

COASTAL OCEAN OPTICS AND DYNAMICS |



The New Age of
Hyperspectral
Oceanography

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Introduction

A multispectral optical sensor collects data at select wavebands or channels. An example is the Sea-viewing Wide-Field-of-view Sensor (SeaWiFS) ocean color satellite, which measures eight wavebands between 402 and 885 nm (20-40 nm bandwidth with peaks centered around 412, 443, 490, 510, 555, 670, 765, and 865 nm). Optical oceanographers have been using multispectral sensors since the 1980s with great success¹.

A hyperspectral sensor gives continuous spectral coverage over a broad wavelength range [at least over visible wavelengths, and preferably from near ultraviolet (UV) to near infrared (IR)] with better than 10 nm resolution. The utility of hyperspectral measurements has long been recognized in fields as diverse as geology and astronomy, and hyperspectral instruments have been used in oceanographic research for about 30 years. However, most of these instruments have been laboratory bench-top spectrophotometers and radiometers that measure absorption and radiance or irradiance at <10 nm continuous spectral resolution from the UV to IR wavelengths. These instruments were relatively slow with sample scan rates on the order of minutes to maximize signal to noise. Just a decade ago, computational limitations also made processing and storage of large amounts of hyperspectral data difficult. However, within the last five years, high sample rate (less than seconds) *in situ* and remote sensing hyperspectral sensors have been developed and utilized for various

coastal and open-ocean studies. Advances in computer technology in the last decade have enabled more rapid processing of hyperspectral data and greatly improved the storing and archiving capability of these large, and often difficult-to-manage data sets.

Hyperspectral technology has expanded from hand-held radiometers to submerged sensors for measurements of inherent optical properties (IOPs), optical properties that depend on only the aquatic medium itself (e.g., absorption and scattering; Mobley, 1994) and apparent optical properties (AOPs), which depend on the IOPs and the geometry of the light field. Recently, hyperspectral airborne detectors have been enhanced for high spectral and spatial resolution measurements of ocean radiance and reflectance. Although multispectral sensors have a higher signal to noise ratio for the same quality of optical components (because they integrate over a larger bandwidth and thus collect more photons each band), the sensitivity and data quality of hyperspectral sensors are rapidly increasing and costs are coming down. Thus the shift from multispectral to hyperspectral systems will continue. The availability of hyperspectral sensors opens a new door for optical oceanography and related fields that make use of optical remote sensing of the oceans. Here, we discuss a few of the scientific advantages to using high spectral resolution sensors and describe valuable hyperspectral applications in the marine environment.

¹See special issues: "Hydrologic Optics" in *Limnology and Oceanography*, 34(8), 1989; "Ocean Color From Space: A Coastal Zone Color Scanner Retrospective" in *Journal of Geophysical Research*, 99(C4), 7291-7270, 1994; and "Ocean Optics" in *Journal of Geophysical Research*, 100(C7), 13,133-13,372, 1995).



Spectral Techniques

Traditionally, multispectral remote sensors have been utilized for characterizing open-ocean waters. Some results have shown that a few, wide, carefully selected bands may be all that is needed to monitor these water bodies whose optical signatures are dominated by chlorophyll *a* and co-varying optically significant constituents. However, when these open ocean algorithms (O'Reilly et al., 1998) are applied to coastal areas, the results are less useful, if not altogether inapplicable (Hu et al., 2000; Lee and Carder, 2002). The coastal ocean is an optically complex environment. For example: (1) phytoplankton

