etc), hydrology (precipitation, flow, runoff, etc), water quality (salinity, dissolved oxygen, etc) and aquatic optical components (chlorophyll and sediments). Especially, the Vegetation-CO2-DOC-CDOM chain relationship may give us a whole picture of DOC dynamic, transportation and cycle on regional watershed ecosystem, as well as the possible reason and impact of anthropogenic activities on water quality. The SWAT (Soil and Water Assessment Tool) model will serve as a good tool to model the interactions between watershed features, environmental factors, and land use practice. This objective is challenging since the related systems are fairly complex.
However, our goal is to build a model capturing the major factors controlling CDOM flux from Neponset River to Boston Harbor.

Methodology:

(1) In situ measurement:

Our field data collection was conducted in Sept. 25 and Nov. 04, 2009. The in situ CDOM concentration and spectral data were measured on the vessel R/V Neritic, cooperating with researchers of UMass Boston, over the low Neponset River and Boston Harbor (Fig. 1). The data acquisition activities include (1) continuous above-surface hyperspectral measurements, (2) continuous underwater measurements of the IOPs (attenuation and absorption coefficients), salinity, density, dissolved oxygen, UV radiance, CDOM fluorescence, chlorophyll fluorescence, and optical backscattering for suspended sediments, and (3) discrete water sampling and analysis in laboratory.

The water above-surface remote-sensing reflectance was measured by a portable spectroradiometer (ASD FieldSpec®), with a full spectral range (350 – 2500 nm). The spectral sampling interval of output is 1 nm. In the entire cruise, we collected approximate 1,500 hyperspectral samples. The underwater measurements were carried out by the MiniShuttle, a towed, undulating vehicle based on the Nu-Shuttle manufactured by Chelsea Instruments. It is a synthetic function instrument with multiple devices, including a SeaTech fluorometer measuring the fluorescent dissolved organic matter. The resolution of our underwater measurements is very high and we consequently made a large dataset containing about 45,000 samples. In addition, about 25 discrete water samples were also collected and analyzed to calibrate the real time underway measurements.

The EO-1 Hyperion images in the same regions were requested during fieldtrip dates. The image acquired in Nov. 04 is cloud free. Hyperion images provide a high spectral resolution 400 – 900 nm with 10 nm interval, and a high spatial resolution 30 m. We also acquired a latest WorldView-2 (WV2) image covering our study site. WorldView-2 is a multispectral sensor which bears 8 bands, including a coastal blue band (400 – 450 nm), and also is with very high spatial resolution (~1.8 m).

(2) Remote sensing inversion algorithm and processing:

The whole processing of CDOM remote sensing inversion from WV2 can be referred to the Fig. 2(a). Given a WV2 image, we need to convert the digital number (DN) to the radiance and then make an atmospheric correction, using FLAASH module provided by ENVI®, to obtain the total reflectance, and then compute the remote sensing reflectance, $R_{rs}$, using HydroLight simulation to remove the water
surface reflectance, and finally input these \( R_{rs} \) into remote sensing inversion model to derive CDOM concentration \( a_g(440) \) (absorption coefficient at 440 nm). For Hyperion images, some additional preprocessing are needed, including replacing dark lines, destriping and denosing.

To retrieve CDOM’s \( a_g(440) \), we developed a QAA-CDOM algorithm (Fig. 2(b)). QAA-CDOM is based on Lee’s QAA algorithm and its extension, QAA-E. QAA is a quasi-analytical level-by-level algorithm combining a series of empirical, semi-analytical, and analytical algorithms. QAA only requires \( R_{rs} \) at several wavelengths (410, 440, 490, 555, and 640 nm) as input data, and at different levels, it outputs \( r_{rs} \), absorption and backscattering coefficients of water’s total (\( a_t, b_{tp} \)), chlorophyll (\( a_{ph}, b_{ph} \)) and CDM (\( a_{dg}, b_d \)) (CDOM and NAP together) for all given \( R_{rs} \)’ wavelengths. QAA has been tested and used in many applications. QAA’s output \( a_{dg}(440) \), however, has been proven too rough to represent \( a_g(440) \) in estuarine and coastal turbid waters, so that QAA’s extension, QAA-E, has been developed, in which \( a_g(440) \) is exactly derived, using either \( a_d \)-based or \( a_g \)-based methods. Recently, QAA-E has been further improved to QAA-CDOM in which a QAA’s original function and a few parameters has been optimized by integrating synthetic data, very high spatial resolution \textit{in situ} data from our Mississippi cruise and other field data (NOMAD) collected globally during the last decades. QAA-CDOM has been tested with not only excellent inversion accuracy (<25%), but also suitable for high CDOM variability (0.01 – 13.3 m\(^{-1}\)).

