Quantifying the Spectral Absorption Coefficients of Phytoplankton and Non-Phytoplankton Components of Seawater from in Situ and Remote-Sensing Measurements

Dariusz Stramski (PI)
Rick A. Reynolds (Co-PI)

Scripps Institution of Oceanography
University of California San Diego

NASA PACE Science Team Meeting
Harbor Branch Oceanographic Institute, 17–19 January 2017

Objectives

- **IOP METHODOLOGY**: Develop consensus recommendations for improved methodology for hyperspectral measurements of particulate absorption coefficient with a filter-pad technique.

- **IOP INVERSION**: Develop community-endorsed retrieval algorithm for partitioning the total absorption coefficient of seawater into the contributions of phytoplankton, nonalgal particles, and colored dissolved organic matter (CDOM) with a key novel aspect of separating non-algal particles from CDOM.

- **WATER-LEAVING RADIANCE**: Improve an understanding of determinations of water-leaving radiance from extrapolation of underwater radiometric measurements and provide recommendations for improved methodology.

Objective 1: IOP Methodology

Research Article Vol. 54, No. 22 / August 1 2015 / Applied Optics 6763

applied optics

Correction of pathlength amplification in the filter-pad technique for measurements of particulate absorption coefficient in the visible spectral region

Dariusz Stramski,[1,*] Rick A. Reynolds,[1] Sławomir Kaczmarek,[2] Julia Uitz,[1,3] and Guangming Zheng[1,4,5]

[1]Marine Physical Laboratory, Scripps Institution of Oceanography, University of California San Diego, La Jolla, California 92093-0238, USA
[2]Institute of Oceanology, Polish Academy of Sciences, Powstancow Warszawy 55, 81-712 Sopot, Poland
[3]Currently at Sorbonne Universités, UPMC Université Paris 06, CNRS, Observatoire Océanologique de Villefranche (OOV), Laboratoire d'Océanographie de Villefranche (LOV), 181 Chemin du Lazaret, 06 230, Villefranche-sur-Mer, France
[4]Currently at NOAA/NESDIS/Center for Satellite Application and Research, 5830 University Research Court, College Park, Maryland 20740, USA
[5]Currently at Global Science & Technology, Inc., 7855 Walker Drive, Suite 200, Greenbelt, Maryland 20770, USA
*Corresponding author: dstramski@ucsd.edu

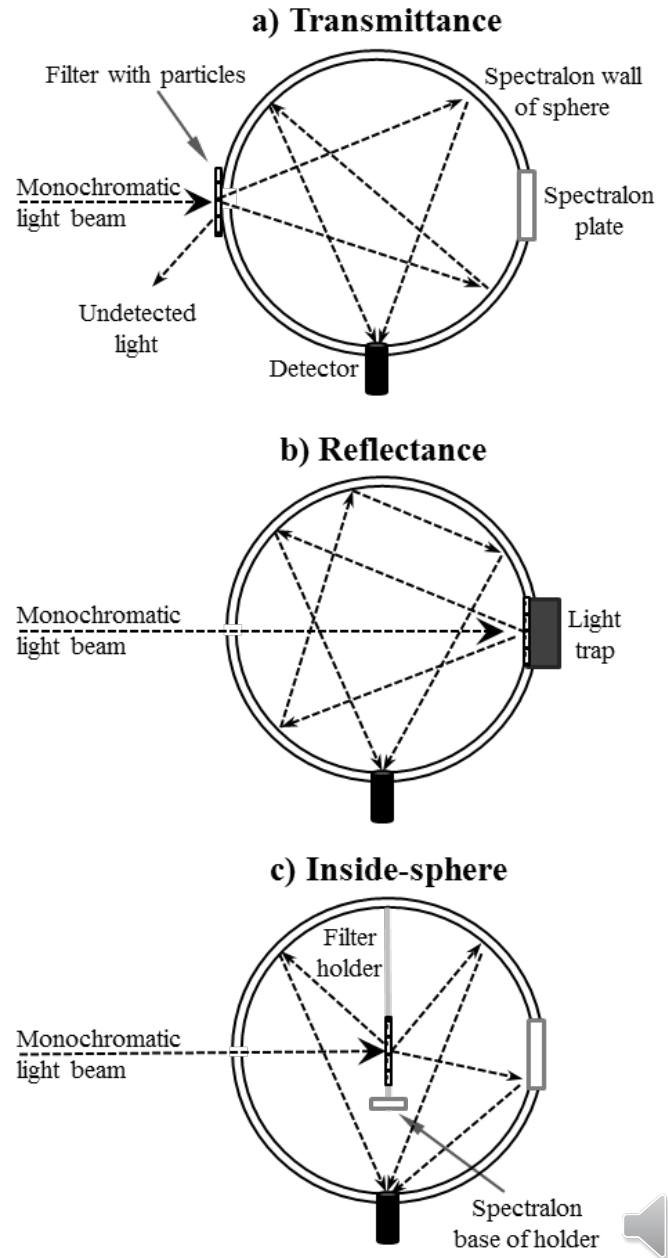
Received 2 April 2015; revised 26 June 2015; accepted 1 July 2015; posted 1 July 2015 (Doc. ID 237332); published 27 July 2015

Spectrophotometric measurement of particulate matter retained on filters is the most common and practical method for routine determination of the spectral light absorption coefficient of aquatic particles, $a_p(\lambda)$, at high spectral resolution over a broad spectral range. The use of differing geometrical measurement configurations and large variations in the reported correction for pathlength amplification induced by the particle/filter matrix have hindered adoption of an established measurement protocol. We describe results of dedicated laboratory experiments with a diversity of particulate sample types to examine variation in the pathlength amplification factor for three filter measurement geometries; the filter in the transmittance configuration (T), the filter in the transmittance-reflectance configuration (T-R), and the filter placed inside an integrating sphere (IS). Relationships between optical density measured on suspensions (OD_s) and filters (OD_f) within the visible portion of the spectrum were evaluated for the formulation of pathlength amplification correction, with power functions providing the best functional representation of the relationship for all three geometries. Whereas the largest uncertainties occur in the T method, the IS method provided the least sample-to-sample variability and the smallest uncertainties in the relationship between OD_s and OD_f. For six different samples measured with 1 nm resolution within the light wavelength range from 400 to 700 nm, a median error of 7.1% is observed for predicted values of OD_s using the IS method. The relationships established for the three filter-pad methods are applicable to historical and ongoing measurements; for future work, the use of the IS method is recommended whenever feasible.