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populations are generally more abundant and less diverse, (2) terrestrial influences [high concentrations of colored dissolved organic matter (CDOM) and particles] cannot be ignored, (3) the influence of the ocean bottom (bottom reflectance and sediment resuspension) is important, and (4) high temporal and spatial variability collude to create an optically diverse environment. Not only do these influences complicate the characterization of the water and bottom types, but also make the atmospheric correction of these scenes difficult. Traditional blue water atmospheric corrections (e.g., “black pixel” assumptions; Siegel et al., 2000) are no longer valid. These correction methods assume that any remote sensing signal at the IR wavelengths is due to the atmosphere, but this assumption does not hold in high sediment or optically shallow coastal waters. Thus, the successful removal of the atmospheric interference in the water-leaving radiance signal within the coastal environment requires *a priori* knowledge of a host of atmospheric constituents (e.g., water column vapor, aerosol type and density, ozone concentration). Without *a priori* knowledge, these constituents must be derived from the spectral data stream itself, decreasing the degrees of freedom with which to resolve the water leaving radiance signal. Additionally, the increased development along the world’s coastal boundaries adds a degree of complexity in the determination of concentration and interactions between the marine and terrestrial aerosols, such that the atmospheric parameterization may change dramatically within a single scene. Hyperspectral information provides optical oceanographers the potential to accurately correct remote sensing images and classify complex oceanic environments, finer-scale features (e.g., bottom type and characteristics and phytoplankton blooms), and depth-dependent IOPs.

With higher spectral resolution data (i.e., more wavelengths) come more degrees of freedom for optical models and empirical algorithms. Many ocean color algorithms in use today involve empirical relationships between the property of interest (i.e., chlorophyll *a* concentration, IOPs, etc.) and waveband ratios of remote sensing reflectance or water-leaving radiance (O'Reilly et al., 1998). Most of these algorithms are derived by regressions of radiance at select (or available) wavebands or waveband ratios versus the property of interest. Naturally, the regression results are maximized at the highest number of statistically independent wavelengths available. Also, the spectral resolution of derived IOPs is limited by the number of wavebands of the ocean color remote sensing data used in the regression.

Multispectral measurements of absorption are useful for determining the relative concentrations and variability of the different constituents in the water column: water itself, phytoplankton, CDOM, and inorganics (Schofield et al., In press and references therein). Absorption peaks of chlorophyll *a*, non-pigmented troughs, and the exponential slopes of CDOM and inorganic material are well distinguished in absorption spectra collected by most multispectral sensors. However, in order to identify phytoplankton by taxonomic group or species, quantification of the absorption by accessory or marker pigments beyond chlorophyll *a* is oftentimes necessary. Some accessory pigments are unique to individual phytoplankton taxa and usually cannot be discerned in absorption spectra with a limited number of wavelengths or wavebands (accessory pigment peaks are generally narrow), but can be discriminated in hyperspectral data. This discrimination can be accomplished with various methods such as spectral unmixing and deconvolution, Gaussian decomposition, and derivative analysis (usually taken

to the fourth derivative) together with similarity index analysis (e.g., Millie et al., 1997; Schofield et al., In press). These decomposition analyses are techniques that separate pigment peaks and shoulders from troughs in phytoplankton absorption curves of mixed assemblages. The similarity index is typically used to correlate measured absorption with known phytoplankton absorption

“Hyperspectral information provides optical oceanographers the potential to accurately correct remote sensing images and classify complex oceanic environments, finer-scale features..., and depth-dependent [inherent optical properties].”

curves for identification purposes by taking into account the differences in shapes between two spectra based on the peaks and troughs of each spectrum. These identification techniques usually cannot be applied to multispectral data because the required features (i.e., peaks and troughs) are not well resolved.

While the absorption properties of numerous planktonic species and other water column constituents have been studied extensively, the same cannot be said for their backscattering properties. Backscattering properties must be known in order to accurately interpret ocean color measurements because the reflectance of the upper ocean is directly related to the ratio of the backscattering coefficient to the absorption coefficient. Hyperspectral backscattering measurements can be used to distinguish phytoplankton populations from co-varying seawater constituents because the spectral dependence of backscattering by algal cells is different from that of other particles (Bricaud et al., 1983; Stramski et al., 2001). Also, hyperspectral backscatter measurements in the laboratory have revealed that some phytoplankton species may show complex, high-

ly distinct backscattering spectra between species (cultured) (Bricaud et al., 1983; Ahn et al., 1992) whereas other microorganisms, such as bacteria and flagellates, show wavelength independent backscatter (Morel and Ahn, 1990, 1991). These studies and the results of numerous modeling efforts (see Stramski et al., 2001 and references therein) demonstrate that backscatter is not spectral-

ly flat (as it is oftentimes modeled) or easily predicted for all particles. Therefore, backscatter has the potential to provide a means to identify phytoplankton by group or species and to determine particle characteristics. This provides incentive for the development of *in situ* hyperspectral backscatter sensors and algorithms.