Figure 2. The simple flow charts of (a) whole processing of WV2 satellite images and (b) QAA-CDOM algorithm.
Principal Findings and Significance:

(1) In situ CDOM concentration

According to our measurements in Nov. 4, 2009, CDOM in the Neponset River and Boston Harbor regions ranged from 8.17 to 86.75 QSU, with mean value 34.7 QSU. This wide range shows CDOM in the Neponset River is highly varied complicated. Also, CDOM and salinity demonstrate high negative correlation (Fig. (3)). However, their correlation coefficients change at different times (Sept. 25, 2009 vs. Nov. 04, 2009) but are similar at different locations (upstream vs. downstream), indicating that CDOM seasonal or temporal variations are more significant than its spatial variations.

(2) CDOM high-resolution remote sensing inversion.

CDOM distribution in the low Neponset River and Boston Harbor has been mapped in very high spatial resolution (~ 1.8 m) from a WV2 image, see Fig. 4. This resultant image and statistical comparisons (Fig. 5) show that QAA-CDOM is able to invert CDOM absorption coefficients with excellent accuracy ($RMSE = 0.11, R^2 = 0.73$). Our results also indicate that $a_d(440)$ in the Neponset River and Boston Harbor is slightly underestimated, particularly for the fresh water in the upstream. According to our analysis, this underestimation is possibly due to the interference of very high concentrations of phytoplankton (chlorophyll) growing in the same regions.
Figure 4. CDOM distribution in the Low Neponset River and Boston Harbor regions, derived from WV2 satellite images.

Figure 5. Derived CDOM and properties of other in-water components. (a) Satellite-derived CDOM and in situ measured concentration of CDOM, CHL, and non-algal particles, and water depth and salinity, along our tracks. (b) Comparisons between derived and measured CDOM in six locations, including the Neponset River.
Uncertainty of in situ measurement and remote sensing inversion

The uncertainties related to the whole inversion processing were analyzed in three levels: uncertainties in the processing of in situ measurement (level 1), satellite image preprocessing (level 4) and remote sensing inversion model (level 5), respectively. We found that in the level 1, the uncertainties of the in situ CDOM measurement in the Neponset River and Boston Harbor is approximately 1.547, which is about 10 times larger than our other study sites in the Mississippi River plumes and Hudson River estuary. This result indicates that the true CDOM distribution in the Neponset River is complex and highly varied even in a small water volume. The overall average level 1 uncertainty of our three study sites is 0.262%. This normalized uncertainty is stood on the unit of volts. If we convert it to QSU by multiplying 30, then we get 7.86%. This value, closing to 0.1, implies that in the unit of QSU, keeping 1 digital number is significant for shuttle’s measurement. If we further convert it to absorption coefficient, then we obtained for $a_d(440)$, the normalized uncertainty is about 0.32%. Similarly, it indicates that in the unit of absorption coefficient (m$^{-1}$), the first two digits are significant. If we exclude the Neponset data, the normalized uncertainties for volts, QSU, and absorption coefficient are 0.122%, 3.66%, and 0.22%, respectively.

The uncertainties of level 4 and level 5 are listed in the Table 1 and Table 2, respectively.

Table 1. Uncertainties of above surface spectrum. Star symbol indicates the results were calculated from strong wave areas. The values in the ‘Err’ columns multiple 100 is the error percentage. The $Err_4$ and $Err_{49}$ are the mean value of the 4 bands (440, 490, 555, 640) and the 49 bands of Hyperion sensor.

<table>
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<th>$Err_{49}$</th>
<th>$Err_4$</th>
<th>$Err$ (440)</th>
<th>$Err$ (490)</th>
<th>$Err$ (555)</th>
<th>$Err$ (640)</th>
<th>$U_A$ (440)</th>
<th>$U_A$ (490)</th>
<th>$U_A$ (555)</th>
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Table 2. Uncertainty of QAA-CDOM remote sensing inversion model.

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<th>Derived</th>
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<th>$U_{A2}$</th>
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<th>$Err%$ Abs mean</th>
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Publications and Conference Presentations:

Provide citations for publications resulting from all projects supported using your grant and required matching funds, including base grants. Please provide the citations in the format requested.

a. Articles in Refereed Scientific Journals

b. Book Chapter
c. **Dissertations**

Weining Zhu, Dept. of Geosciences, Inversion And Analysis of Chromophoric Dissolved Organic Matter In Estuarine And Coastal Regions Using Hyperspectral Remote Sensing

d. **Water Resources Research Institute Reports**

e. **Conference Proceedings**

f. **Other Publications**


**Student Support**

Number of students supported by grant or matching funds, the degree they are pursuing, and their major.

- Name: Weining Zhu
- Degree: Ph.D. candidate
- Major: Geosciences

**Notable Achievements and Awards**

Provide a brief description of any especially notable achievements and awards resulting from work supported by section 104 and required matching funds and by supplemental grants during the reporting period.

Using this grant as seed fund and preliminary study, we submitted a NSF proposal and it was successfully funded.

Qian Yu (PI), Co-PI: Anna Liu, Collaborated with Yong Tian and Robert Chen at UMass-Boston, **Collaborative Research: Modeling DOC dynamics from landscapes to coasts: hydrological connectivity and estuary processes**, NSF Collaboration in Mathematical Geosciences (CMG), #1025547, $517,987 ($329,346 on Amherst Campus), Sept 2010 - Aug 2013.