OCIS codes: (010.1030) Absorption; (010.4450) Oceanic optics.

http://dx.doi.org/10.1364/AO.54.006763

Three filter-pad methods



Laboratory β-experiments to determine the pathlength amplification factor

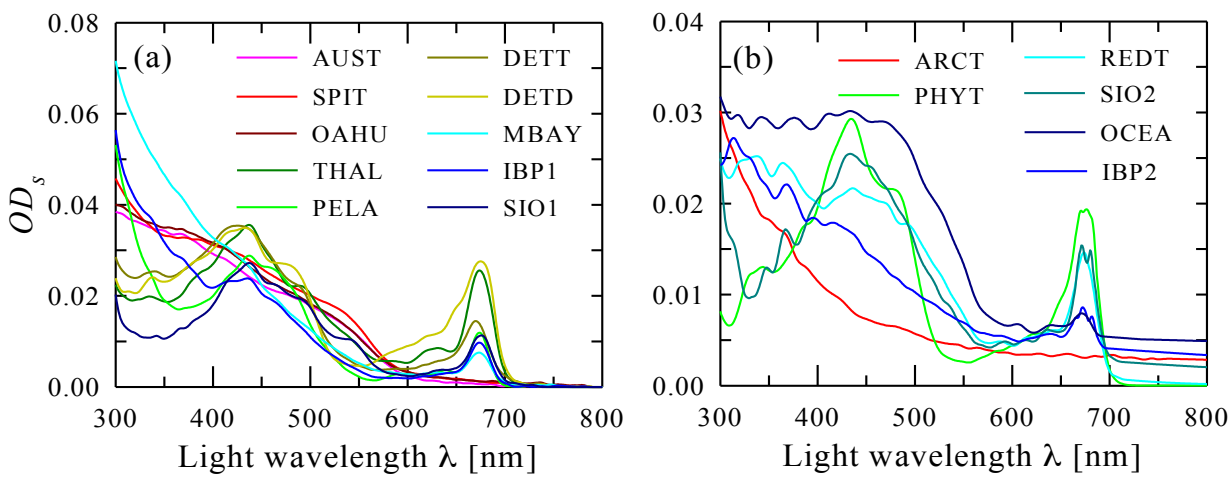
Description of samples used in two sets of β-experiments

Sample	Sample description	Filtration volumes [mL]
AUST	Surface soil dust from Australia	5, 8, 20, 35
SPIT	Ice-rafted particles from Spitsbergen	5, 10, 15
OAHU	Surface soil dust from Oahu, HI	5, 10, 20, 35
THAL	Thalassosira weissflogii culture	5, 10, 20, 35
PELA	Pelagomonas calceolata culture	8, 12, 20, 25
DETT	Phytodetritus from Thalassosira weissflogii	9, 14, 20, 35
DETD	Phytodetritus from Dunaliella tertiolecta	9, 14, 20, 30
MBAY	Seawater from Mission Bay, CA	4, 10, 18, 28
SIO1	Seawater from Scripps Pier, CA	4, 20
IBP1	Seawater from Imperial Beach Pier, CA	4, 10, 20, 30

Sample	Sample description	Filtration volumes [mL]	
		IS method	T, T-R method
ARCT	Particles from melted Arctic sea-ice	9, 19, 41	41, 41
PHYT	Mixture of four phytoplankton cultures	3, 9, 15	n/a†, n/a
REDT	Red tide from Scripps Pier (L. polyedrum)	3, 7, 15, 23	15, n/a
SIO2	Seawater from Scripps Pier	5	5, 5
OCEA	Seawater from offshore San Diego	9, 14.5	14.5, 14.5
IBP2	Seawater from Imperial Beach Pier	5, 10, 17, 25	25, 25

†"n/a" refers to not applicable as the measurement was not performed.

Reference absorption spectra for all samples measured on suspensions inside the sphere