Examples of Hyperspectral Analyses

Hyperspectral data used in combination with spectral techniques such as derivative analysis, spectral angle mapping, spectral deconvolution, and similarity indices can aid in the characterization of marine ecosystems including the detection and identification of harmful algal blooms, an increasing problem in the world's coastal oceans (Millie et al., 1997; Lohrenz et al., 1999). For example, Figure 1 shows phytoplankton absorption spectra for a red tide species, *Karenia brevis*, measured with a multispectral sensor, a hyperspectral sensor, and modeled using Mie theory (following Mahoney, 2001). *K. brevis* can be identified by its accessory pigment, Gyroxanthin—diester, which has unique absorption peaks at 444 and 469 nm



(Örnólfssdóttir et al., 2003). As seen in Figure 1, the multispectral spectrum lacks detailed absorption information, i.e., pigment peaks by distinguishing accessory pigments, due to a limited number of wavebands. Hyperspectral data allow for the detection of species-discriminating accessory pigments and are more adequate for comparing measured spectra to a reference spectrum for similarity index analysis (Figure 1). Wood et al. (2002) have also used these techniques and presented evidence that distinctive hyperspectral signatures are associated with *Synechococcus* blooms in upwelling and nutrient enrichment systems in the Gulf of California. Cannizzaro et al. (2002) show that it is possible to utilize multispectral techniques (SeaWiFS) to detect *K. brevis*. However, their method works only for waters under certain optical conditions (low concentrations of CDOM and suspended sediments relative to chlorophyll *a* or low backscattering relative to absorption) as different ocean color products (particulate backscattering and its relationship to chlorophyll *a*) are used as proxies for *K. brevis* abundance.

In the past, multispectral techniques have been used for the derivation of water depth and bottom bathymetry (e.g., Philpot, 1989; Maritorena et al., 1994), and more recently for characterization of bottom type (see “Light in Shallow Waters” in *Limnology and Oceanography*, 48(2), 2003). These analyses generally involve empirical algorithms, where reflectance waveband ratios are regressed against water depth. Wavelength limitations and commonly employed assumptions that the water optical properties are vertically uniform and constant over the area being mapped can lead to inaccurate retrievals of bottom depth and characteristics under certain conditions. These retrievals can be improved with hyperspectral data (Lee and Carder, 2002 and references therein). For example, Figure 2 shows hyperspectral

remote sensing reflectance spectra for two water types generated by the Hydrolight radiative transfer model (Mobley, 1994). Water 1 is 6.5 m and has low chlorophyll *a* and CDOM concentrations with a bottom type of a mixture of soft coral and *Sargassum*, while Water 2 is 13 m deep, “pure water” with a flat green sponge bottom type. By inspection of the hyperspectral spectra, the difference between the two curves is obvious in the 500–600 nm range. However, spectra for the two water types produced using only the SeaWiFS wavebands appear almost identical (note: the SeaWiFS spectra were derived by applying the SeaWiFS spectral response function to the hyperspectral signatures). A second example, Figure 3, shows 122 remote sensing reflectance spectra generated by Hydrolight for various combinations of nine different sets of IOPs, 32 different bottom reflectances, and 22 depths between 5.5 and 50 m. These spectra are clearly unique. However, every spectrum has nearly the same remote sensing reflectance wavelength ratio: $R_{rs}(490)/R_{rs}(555) = 1.71 \pm 0.01$. This ratio, if used in the SeaWiFS Ocean Chlorophyll 2 (OC2) band-ratio algorithm (O’Reilly et al., 1998, as revised on http://seawifs.gsfc.nasa.gov/SEAWIFS/RECAL/Repro3/OC4_reprocess.html), gives a chlorophyll concentration of 0.59 ± 0.01 mg Chl m^{-3} . Thus these simulated water bodies, which have IOPs corresponding to chlorophyll concentrations between 0.0 (pure water) and 0.2 mg Chl m^{-3} , are all viewed as the same by the OC2 algorithm. The OC2 algorithm fails here because of bottom effects in optically clear waters simulated by Hydrolight.

