



**TÉLÉDÉTECTION OPTIQUE DES EAUX CÔTIÈRES OPTIQUEMENT
COMPLEXES ET PEU PROFONDES : APERÇU DE LA QUALITÉ DE L'EAU, DE
LA HAUTEUR DE LA COLONNE ET DE LA COMPOSITION BENTHIQUE**

**Optical remote sensing of optically complex and shallow coastal waters: insight into water
quality, column height and benthic composition**

Thèse présentée

dans le cadre du programme de doctorat en sciences de l'environnement

en vue de l'obtention du grade de Philosophiae Doctor (Ph.D.)

PAR

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Mai 2025

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Dépôt initial le 14 Janvier 2025

Dépôt final le 28 Mai 2025

UNIVERSITÉ DU QUÉBEC À RIMOUSKI

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তোমার জন্য...

In loving memory of my **Mā**,
whose strength carried me here

ACKNOWLEDGMENTS

With immense gratitude and a profound sense of fulfilment, I take this opportunity to express my heartfelt thanks to all those who have contributed to this journey of not only obtaining a doctorate, but also for discovery, growth, and achievement.

First and foremost, I am deeply indebted to my esteemed supervisor, Dr. Simon Bélanger, whose unwavering support, visionary guidance, exceptional mentorship, and unfathomable freedom in doing research have been the cornerstone of this work. Your insights, patience, and dedication have not only enriched this research but also inspired me to strive to get into the core concepts.

I extend my sincere appreciation to my co-supervisor Dr. Cédric Fichot and esteemed collaborator Dr. John Hedley for their invaluable contributions in teaching me the core concepts of optics in coastal waters, constructive feedback in writing the articles, and most importantly constant encouragement. Your expertise and generosity in sharing knowledge have significantly shaped the course and outcomes of this thesis.

I am profoundly grateful to UQAR for providing the resources and infrastructure essential for the successful completion of this research. I also express my gratitude to all the staff and personnel at the Département de Biologie, Chimie et Géographie for the access to laboratory facility and materials, helping with fieldwork equipment and streamlining the official formalities.

My heartfelt thanks to all my friends and colleagues in the AQUATEL lab for helping me greatly with learning French, informing me about the local culture and lifestyle, helping me greatly with field visits and university formalities and also teaching me how to party till 4h in the morning ! I wanna extend my token of appreciation to my dear friend and colleague Dr. Rakesh Kumar Singh, for not only teaching me very key concepts for the successful completion of this thesis but also for realising the epistemological aspects of doing research.

On a deeply personal note, I wish to dedicate this thesis to my late mother Chumki Mazumder Mukherjee, whose indomitable spirit and unwavering belief in me have been my guiding light, not only in the course of this thesis but at every point in my life. Her memory lives on in every word and every endeavour within these pages.

To my close circle, who have been my constant companions through the highs and lows, thank you for your humour, empathy, and countless moments of joy that have kept me balanced and grounded. I express my heartfelt appreciation to my dear friend Utsab for letting me stay at his apartment during a difficult stretch this year, which helped me in wrapping up the thesis adequately.

I extend my deepest gratitude to BAM for standing by my side during challenging times and inspiring me to keep moving forward. The discussions of the struggles of life and work among us have been a source of strength, and I thank you from my heart for your cooperation in this journey.

To Rachana, the brightest star in my mindscape, thank you for your unconditional love, patience, and encouragement for the last six years. The overwhelming geographic distance between us has been difficult and tedious at times, but your unconditional faith in me has been my sanctuary during moments of doubt and despair and my motivation to persevere.

This thesis is not merely a culmination of my academic pursuits but also a reflection of the collective efforts, kindness, and support of everyone who has walked alongside me on this path. To all of you, I owe a debt of gratitude that words can scarcely convey.

FOREWORD

The successful development of this thesis was made possible through the invaluable support provided by research projects conducted by, or in collaboration with, the Laboratoire d'optique aquatique et de télédétection (AQUATEL) at the Université du Québec à Rimouski (UQAR). Funding from different projects, combined with generous scholarship grants awarded to the author, have played a pivotal role in facilitating the research and achieving the milestones outlined in this work, as detailed below.

The objectives in this thesis are achieved for the partial fulfilment of the “WaterSat Imaging Spectrometer Experiment (WISE) for optically shallow inland and coastal waters assessment (WISE-Man)” project funded by the Canadian Space Agency (CSA) under the “Flights and Fieldwork for the Advancement of Science and Technology (FAST-2017)”, Fisheries and Oceans Canada via the Coastal Environmental Baseline Program, and Québec-Ocean. Specifically, this thesis addressed the research questions in WP2 in the FAST-2017, i.e. Hyperspectral inversion for bathymetry, water constituents and bottom-type mapping. Additional funding was also provided from the Algae-WISE project, approved by CSA under FAST-2019 proposal. The scholarships were obtained from the Fondation de l'UQAR, through a Research Merit Scholarship and Québec-Ocean for publication grant.

ABSTRACT

In the 21st century, coastal regions have become global hotspots for human settlements due to their unique environmental, social, and economic benefits. These areas serve as sinks for substantial organic matter from riverine and terrigenous sources, along with sedimentary mineralization, which influence coastal water quality in addition to anthropogenic stressors. However, global warming—manifested in rising sea levels, increasing temperatures, and sea ice melting—has profoundly impacted coastal ecosystems and water quality, especially in northern temperate regions. In shallow coastal zones, these changes also alter water depth and benthic structures, threatening numerous lifeforms. Monitoring water quality and benthic composition in such dynamic environments is challenging due to the vast spatial and temporal scales involved. Conventional biogeochemical and bio-optical sampling methods are often inadequate. To address this, remote sensing reflectance (R_{rs}) derived from airborne or satellite observations is widely used to estimate optically significant constituents (OSCs), such as chlorophyll-a concentration ($[chl]$), suspended particulate matter (SPM) and coloured dissolved organic matter (CDOM). In optically shallow waters, water depth and benthic substrate composition are also derived apart from the OSCs. In the 1980s, these parameters were retrieved using empirical approaches such as simple ratios of the spectral bands of a sensor; however, in recent times, semi-analytical (SA) inversion models based on radiative transfer (RT) theory for shallow waters are more frequently used. However, the SA models typically neglect naturally occurring inelastic scattering processes, such as sun-induced fluorescence (SIF) from $[chl]$ and CDOM, which can significantly contribute to R_{rs} in CDOM-rich waters. Moreover, RT inversion is an "ill-posed" problem, where multiple combinations of OSCs, water depth, and benthic types can yield similar R_{rs} spectra, making the retrieval process ambiguous. Additionally, existing inversion models lack robust methods to quantify the uncertainty associated with retrieved parameters. The main objective of this thesis was to improve our understanding of dominant optical processes (scattering, absorption) in CDOM-rich optically shallow coastal waters (specifically at the Manicouagan Peninsula (MP) in Côte-Nord, Québec, where an extensive fieldwork campaign was carried out in Summer 2019 as part of the WISE-Man project) and develop a robust method to retrieve both estimates and associated uncertainty of OSCs and benthic information from spectral R_{rs} .

The first article evaluated optical closure through extensive RT simulations using *in situ* inherent optical properties (IOPs) collected in MP's CDOM-rich waters. The analysis revealed significant uncertainties in measurements from the A-Sphere absorption meter and the BB9 volume scattering function (VSF) meter. The A-Sphere's absorption values were spectrally biased, potentially due to inelastic scattering effects of $[chl]$ and CDOM within the integrating sphere in the presence of a monochromatic light source, while the BB9 struggled with weak light scattering by organic particles. The study also demonstrated that SIF from $[chl]$ and CDOM contributes approximately 20% to the green and red spectral regions of measured R_{rs} .

The second article introduced a novel probabilistic inversion framework called Semi-Analytical Bayesian Error Retrieval (SABER). SABER employed Markov Chain Monte Carlo (MCMC) sampling to retrieve posterior distributions of OSCs, water depth, and benthic properties while quantifying retrieval uncertainties using the Maximum-a-Posterior (MAP) approach. The algorithm was tested on global *in situ* and synthetic datasets spanning eight optical water types, demonstrating robust performance in optically deep and shallow waters. Retrieval uncertainty was highest for chlorophyll concentration and lowest for particulate backscatter.

The third article focused on SABER's performance and uncertainty sources in MP's optically complex waters. A sensitivity analysis revealed that the spectral slope of detrital absorption (s_{dg}) and the presence of dark benthic substrates, such as eelgrass, were key drivers of retrieval uncertainty. By subtracting SIF-equivalent R_{rs} , estimated using a separate SA model, from observed R_{rs} before inversion, the accuracy of retrieved OSCs was improved. Water depth estimates were highly accurate when depths were within the optical penetration range. For benthic types, the region predominantly featured sand interspersed with eelgrass patches. Retrievals for sand were robust, but uncertainties for eelgrass presence were nearly tenfold higher due to weak signal strength.

Overall, this thesis advanced the forward and inverse RT modeling for OSC and benthic property retrieval in optically complex, CDOM-rich shallow waters. While challenges remain, such as refining SA assumptions for shallow waters and adapting methodologies for satellite sensors, this work represents a significant step towards understanding radiative transfer in nearshore ecosystems. It lays the foundation for more robust monitoring and management of these vital coastal regions.

Keywords : coastal ecosystem, CDOM, optically shallow, radiative transfer, inverse problem, Sun-Induced Fluorescence, uncertainty, benthic reflectance, Saint Lawrence Estuary

RÉSUMÉ

Au 21^{ème} siècle, les régions côtières sont devenues des centres névralgiques pour les établissements humains à l'échelle mondiale, en raison de leurs avantages environnementaux, sociaux et économiques uniques. Ces zones servent de réceptacles pour une quantité importante de matière organique provenant de sources fluviales et terrigènes, ainsi que de la minéralisation sédimentaire, influençant la qualité de l'eau côtière en plus des pressions anthropiques. Cependant, le réchauffement climatique — marqué par l'élévation du niveau de la mer, l'augmentation des températures et la fonte des glaces — a eu un impact profond sur les écosystèmes côtiers et la qualité de l'eau, en particulier dans les régions tempérées nordiques. Dans les zones côtières peu profondes, ces changements modifient également la profondeur de l'eau et les structures benthiques, menaçant de nombreuses formes de vie. Surveiller la qualité de l'eau et la composition benthique dans de tels environnements dynamiques est un défi, en raison des vastes échelles spatiales et temporelles des processus océanographiques. Les méthodes conventionnelles d'échantillonnage biogéochimique et bio-optique se révèlent souvent inadéquates. Pour y remédier, la réflectance mesurable par télédétection (R_{rs}), dérivée d'observations radiométriques aéroportées ou satellitaires, peut être utilisée pour estimer les constituants optiquement significatifs (OSC), tels que la concentration en chlorophylle-a ($[chl]$), les matières en suspension (SPM), la profondeur de l'eau et la composition benthique. Ces paramètres sont obtenus par inversion mathématique de modèles semi-analytiques (SA) basés sur une approximation des équations de transfert radiatif (RT) pour les eaux peu profondes. Cependant, les modèles traditionnels négligent généralement les processus de diffusion inélastique naturels, tels que la fluorescence induite par le soleil (SIF) provenant du $[chl]$ et de la matière organique dissoute colorée (CDOM), qui peuvent contribuer de manière significative au R_{rs} dans les eaux riches en CDOM. De plus, l'inversion RT est un problème « mal posé » : de multiples combinaisons d'OSCs, de profondeurs d'eau et de types benthiques peuvent produire des spectres R_{rs} similaires, rendant le processus d'inversion ambigu. Par ailleurs, les modèles actuels d'inversion manquent de méthodes robustes pour quantifier l'incertitude associée aux paramètres estimés. L'objectif principal de cette thèse était d'améliorer notre compréhension des processus optiques dominants (diffusion, absorption) dans les eaux côtières optiquement peu profondes riches en CDOM (notamment dans la péninsule de Manicouagan (MP) en Côte-Nord, Québec, où une vaste campagne de terrain a été menée à l'été 2019 dans le cadre du projet WISE-Man) et de développer une méthode robuste permettant d'estimer les caractéristiques optiques de la colonne d'eau (OSC) ainsi que les propriétés benthiques à partir des spectres de R_{rs} , tout en quantifiant l'incertitude associée à ces estimations.

Le premier article évalue la fermeture optique à travers des simulations RT approfondies utilisant des propriétés optiques intrinsèques (*in situ*) collectées dans les eaux riches en CDOM de la MP. L'analyse a révélé des incertitudes importantes dans les mesures des instruments A-Sphere et BB9. Les valeurs d'absorption de l'A-Sphere étaient biaisées, probablement en

raison des effets de diffusion inélastique dans la sphère intégrante, tandis que le BB9 avait des difficultés à mesurer la fonction de diffusion volumique (VSF) pour les particules organiques faiblement diffusantes. L'étude a également démontré que la SIF provenant du $[chl]$ et du CDOM contribue à environ 20 % aux régions spectrales verte et rouge de la R_{rs} mesurée. Le deuxième article introduit un cadre d'inversion probabiliste novateur appelé SABER (*Semi-Analytical Bayesian Error Retrieval*). SABER utilise l'échantillonnage par chaîne de Markov (MCMC) pour restituer les distributions postérieures des OSCs, des profondeurs d'eau et des propriétés benthiques, tout en quantifiant les incertitudes grâce à l'approche du *Maximum a Posteriori* (MAP). L'algorithme a été testé avec succès sur des ensembles de données *in situ* et synthétiques mondiaux couvrant huit types d'eau optique, montrant des performances solides dans les eaux profondes et peu profondes. L'incertitude des estimations était la plus élevée pour la concentration en chlorophylle et la plus faible pour la rétro-diffusion particulière. Le troisième article se concentre sur les performances de SABER et les sources d'incertitude dans les eaux optiquement complexes de la MP. Une analyse de sensibilité a révélé que la pente spectrale de l'absorption détritique (s_{dg}) et la présence de substrats benthiques sombres, comme les herbiers de zostères, étaient les principaux facteurs d'incertitude. Nous avons observé une amélioration de du modèle SABER quand la SIF, estimée de manière semi-analytique a priori, était soustraite de la R_{rs} . Les estimations de profondeur d'eau étaient précises lorsque les profondeurs étaient inférieures ou égales à la profondeur de pénétration optique. Pour les types benthiques, la région présentait principalement du sable avec des patchs intermédiaires de zostères. Les estimations pour le sable étaient robustes, mais les incertitudes pour les zostères étaient environ dix fois plus élevées, en raison d'un signal faible. Dans l'ensemble, cette thèse fait progresser les modèles RT directs et inverses pour la restitution des OSCs et des propriétés benthiques dans les eaux peu profondes complexes riches en CDOM. Bien que des défis subsistent, tels que l'amélioration des hypothèses SA pour les eaux peu profondes et l'adaptation des méthodologies aux capteurs satellitaires, ce travail représente une étape importante vers une meilleure compréhension du transfert radiatif dans les écosystèmes côtiers.

Mots clés : Écosystème côtier, CDOM, eaux optiquement peu profondes, transfert radiatif, problème inverse, fluorescence induite par le soleil, incertitude, réflectance benthique, Estuaire du Saint-Laurent

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GENERAL INTRODUCTION

Modeling the coastal ecosystem

Ecosystems are dynamic and interconnected systems comprising living components, such as vegetation, animals, and microorganisms, interacting with non-living elements, including water, sediment, and minerals. These systems function as cohesive units through bi-directional exchanges of mass and energy (Weathers et al., 2013). Ecosystem stability and productivity rely heavily on external inputs like solar radiation or organic matter transported through riverine plumes. Quantifying these mass-energy fluxes is critical for understanding ecosystem health and predicting their responses to natural and anthropogenic disturbances (Doney et al., 2001).

Among global ecosystems, marine and coastal ecosystems stand out for their ecological and socio-economic significance. The oceanic/marine systems interact with terrestrial land through oceanic currents. The variation in water properties such as salinity, density, temperature, as well as waves and currents, creates stratified layers in the water column; however, upwelling in the ocean breaks the stratified layers and vertically mixes the water layers (Yang, 2014). It increases productivity in the ocean, supporting various living organisms that eventually create a heterogeneous family of species, implicitly thriving on the neighbouring abiotic compounds, resulting in the creation of a marine ecosystem. Marine ecosystems play a vital role in maintaining global temperature, pH level, dissolved gas concentration and biogeochemical (BGC) cycles.