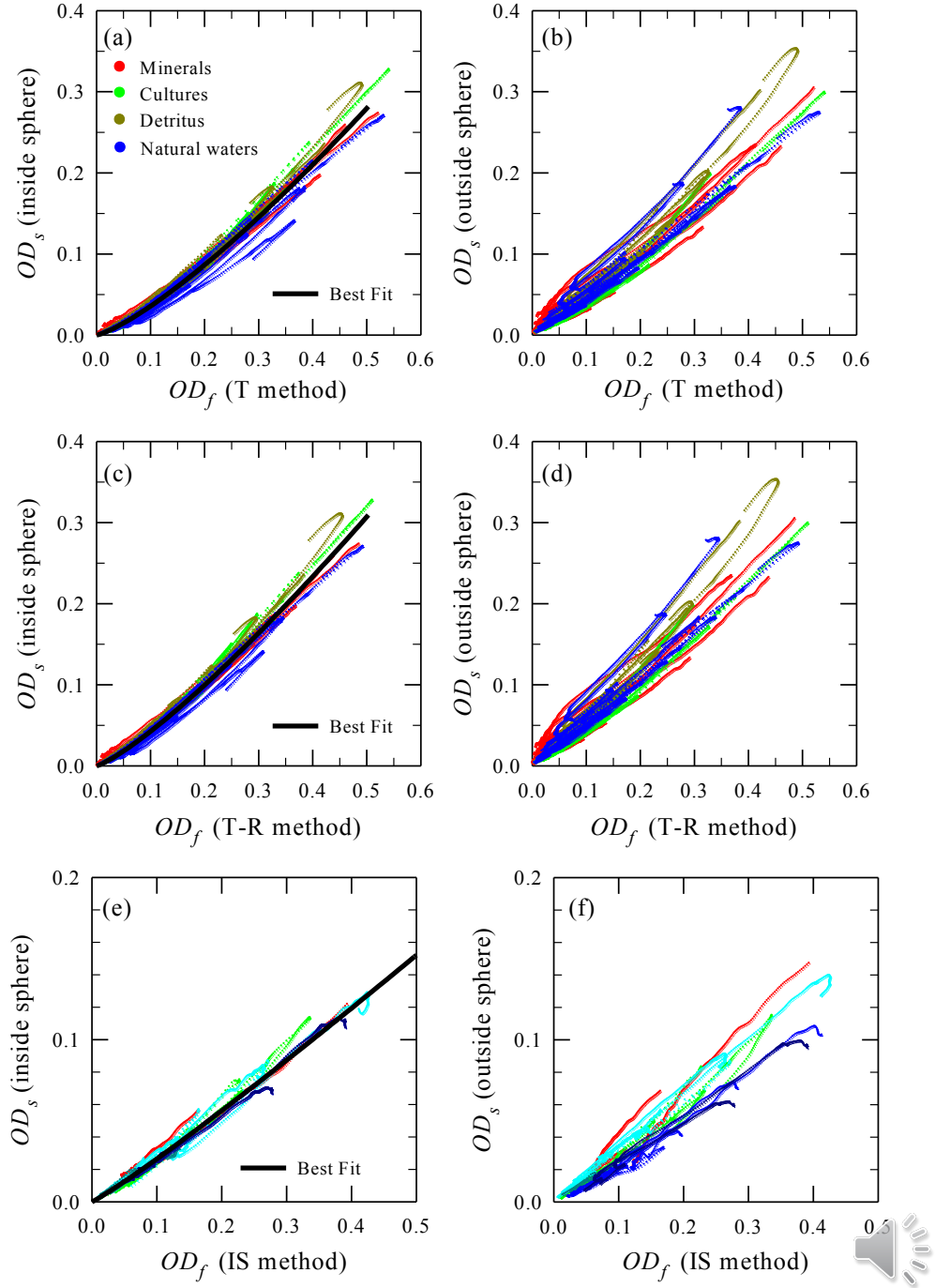


Results for β-relationship (OD_s vs. OD_f) for different measurement configurations based on data within the visible spectral region 400 – 700 nm

Reference absorption of suspension must be measured very accurately, e.g., inside the integrating sphere

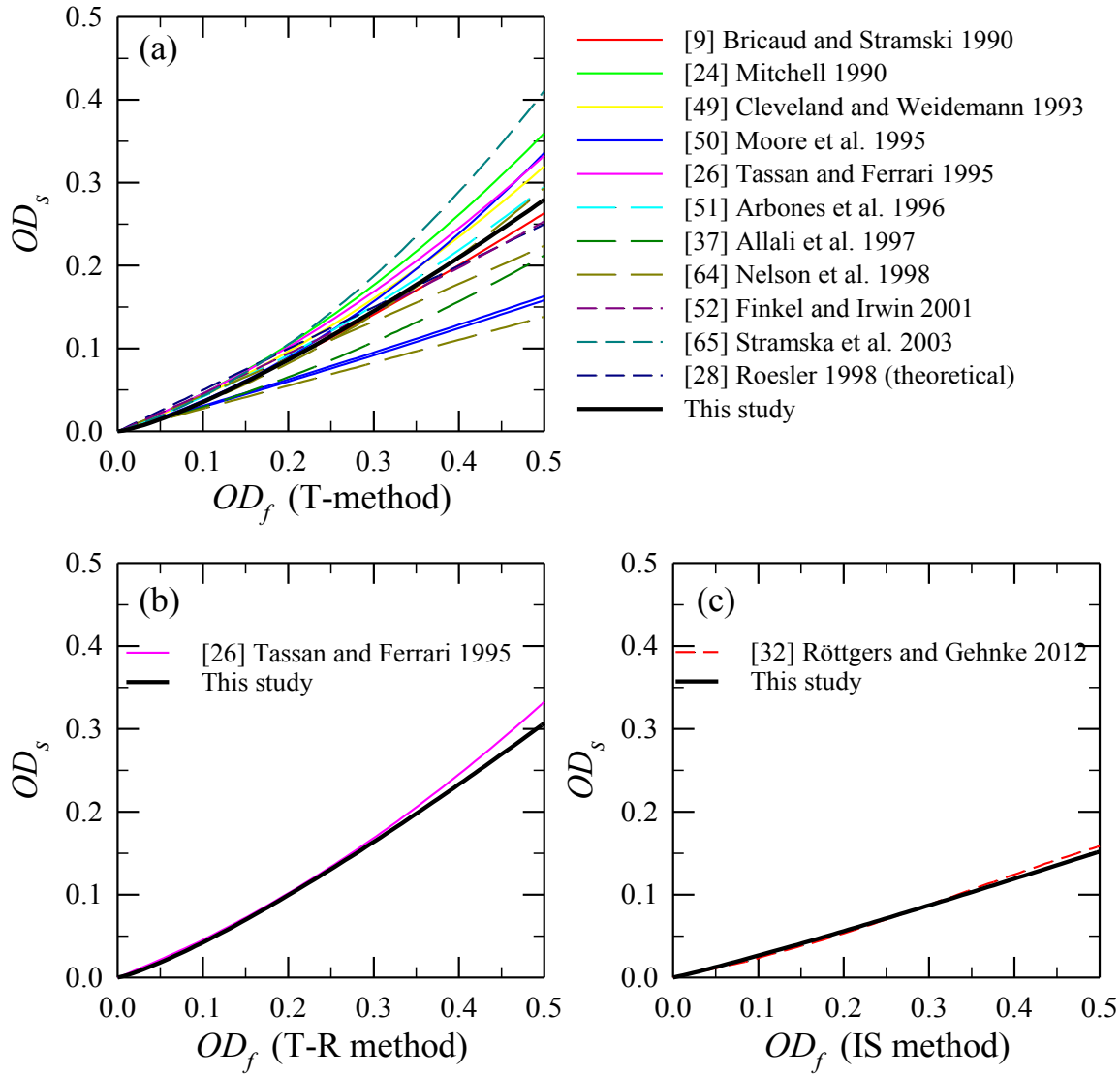
The best measurement configuration for the filter-pad technique is inside the integrating sphere (IS method, see panel e). The traditional T and T-R methods are inferior