While much of the interest in hyperspectral approaches relates to the visible wavebands, several oceanic constituents of interest have distinct spectral signatures in the UVA/UVB (e.g., Ogura and Hanya, 1966). Chief among these is nitrate, a major plant nutrient that limits the primary

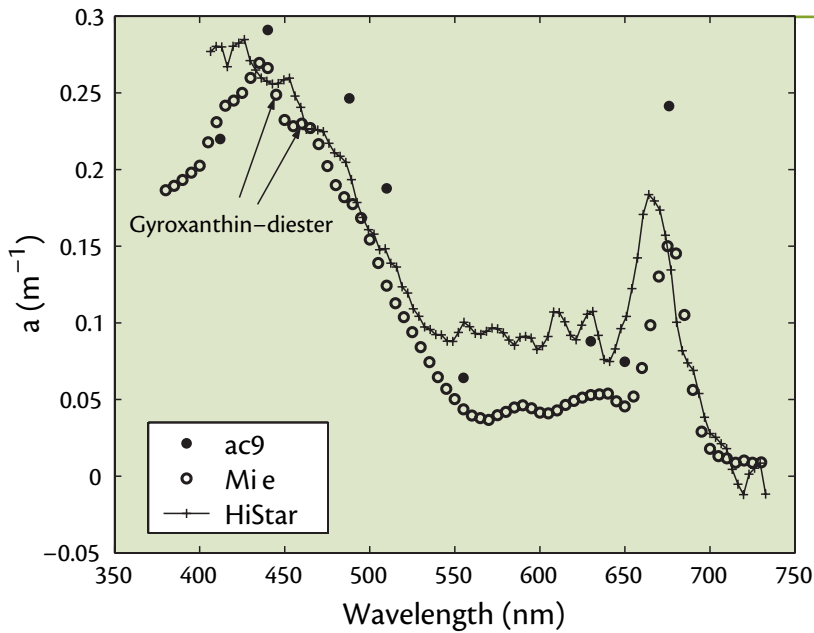


Figure 1. Phytoplankton taxonomic group or species identification is now achievable with the development of hyperspectral instruments; generally narrow accessory pigment absorption wavelength peaks that are unique to specific species can be discerned. Shown here are three different methods used to measure phytoplankton absorption spectra for a red tide species, *Karenis brevis*, on the west Florida shelf. Closed circles symbolize absorption measured with a multispectral sensor (ac-9). Open circles signify data modeled using Mie theory (following Mahoney, 2001), and plus signs represent data measured with a hyperspectral sensor (HiStar). It is apparent in this figure that the multispectral spectrum lacks the distinguishing accessory pigment peaks due to a limited number of wavebands. Hyperspectral data, however, allow for the detection of species-discriminating accessory pigments and are more adequate for comparing measured spectra to a reference spectrum and thus phytoplankton species identification. *K. brevis* can be identified by its accessory pigment, Gyroxanthin-diester, which has unique absorption peaks at 444 and 469 nm (Örnólfssdóttir et al., 2003). (Multispectral data were provided by Oscar Schofield and John Kerfoot, Rutgers University and hyperspectral data were provided by Steven Lohrenz, University of Southern Mississippi.)