In an interconnected ecosystem, the heterogeneity and complexity of different species and the mass-energy exchange are more profoundly observed in coastal areas compared to deep oceans. Coastal ecosystems, though covering less than 10% of Earth's surface, contribute disproportionately to global productivity. They account for 30% of marine primary production and 90% of marine fisheries (Millennium Ecosystem Assessment, 2005). They also serve as

hotspots for biogeochemical cycling, sediment deposition, and nutrient mineralization, supporting some of the highest biodiversity on Earth (Martin, 2013). At the same time, these regions are highly vulnerable to anthropogenic pressures due to their proximity to human populations—60% of humanity resides within 50 km of the coast (Watson et al., 1996). Understanding and mitigating the impacts of these pressures are essential for maintaining biodiversity and ecosystem services.

The dynamic and heterogeneous nature of coastal ecosystems makes them inherently difficult to monitor and model. The high spatial and temporal variability in physical, chemical, and biological processes challenges researchers to collect sufficient *in situ* data from field sampling to represent these systems accurately. Traditional modelling approaches involve simplifying complex systems into mathematical or numerical frameworks, focusing on key processes and variables while discarding less influential ones (Jørgensen and Bendoricchio, 2001). However, these models rely on *in situ* observations for calibration and validation, but logistical, financial, and technical constraints often limit the availability of such data, particularly at scales commensurate with the variability of coastal processes.

In response to these challenges, remote sensing (RS) has emerged as a transformative tool for studying coastal ecosystems. RS is the science of acquiring data about Earth's surface using sensors that operate at various wavelengths, from visible light to microwaves (Wright et al., 1980). Satellite-mounted sensors provide synoptic, repetitive coverage at scales that are impossible to achieve with field surveys alone. This capability makes RS particularly valuable for capturing the dynamic processes characteristic of coastal ecosystems, such as wave propagation, sediment transport, organic plumes and phytoplankton blooms (Klemas, 2010).

Remote sensing can contribute to coastal ecosystem studies in two primary ways. First, it can serve as an environmental modeling tool to derive biogeochemical datasets that can replace or supplement *in situ* measurements. For instance, bio-optical algorithms applied to satellite-derived reflectance data can estimate key biogeochemical variables such as chlorophyll-

a concentration, suspended sediment, or coloured dissolved organic matter (Arsanjani et al., 2009). These data can be used to calibrate and validate ecosystem models, reducing uncertainties in regions where field data are scarce. Second, RS can directly infer ecological and biophysical dynamics without the need for intermediary bio-optical models. For example, time-series analyses of satellite imagery can reveal trends in coastal productivity, habitat degradation, or the impacts of climate change, providing actionable insights for policymakers and conservationists (Jensen, 2014). The next subsection discusses the formal theory of aquatic RS applicable to marine and coastal ecosystems.

Optical Remote Sensing of coastal waters

Historical overview : Optical RS spanning in the Visible and Near Infra-Red (Vis-NIR) spectral region of the electromagnetic spectrum has shown great potential to be used with marine and coastal ecosystem models (Klemas, 2010). Optical sensors, such as spectroradiometers and imaging cameras, are mounted on satellites to provide repeated observations and a wide field of view, depending on the satellite's orbit and altitude. The diversity in sensor configuration and spectral channels makes it useful in multidisciplinary aspects of studying coastal ecosystems (Jensen, 2014). Aquatic Space borne RS, specifically Ocean Colour Remote Sensing (OCRS) started with the “Coastal Zone Color Scanner Experiment” (CZCS) experimental sensor for coastal and open oceanic observation, that was in service between 1978 and 1986 (Hovis et al., 1980; McClain, 2009). The successful CZCS campaign led to the launch of several multispectral (MS) OCRS sensors in the 1990s, such as the Modular Optoelectronic Scanner (MOS) (Zimmermann et al., 1993), the Sea-viewing Wide Field-Of-View Sensor (SeaWiFS) (Hooker and Esaias, 1993), the Moderate Resolution Imaging Spectrometers (MODIS) (Pagano and Durham, 1993) and the Medium Resolution Imaging Spectrometer (MERIS) (Rast et al., 1999). These sensors had spatial resolution > 300 m, which limited their ability to resolve fine-scale events in coastal and inland waters.

The USGS Landsat satellite series, including the Thematic Mapper (TM) on Landsat 4-5, the Enhanced TM+ (ETM+) on Landsat 7, the Operational Land Imager (OLI) on Landsat 8, and OLI-2 on Landsat 9 offers high spatial resolution data. Although originally designed for terrestrial applications, these satellites have been widely utilized for mapping coral reefs in optically shallow waters (Jupp and Mayo, 1982; Jupp et al., 1985; Bello-Pineda et al., 2005; Roelfsema et al., 2018; Kovacs et al., 2018) and extensively for assessing coastal water quality (Giardino et al., 2001; Dörnhöfer and Oppelt, 2016; Wei et al., 2019; Sharaf et al., 2019; Pahlevan et al., 2021; Smith et al., 2021; Pahlevan et al., 2022). Similarly, the European Copernicus program's Sentinel satellite series, particularly Sentinel-3A and 3B equipped with the Ocean and Land Colour Instrument (OLCI), has been actively employed in coastal water quality studies and benthic mapping due to OLCI's 21 spectral bands with multiple bands in visible domain tailored for OCS (Salama and Verhoef, 2015; Eleveld et al., 2017; Barnes et al., 2018; Blix et al., 2018; Xue et al., 2019; Werther et al., 2022b; Pahlevan et al., 2022; Jiang et al., 2023).

Hyperspectral (HS) sensors with a high count of spectral bands enabled the contiguous acquisition of high-quality spectral signatures for different Optically Significant Constituents (OSCs) in the coastal waters. In optically shallow waters, water column height and benthic substrate composition have also been additionally derived from space-borne HS sensors such as PRISMA (Alevizos et al., 2022; Minghelli et al., 2021; Chan, 2022). HS aquatic data is also available from the HICO and DESIS sensors, mounted on the International Space Station (ISS) and have been successfully applied in bathymetry estimation and benthic mapping (Garcia et al., 2014a,b). NASA has recently launched the Plankton, Aerosol, Cloud, ocean Ecosystem (PACE) satellite with an HS spectroradiometer named the Ocean Color Instrument (OCI) acquiring high-quality ocean colour data between 320-895 nm wavelength with 1.25-2.5 nm intervals (Werdell et al., 2024). Similarly, many airborne HS sensors (AVIRIS-NG, APEX, CASI, HyMAP, PHILLS, PRISM etc.) with a high spatial-spectral resolution (< 10 m spectral interval and < 2 m pixel size) have been flown over aquatic targets to address the sensor capability, both for water quality detection (O'Shea et al., 2021, 2023;

Jay and Guillaume, 2016) and bathymetry and benthic mapping (Klonowski, 2007; Marcello et al., 2018; Garcia et al., 2018; Hedley et al., 2017; Uhl et al., 2016).

Technical overview : The spectral radiance signal emerging from the water, measured by OCRS sensors, originates from a series of interactions involving : **1.** the aquatic medium and optically significant constituents (OSCs) within the water column (Werdell et al., 2018), **2.** the air-water interface resulting in specular reflection (glint) and **3.** the atmospheric components, such as gas molecules and aerosols, through which the upwelling radiation travels before reaching the sensor (Singh and Shanmugam, 2014). To accurately retrieve aquatic information, the sensor-acquired signal must undergo corrections for **I.** atmospheric path radiance, **II.** spectral absorption by gases such as water vapour and ozone, and **III.** specular reflection of solar radiation ; i.e., glint at the water surface (Mobley et al., 2016). This correction process, known as atmospheric correction (AC), is crucial for ensuring accurate representations of aquatic targets in OCRS. However, the radiometric datasets utilized in this thesis are derived from vertically binned, sub-surface, or surface measurements. As such, the implementation of AC techniques was not required. Consequently, this thesis does not provide a detailed discussion on AC methods. Instead, it focuses on the characterization of underwater light field in a manner relevant to OCRS.

The OCRS sensors (space-borne/air-borne/hand-held) measure the water-leaving radiant flux (Φ) with directional dependence using photodetectors. The spectral dependence is determined using a filter and diffuser setup preceding the photodetector. These sensors scale Φ using mainly two radiometric quantities, radiance and irradiance, mainly to measure the radiant energy and quantitatively describe the aquatic light field (Kirk, 1983; Mobley, 1994). Radiance (L , $\mu\text{W m}^{-2} \text{ nm}^{-1} \text{ sr}^{-1}$), as shown in Fig. 1a, is the radiant flux (Φ) in a given direction per unit solid angle (Ω) per unit projected area (A) at a spectral wavelength (λ) at right angles to the direction of propagation (Kirk, 1983). Irradiance (E , $\mu\text{W m}^{-2} \text{ nm}^{-1}$) is measured using a planar cosine collector as Φ incident perpendicularly on or emitted from water surface with the projected area (A) for varying λ (Kirk, 1983). Irradiance can be divided into two-flow components; downwelling irradiance (E_d) and upwelling irradiance (E_u) (Kirk, 1983) (Fig.

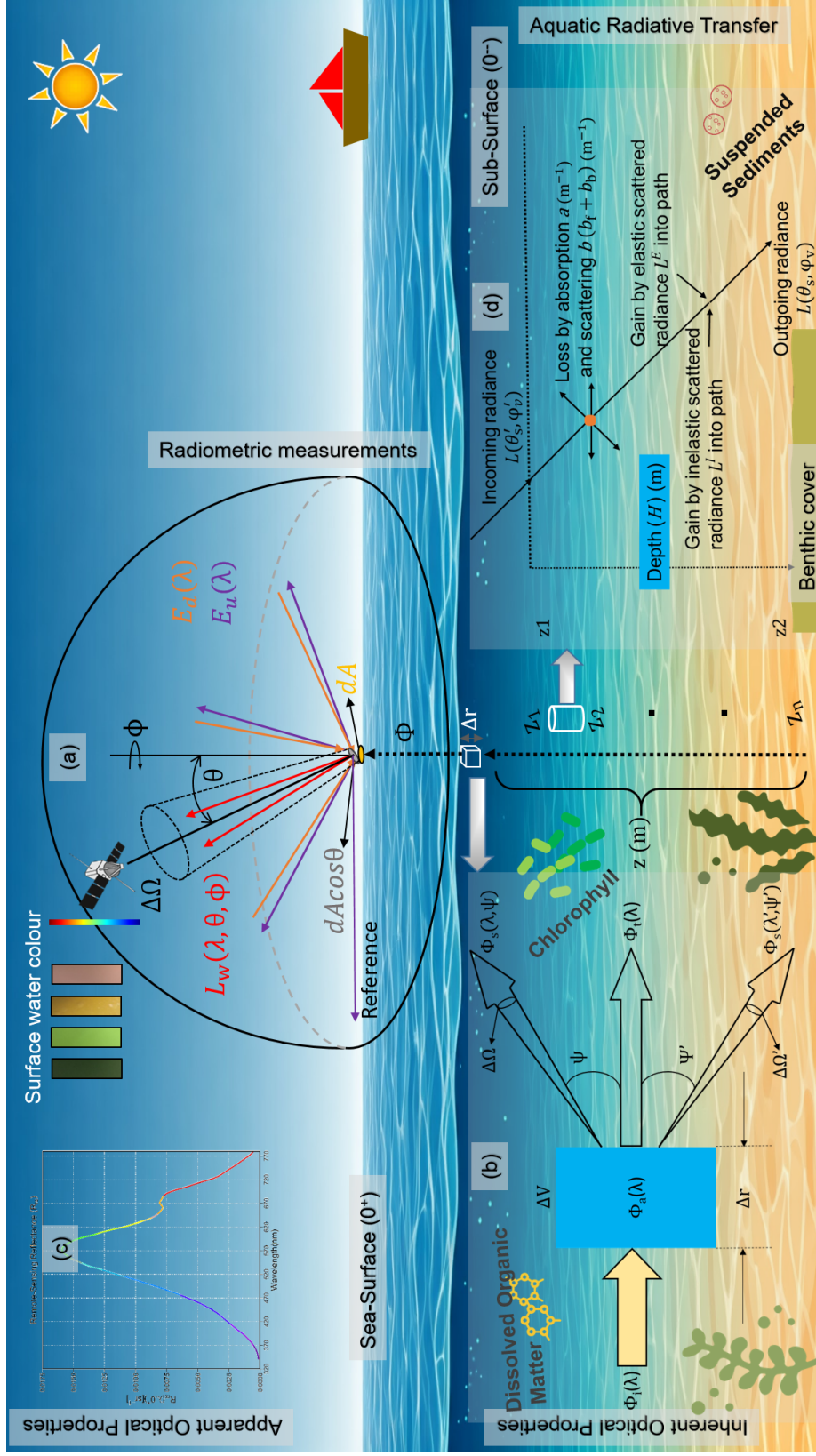


FIGURE 1 – Schematic Diagram of the fundamentals of OCERS. (a) shows the acquisition of radiometric variables (RV), such as upwelling radiance and irradiance for both up and down-welling directions, (b) shows how the Inherent Optical Properties (IOPs) of the water column affect the incident radiant flux (Φ), (c) shows the most commonly used Apparent Optical Property (AOP), i.e., water-leaving R_{rs} [sr^{-1}], derived from radiometric variables shown in a. (d) is the illustration of radiative transfer in optically shallow waters; how the IOPs in water column and benthic contribution affects the water-leaving RV/AOP. b and d panels are redrawn with modifications from Mobley (1994) and Albert (2004), respectively, under the common creative license.

1a). These irradiances are specifically related to radiance as shown in Eq. 1 c,d (λ is omitted in following for simplicity).

$$L(\theta, \phi, \lambda) = \frac{\Phi}{A \cdot \Omega \cdot \lambda} \quad (1a)$$

$$E(\lambda) = \frac{\Phi}{A \cdot \lambda} \quad (1b)$$

$$E_d = \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi/2} L(\theta, \phi) \cos \theta \sin \theta d\theta d\phi \quad (1c)$$

$$E_u = - \int_{\phi=0}^{2\pi} \int_{\theta=\pi/2}^{\pi} L(\theta, \phi) \cos \theta \sin \theta d\theta d\phi \quad (1d)$$

When sunlight propagates through water, it interacts with both the water and the optically significant constituents (OSCs), undergoing two primary processes : absorption and scattering. These interactions are quantified by the absorption coefficient and the Volume Scattering Function (VSF), which together are known as Inherent Optical Properties (IOPs). IOPs depend solely on the composition of the aquatic medium and not on the geometry of the incident light field (Preisendorfer, 1976). Formally, for an incident monochromatic light such as sunlight with spectral radiant power $\Phi_i(\lambda)$ passing through a small water volume ΔV of thickness Δr , a portion of the incident power, $\Phi_a(\lambda)$, is absorbed by the water and its OSCs (Fig. 1b). This absorption occurs when the vibrational frequencies of water or OSC molecules resonate with the frequency of the incident radiation. The absorbed energy, $\Phi_a(\lambda)$, is subsequently transformed into heat, emitted at different wavelengths, or utilized in biological or chemical processes such as photosynthesis by phytoplankton. The absorbance $[A(\lambda)]$ derived absorption coefficient; $a(\lambda)$ (m^{-1}) quantify the fraction of light absorbed as :

$$A(\lambda) = \frac{\Phi_a(\lambda)}{\Phi_i(\lambda)}, \quad a(\lambda) = \frac{dA(\lambda)}{dr} \quad (2)$$

Scattering occurs when absorbed photons are re-emitted. If the re-emission wavelength matches the incident wavelength, the process is termed *elastic scattering*; otherwise, it is *inelastic scattering* such as Sun Induced Fluorescence (SIF) from Chlorophyll-a and coloured dissol-

ved organic matter, respectively (Albert, 2004). The scattered light changes direction and is described by the volume scattering function (VSF); $\beta(\psi, \lambda)$ ($\text{m}^{-1} \text{sr}^{-1}$), which quantifies scatterance per unit solid angle ($\Delta\Omega$) and per unit volume (ΔV) at a scattering angle ψ , where the scatterance ($B(\lambda)$) is the fraction of the incident light scattered out of the original path at an angle Ψ into a solid angle $\Delta\Omega$ including all directions centered on scattering angle Ψ (Fig. 1b) :

$$B(\lambda) = \frac{\Phi_s(\lambda)}{\Phi_i(\lambda)}, \quad \beta(\psi, \lambda) = \frac{B(\lambda)}{\Delta r \Delta\Omega} = \frac{\Phi_s(\psi, \lambda)}{\Phi_i(\lambda) \Delta r \Delta\Omega} \quad (3)$$

Integrating $\beta(\psi, \lambda)$ over all solid angles (Ω) provides the scattering coefficient; $b(\lambda)$ (m^{-1}) :

$$b(\lambda) = \int_{\Omega} \beta(\psi) d\Omega = 2\pi \int_0^{\pi} \beta(\psi) \sin \psi d\psi \quad (4)$$