The use of inside-sphere method is recommended whenever feasible



Our final recommended β-relationships for T, T-R, and IS methods (black solid lines) which are proposed as a community standard for pathlength amplification correction in the visible spectral region.

Literature data are shown for comparison.



Objective 2: IOP Inversion

Partitioning of the Absorption Coefficient of Seawater

Pure Seawater — Phytoplankton — Non-algal Particles — CDOM (Colored Dissolved Organic Matter)

$$\text{Total } a(\lambda) = a_w(\lambda) + a_{ph}(\lambda) + \underbrace{a_d(\lambda) + a_g(\lambda)}_{a_{dg}(\lambda)}$$

$$\underbrace{a_{ph}(\lambda) + a_{dg}(\lambda)}_{\text{Total non-water } a_{nw}(\lambda)}$$

AGU PUBLICATIONS

JGR

Journal of Geophysical Research: Oceans

RESEARCH ARTICLE

10.1002/2014JC010604

Key Points:

- A partitioning model for light absorption coefficient of natural waters
- Nonalgal particulate and CDOM components are separated
- No restrictive assumptions about absorption coefficients are required

Supporting Information:

- Supporting Information S1

Correspondence to:
G. Zheng,
guangming.zheng@noaa.gov

Citation:
Zheng, G., D. Stramski, and P. M. DiGiacomo (2015), A model for partitioning the light absorption coefficient of natural waters into phytoplankton, nonalgal particulate, and colored dissolved organic components: A case study for the Chesapeake Bay, *J. Geophys. Res. Oceans*, *120*, 2601–2621, doi:10.1002/2014JC010604.

Received 19 NOV 2014
Accepted 22 JAN 2015
Accepted article online 27 JAN 2015
Published online 3 APR 2015

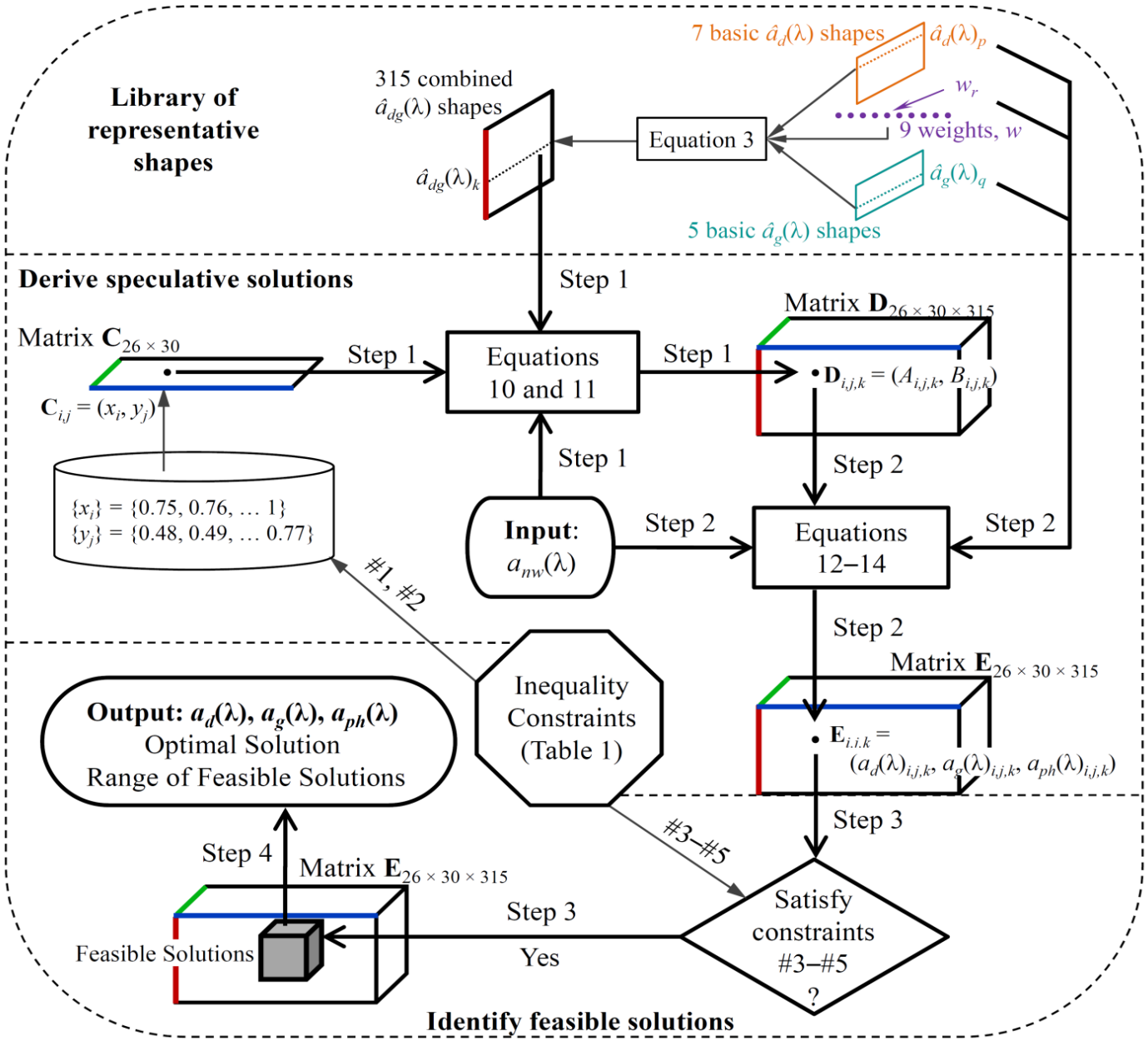
A model for partitioning the light absorption coefficient of natural waters into phytoplankton, nonalgal particulate, and colored dissolved organic components: A case study for the Chesapeake Bay