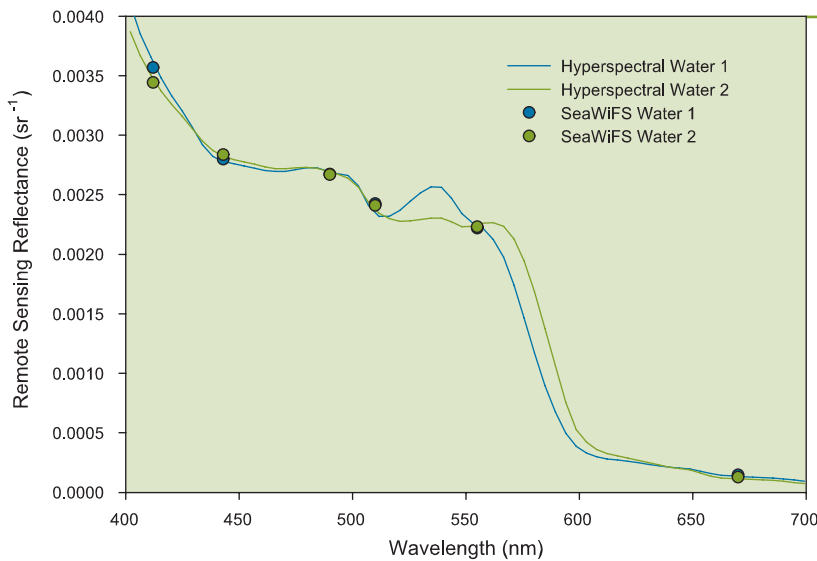


Figure 2. Bottom effects in shallow coastal waters may lead to inaccurate remote sensing retrievals of bottom depth if limited spectral bands are utilized for analysis. This figure shows modeled hyperspectral (solid lines) and multispectral (SeaWiFS wavebands; circles) spectra for two water types, generated by the Hydrolight radiative transfer model (Mobley, 1994). Water 1 (blue) is 6.5 m deep and has low chlorophyll-*a* and CDOM concentrations with a bottom type of a mixture of soft coral and *Sargassum*, while Water 2 (green) is 13 m deep, "pure water" with a flat green sponge bottom type. By inspection of the hyperspectral spectra, the difference between the two curves is obvious in the 500-600 nm range. However, spectra for the two water types produced using only the SeaWiFS wavebands appear almost identical. (SeaWiFS spectra in this figure were derived by applying the SeaWiFS spectral response function to the hyperspectral signatures).