This total scattering coefficient can be further divided into forward ($0 \leq \psi \leq \pi/2$) and backward ($\pi/2 \leq \psi \leq \pi$) directions :

$$b(\lambda) = b_f(\lambda) + b_b(\lambda) = 2\pi \int_0^{\pi/2} \beta(\lambda, \psi) \sin \psi d\psi + 2\pi \int_{\pi/2}^{\pi} \beta(\lambda, \psi) \sin \psi d\psi \quad (5)$$

Apparent Optical Properties (AOP) are properties that depend on both the medium properties and geometrical structure of the aquatic light field (Kirk, 1983). Therefore, AOPs can be efficiently used to derive abundance of an OSC, such as the Chlorophyll-a concentration in water column or the benthic substrate in optically shallow water. The most commonly used AOP in OCRS is the Remote Sensing reflectance (R_{rs} ; [sr^{-1}]) (Mobley, 1999) (Fig. 1c) and it is defined as ratio of water-leaving upwelling radiance (L_u) to downwelling plane irradiance (E_d) (Mobley, 1994). R_{rs} serves as a proxy of how much of the downwelling light incident onto the water surface is returned through the surface in a particular viewing direction. The spectral R_{rs} just above the water surface (0^+) is obtained as :

$$R_{rs}(0^+, \lambda, \theta, \phi) = \frac{L_w(0^+, \lambda, \theta, \phi)}{E_d(0^+, \lambda, \theta, \phi)} \quad (6)$$

Radiative transfer (RT) theory establishes the connection between the IOPs and AOPs by solving equations that describe the underwater light field, while incorporating boundary conditions at the air-sea interface and the seafloor. As illustrated in Fig. 1d, radiance $L(\theta', \phi')$ traveling through a water column of depth Δz (from z_1 to z_2) and emerging as $L(\theta, \phi)$. Within the water column, absorption $a(\lambda)$ and scattering $b(\lambda)$ govern the modification of the light field. RT theory accounts for the attenuation of radiance due to the extinction caused by $a(\lambda)$ and $b(\lambda)$, as well as the addition of radiance along the propagation path. This added radiance originates from elastic (L^E) and inelastic (L^I) scattering, which redistribute energy into the observed direction. The RT framework thus quantifies both the loss and gain of radiance in the light field as a function of the water column's IOPs (Mobley, 1994). The net change in radiance is calculated as following Mobley (1994) :

$$\cos \theta \frac{dL}{dz} = -(a + b) \cdot L + L^E + L^I \quad (7)$$

Integrating Eq. 7 over all the possible scattering angles give the RT equation for radiance over all directions, i.e. irradiance in water :

$$\int_{\Omega} \cos \theta \frac{dL}{dz} d\Omega = -(a + b) \cdot \int_{\Omega} L d\Omega + \int_{\Omega} L^E d\Omega + \int_{\Omega} L^I d\Omega \quad (8)$$

Traditionally, in OCRS the integral is performed while setting the $L^I = 0$ to only account for the elastic scattering, as it majorly determines the direction of the photon and shape of the water leaving AOPs. The integral of L^E over all directions is further divided into the upward (Ω_u) and downward (Ω_d) directions to account for the hemispherical dependence. The integral of the elastic scattered radiance towards the up and down direction is given as :

$$\int_{\Omega_u} \mu \frac{dL}{dz} d\Omega_u = -(a + b) \cdot \int_{\Omega_u} L d\Omega_u + \int_{\Omega_u} L^E d\Omega_u \quad (9a)$$

$$\int_{\Omega_d} \mu \frac{dL}{dz} d\Omega_d = -(a + b) \cdot \int_{\Omega_d} L d\Omega_d + \int_{\Omega_d} L^E d\Omega_d \quad (9b)$$

Here, $\mu = \cos \theta$, represents the cosine of the Sun Zenith angle (Mobley, 1994). By reformu-

lating Eq. 9a and b using the formula of the mean cosine ($\bar{\mu}$), as introduced by Preisendorfer (1976), and further segregating the scattering coefficient b for each hemisphere into upward and downward components, the equations can be rewritten as follows :

$$-\frac{d}{dz}E_u = -\frac{a}{\bar{\mu}_u} \cdot E_u - \frac{b_{ud}}{\bar{\mu}_u} \cdot E_u + \frac{b_{du}}{\bar{\mu}_d} \cdot E_d \quad (10a)$$

$$\frac{d}{dz}E_d = -\frac{a}{\bar{\mu}_d} \cdot E_d - \frac{b_{du}}{\bar{\mu}_d} \cdot E_d + \frac{b_{ud}}{\bar{\mu}_u} \cdot E_u \quad (10b)$$

Here, the diffused scattering for upwelling radiance (b_u) has been separated into upward directed hemisphere b_{uu} and to the downwards direction b_{ud} . This separation also holds for b_d . The change in the diffused radiance integrated over Ω is given by diffused attenuation coefficients (K) (Mobley, 1994; Albert, 2004), assumed constant for the up and down-welling directions, respectively ($K \equiv K_u \equiv K_d$). Similarly to obtain analytical solution of Eq. 10a,b, the mean cosines are also assumed to be in very close proximity for upwelling and downwelling directions ($\bar{\mu}_0 \equiv \bar{\mu}_u \equiv \bar{\mu}_d$). Also, it is assumed that the last state of a photon in the downwelling direction is heavily influenced by the light scattered by the water and OSCs perpendicular to the direction of radiation propagation ($b_{ud} \equiv b_{du} \equiv b_b$). With these approximations, Eq. 10a, b can be rewritten as :

$$-\frac{d}{dz}E_u = -\frac{a}{\bar{\mu}_0} \cdot E_u - \frac{b_b}{\bar{\mu}_0} \cdot E_u + \frac{b_b}{\bar{\mu}_0} \cdot E_d \quad (11a)$$

$$\frac{d}{dz}E_d = -\frac{a}{\bar{\mu}_0} \cdot E_d - \frac{b_b}{\bar{\mu}_0} \cdot E_d + \frac{b_b}{\bar{\mu}_0} \cdot E_u \quad (11b)$$

Summing and rearranging Eq. 11a and b, The Irradiance reflectance ($R = E_u/E_d$) is obtained as :

$$\begin{aligned} R &= \frac{\bar{\mu}_0 K - a}{\bar{\mu}_0 K + a} = \frac{(\bar{\mu}_0 K)^2 - a^2}{(\bar{\mu}_0 K)^2 + a^2 + 2\bar{\mu}_0 a K} \\ &= \frac{b_b}{a + b_b + \sqrt{a(a + 2b_b)}} = \frac{1}{1 + \frac{\sqrt{a(a + 2b_b)}}{a + b_b}} \cdot \frac{b_b}{a + b_b} = f^\circ \cdot \frac{b_b}{a + b_b} \end{aligned} \quad (12)$$

Here, $K = \frac{\sqrt{a(a + 2b_b)}}{\bar{\mu}_0}$ and f° is the proportionality factor (Albert, 2004). This quantity can be

converted to R_{rs} as :

$$R_{rs} = \frac{f^\circ}{Q} \cdot \frac{b_b}{a + b_b} \quad (13)$$

Q , the anisotropic measure of the aquatic light field (here relevant for the water surface) is defined as $1 \leq Q = (E_u/L_u) \leq \infty$. To incorporate benthic dependence in optically shallow environment, the differential equations in Eq. 10a, b are constrained with water depth H [m] and benthic irradiance reflectance R_B , such as $E_u(H_B) = R_B \cdot E_d(H)$. In presence of the benthic cover, the irradiance values are redetermined as exponentially decaying functions with increasing H :

$$E_u(H) = \mathbf{A}e^{-KH} + \mathbf{B}e^{KH} \quad (14a)$$

$$E_d(H) = \mathbf{C}e^{-KH} + \mathbf{D}e^{KH} \quad (14b)$$

The **A, B, C, D** are place holder coefficients for rearranged expressions, included for brevity. See into Albert (2004) for details on these coefficients. Taking out the ratio of Eq. 14 a and b gives the irradiance reflectance at a given H :

$$R(H) = \frac{R_\infty (1 - R_\infty R_B) + (R_B - R_\infty) e^{-2K(H_B-H)}}{1 - R_\infty R_B + R_\infty (R_B - R_\infty) e^{-2K(H_B-H)}} \quad (15)$$

R_∞ is equivalent to the irradiance reflectance in presence of an infinite depth bottom. Interestingly, setting $H = 0$ in Eq. 14 gives the irradiance reflectance just under the water surface (subsurface, 0^-). Now, these reflectance values are very small for aquatic targets, and taking quadratic terms of R as a product would obtain estimates negligibly deviating from 0, giving the denominator in Eq. 15 as $\equiv 1$. The simplified subsurface irradiance reflectance in optically shallow water is given as :

$$R(0^-) = R_\infty(1 - e^{-2KH}) + R_B e^{-2KH} = R_\infty(1 - e^{-2KH}) + \left(\sum_{i=1}^n f_{a,i} \cdot R_{B,i} \right) \cdot e^{-2KH} \quad (16)$$

The benthic reflectance is expressed as a linear mixture model of reflectances measured over n types of substrates, e.g., sand, mud, seagrass etc. The abundance of each class can be represented by the aerial fraction $f_{a,i}$ constrained to be unity when summed. Finally, the subsurface R_{rs} in optically shallow water, the major AOP of interest in the thesis is given by :

$$R_{rs}(0^-) = R_{rs,\infty}(1 - e^{-2KH}) + \left(\sum_{i=1}^n f_{a,i} \cdot \mathcal{B}_i \cdot R_{B,i} \right) \cdot e^{-2KH} \quad (17)$$

Where, $\mathcal{B}$ is the benthic substrate's bidirectional reflectance distribution function (BRDF), defining the anisotropic nature of the benthic light field. For a perfectly Lambertian substrate, $\mathcal{B}$ would be equal to π (Mobley and Sundman, 2003; Mobley et al., 2003).

Problem Statement and Objectives

Among coastal environments, OCRS in CDOM-rich waters remains particularly challenging due to the strong absorption of light by CDOM, which significantly reduces the water-leaving signal, especially in the blue-green spectral region. These conditions result in a low signal-to-noise ratio (SnR), elevated uncertainty in IOPs, and a poor correlation between *in situ* IOPs and AOPs (Araújo and Bélanger, 2022; Mukherjee et al., 2023). While many studies have focused on turbid and scattering-dominated coastal waters, relatively few have addressed CDOM-dominated systems, despite their relevance to biogeochemical and optical variability in freshwater-influenced coastal zones. Bridging this research gap is therefore critical for advancing coastal remote sensing and expanding its applications.

In this context, the Manicouagan Peninsula (MP) in Côte-Nord, Québec, located near the lower Estuary of the St. Lawrence (ESL) river, was selected as the primary study area for this thesis. Extensive field campaigns were conducted in the region in 2019 (see Fig. 2 and 19). The MP waters are optically complex and dominated by terrestrial and riverine CDOM input, leading to absorption-driven R_{rs} spectra with less than 2% signal strength. In such conditions, inelastic scattering processes, particularly Sun-induced CDOM fluores-

cence (f_{DOM}), may contribute substantially to R_{rs} in the blue-green region (Gallegos et al., 2008; Lefering et al., 2016a). Thus, quantifying the contribution of f_{DOM} is crucial, and if found significant, necessitates the development of a mechanistic model to represent the inelastic scattering contribution to R_{rs} . Such a model would extend Eq. 17 and its parameterized forms, supporting both forward and inverse radiative transfer simulations in optically shallow, CDOM-rich waters.

The remote sensing reflectance, $R_{\text{rs}}(\lambda)$ as obtained in Eq. 17, is a forward function of the absorption coefficient $a(\lambda)$, the backscattering coefficient $b_b(\lambda)$, water depth H , benthic reflectance $R_B(\lambda)$, and the viewing geometry parameters θ and ϕ (the vector of these variables is referred as Φ_{var} in the Introduction onward). This forward model can accurately represent the RT processes and their dependence on these variables in water; however, in OCRS, the R_{rs} serves as the fundamental quantity to derive OSC concentrations or benthic composition and bathymetry. This is achieved by solving the inverse problem of the forward RT model, $f^{-1}(R_{\text{rs}})$, where R_{rs} is expressed in Eq. 17. However, this inverse problem is mathematically ill-posed (Defoin-Platel and Chami, 2007a), as multiple combinations of variables in Φ_{var} can produce similar R_{rs} spectra. This non-uniqueness and ambiguity contradict the criteria outlined by Hadamard (1902) for a well-posed problem, creating significant challenges in accurately retrieving Φ_{var} .

Additionally, the net uncertainty (variance) associated with the retrieved estimates of Φ_{var} consists of uncertainties propagated from the radiometric acquisition deriving the R_{rs} , the atmospheric perturbations along the path length, approximations made to solve the RT for shallow water and the random error (noise) present in the process (Mélin, 2019). This is particularly important for optically shallow R_{rs} inversions, which are sensitive to multiple local minima and often rely on complex bio-optical formulations (Defoin-Platel and Chami, 2007a). Traditional noise estimation methods, such as those based on spectrally dependent sensor-environmental noise equivalent reflectance ($\text{NE}\Delta R_{\text{rs}}$), have been used to scale retrieval outputs (Brando and Dekker, 2003; Hedley et al., 2012), yet they fail to provide bounded or

parameter-specific uncertainty estimates (Jay et al., 2017b; Garcia et al., 2020). While bootstrapping techniques randomly perturb input reflectance to assess output variability, they do not capture uncertainties arising from model structure or inversion logic. Alternative methods using Cramér-Rao bounds (CRB) have been applied to estimate uncertainty based on Fisher information from R_{rs} (Jay et al., 2017a; Guillaume et al., 2023), but these require a separate post-retrieval step and assume unbiased estimators. These limitations highlight a research gap in developing methodologies for optically shallow water that can simultaneously yield the least ambiguous estimates of Φ_{var} and assess the uncertainties propagated to each estimate from the ill-posed inversion process.

Therefore, the overarching goal of this thesis is to improve our understanding of dominant optical processes such as scattering and absorption in the optically shallow coastal CDOM-rich waters and develop a new robust method to retrieve OSCs and benthic information (and their uncertainties) from R_{rs} for not only MP, but applicable to globally varying coastal waters. Three major chapters have been proposed :

In Chapter **I**, a comprehensive optical closure exercise was performed for the nearshore waters at MP to determine the consistency between observed R_{rs} and *in situ* IOP data, which was mainly collected in the scope of the current project. This exercise revealed that inelastic scattering components contribute significantly (18% and 20%) at green and red spectral regions of the measured R_{rs} for the highly absorptive coastal waters. To account for this contribution from inelastic scattering, the conventional forward RT model was extended with two analytical parametrizations to account for the SIF from [chl] and CDOM, respectively. Chapter I addresses the following research questions :

1. What are the specific recommendations in measuring IOPs and radiometric measurements in CDOM-rich absorptive waters ?
2. What is the relative contribution (%) of inelastic scattering in the water-leaving R_{rs} in CDOM-rich absorptive waters ?

In Chapter **II**, A novel Bayesian inversion approach, Semi-Analytical Bayesian Error Re-

trieval (SABER), has been developed for remote sensing of coastal waters, applicable to both optically deep and shallow environments. SABER utilizes a Markov Chain Monte Carlo (MCMC) sampling framework to retrieve posterior distributions of Φ_{par} , moving beyond traditional methods that provide point estimates without quantifying uncertainty. The model employs log-normal priors (and uniform priors for benthic reflectance fractions) and Gaussian likelihoods, with Maximum-a-Posterior (MAP) estimates on the retrieved posterior identifying the least ambiguous solutions. Uncertainties are quantified as posterior variances. SABER was validated using synthetic datasets and global *in situ* observations, demonstrating reduced mean uncertainties in OSC retrievals and benthic estimates. Chapter II addresses the following research questions :

1. Can SABER, a Bayesian probabilistic approach, using MCMC sampling, improve the retrieval accuracy of OSCs and benthic variables in optically shallow water compared to conventional inversion methods ?
2. Among Φ_{var} , which retrieved variables have the highest and lowest retrieval uncertainty, and why ?
3. Can SABER be applied to different Optical Water Types (OWTs) at a global scale of observations ?