Guangming Zheng[1,2,3], Dariusz Stramski[4], and Paul M. DiGiacomo[1]

[1]NOAA/NESDIS/Center for Satellite Application and Research, College Park, Maryland, USA, [2]Earth System Science Interdisciplinary Center, University of Maryland, College Park, Maryland, USA, [3]Now at Global Science and Technology Inc., Greenbelt, Maryland, USA, [4]Marine Physical Laboratory, Scripps Institution of Oceanography, University of California San Diego, La Jolla, California, USA

Abstract We present a model, referred to as Generalized Stacked-Constraints Model (GSCM), for partitioning the total light absorption coefficient of natural water (with pure-water contribution subtracted), $a_{nw}(\lambda)$, into phytoplankton, $a_{ph}(\lambda)$, nonalgal particulate, $a_d(\lambda)$, and CDOM, $a_g(\lambda)$, components. The formulation of the model is based on the so-called stacked-constraints approach, which utilizes a number of inequality constraints that must be satisfied simultaneously by the model outputs of component absorption coefficients. A major advancement is that GSCM provides a capability to separate the $a_d(\lambda)$ and $a_g(\lambda)$ coefficients from each other using only weakly restrictive assumptions about the component absorption coefficients. In contrast to the common assumption of exponential spectral shape of $a_d(\lambda)$ and $a_g(\lambda)$ in previous models, in our model these two coefficients are parameterized in terms of several distinct spectral shapes. These shapes are determined from field data collected in the Chesapeake Bay with an ultimate goal to adequately account for the actual variability in spectral shapes of $a_d(\lambda)$ and $a_g(\lambda)$ in the study area. Another advancement of this model lies in its capability to account for potentially nonnegligible magnitude of $a_d(\lambda)$ in the near-infrared spectral region. Evaluation of model performance demonstrates good agreement with measurements in the Chesapeake Bay. For example, the median ratio of the model-derived to measured $a_d(\lambda)$, $a_g(\lambda)$, and $a_{ph}(\lambda)$ at 443 nm is 0.913, 1.064, and 1.056, respectively. Whereas our model in its present form can be a powerful tool for regional studies in the Chesapeake Bay, the overall approach is readily adaptable to other regions or bio-optical water types.

Flowchart of the Generalized Stacked-Constraints Model

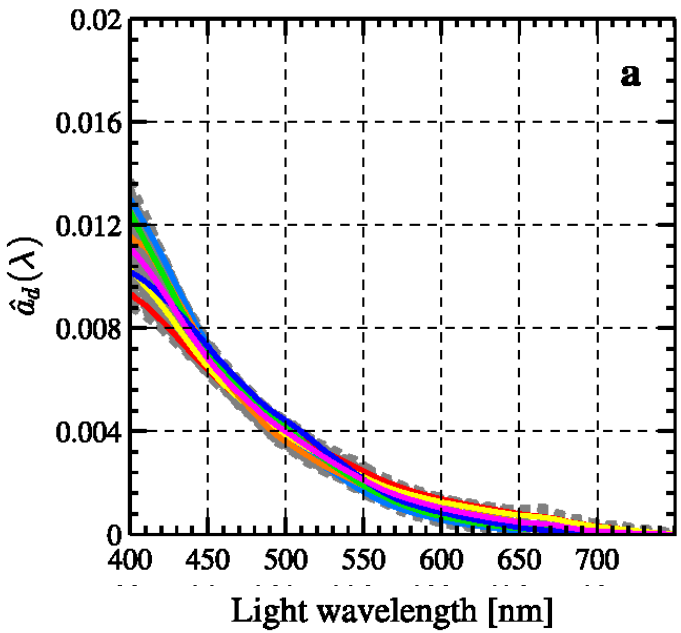


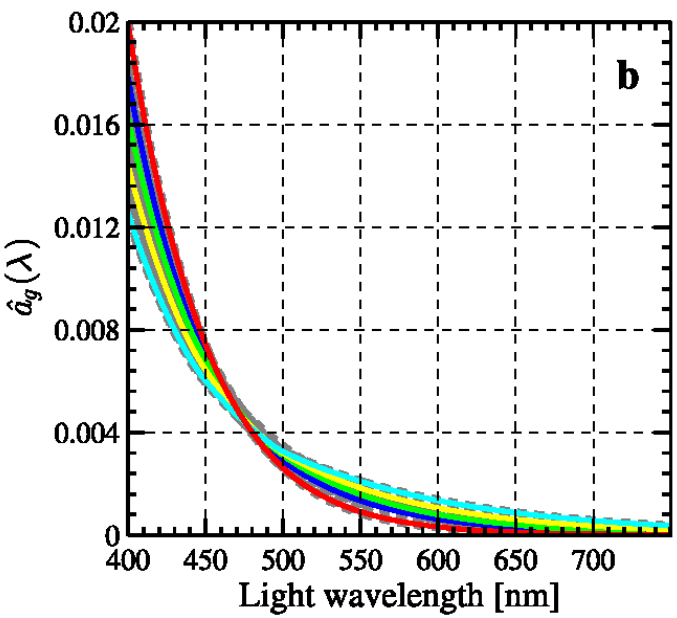
Inequality constraints used in the Generalized Stacked-Constraints Model