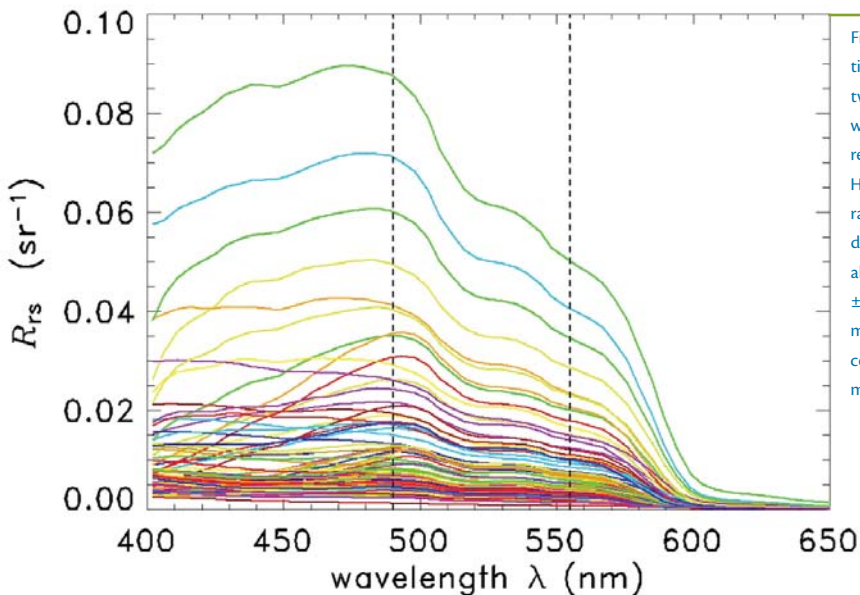


Figure 3. Chlorophyll concentration algorithms designed for multispectral instrumentation may not be useful for shallow, optically clear waters. Shown here are one hundred twenty two Hydrolight-generated remote sensing reflectance (R_{rs}) spectra for Bahamian waters using various combinations of nine different sets of IOPs, 32 different bottom reflectances, and 22 depths between 5.5 and 50 m. These spectra are clearly unique. However, every spectrum has nearly the same remote sensing reflectance wavelength ratio: $R_{rs}(490)/R_{rs}(555) = 1.71 \pm 0.01$ (490 and 555 nm are indicated by the vertical black dashed lines). If this ratio were applied to the commonly used SeaWiFS band-ratio algorithm (OC2; O'Reilly et al., 1998), it would give a chlorophyll concentration of 0.59 ± 0.01 mg Chl m^{-3} . In other words, the same chlorophyll concentration would be determined for all 122 spectra despite the fact that these simulated water bodies have IOPs corresponding to chlorophyll concentrations between 0.0 (pure water) and 0.2 mg Chl m^{-3} . The OC2 algorithm fails here because of bottom effects in optically clear waters.



ABOVE AND PRECEDING THREE SPREADS: Three bands (RGB= 666, 547, 439 nm) from a March 23, 1996 Air borne Visible/Infrared Imaging Spectrometer (AVIRIS) image taken over the Florida Keys from an ER-2 aircraft at 20 km above ground. The top of the image is near the eastern end of the Keys; the bottom of the image is near the western end. The rough heading is 260 degrees (clockwise from north) top to bottom (i.e., just south of west). AVIRIS is an optical sensor that delivers calibrated images of upwelling spectral radiance in 224 contiguous spectral channels (bands) with wavelengths from 400 to 2500 nanometers. Note that this image is not atmospherically corrected. It is $\pi \times \text{radiance} / [\text{mean_solar_ir_radiance_at_the_top_of_the_atmosphere} \times \cos(\text{solar_zenith_angle})]$. Original data courtesy of NASA/JPL. Caption courtesy of Marcos Montes of Naval Research Laboratory, Washington D.C.

production of organic matter in many regions of the world's oceans. The net vertical transport of nitrate, for example, constrains the export flux of organic matter from the surface ocean in a steady-state sense. Nitrate dissolved in seawater exhibits a broad absorption maximum centered at ~210 nm; it competes with the absorption of bromide, a conservative component of sea-salt, and to a lesser extent, the carbonate ion (Figure 4). In anaerobic areas, sulphide also absorbs in a band around 220 nm and various dissolved organic compounds of oceanographic and practical purposes (e.g., TNT) exhibit absorption maxima in the UV. Past attempts to estimate the concentration of nitrate and other compounds with multispectral instruments have been met with equivocal success. The introduction of a field-deployable hyperspectral UV absorption spectrometer, i.e., the *In Situ* Ultraviolet Spectrometer (ISUS), coupled with advanced spectroscopic deconvolution techniques, has made routine spectral measurements of nutrients possible (Johnson and Coletti, 2002; Figure 4). Oceanographers are now able to resolve nitrate concentrations in the ocean at temporal and spatial scales consistent with measurements of temperature and salinity and to an accuracy and precision more than acceptable for oceanographic biogeochemical investigations, as a direct result of a hyperspectral approach to the problem.