In Chapter **III**, the SABER model was first optimized to evaluate the propagation of uncertainties from free parameters, such as the spectral slopes of detrital absorption and backscattering in the water column, as well as the benthic classes used in the inversion. The refined model was then applied to R_{rs} measurements collected in the optically shallow waters of the Manicouagan Peninsula (MP) during 2019 field campaigns. The input R_{rs} was corrected for inelastic scattering, and the impact of this correction on inversion outcomes was assessed. The retrieved OSCs and benthic parameters showed strong agreement with *in situ* observations. However, the retrieval uncertainties increased significantly, except for detrital absorption in the presence of dark benthic substrates, such as eelgrass (*Zostera marina* L.). A detailed analysis revealed that the spectral slope of detrital matter and dark benthic substrate, specifically

eelgrass, contributed the largest fractions to the overall uncertainty in the SABER estimates.

The associated research questions are formulated as :

1. How uncertainty is propagated into SABER estimates from free model parameters such as the spectral slopes of detrital absorption and backscattering in the water column, as well as the benthic classes used ?
2. What is the effect of correcting the input R_{rs} for inelastic scattering equivalent signal on the SABER retrieved quantities ?
3. What is the uncertainty budget for all the SABER retrieved Φ_{var} and which model parameter had the highest influence ?

Outline of the thesis

The thesis is divided into a general introduction, followed by the three chapters mentioned above and a general conclusion. The general introduction provides a brief background of modeling coastal ecosystems, summarizes the fundamental concepts used in OCRS and finds the research gap in OCRS for optically shallow water. Chapter I-III are self-contained research articles, either published in peer-reviewed journal or ready for submission for peer-review. The general conclusion draws the major points from the three chapters in an interconnected manner while the answers to the formulated research questions are also discussed.

ARTICLE 1

OPTICAL CLOSURE IN HIGHLY ABSORPTIVE COASTAL WATERS : SIGNIFICANCE OF INELASTIC SCATTERING PROCESSES

Published in **Optics Express** (2023), 31 :21.

<https://doi.org/10.1364/OE.501732>

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1.1 ABSTRACT

In hydrological optics, "optical closure" means consistency between the apparent optical properties (AOPs) determined from radiometric measurements and those derived from radiative transfer modelling based on concurrently measured Inherent optical properties (IOPs) and boundary conditions (sea and sky states). Good optical closure not only provides confidence in the data quality but also informs on the adequacy of the radiative transfer parameterization. Achieving optical closure in highly absorptive coastal waters is challenging due to the low signal-to-noise ratio of radiometric measurements and uncertainties in the measurements of IOPs, namely the spectral absorption and backscattering coefficients. Here, we present an optical closure assessment using a comprehensive set of *in situ* IOPs acquired in highly absorptive coastal waters optically dominated by chromophoric dissolved organic matter (CDOM). The spectral remote sensing reflectance, $R_{rs}(\lambda)$, was modeled using the software HydroLight (HL) with measured IOPs and observed boundary conditions. Corresponding in-water *in situ* $R_{rs}(\lambda)$ was derived from radiometric measurements made with a Compact Optical Profiling System (C-OPS ; Biospherical). The assessment revealed that the inclusion of inelastic scattering processes in the model, specifically Sun-induced CDOM Fluorescence (f_{DOM}) and Sun-Induced Chlorophyll Fluorescence (SICF) from Chlorophyll-a ($[chl]$), significantly improved the optical closure and led to good agreement between measured and modeled R_{rs} (i.e., for $440 \leq \lambda \leq 710$ nm with no inelastic processes : $R^2=0.90$, slope=0.64 ; with inelastic processes : $R^2=0.96$, slope=0.90). The analysis also indicated that f_{DOM} and SICF contributed a substantial fraction of the green-red wavelength R_{rs} in these waters. Specifically, f_{DOM} contributed $\sim 18\%$ of the modeled R_{rs} in the green region and SICF accounted for $\sim 20\%$ of the modeled R_{rs} in the red region. Overall, this study points out the importance of accounting for f_{DOM} in remote sensing applications in CDOM-dominated waters.

1.2 RÉSUMÉ

En optique hydrologique, le terme “fermeture optique” (“*optical closure*”) désigne la cohérence entre les propriétés optiques apparentes (AOPs) issues de mesures radiométriques et celles dérivées de la modélisation du transfert radiatif basée sur les propriétés optiques intrinsèques (IOPs) mesurées simultanément ainsi que sur les conditions observées aux limites (états de la mer et du ciel, type de fond). Une fermeture optique efficace garantit la qualité des données tout en évaluant l’adéquation de la paramétrisation du transfert radiatif. Cependant, l’obtenir dans les eaux côtières fortement absorbantes est difficile en raison du faible rapport signal/bruit des mesures radiométriques et des incertitudes sur les IOPs, notamment les coefficients d’absorption spectrale et de rétrodiffusion. Dans cette étude, une fermeture optique a été réalisée à l’aide d’un ensemble complet d’IOPs et l’AOPs *in situ* collectés dans des eaux côtières fortement absorbantes dominées par la matière organique dissoute chromophorique (CDOM). La réflectance spectrale de l’eau, $R_{rs}(\lambda)$, a été modélisée avec le logiciel HydroLight, en utilisant les IOPs mesurés et les conditions limites observées. Les valeurs de $R_{rs}(\lambda)$ *in situ* ont été obtenues à partir de mesures radiométriques effectuées avec un profileur optique compact (C-OPS ; Biospherical). L’inclusion des processus de diffusion inélastique, notamment la fluorescence du CDOM (f_{DOM}) et celle de la chlorophylle-a ([*chl*]) induites par le Soleil (SICF), a significativement amélioré la fermeture optique, avec une meilleure concordance entre les R_{rs} mesurées et modélisées (sans processus inélastiques : $R^2=0,90$, pente=0,64 ; avec : $R^2=0,96$, pente=0,90). f_{DOM} et SICF ont contribué de manière notable aux R_{rs} dans les longueurs d’onde vert-rouge. Plus précisément, f_{DOM} a représenté environ 18% des R_{rs} modélisés dans la région verte, et SICF environ 20% dans la région rouge. Cette étude souligne ainsi l’importance d’inclure f_{DOM} dans les applications de télédétection des eaux dominées par le CDOM.

1.3 Introduction

Sunlight propagating into the oceanic water column is absorbed and scattered by pure water and optically significant constituents (OSCs), resulting in changes in the underwater light field as a function of depth. OSCs are characterized in terms of Inherent Optical Properties (IOPs), namely the coefficients of spectral absorption $a(\lambda)$ [m^{-1}], backscattering $b_b(\lambda)$ [m^{-1}] and beam attenuation $c(\lambda) = a(\lambda) + b(\lambda)$ [m^{-1}] (where λ is wavelength and b is total scattering). These IOPs depend on the biogeochemical composition of the OSCs (Kirk, 1983). Along with IOPs, viewing geometry and boundary conditions also determine the radiance distribution of the underwater light field (Apparent Optical Property; AOP) (Preisendorfer, 1976; Mobley, 1994). In Ocean Colour Remote Sensing (OCRS), the main AOP of interest is the Remote Sensing reflectance (R_{rs} , sr^{-1}), defined as the ratio of upwelling water-leaving radiance (L_u) and downwelling irradiance (E_d) just above the sea surface (Mobley, 1994). A radiative transfer (RT) model can be used to estimate the AOPs in the water column based on the measured total (bulk) IOPs or by using IOPs constructed as the sum of the individual mass-normalized IOPs for each OSC, multiplied by their corresponding concentrations (Mobley, 1994).

Conversely, in applied remote sensing, an ‘inversion’ of a radiative transfer model is often performed with the aim of retrieving IOPs or OSCs from measured $R_{rs}(\lambda)$ spectra (Lee et al., 2006b). Prior to attempting this inversion, it is a good practice to check the consistency of *in situ* IOP and AOP measurements to assess the degree of uncertainty in the measurements and the model, and also to build confidence in the analysis. One approach to do this is to use vertical profile data; where *in situ* water-column profiles of IOPs are input to the model, with appropriate boundary conditions, to estimate AOPs. These are then compared to AOPs determined from radiometric measurements from the independent deployment of radiometer(s) in close space-time proximity to the acquisition of *in situ* IOP profiles. This consistency check between *in situ* IOPs and AOPs is referred to as testing for “optical closure” (Mobley, 1994; Tzortziou et al., 2006; Gallegos et al., 2008). The degree of optical closure under different

conditions can give insight regarding underlying assumptions in the model, e.g., the shape of the volume scattering function or the significance of inelastic processes (Morel et al., 2002). However, great care must be taken in the interpretation since closure is also dependent on the accuracy of the IOP and AOP measurements.

One application of optical closure is to assess the data corrections that must be applied to IOPs obtained from *in situ* instruments. For example, Lefering et al. (2016a) showed that inadequate scattering corrections of flow-tube AC (absorption - attenuation meter) data can lead up to ~30% error in the simulated R_{rs} . Commercially available *in situ* instruments for IOPs mainly include, among others, the WETLabs AC-S or AC-9, which use a flow-tube design for $a(\lambda)$ and $c(\lambda)$, and the HOBILabs Hydroscat-6 or WETLabs BB-9 for the volume scattering function (VSF) - these measure at a fixed angle in the backward direction allowing an estimation of the $b_b(\lambda)$ following various assumptions. For estimation of non-water absorption, there are also Integrating Cavity Absorption Meters (ICAM), such as Point-Source ICAM (PSICAM) for discrete samples (Röttgers and Doerffer, 2007) or HOBILabs A-Sphere for *in situ* vertical profiles (Bélanger et al., 2017). Unlike flow-tube designs, spherical-cavity ICAM instruments allow absorption measurements with potentially minimal errors from scattering losses (Pope et al., 2000), but to date, they have not been commonly used in optical closure experiments.

Recent research using optical closure showed a significant discrepancy of modelled R_{rs} at green maxima wavelengths (~555 nm) in coastal waters when AC-S is used for $a(\lambda)$ and $c(\lambda)$ Bausell and Kudela (2021); Lefering et al. (2016a). Uncertainty in $a(\lambda)$ from AC-S measurements mainly comes from the uncollected scattered photons inside the reflective a -tube. Several scattering correction schemes have been proposed in the literature (Zaneveld et al., 1994; Gallegos and Neale, 2002; McKee et al., 2008, 2013; Röttgers et al., 2013), which have been the subject of numerous studies in coastal waters (Tzortziou et al., 2006; Lefering et al., 2016a; Tonizzo et al., 2017). Similarly, $b_b(\lambda)$ obtained from a single fixed VSF angle is also subject to corrections, such as to compensate for attenuation along the optical path

length ("sigma" (σ) correction, required especially in coastal waters with high concentrations of OSCs) (Doxaran et al., 2016; Tuchow et al., 2016), or to quantify the uncertainty in $b_b(\lambda)$ from variability in VSF angular distribution (Chami et al., 2006). The first issue is worse for backscatter acquired from instruments with longer path lengths such as the HydroScat (~ 0.15 m vs. ~ 0.04 m for the BB9 (Doxaran et al., 2016)). For example, Tuchow et al. (2016) showed that the σ correction of Doxaran et al. (2016), in which the backscatter is corrected for both absorption and scattering along the path length, improved the optical closure in a plankton bloom in Monterey Bay.

Optical closure studies have also addressed the consequences of the assumed shape of the VSF (equivalently, the phase function : the angular probability distribution of the scattering when it occurs). While Petzold (1972) given phase function has been frequently used in the past for open oceanic waters , newer studies on optical closure in coastal waters imply that the Fournier-Forand (FF) phase function (Fournier and Forand, 1994) is a better choice (Tzortziou et al., 2006; Lefering et al., 2016a; Tuchow et al., 2016; Tonizzo et al., 2017). The FF phase function can be parameterized as a function of the backscatter fraction; $\tilde{B}(\lambda)$, the ratio of backscatter $b_b(\lambda)$ to total scattering coefficient $b(\lambda)$ (Mobley et al., 2002). Tzortziou et al. (2006) compared FF phase function, parameterized by $\tilde{B}$ obtained from the combination of an ECO-VSF-derived b_b and AC-9-derived b , with both the Petzold's and FF phase functions in a closure exercise in Chesapeake Bay. They found that the error was reduced by $\sim 20\%$ when the FF phase function was used over Petzold's one. Tuchow et al. (2016) assessed optical closure for measurements in a plankton bloom in Monterey Bay where the FF phase function was also found to perform better than Petzold's. The optical closure demonstrated by Gallegos et al. (2008) over a range of highly contrasting optical conditions, from lakes dominated by scattering or absorption, highlighted both the importance of the scattering correction of AC-9 data for turbid lakes and the use of the FF phase function with lower $\tilde{B}$ values in humic lakes. Furthermore, Gallegos et al. (2008) recognized the potentially important contribution of CDOM fluorescence in their humic lakes, but the lack of vertical resolution of their AOP measurements prevented the assessment of these inelastic processes.

Here, we examined optical closure in coastal waters dominated by high concentrations of CDOM. Specifically, we assessed how the inclusion of inelastic scattering due to CDOM (f_{DOM}) affects the optical closure in blue and green wavelengths in a coastal absorptive aquatic environment. We also considered sun-induced chlorophyll fluorescence (SICF) to assess its effect on R_{rs} in the red wavelengths. The implications of using *in situ* absorption coefficient acquired using an ICAM integrating sphere in characterizing the optical closure is also explored.

1.4 Materials and Methods

The study area is located in the lower part of the Estuary of St Lawrence (ESL) in Québec, Canada (Fig. 2a). In this region a_{CDOM} is the dominant component of total $a_{\text{t-w}}$, especially in blue and green wavelengths (Araújo and Bélanger, 2022). Two sets of IOP instruments were deployed : 1. WETLabs AC-S & BB9; and 2. HOBILabs A-Sphere & HydroScat6. Each IOP package was accompanied by in-water radiometric profilers (C-OPS) for AOP determinations.

1.4.1 Study area

The Manicouagan Peninsula ($\sim 49^\circ\text{N}$, 68.3°W ; Fig. 2b) is a deltaic formation located on the north shore of the ESL and comprises a cold temperate environment with a rich marine ecosystem (Department of Fisheries and, 2010; Plourde and Runge, 1993). The mixed freshwater flow from three surrounding rivers (Betsiamites, Aux-Outardes, and Manicouagan) with an averaged mean annual discharge of $\sim 1600 \text{ m}^3\text{s}^{-1}$ (Jaegler, 2014), provides large inputs of terrigenous CDOM and makes the coastal waters of the ESL highly absorptive (Cizmeli, 2008; Bélanger et al., 2017; Araújo and Bélanger, 2022). The main area of interest has a bathymetry reaching $\sim 150 \text{ m}$ after a relatively extensive tidal flat ($\sim 2 \text{ km}$). The bottom type of the tidal flat consists of sand with both small and coarse particles, partly covered by

eelgrass meadows (*Zostera marina* L.)(Department of Fisheries and, 2010).