Table 1. Inequality Constraints Used in the Generalized Stacked-Constraints Model (GSCM) for Partitioning the Total Light Absorption Coefficient of Natural Water (With Pure-Water Contribution Subtracted), $a_{nw}(\lambda)$, into Phytoplankton, $a_{ph}(\lambda)$, Nonalgal Particulate, $a_d(\lambda)$, and CDOM, $a_g(\lambda)$, Components

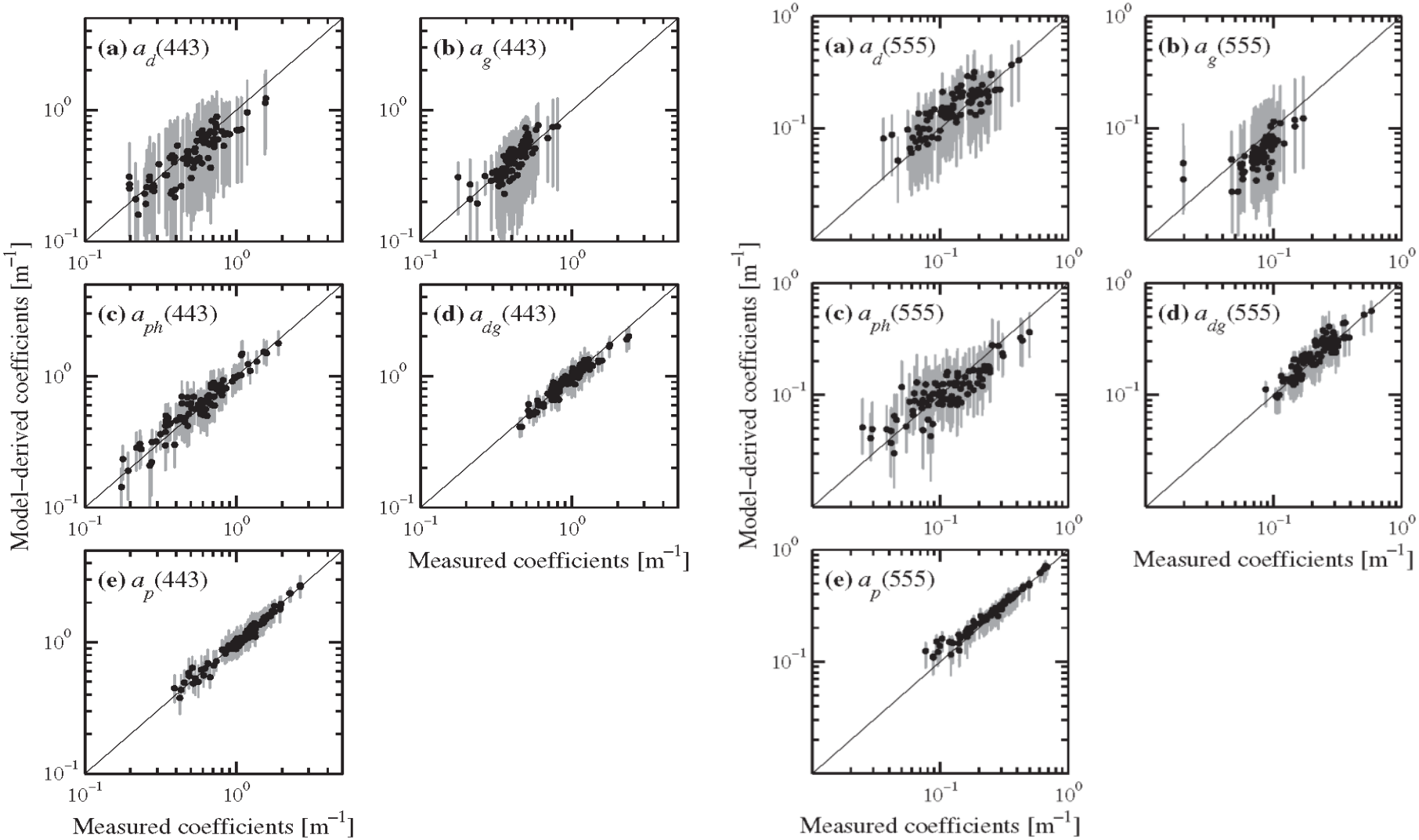
	Constraints	Physical Meaning
#1	$0.75 < a_{ph}(412)/a_{ph}(443) < 1$	The band ratio of phytoplankton absorption characterizing changes within the short-wavelength portion of the major absorption maximum in the blue spectral region
#2	$0.48 < a_{ph}(490)/a_{ph}(443) < 0.77$	Same as above but within the long-wavelength portion of the blue absorption maximum
#3	$0.76 < a_{ph}(469)/a_{ph}(412) < 1.13$	The band ratio of phytoplankton absorption involving both sides of the blue absorption maximum
#4	$0.19 < a_{ph}(555)/a_{ph}(490) < 0.50$	The band ratio of phytoplankton absorption between the green and cyan spectral regions
#5	$0 < a_d(750)/a_d(443) < 0.3$	The band ratio of nonalgal particulate absorption between the NIR and the blue spectral regions