Summary and Conclusions

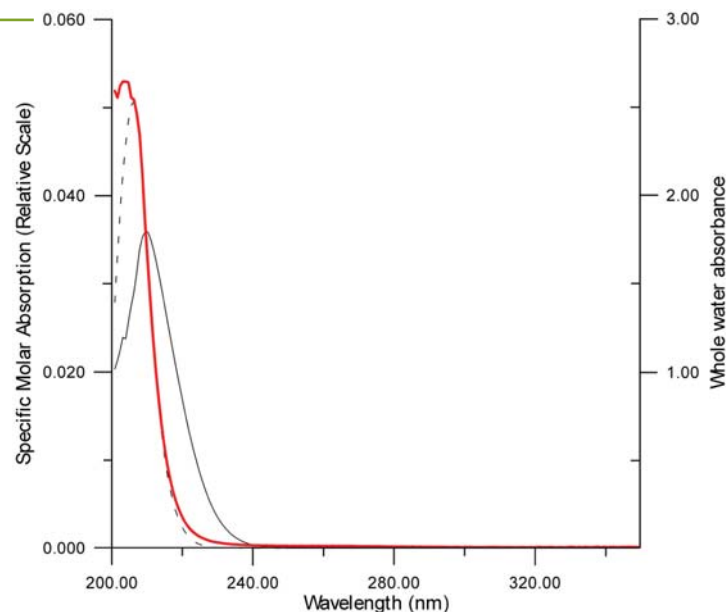
Hyperspectral technology provides a means for optical oceanographers to classify and quantify complex oceanic environments (*in situ* and remotely): bottom depth and type, particle characteristics, depth-dependent IOPs, and specific chemical compounds. Hyperspectral data enable, for the first time, a real attempt at environmental spectroscopy. *In situ* and remote phytoplankton taxonomic group or species identification

is now achievable with the development of hyperspectral instruments; generally narrow accessory pigment absorption wavelength peaks that are unique to specific species can be discerned. High spectral resolution back-scattering spectra are unique to some phytoplankton species and can aid in the characterization of oceanic particles. One other exciting aspect of hyperspectral technology is the development of optically based chemical sensors. These sensors allow for long-term monitoring of ecologically important nutrients and potentially harmful pollutants at unprecedented time and space scales.

Hyperspectral instrumentation is becoming increasingly important to oceanographic research as coastal and open ocean observing systems are rapidly developing into key elements for scientific research, monitoring, decision-making, science education, and outreach. Some concerns of these observatories are that autonomous sampling platforms can be limited by weight and volume and data bandwidth capabilities. The incorporation of hyperspectral sensors to autonomous sampling platforms of an observing system can expand the amount of information gained from one instrument without compromising platform payload. High spectral resolution sensors provide a greater number of wavelengths for various analysis techniques, particularly in optically complex coastal environments. In addition, emerging cabled observatories offer exceptional power and data bandwidth for hyperspectral sensors.

Optical oceanographers have been posing hyperspectrally-related questions since the popularity of ocean exploration expanded in the 1950s. However, technological and computing constraints limited us to the use of multispectral or even single wavelength sensors in our field studies. Now that computing power has become more than adequate to handle large quantities of data

Figure 4. Nitrate is a major plant nutrient that limits the primary production of organic matter in many regions of the world's oceans. Nitrate dissolved in seawater exhibits a broad absorption maximum centered at ~210 nm. The introduction of a field-deployable hyperspectral UV absorption spectrometer, known as *In Situ* Ultraviolet Spectrometer (ISUS), coupled with advanced spectroscopic deconvolution techniques, has made routine spectral measurements of nutrients possible at unprecedented time and space scales. The specific molar absorption of bromide (black, dotted line) and nitrate (black, solid line) are shown with the absorption spectrum of whole water (red line; 1 nm resolution) measured with the ISUS (MBARI/Satlantic Inc.) deployed on a Conductivity-Temperature Depth profiler (CTD) at 150 m depth in the western Equatorial Pacific. Most of the variance in absorption is explained by bromide; advanced deconvolution techniques are required to extract the concentration of nitrate (here 14.9 μM) based on its absorption.



and technology has allowed miniaturization of *in situ* and remotely sensed optical sensors, we have been able to utilize hyperspectral instruments in the field to answer a host of scientific questions that were never before possible. This is an exciting time for oceanographers. New spectral algorithms and techniques will be further developed and refined as high spectral resolution technologies are improved for IOP sensors for measurements of absorption, attenuation, scattering, backscattering, and the volume scattering function. Potentially, a suite of relatively small, robust hyperspectral instruments will be available to measure and resolve bottom depth and type, particle size and type (including phytoplankton species identification), and micro- and macro-nutrient concentrations *in situ* in the very near future. ☒

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