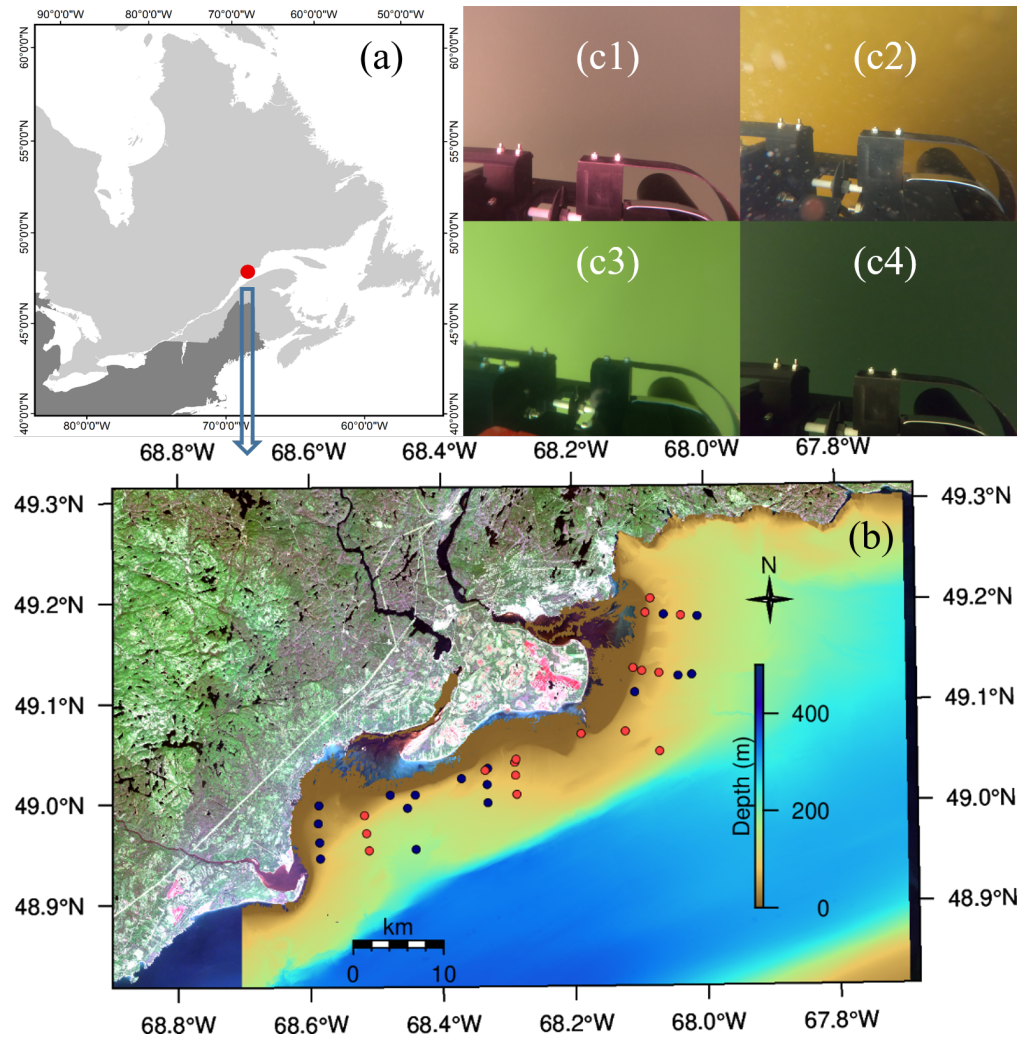


FIGURE 2 – Illustration of the study area for chapter one : (a) Map of Québec province in Canada where the red dot represents the location of the study area, (b) study area at a finer scale; Manicouagan Peninsula situated in the Lower Estuary of Saint Lawrence. The blue points show the sampling locations for boat Kildir (A-Sphere and HydroScat) and the red ones show the same for FJ Saucier (AC-S and BB9). The points are overlaid on CHS NONNA-10 bathymetry data and the land area is a true colour composite of R_{rs} obtained from Sentinel-2 multi-spectral data acquired on July 2019. (c1-c4) C-OPS mounted Go-Pro acquired RGB images showing the variability of water colour among all sampling sites in the study area (both optically deep and shallow).

1.4.2 *In situ* data sets

1.4.2.1 Sampling strategy

An intensive interdisciplinary fieldwork campaign was carried out in August 2019 as part of the **WaterSat Imaging Spectrometer Experiment** (the *WISE-Man* project). The main objective of the fieldwork was to collect high-quality optical and biogeochemical measurements for the calibration and validation of WISE, a hyperspectral prototype camera developed by ITRES Inc (Calgary, Canada) for coastal and inland water assessment (see also Araújo and Bélanger (2022); Mabit et al. (2022); Mukherjee et al. (2021)).

The *in situ* sampling was performed using two small boats, *FJ Saucier* and *Kildir* (Fig. 2b). The boats were used to deploy instruments measuring conductivity-temperature-depth (CTD), radiometric quantities and IOPs, and to collect discrete water samples for the determination of biogeochemical constituents and properties. A total of 65 stations were visited over a 9-day period from August 17th to 25th in 2019. Among these, 36 stations had depths greater than 10 m. The remaining 29 stations were shallower.

Each boat was equipped with a Compact Optical Profiling System (C-OPS) for measuring in-water radiometric profiles to facilitate the estimation of $R_{rs}(\lambda)$. For the IOPs, the *Kildir* deployed an optical package consisting of an A-Sphere (ASPH) and a HydroScat-6p (HS6) from HOBILabs, as well as a Seabird SBE19+ CTD for synchronous data acquisition. A total of 30 profiles were performed with this setup. The *FJ Saucier* was equipped with an AC-S and BB9 from WETLabs along with a Seabird SBE19+ CTD. This package was used to acquire data at 32 stations (Fig. 2b). Discrete water samples were also collected at each station for laboratory analysis of OSCs. Specifically, the water was sampled using a 5-L Niskin or a 4.2-L Wildco Beta horizontal sampler at ~0.5 m depth (“surface”) at all stations ($N=64$). Samples were also collected at ~5 m depth (“sub-surface”) at some selected stations ($N=15$). The discrete water samples were stored in clean, 20-L insulated carboys rinsed three times with sample water.

1.4.2.2 Remote sensing reflectance

The C-OPS measured downwelling irradiance $E_d(z, \lambda)$, upwelling irradiance $E_u(z, \lambda)$ and upwelling radiance $L_u(z, \lambda)$ in the water column (where z is depth) at 19 wavelengths across 305-780 nm spectral domain (λ), at a frequency of 15 Hz (Hooker et al., 2013; Morrow et al., 2010). Simultaneous above-surface downward irradiance, $E_d(0^+, \lambda)$, was measured with a radiometer attached to the top of the boat, making sure there were no obstructions in the field of view. The C-OPS was deployed for 3-to-5 vertical profiles at each station, and care was taken to avoid the boat shadow and limit boat pitching and rolling (Araújo and Bélanger, 2022).

The C-OPS data were processed using the software R and the Cops package (<https://github.com/belasi01/Cops>); (Bélanger et al., 2017; Mabit et al., 2022; Araújo and Bélanger, 2022)). The data was processed following the NASA radiometric protocols (Mueller et al., 2003), with some modifications. Radiometric measurements with high tilt, i.e. $> 5^\circ$ were discarded, although the tilt threshold was increased to 7° or 8° near the surface and in highly stratified waters, to account for the extra turbulent nature of the air-water interface. Data collected near the air-water interface was typically noisy and was therefore discarded and replaced by extrapolating the radiometric data from the sub-surface to just below the air-water interface (see description below). A wavelength-specific detection limit threshold was used to remove noisy radiometric measurements (i.e., when the C-OPS is just measuring noise). Normalization to account for changing incident surface irradiance during the vertical profiles was done by multiplying $E_d(z, \lambda)$, $E_u(z, \lambda)$, and $L_u(z, \lambda)$ by the ratio $\hat{E}_d(0^+, \lambda, t)/E_d(0^+, \lambda, t_0)$, where $\hat{E}_d(0^+, \lambda, t)$ refers to the mean in-air surface irradiance over time t in the profile, and t_0 is the time reference of a particular observation in the same profile (Mueller et al., 2003). After normalization, the data was fitted using a linear regression applied to the log-transformed radiometric quantity versus depth. This allowed extrapolation of the quantities of interest to just below the sea surface ($z = 0^-$). An instrument self-shading correction was also applied to the normalized $L_u(0^-, \lambda)$, using the total absorption coefficient

at each C-OPS wavelength measured coincidentally with the ASPH or the AC-S (Gordon and Ding, 1992; Zibordi et al., 2015). Finally, the surface remote sensing reflectance, i.e. $R_{rs}(0^-, \lambda)$ was calculated as :

$$R_{rs}(0^-, \lambda) = \frac{L_u(0^-, \lambda)}{E_d(0^-, \lambda)} \quad (1.1)$$

1.4.2.3 IOP data

Vertical profiles of IOPs were collected using two separate instrument setups (referred to here as “IOP packages”) consisting of an ASPH and a HydroScat on the *Kildir* and an AC-S and BB9 on the *FJ Saucier*, each integrated with a Seabird SBE19+ CTD in the IOP package. Each package was vertically deployed using a mechanical pulley attached to the deployment cable, which was only ~ 5 m in length for the *FJ Saucier*, limiting the IOP acquisition to sub-surface waters only.

All instruments were calibrated by the manufacturer, but additional calibration checks were performed prior to the fieldwork. Blank measurements with the ASPH, a submersible Teflon ICAM, were checked before the field campaign using nano-pure water. The instrument measures the absorption at 1,500 wavelengths between 360 and 764 nm, which are binned at 1-nm spectral resolution. Raw data were converted into non-water absorption coefficients (a_{t-w}) using the manufacturer software and the calibration file that was included for the pure water offset. Absorption coefficients were corrected for temperature (T) and salinity (S) differences relative to the calibration using data from the CTD at the same depth, using the coefficients published by Röttgers et al. (2014).

The AC-S instrument measured *in situ* non-water absorption (a_{t-w}) and attenuation coefficients (c_{t-w}) at a frequency of 5 Hz. The instrument uses a pump to pull water through two flow tubes, each having a path length of ~ 25 cm and an integrated light source, detector and filter wheel. a_{t-w} and c_{t-w} were measured at 81 wavebands between 400 and 756 nm. The field-acquired binary data was converted to raw text data using the manufacturer’s soft-

ware (WETLabs, WAP). The raw data were converted into engineering units by applying a calibration file obtained from the manufacturer after the fieldwork (post-cruise calibration) (Ciochetto, 2017). Corrections for the effects of temperature and salinity, as measured by the CTD, were applied following the manufacturer's standard recommendations (Röttgers et al., 2014). Pure water calibration files required for the data processing were obtained in the laboratory before and after the fieldwork, and the average of the two calibrations was used.

The AC-S data were also corrected for scattered photons failing to be detected in the *a*-tube and *c*-tube. Several scattering correction methods were tested, including Zaneveld et al. (1994); Twardowski et al. (1999), Röttgers et al. (2013), McKee et al. (2008), and McKee et al. (2013). A detailed comparison of the implemented scattering correction methods and their respective effect on the radiative transfer modeling is presented in Section 4.1 in the Annex-I. Based on this analysis, the McKee et al. (2008) method, which uses measured b_{bp} as ancillary input for the correction, was judged to perform best, however, the use of potentially overestimated VSF from BB9 (See 1.5.2.1 afterwards) might have introduced uncertainty in this choice of scatter correction.

The total backscattering coefficient, b_b , at selected wavelengths was measured using the HydroScat and BB9 instruments. The HydroScat was calibrated by HOBI Service Inc. prior to the fieldwork following the method of Maffione and Dana (1997). The BB9 was sent to the manufacturer (SeaBird/WetLabs) for calibration after the cruise (post-calibration), and the data were processed using the post-calibration coefficients. The HydroScat measured the VSF at 140° at 6 wavebands centered at 394, 420, 470, 532, 620 and 700 nm. The HydroScat has an effective optical path length of ~ 15 cm. A first-order correction factor, σ , for attenuation along this long path was derived using the a_{t-w} measured coincidentally by the ASPH, as recommended by Doxaran et al. (2016). Finally, the particulate backscattering coefficient, b_{bp} , was derived as following :

$$b_{bp} = 2\pi\chi_p(\beta(\theta^\circ) - \beta_w(\theta^\circ)) \quad (1.2)$$

where $\chi_p = 1.08$ is a value provided by the manufacturer assuming a VSF shape estimated from a specific backscatter fraction value at $\theta = 140^\circ$ (Maffione and Dana, 1997). $\beta_w(\theta)$ is the pure seawater VSF at 140° computed following Zhang and Hu (2009) using the T and S measured at the same depth with the CTD. The BB9 measures the VSF at an effective scattering angle of 117° , $\beta(117^\circ)$, for wavebands centered at 412, 440, 488, 510, 532, 595, 650, 676 and 715 nm. The effective pathlength is ~ 3.9 cm and $\beta(117^\circ)$ was σ -corrected using a_{t-w} values obtained from adjacent AC-S following Doxaran et al. (2016). Finally, b_{bp} was calculated using the same equation (Eq. 1.2) above but with $\chi_p = 1.1$ (Boss and Pegau, 2007).

The ASPH and HydroScat package did not include any measurement of beam attenuation (c). As a result, non water beam attenuation (c_{t-w}) could not be measured directly at the stations visited by the *Kildir*. Instead, c_{t-w} was estimated by calculating $c_{t-w}(\lambda) = a_{t-w}(\lambda) + b_{bp}(\lambda)/\tilde{B}$, where $\tilde{B}$ is an assumed and spectrally constant value of the backscatter fraction derived from three possible options :

1. The Petzold phase function value of 0.018 (Petzold, 1972);
2. The mean $\tilde{B}(532)$ derived from BB9 and AC-S data (this was 0.013, see results);
3. A value was estimated from HydroScat and AC-S data from two physically close stations.

The latter value was based on HydroScat-derived b_{bp} and AC-S-derived b_p at two nearby offshore stations sampled simultaneously on August 23rd 2019. Assuming spatial homogeneity between stations, a $\tilde{B}(532)$ value of 0.0105 ± 0.006 was obtained. Similar values have been reported in the literature for CDOM-rich waters. For example, Gallegos et al. (2008) reported a constant $\tilde{B} = 0.0115$ for humic-rich lakes. In addition, it has been shown that nearshore ESL particles were organic-rich and had low b_{bp} to suspended particulate matter ratio but high for the ratio with both organic dominated non-algal particulate absorption and particulate organic matter in ESL waters (Araújo and Bélanger, 2022; Mabit et al., 2022). Similarly, some studies have also shown that the organic-rich particles generally present low

$\tilde{B}$ (Twardowski et al., 2001) as well as b_{bp} (Reynolds et al., 2016). These three values of $\tilde{B}$ were retained as potential candidates and applied in a sensitivity analysis as part of the optical closure experiment.

Finally, all the corrected IOP values were binned at 0.5m depth intervals for stations deeper than 10 m, and at 0.1m depth intervals for shallower stations. Binning was performed using a non-linear LOESS smoothing function implemented in R using the open source package Riops (for details, see <https://github.com/belasi01/Riops>).

1.4.2.4 Laboratory analysis

Several measurements of spectrophotometric IOPs and biogeochemical variables were determined from the discrete water samples, i.e., CDOM spectral absorption ($a_{CDOM}(\lambda)$), total particulate and non-algal particulate spectral absorption ($a_p(\lambda)$ and $a_{NAP}(\lambda)$), Chlorophyll-a concentration [*chl*] and Suspended particulate matter (SPM) concentration.

The CDOM spectral absorption coefficient, $a_{CDOM}(\lambda)$, was measured for water samples filtered under low vacuum using 47-mm Nucleopore filters (Whatman, 0.2 μ m nominal pore size) (Mabit et al., 2022). CDOM absorbance (A) was measured between 220 and 800 nm using a Perkin Elmer double-beam Lambda-850 spectrophotometer, 10 cm quartz cells, and nano-pure water as the reference. A baseline correction was applied on the measured A values by subtracting the average values over a spectral window of 5 nm centred at 685 nm (Babin, 2003). Finally, a_{CDOM} was calculated by normalizing the corrected absorbance values by the path length of the quartz cells ($L = 0.1$ m) and converting to a Napierian logarithm scale : $a_{CDOM}(\lambda) = 2.303A(\lambda)/L$.

Particulate spectral absorption coefficient, $a_p(\lambda)$, was measured following the filter-pad technique as described in Röttgers and Gehnke (2012). First, a known volume of sampled water (replicates between two and five) was filtered through Whatman GF/F glass fibre filters shortly after sampling (< 3h). The filters were placed inside a 150-mm integrating sphere fit-

ted to the Perkin Elmer Lambda-850 spectrophotometer. Absorbance was scanned from 300 to 800 nm at every 1 nm. The absorbance of a blank filter was subtracted from total absorbance (Röttgers and Gehnke, 2012). Blank-corrected absorbance values were corrected for path length amplification and converted to a_p using eq. 1 in Stramski et al. (2015). Similarly, a_{NAP} was measured by placing the filters inside the sphere after extraction of the phytoplankton pigments using methanol 90% for ~18 to 24 hours (Kishino et al., 1985). Chlorophyll-a concentration [*chl*] was determined fluorometrically from triplicate sub-samples filtered onto 25-mm Whatman GF/F filters (varied known volumes between 200-550 ml). [*chl*] values were measured using a Turner Designs 10-AU fluorometer, following a 24-hour extraction in 90% acetone at 4 °C in the dark following the acidification method of Parsons (2013).

SPM concentration was measured following the recommendations of Neukermans et al. (2012). Known volumes (V) of seawater (varies between 500-1250 ml) were filtered in water sample triplicates through pre-ashed (1 hour at 450 °C), pre-rinsed and pre-weighed (mass M_0 mg) 47-mm GF/F filters. Each filter was then rinsed with Milli-Q water and dried for 24 hours at 60 °C prior to weighing under a dry atmosphere (mass M_1 , mg) to obtain the SPM concentration as $\text{SPM} = (M_1 - M_0)/V$. The final value from triplicates [*chl*] and SPM was determined considering their average, within a confidence interval of 95%.

1.4.3 Radiative transfer simulations

The radiative transfer model HydroLight version 6.0 (Mobley, 1994) was used to simulate surface remote sensing reflectance, $R_{\text{rs}}(0^-, \lambda)$. HydroLight models directional radiance in the water column and irradiance above the surface using an invariant embedding approach to solve the radiative transfer equation. The details of this model can be found in Mobley (1994).