Representative absorption spectra of non-algal particles and CDOM for the Chesapeake Bay





Comparison of model-derived and measured absorption coefficients for 443 and 555 nm for the data set from the Chesapeake Bay

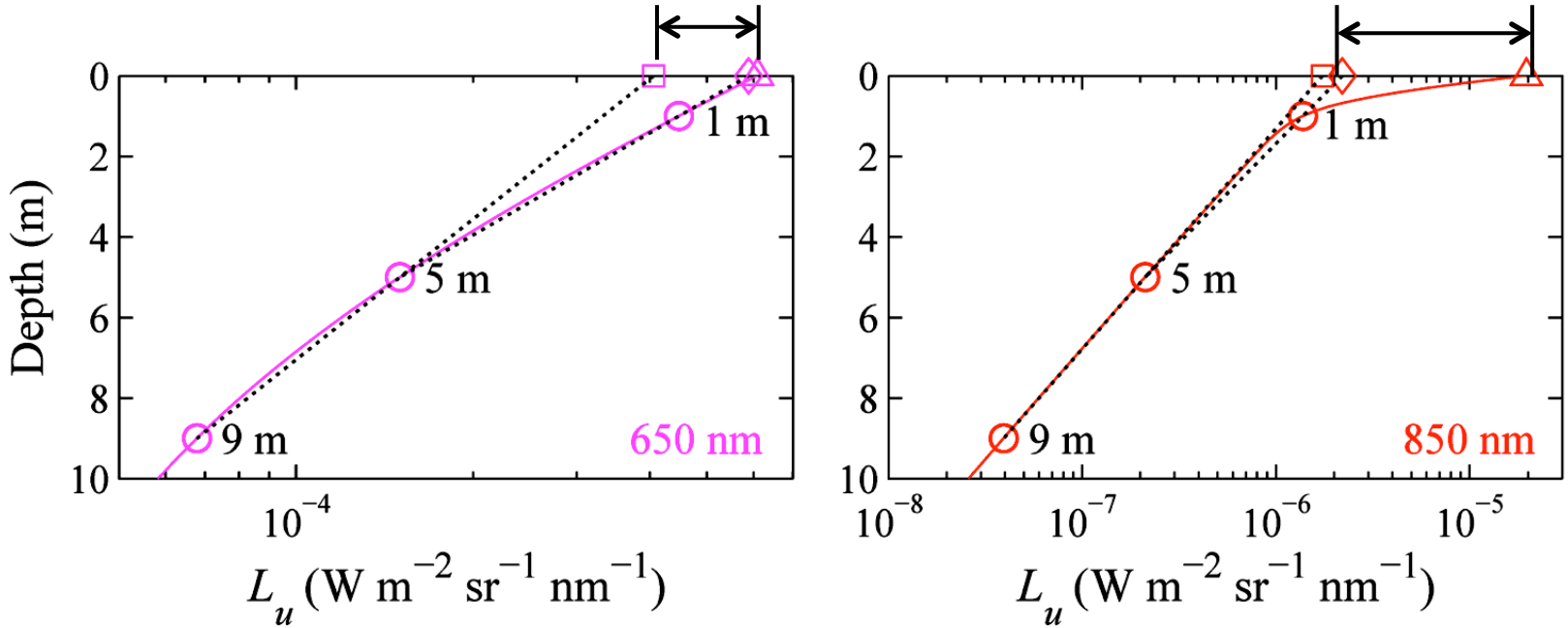


The model performs generally well, for example in the blue the median ratio of model-derived to measured values is less than 10% and the median absolute percent difference less than 20%

Objective 3: Water-leaving radiance from in situ measurements

Extrapolation issue for the long-wavelength portion of the spectrum caused by inelastic radiative process of Raman scattering

Solid lines – actual depth profiles of L_u simulated with radiative transfer model
Dotted lines – extrapolated depth profiles of L_u



- At 650 nm
  - Underestimation by **3.4%** using 1 and 5 m
  - Underestimation by **33.4%** using 5 and 9 m
- At 850 nm
  - Underestimation by **88.8%** using 1 and 5 m
  - Underestimation by **91.2%** using 5 and 9 m

Desired error is ⩽ 5%

applied optics

Effects of inelastic radiative processes on the determination of water-leaving spectral radiance from extrapolation of underwater near-surface measurements

Linhai Li,* Dariusz Stramski, and Rick A. Reynolds

Marine Physical Laboratory, Scripps Institution of Oceanography, University of California San Diego, La Jolla, California 92093-0238, USA
**Corresponding author: lil032@ucsd.edu*

Received 20 May 2016; revised 14 July 2016; accepted 24 July 2016; posted 28 July 2016 (Doc. ID 266597); published 29 August 2016

Extrapolation of near-surface underwater measurements is the most common method to estimate the water-leaving spectral radiance, $L_w(\lambda)$ (where λ is the light wavelength in vacuum), and remote-sensing reflectance, $R_{rs}(\lambda)$, for validation and vicarious calibration of satellite sensors, as well as for ocean color algorithm development. However, uncertainties in $L_w(\lambda)$ arising from the extrapolation process have not been investigated in detail with regards to the potential influence of inelastic radiative processes, such as Raman scattering by water molecules and fluorescence by colored dissolved organic matter and chlorophyll-*a*. Using radiative transfer simulations, we examine high-depth resolution vertical profiles of the upwelling radiance, $L_u(\lambda)$, and its diffuse attenuation coefficient, $K_{L_u}(\lambda)$, within the top 10 m of the ocean surface layer and assess the uncertainties in extrapolated values of $L_w(\lambda)$. The inelastic processes generally increase L_u and decrease K_{L_u} in the red and near-infrared (NIR) portion of the spectrum. Unlike K_{L_u} in the blue and green spectral bands, K_{L_u} in the red and NIR is strongly variable within the near-surface layer even in a perfectly homogeneous water column. The assumption of a constant K_{L_u} with depth that is typically employed in the extrapolation method can lead to significant errors in the estimate of L_w. These errors approach ~100% at 900 nm, and the desired threshold of 5% accuracy or less cannot be achieved at wavelengths greater than 650 nm for underwater radiometric systems that typically take measurements at depths below 1 m. These errors can be reduced by measuring L_u within a much shallower surface layer of tens of centimeters thick or even less at near-infrared wavelengths longer than 800 nm, which suggests a requirement for developing appropriate radiometric instrumentation and deployment strategies.