Vertical profiles of $a_{\text{t-w}}(\lambda)$, $c_{\text{t-w}}(\lambda)$ and $b_{\text{bp}}(\lambda)$ for each station were input into HydroLight with 0.25 m depth interval obtained by fitting a spline interpolation to bin the actual

IOP profiles. The phase function was modelled using the Fournier–Forand (FF) phase function with shape specified by $\tilde{B}(\lambda)$ (Mobley et al., 2002). The pure water absorption coefficients from Pope and Fry (1997) and pure water scattering coefficients from Morel (1974) were used in the model configuration to yield the total IOPs. The RADTRAN-X routine was used to model the sky radiance distribution with viewing geometry and atmospheric transmittance calculated from field-acquired time, location and approximate cloud cover. The water surface roughness model of Cox and Munk (1954) was used with wind speeds measured by a hand-held anemometer (always $< 5 \text{ ms}^{-1}$). The water column was considered infinitely deep, as only stations with a physical depth greater than 10 m were used in the modeling. Since these waters are optically deep ($c(\lambda) > 1.3 \text{ m}^{-1}$), the effect of bottom reflectance could be considered negligible.

HydroLight simulations were performed with and without inelastic scattering, with both f_{DOM} and SICF included in the inelastic scattering treatment. To include inelastic scattering in the simulations, two additional depth-dependent input variables must be provided, i.e. $[chl]$ and $a_{\text{CDOM}}(443)$. These were obtained from the surface (0.5 m) discrete water samples as described in the previous sections. For consistency between in-water $a_{\text{t-w}}(443)$ profile measurements and benchtop spectrophotometric measurements, we estimated the profile $a_{\text{CDOM}}(443)$ as :

$$\widehat{a}_{\text{CDOM}}(z, 443) = a_{\text{t-w}}(z, 443) \times \frac{a_{\text{CDOM}}(443)}{a_{\text{CDOM}}(443) + a_{\text{p}}(443)} \quad (1.3)$$

where $\widehat{a}_{\text{CDOM}}(z, 443)$ is the estimated $a_{\text{CDOM}}(443)$ at depth z , $a_{\text{t-w}}(z, 443)$ is the *in situ* non water absorption (ASPH or AC-S derived), and $a_{\text{CDOM}}(443)$ and $a_{\text{p}}(443)$ are the spectrophotometrically determined absorption coefficients. The relative CDOM contribution to non-water absorption is therefore assumed constant in the water column. Vertical profiles of $[chl]$ were assumed constant and equivalent to the surface $[chl]$ values obtained from the laboratory analysis. In HydroLight, inelastic scattering equivalent radiance is calculated via integrating the volume inelastic scattering function given as $\beta_{\text{g}}(\psi, \lambda^*, \lambda) = b_{\text{g}}(\lambda^*)f_{\text{g}}(\lambda^*, \lambda)\beta_{\text{g}}(\psi)$.

Here $b_g(\lambda^*)$ is loss of photon at excitation wavelength (λ^*), $\beta_g(\psi)$ is scattering phase function set to $1/4\pi$, $f_g(\lambda^*, \lambda)$ is the wavelength redistribution function (WRF) calculated as, $f_g(\lambda^*, \lambda) = \eta_g(\lambda^*, \lambda) \frac{\lambda^*}{\lambda}$, where, $\eta_g(\lambda^*, \lambda)$ is the shape of quantum efficiency, for which the parameterization of Hawes et al. (1992) and Mobley (1994) were used for f_{DOM} and SICEF, respectively along with HydroLight set default quantum yield. HydroLight runs were performed for the wavelength range 360 - 800 nm (interval 5 nm, the IOPs were spectrally extrapolated where necessary) with the lower bound set to ensure the excitation range of fluorescence was included.

1.4.4 Statistical metrics used

The following statistical metrics were used in the various comparisons between IOPs and measured and modeled R_{rs} : Median Absolute Percentage Error MDAPE(%), median %-Bias and Root Mean Square Percentage Error, RMS%E. These are defined as :

$$\text{MDAPE}(\%) = \text{median}(|\delta \overline{y}_i|) \times 100 \quad (1.4a)$$

$$\% - \text{Bias} = \text{median}(\delta \overline{y}_i) \times 100 \quad (1.4b)$$

$$\text{RMS}\%E = \sqrt{\frac{1}{n} \sum_{i=1}^n (\delta \overline{y}_i)^2} \times 100 \quad (1.4c)$$

In general, y_i is the observed or actual value, and $\hat{y}_i$ is the predicted value, i is a specific observation where n is the number of observations, so $\delta \overline{y}_i = \frac{(\hat{y}_i) - y_i}{y_i}$ is the relative difference for one observation. In different contexts the values in question could be $a_{t-w}(\lambda)$, $b_{bp}(\lambda)$ or $R_{rs}(\lambda)$.

1.5 Results

1.5.1 Optical and biogeochemical conditions of the study area

The sampled surface waters (0.5 m depth) were typically brackish with a salinity of 22.74 ± 4.65 (st.dev.) PSU (Practical Salinity Units) and with a temperature of 10.66 ± 1.85 °C (Table 1). Chlorophyll-a concentration ranged from 1.05 to 5.3 mg m⁻³ indicating moderate phytoplankton biomass. High absorption coefficients ($\sim 1.00 \pm 0.31$ m⁻¹ at 443 nm) and low backscattering coefficients (0.007 ± 0.002 m⁻¹ at 532 nm) resulted in visually dark waters (Fig. 2c, Fig. 6a).

TABLE 1 – Descriptive statistics of IOPs and relevant BGC data used for HL simulation. The data here is from *Kildir* collected samples for deep stations (depth ≥ 10 m). statistical parameters are **min**; minimum, **max**; maximum, **med**; median and **sd**; standard deviation.

	Min	Max	Med	sd(±)
$a_{t-w}(443)[m^{-1}]$	0.51	1.50	0.94	0.31
$c_{t-w}(443)[m^{-1}]$	1.33	2.52	1.68	0.42
$b_{bp}(532)[m^{-1}]$	0.004	0.010	0.007	0.002
$[chl][mg\ m^{-3}]$	1.05	5.30	2.68	1.15
SPM[mg ¹ L ⁻¹]	2.51	18.40	7.90	5.14
Salinity [PSU]	11.34	27.80	22.74	4.65
Temperature [°C]	7.60	12.80	10.66	1.85

1.5.2 IOP consistency evaluation

First, we examined the consistency between the laboratory determined coefficients and biogeochemical quantities from the water samples and the *in situ* IOP data collected from the two IOP packages, the ASPH and HydroScat ($n = 12$), and the AC-S and BB9 ($n = 15$).

1.5.2.1 Particulate backscattering coefficient

On average, $b_{bp}(532)$ values for the HydroScat and BB9 showed different ranges of variability with medians of 0.007 m^{-1} (0.004 to 0.010 m^{-1}) and 0.015 m^{-1} (0.012 to 0.026 m^{-1}), respectively (Fig. 3). A discrepancy in spectral shape was also observed between the sensors, with noisier spectra for BB9 relative to the HydroScat (Fig. 3a). To get more insight on the reliability of *in situ* $b_{bp}(\lambda)$, we examined the relationship between $b_{bp}(555)$ and both the SPM and the non-algal absorption coefficients. These can be treated as independent proxies for particulate matter as they have frequently been demonstrated to co-vary with backscattering (Matsuoka et al., 2007; Reynolds et al., 2016; Araújo and Bélanger, 2022). The BB9 data showed greater spread and a systematically higher magnitude than the HydroScat data for a similar range of $a_{NAP}(443)$ (Fig. 3b). Similarly, there was only a weak relationship between SPM and BB9-derived $b_{bp}(555)$ (Fig. 3c), whereas the HydroScat data was much better correlated to SPM (correlation coefficient, r , of -0.26 and $+0.58$ for the BB9 and HydroScat, respectively).

Additional comparisons were performed to determine which backscatter instrument yielded more reliable results. First, we have used the QAA v5 (Lee et al., 2002) to roughly estimate b_{bp} from the C-OPS R_{rs} as an independent measurement (Fig.4a). A good agreement is obtained for HS6 values with $\delta \bar{b}_{bp}(532) \approx 9\%$. In contrast, BB9 values are overestimated and sparsely scattered relative to QAA-derived $b_{bp}(532)$ values, with a mean $\delta \bar{b}_{bp}(532)$ of $\sim 30\%$, with three stations showing discrepancy larger than 70% (Fig.4b). This discrepancy, along with the noisy spectral shape, can be possibly attributed to raw data discretization errors or attenuation correction factors. It is to be noted that to ensure data quality, the BB9 was post-calibrated just after the fieldwork, which improved the spectral shape in blue wavelengths much relative to the original pre-field calibration, however, an increase in magnitude is also observed across the BB9 channels (Not shown).

Finally, when the data from the nine stations with concurrently acquired AC-S and BB9 profiles was propagated through the optical closure experiment, there was a constant ove-

restitution of R_{rs} regardless of the modeling treatment applied (Fig. 33 in Section 4.2). The overall conclusion of these results was that BB9 data were mostly erroneous, with b_{bp} being systematically overestimated. Therefore, only the data from the ASPH and HydroScat optical package was further considered in this paper.

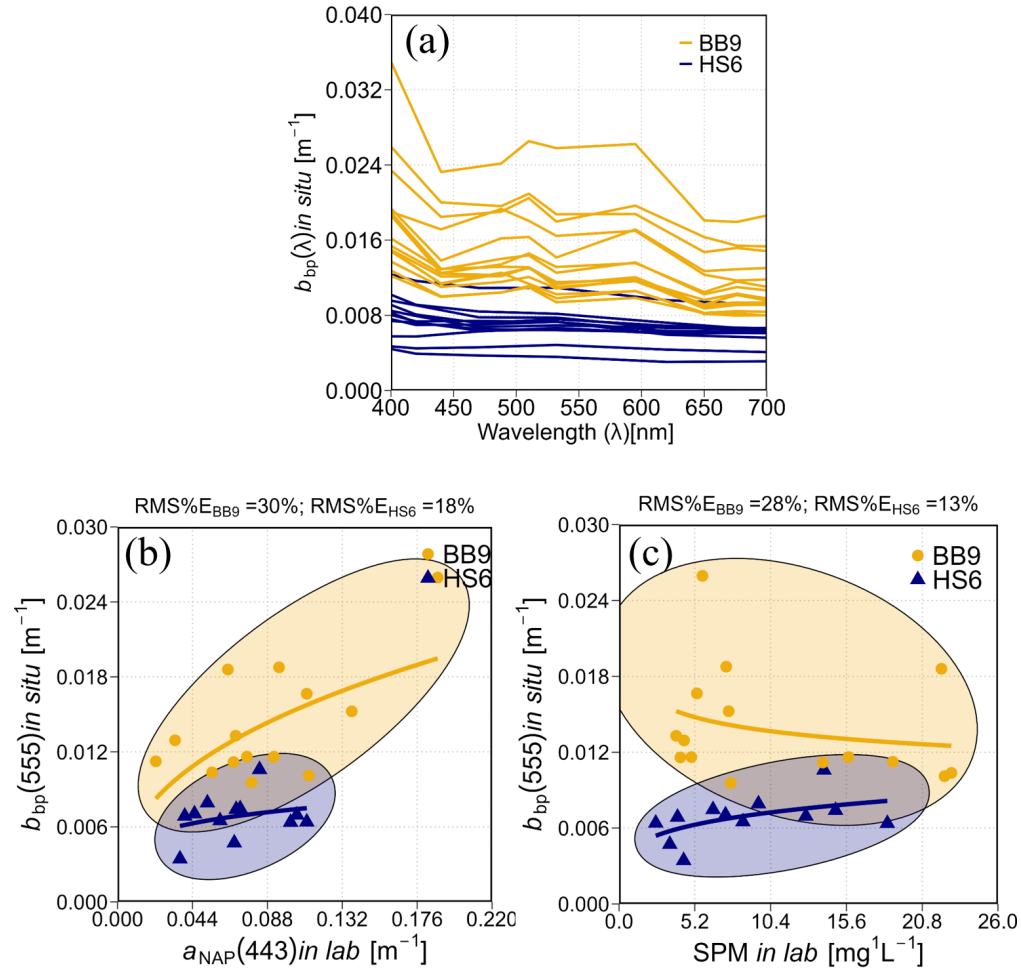


FIGURE 3 – Consistency check of measured particulate backscattering coefficient (b_{bp}) : (a) Spectral particulate backscattering from the HydroScat and BB9 for deep water stations (water depth ≥ 10 m). General relationships between $b_{bp}(0^-, 555)$ (as Y-axis) from both b_b sensors and (b) non-algal particulate absorption coefficient at 443 nm, $a_{NAP}(443)$, and (c) corresponding suspended particulate matter (SPM) concentration (both as X-axis). The elliptical clusters are drawn to provide a visual estimate of the trend and its variability. The solid lines represent the power regression ($y = a \cdot x^b$) fitted line for each b_{bp} sensor.

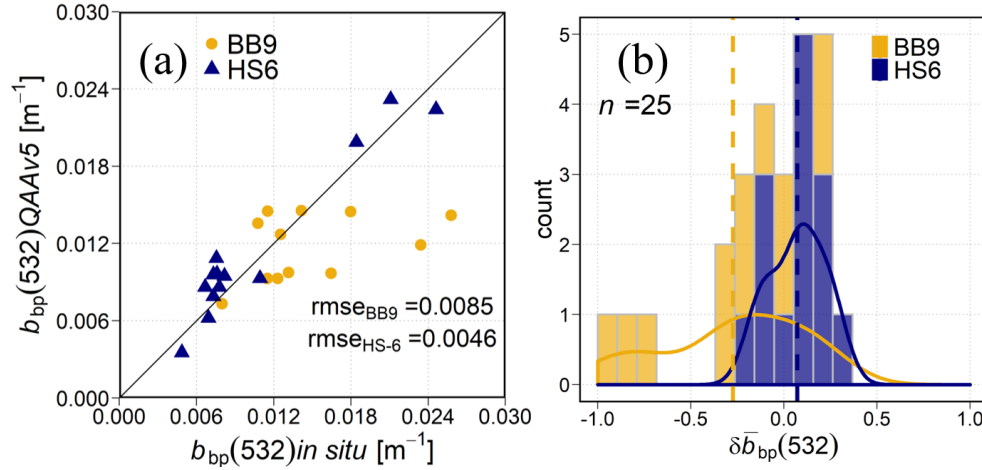


FIGURE 4 – consistency of processed backscatter; **(a)** scatterplot of *in situ* $b_{bp}(0^-, 532)$ (X-axis) with QAA obtained $b_{bp}(0^-, 532)$ values (Y-axis). **(b)** The right-hand side figures show the histogram of normalized bias; $\delta \bar{b}_{bp}(532)$ for *in situ* backscatter at 532nm. It is calculated as $\frac{b_{bp}(532)_{QAA} - b_{bp}(532)_{in situ}}{b_{bp}(532)_{QAA}}$. The dashed vertical lines on panel **(b)** denote sensor-specific mean $\delta \bar{b}_{bp}(532)$. The validation metric for b_{bp} consistency used here is Root mean square error (rmse)[m⁻¹].

1.5.2.2 Non-water absorption coefficient

The ASPH-derived a_{t-w} was systematically lower than spectrophotometric absorption measured on the discrete samples, $a_{t-w}^{spec} = a_{CDOM} + a_p$, except for one station (OUT-R03) (Fig. 5a). The %-Bias peaks at ~30% around 570 nm and drops sharply to ~10% around 670 nm before increasing again toward 700 nm (Fig. 5b). Interestingly, the inverted spectral shape of the %-Bias suggests that part of the relative ASPH underestimation may be due to CDOM and chlorophyll-a fluorescence taking place inside the ICAM. Fluorescence in the ICAM would be stimulated by the continuous spectral LED source ranging from 360 nm to 764 nm (see Discussion). Assuming the spectrophotometric measurements can be used as the reference, we applied a bias correction to all ASPH spectral a_{t-w} . The implications of the a_{t-w} underestimation and the bias correction on the optical closure results are presented in the next section.

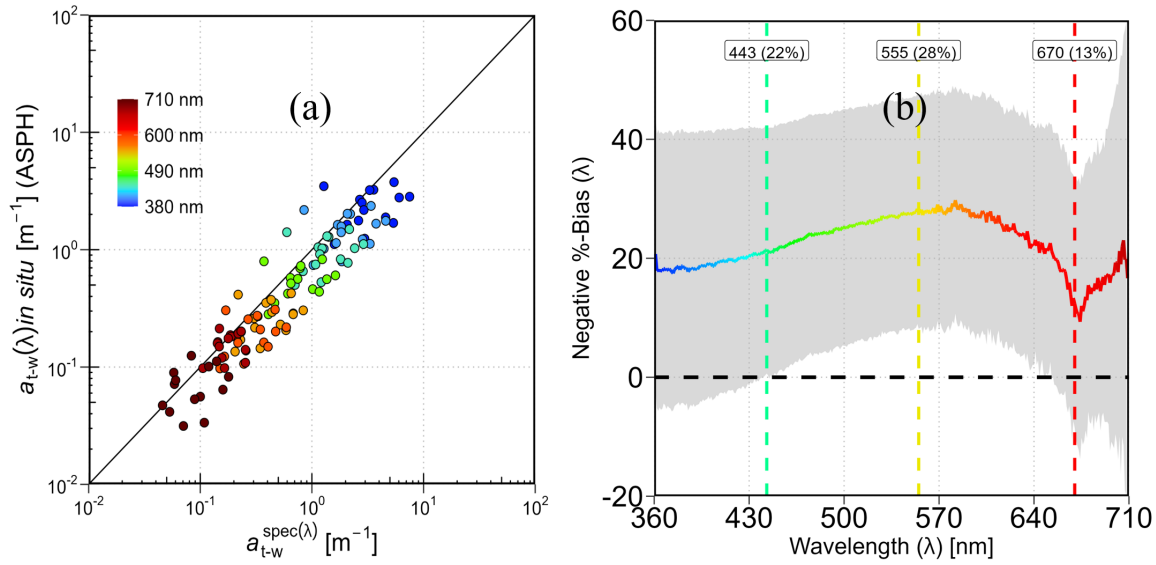


FIGURE 5 – Consistency check for the ASPH absorption data : **(a)** The comparison of ASPH $a_{t-w}(0^-, \lambda)$ with a_{t-w}^{spec} from the surface waters. **(b)** %-Bias (sign inverted) between ASPH and a_{t-w}^{spec} values plotted against λ . The sign is inverted for ease of comparison with the shape of fluorescence. The shaded region shows a 95% Confidence Interval calculated between 360-710 nm for each λ . The vertical dotted lines show the %-Bias for three distinct λ (blue, green, red).

1.5.3 Optical closure

The assessment of optical closure was performed for the 12 stations where simultaneously acquired data from the ASPH, HydroScat and C-OPS were available. Modeled $R_{rs}(0^-, \lambda)$ from HydroLight were compared to the $R_{rs}(0^-, \lambda)$ derived from C-OPS measurements (Fig. 6a). HydroLight simulations were performed using *in situ* IOPs (Fig. 6b,c,d) to obtain $R_{rs}(0^-, \lambda)$ with both only elastic scattering (denoted HL_{el}), as well as for elastic and inelastic scattering combined (denoted $HL_{el+inel}$).

1.5.3.1 Sensitivity to backscatter fraction

From the sensitivity analysis for $\tilde{B}$, we found that the simulated R_{rs} with $\tilde{B} = 0.018$ and $\tilde{B} = 0.013$ were similar in shape and magnitude with each other (spectral % difference for all

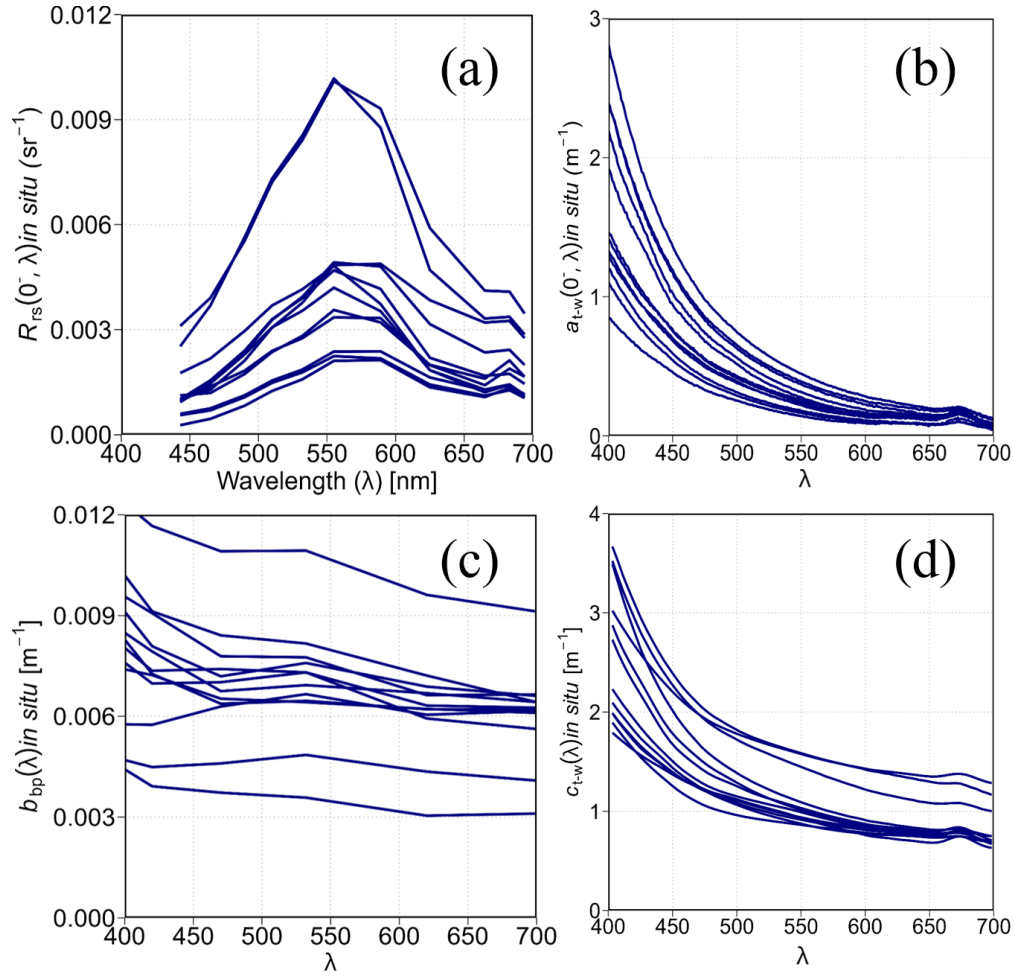


FIGURE 6 – *In situ* R_{rs} and IOP data for 12 *Kildir* stations used in optical closure. In (a) The R_{rs} here is shown for subsurface depth (~ 0.5 m inside water, $z = 0^-$). The corresponding IOP data, i.e. a_{t-w} , b_{bp} and c_{t-w} (b, c, d) are also shown for subsurface depth ($z = 0^-$).

λ of 2.8%). In both cases, simulated R_{rs} were higher than the *in situ* values (spectral %-Bias over all λ , +8.33% and +11%). $\tilde{B} = 0.010$ generated comparatively lower values of R_{rs} by 4 to 10% relative to Petzold's $\tilde{B}$ (0.018) and the resulting R_{rs} were in better agreement with the *in situ* R_{rs} . These results are consistent with the previous interpretation of the BB9-derived b_{bp} being overestimated (giving the value of $\tilde{B} = 0.013$) and since that instrument's data was discarded in the remainder of the study, it was applied in this context also. The value of $\tilde{B} = 0.018$ was just based on the assumption of Petzold's phase function, whereas the value

$\tilde{B} = 0.010$ was obtained from measurements in the study area using the HydroScat. Thus, $\tilde{B} = 0.010$ was preferred for the APSH and HydroScat stations and the other values were not propagated further in the analysis.

1.5.3.2 Impact of the ASPH bias correction

The impact of the a_{t-w} underestimation by the ASPH on the optical closure was investigated. HydroLight was run using four configurations : 1) bias-corrected and HL_{el} , 2) bias-corrected and $HL_{el+inel}$, 3) bias-uncorrected and HL_{el} , and 4) bias-uncorrected and $HL_{el+inel}$. The corresponding σ -corrected b_{bp} from the HydroScat was used in all cases. The modeled $R_{rs}(0^-, \lambda)$ were compared to the corresponding *in situ* $R_{rs}(0^-, \lambda)$ and the spectral %-Bias was used as the evaluation metric.

For $R_{rs}(0^-, \lambda)$ governed by elastic scattering components, i.e. a_{t-w} and b_{bp} mainly, an underestimation in magnitude was observed for both bias-corrected and bias-uncorrected absorption. The underestimation was dependent on λ and reached maximum values in the “green maxima” ($555 \leq \lambda(\text{nm}) \leq 560$) (Fig.7a). However, the underestimation of $R_{rs}(0^-, \lambda)$ was almost twice higher when using bias corrected ASPH absorption than when using their uncorrected version. A similar pattern was observed when inelastic scattering was included in the simulations. However, the underestimation of $R_{rs}(0^-, \lambda)$ at “green maxima” was much lower when the $HL_{el+inel}$ used bias-uncorrected ASPH absorption as an input (Fig. 7b). Aggregating the results for the 12 stations revealed that the $R_{rs}(0^-, \lambda)$ at “green maxima” simulated using the bias-corrected absorption led to a worse %-Bias (HL_{el} : -45.5%, $HL_{el+inel}$: -30%) compared to those generated with the bias-uncorrected absorption (HL_{el} : -16%, $HL_{el+inel}$: -1.5%) (Fig. 7c). Compiling the results at all λ , the precision and linearity of the fit were also better when the bias-uncorrected absorption was used, especially for $HL_{el+inel}$ (bias uncorrected : $R^2 = 0.96$; bias corrected : $R^2 = 0.84$)(Fig. 8).

As a result of these comparisons, the bias-uncorrected ASPH a_{t-w} was used in the rest of this study. However, these comparisons also suggest some possible discrepancies (See 1.6.1)

in the a_{t-w}^{spec} apart from the internal fluorescence inside ASPH previously discussed. Regardless of the a_{t-w} used, the inclusion of inelastic scattering considerably reduced the severity of the underestimation in simulated R_{rs} relative to the reference *in situ* $R_{rs}(0^-, \lambda)$. The next section further analyzes the importance of inelastic scattering in a more detailed manner.

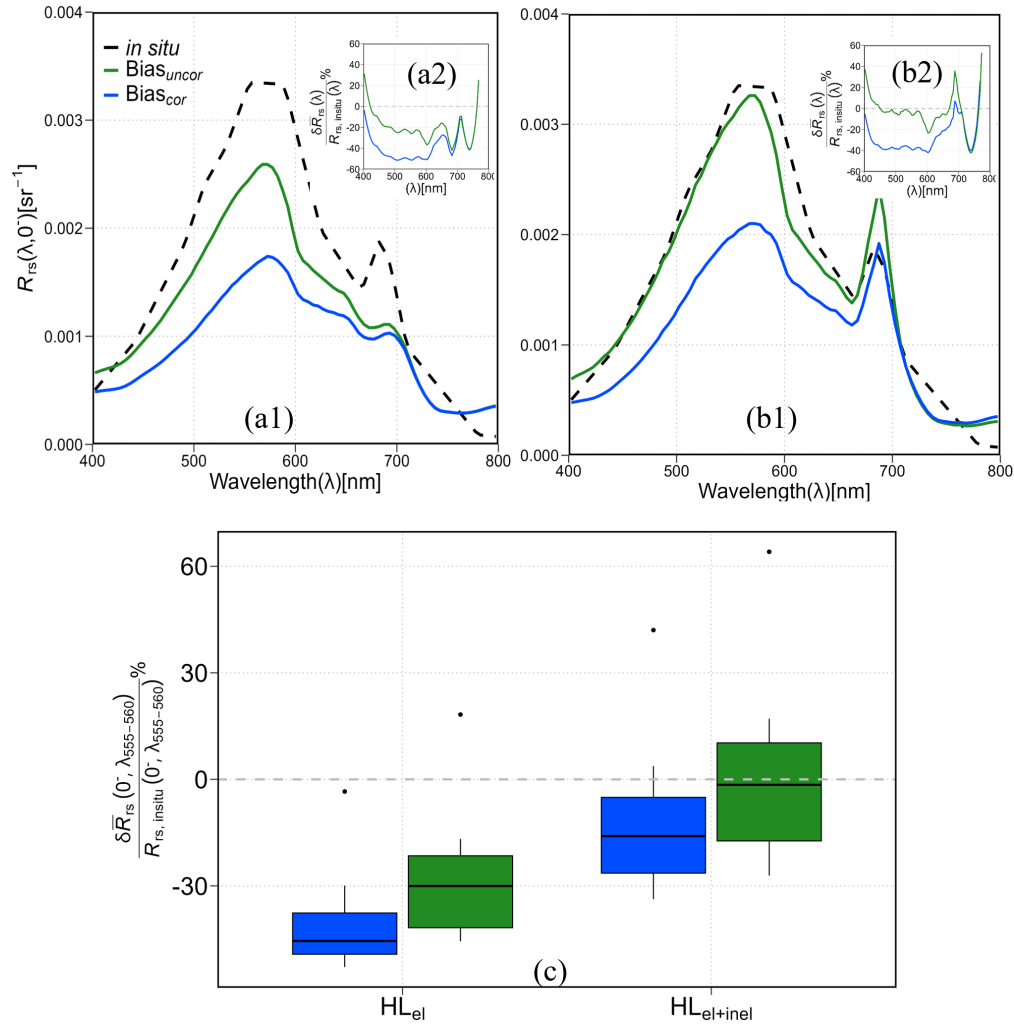


FIGURE 7 – **(a1.)** Spectral plots of variation in HydroLight modeled $R_{rs}(0^-, \lambda)$ from HL_{el} for bias-corrected and bias-uncorrected ASPH a_{t-w} data along *in situ* $R_{rs}(0^-, \lambda)$ derived from the C-OPS (solid black line). The encapsulated plot **(a2.)** shows the spectral %-Bias between C-OPS acquired $R_{rs}(0^-, \lambda)$ and modeled $R_{rs}(0^-, \lambda)$ for bias-corrected and bias-uncorrected ASPH a_{t-w} respectively. **(b1,b2)** Same as **(a1,a2)** but obtained with $HL_{el+inel}$. **(c)** Boxplot of %-Bias at "green-maxima" for modeled $R_{rs}(0^-, \lambda)$ for both elastic and inelastic scattering including bias-corrected and bias-uncorrected ASPH a_{t-w} respectively for all 12 stations.

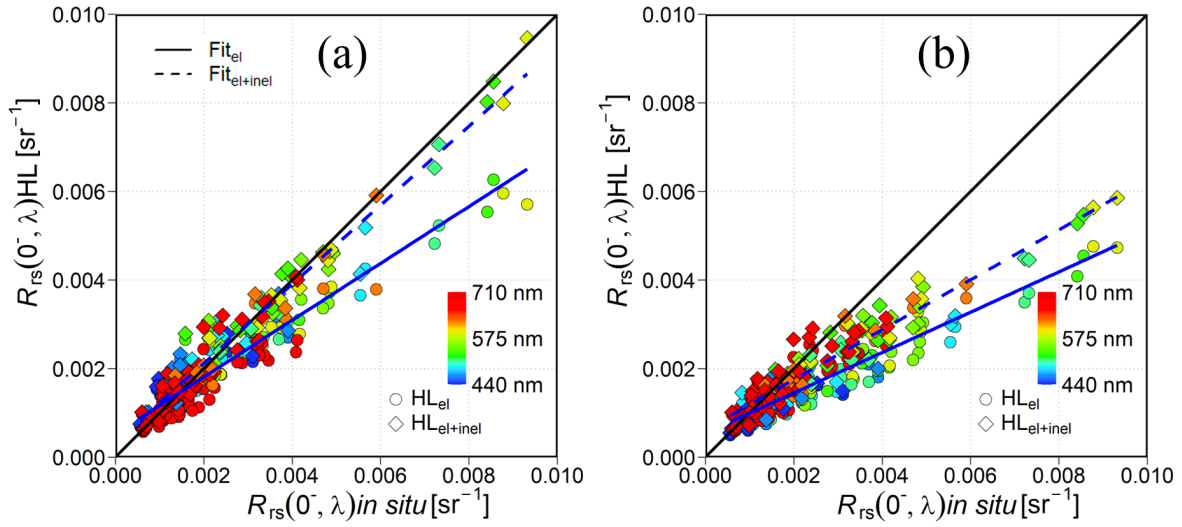


FIGURE 8 – Scatterplot of *in situ* versus modeled $R_{rs}(0^-, \lambda)$ using a_{t-w} and corresponding σ -corrected b_{bp} from the HydroScat using (a) bias-uncorrected ASPH a_{t-w} . (b), bias-corrected a_{t-w} . In both panels, diamonds and circles are for HydroLight simulations with and without inelastic scattering, (HL_{el} and $HL_{el+inel}$) respectively.