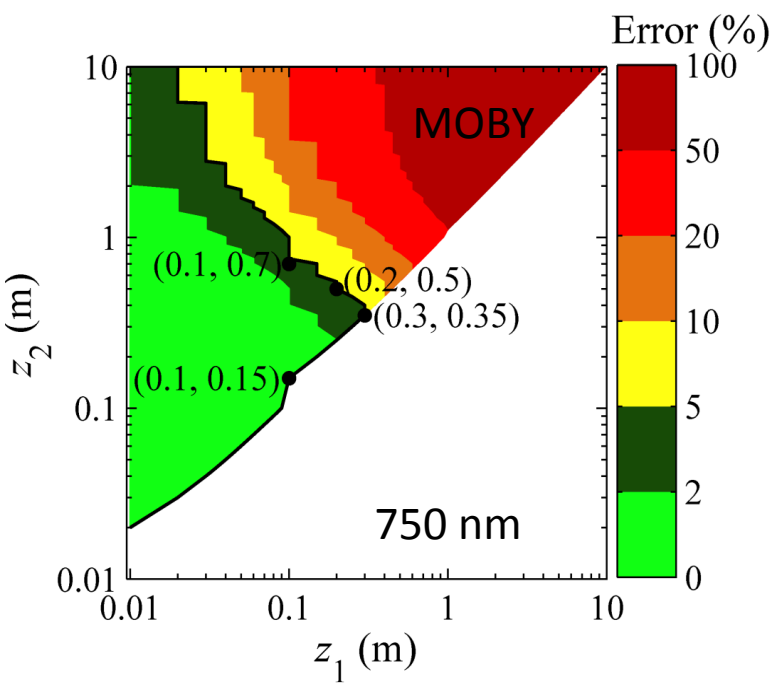
OCIS codes: (010.4450) Oceanic optics; (010.5630) Radiometry; (010.5620) Radiative transfer; (280.4788) Optical sensing and sensors.

http://dx.doi.org/10.1364/AO.55.007050

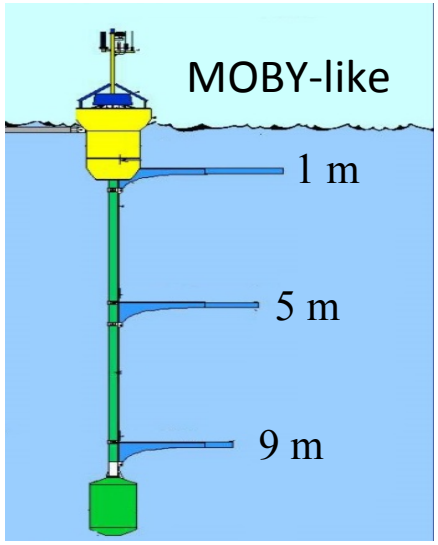
Because of inelastic radiative processes the diffuse attenuation coefficient of upwelling radiance in the red and near-IR varies strongly with depth in the near-surface layer.

In the red and near-IR the errors in water-leaving radiance determined from extrapolation of near-surface underwater measurements taken at depths ≥ 1 m can be very large (tens of percent).

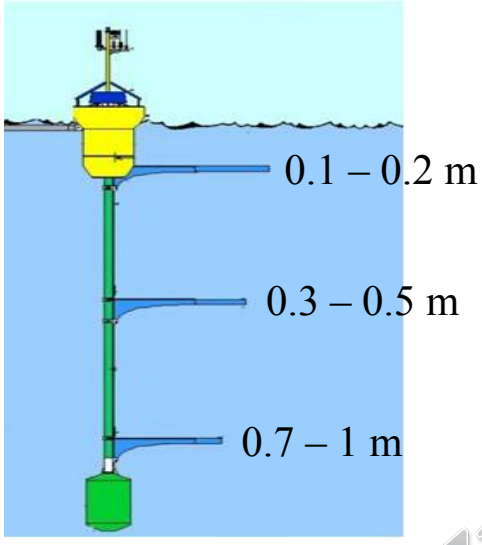
Measurements must be made within the top ~0.5 – 1 m of the water column to ensure errors less than 5%, for example at 0.2 and 0.5 m to ensure that the error at 750 nm is less than 5%.



Unacceptable configuration



Required configuration



Current and near-future work

- **IOP METHODOLOGY**: Determination of pathlength amplification factor for measurements of particulate absorption coefficient using filter-pad technique in the UV spectral region.

- **IOP INVERSION:** Evaluation of the prototype (based on the Chesapeake Bay case study) absorption partitioning model with different data sets shows inconsistent performance, for example good for Puget Sound data and not good enough for the global data set. The development of another version of partitioning model based on different concept is underway. The initial tests are very promising.

- **WATER-LEAVING RADIANCE**: Theoretical study is completed. A proposal to develop a radiometric system with appropriate configuration for near-surface measurements was declined by NASA three times. The reviews did not, however, identify any significant issues in the proposed development.