1.5.3.3 Significance of inelastic scattering

At blue wavelengths (440-490 nm), modeled $R_{rs}(0^-, \lambda)$ with and without inelastic scattering had approximately the same precision; $R^2 = 0.84$ and 0.85 respectively (Fig. 9a, Table 9). The regression slope improved slightly (0.62 to 0.75) when inelastic scattering was included. The MDAPE, RMS%E and %-Bias metrics showed slightly better results without inelastic scattering (Table 9). In particular, there was a decreasing trend in %-Bias (overestimation of $R_{rs}(0^-, \lambda)$) with increasing λ . At 443, 465, and 490 nm %-Bias without inelastic scattering was 20%, 13% and -3%; vs. with inelastic scattering, 28%, 24% and 11%, respectively (Fig. 10b). Note however that $R_{rs}(0^-, 443)$ values were very low (≤ 0.002 sr⁻¹), making it prone to high relative errors. In addition, there is relatively less contribution from inelastic scattering by CDOM and chlorophyll-a at blue wavelengths in this study, which explains the small differences observed between the two sets of simulations (Fig. 9a, 10b).

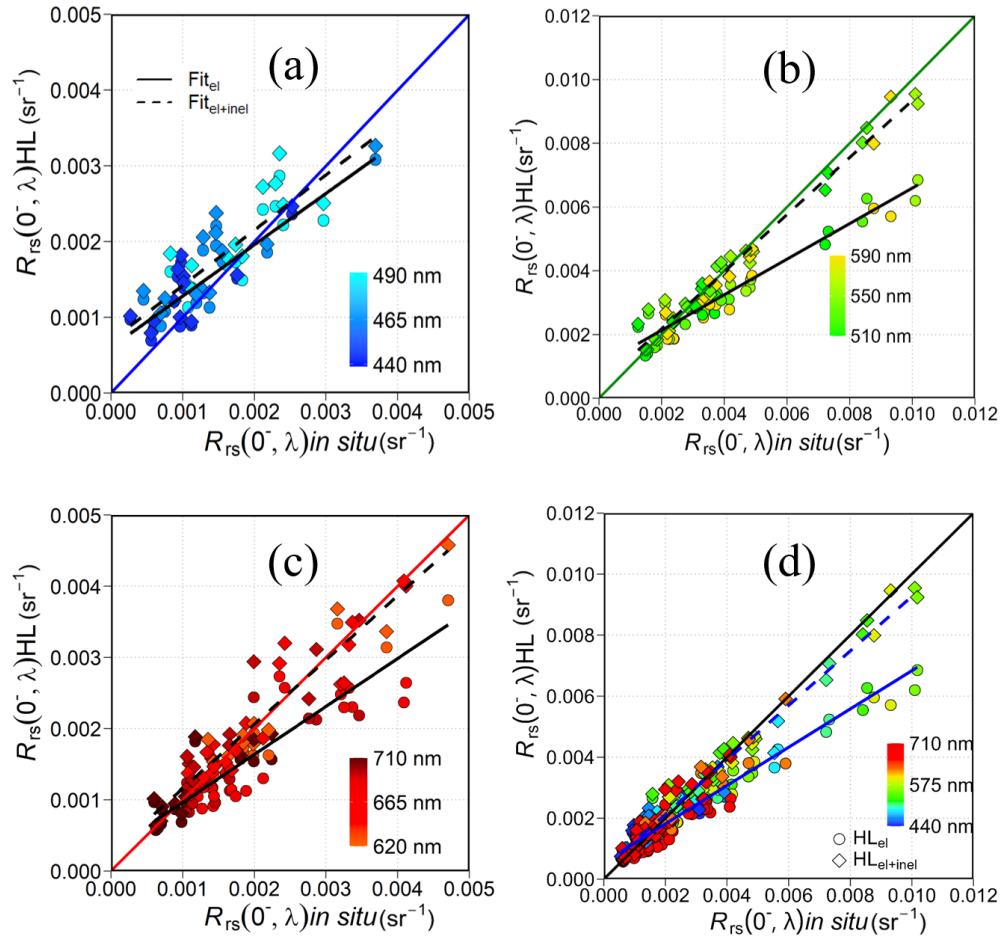


FIGURE 9 – Scatterplots for optical closure obtained for three spectral groups, i.e. **(a)** Blue (440-490nm), **(b)** Green (510-590nm), **(c)** Red (620-710nm) and **(d)** RGB (440-710nm). The solid-coloured diagonal line (slope; $m = 1$) in each plot is the 1 : 1 line. The black solid lines (Fit_{el}) show the linear fit between *in situ* $R_{rs}(0^-, \lambda)$ and HL simulated $R_{rs}(0^-, \lambda)$ with elastic scattering (HL_{el}) whereas, the black dashed lines ($Fit_{el+inel}$) represent linear fit between *in situ* $R_{rs}(0^-, \lambda)$ and HydroLight modeled $R_{rs}(0^-, \lambda)$ with both elastic and inelastic scattering ($HL_{el+inel}$).

At green wavelengths (510-590 nm), where inelastic scattering is primarily from CDOM fluorescence, the inclusion of inelastic scattering improved the agreement with *in situ* $R_{rs}(0^-, \lambda)$ in all stations significantly (Fig. 9b), the precision improved by 7% ($R^2 = 0.97$ from 0.90) and the regression slope increased considerably from 0.57 to 0.91. Accuracy was also signi-

TABLE 2 – Statistics on the goodness of fit between C-OPS acquired *in situ* $R_{rs}(0^-, \lambda)$ data and HydroLight modeled $R_{rs}(0^-, \lambda)$ with (**inel**) and without (**el**) inelastic scattering. Statistical metrics are the coefficient of determination (R^2), the slope of the linear fit (m) along with **MDAPE (%)**, **RMS %E** and **%-Bias** defined in equations (4a-4c). The R^2 and m are obtained with the Major Axis regression of the Type-II family.

λ	R^2		Slope (m)		MDAPE(%)		RMS %E		%Bias	
	el	inel	el	inel	el	inel	el	inel	el	inel
Blue	0.84	0.85	0.62	0.75	22	28	29	35	+11	+21
Green	0.90	0.97	0.57	0.91	21	0.05	23	14	-14	+1
Red	0.81	0.92	0.69	0.95	22	9	21	13	-13	+7
RGB	0.90	0.96	0.64	0.90	21	12	26	22	-8	+6

ificantly improved; MDAPE and RMS%E were reduced to $< 1\%$ and 14% , respectively, and the %-Bias was almost null (i.e., 1%). The best improvements were observed at 555 and 589 nm, with the %-Bias decreasing from -16% to -1.1% at 555 nm, and from -17% to -3.9% at 589 nm (Fig. 10b). These results revealed the importance of f_{DOM} for attaining good optical closure in CDOM-rich, highly absorptive waters.

At red wavelengths (620-710 nm), the sun-induced chlorophyll-a fluorescence (SICF) made a large contribution to inelastic scattering, and the optical closure was considerably improved when this process was included in the simulations (Fig. 9c, Table 9). Both precision and linearity increased (i.e. R^2 and m), the MDAPE decreased from 22% to 9% , the RMS%E improved by 8% , and the %-Bias changed from a large underestimation (-13%) to a moderate overestimation (7%). The highest reductions in %-Bias were observed at 667 nm and 685 nm. At 667 nm, the %-Bias dropped from -13% to -1% . At 685 nm, which corresponds to the SICF emission peak (Mobley, 1994), the large underestimation of -27% changed to a small overestimation of 6% (Fig. 10b). These results strongly imply that the omission of SICF in the radiative transfer simulations was responsible for the underestimation of R_{rs} in the red region.

Finally, the contributions of f_{DOM} and SICF to the modeled $R_{\text{rs}}(0^-)$ were estimated (Fig. 10a) by using HydroLight configurations that enabled the calculation of inelastic scattering contributions. When including all stations, the mean contribution from f_{DOM} was $\sim 18\%$ in the green region and was highest at 555 nm ($\sim 21\%$). Similarly, the mean contribution of SICF in red wavelengths was $\sim 20\%$, with the highest contribution being $\sim 30\%$ at 685 nm (Fig. 10a).

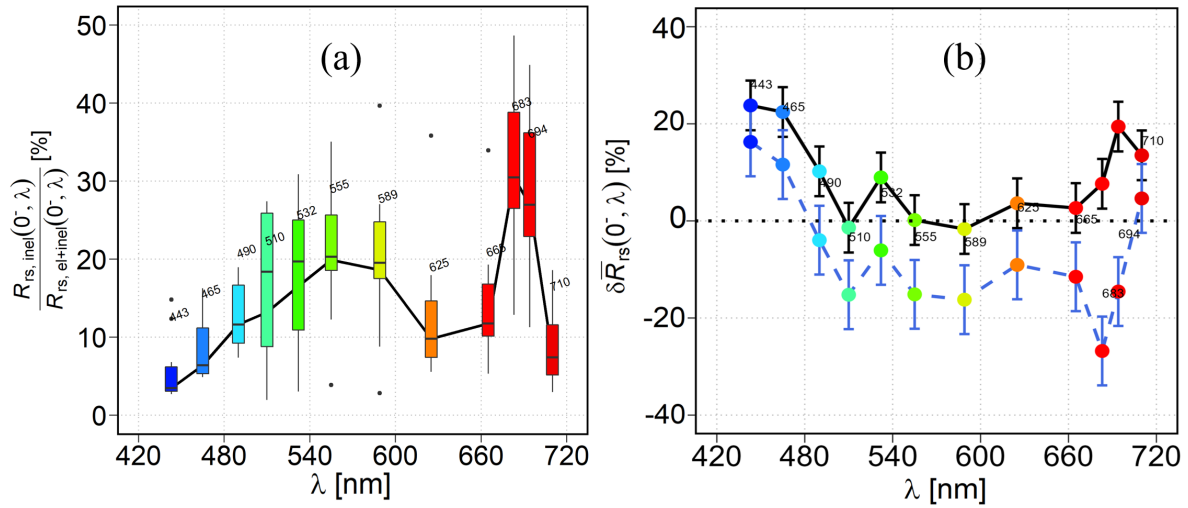


FIGURE 10 – Contribution of inelastic scattering (in %) to $R_{\text{rs}}(0^-, \lambda)$ from HydroLight simulations : **(a)** Spectral box-plots from modeled outputs across C-OPS λ . The solid black line shows the mean contributions of inelastic scattering. **(b)** Mean $\delta \bar{R}_{\text{rs}}$ (in %) compared to *in situ* measurements from all stations for both HL_{el} (Blue dotted line) and $HL_{\text{el+inel}}$ (Black solid line) (+ is overestimation in simulation and - is underestimation). The vertical whiskers around each point show a 95% confidence interval of the mean $\delta \bar{R}_{\text{rs}}$ from all stations and for each λ .

1.6 Discussion

1.6.1 IOP determination in absorbing waters

The colour of the water varied between yellowish green to yellowish-brown where R_{rs} peaked between 570 nm and 600 nm for most of the stations (Fig. 6a), suggesting OSCs

absorb the majority of light in blue and green λ . As shown by Araújo and Bélanger (2022), CDOM largely dominates the absorption budget across the whole visible spectrum in these nearshore waters, with a_{CDOM} accounting for $\sim 80\%$ of $a_{\text{t-w}}$ in the blue. Similar CDOM-rich characteristics in ESL have also been reported by multiple studies (Nieke et al., 1997; Bélanger et al., 2017; Jaegler, 2014).

A noticeable result in the current study was the systematic underestimation of *in situ* $a_{\text{t-w}}$ relative to the spectrophotometric reference, in data from both the ASPH and AC-S. One possible explanation is the depth discrepancy between the water sampling and optical package(s). Freshwater lensing of the river outflow could lead to waters very close to the surface being higher in CDOM than subsurface waters. For example, at station OUT-R09, $a_{\text{t-w}}(443)$ dropped by 70% ($\sim 1.4 \text{ m}^{-1}$ to $\sim 0.4 \text{ m}^{-1}$) between 1 m to 2.5 m depth, while the salinity changed from ~ 23 PSU to ~ 28 PSU. However, in general, water was sampled carefully using a Niskin bottle at ~ 0.5 m at most stations without any issues and it should be comparable to the shallowest valid measurements of the IOP package.

The ASPH underestimation relative to spectrophotometric determination was almost systematic and present at 11 out of 12 stations. The underestimation was not spectrally flat and has features that resemble the combined shape of $[chl]$ and CDOM fluorescence contribution to remote sensing reflectance (Fig. 5b, Fig. 10a). The ASPH uses a flow-through ICAM to acquire the $a_{\text{t-w}}$ values, is theoretically free of scattering errors, unlike the AC-S a -tube. However, the finite volume of pumped water inside the sphere is exposed to a continuous polychromatic light field that may be sufficient to excite DOM fluorophores and pigments, which would re-emit some photons in blue-green and red wavelengths, respectively. The re-mitted light would yield lower $a_{\text{t-w}}$ than expected in these spectral ranges. A similar result of ASPH underestimation in the St Lawrence River waters was reported by Bélanger et al. (2014), where both f_{DOM} and SICF were hypothesised to be the cause of ASPH underestimation of $a_{\text{t-w}}$ values by $\sim 20\%$ and $\sim 30\%$ in green and red, respectively, while underestimation was negligible in the Ultra-Violet (UV) range. However, in the current study, the underestima-

tion was non-negligible in the UV (360-400 nm). In these spectral ranges, inelastic scattering within the instrument can not explain this result.

Another source of discrepancy between *in situ* and spectrophotometric a_{t-w} could be linked to scattering by very small particles (VSP) ($\leq 0.2 \mu\text{m}$) in CDOM-rich coastal waters. Balch et al. (2012) stated a 100% increase in b_b values in the Gulf of Maine (GoM), which were associated with flocculation of CDOM under very high river discharge. Moreover, the study by Zhang et al. (2013) in lakes found a significant correlation ($r = 0.59$) between estimated $b_{b\text{VSP}}(532)$ and spectrophotometric $a_{\text{CDOM}}(412)$, which suggest a common DOM origin for both the variables. As a result, if we assume that VSP arising from CDOM in high concentration does scatter light in coastal environments, and these particles are not fully removed by filtering, spectrophotometric *in lab* a_{CDOM} might be overestimated due to the loss of photons by scattering along the 10 cm pathlength. Part of this loss of photons is corrected by subtracting a flat offset by assuming null absorption at 685 nm, but this may be ineffective if the VSP scattering has a steep spectral dependency toward decreasing λ , which is likely since the particles are small.

The filter pad-based spectrophotometric values of particulate absorption (a_p) also have been reported to be affected by the uncertainty from path length amplification factor (βF) and scattering offset (o) even after null correction at the NIR wavelengths. Lefering et al. (2016b) showed an improved regression-based correction to determine optimal βF and o using the regression slopes and intercepts, respectively obtained from the linear relationship between the spectrophotometric values of a_p and the same obtained from a PSICAM. In our study, we did not have concurrent measurements with PSICAM which limits our correction for filter-pad to often used flat offset correction, which might have introduced potential error in our spectrophotometric a_p . This interpretation is consistent with the HydroLight simulations performed using ASPH data corrected to be aligned with the spectrophotometric measurements, which resulted in much lower R_{rs} relative to the ASPH bias uncorrected results, and were further from the C-OPS derived R_{rs} (Fig. 7, 8).

Overall, we hypothesize that ASPH-derived a_{t-w} was underestimated relative to the spectrophotometer measurements due to the combination of both potential fluorescence within the ASPH and uncertainty in spectrophotometric a_{t-w} from the possible uncertainties in a_p and a_{CDOM} discussed above, yet the net contribution of each of these processes remains to be quantified. But, consequentially, neither the uncorrected ASPH nor the spectrophotometer measurements can be definitively treated as a reliable baseline in this study.

1.6.2 Optical closure in absorbing waters : significance of inelastic scattering processes

The best closure results were obtained when IOPs from the ASPH (uncorrected) and HydroScat measurements were used in the modeling, and inelastic scattering of both CDOM and SICF was also included. However, simulated R_{rs} in the blue wavelengths were still overestimated. This might be related to the discrepancy of a_{t-w} by the ASPH discussed above, especially in the blue spectral range. As the absorption budget in our study area is CDOM driven, the uncertainty in the ASPH absorption magnitude can be considered as critical for the closure disparity in the blue range. The corresponding b_{bp} values at blue (420 nm) had higher variability than green λ (sd at 420nm = $\sim 0.0028m^{-1}$; at 532nm = $0.002m^{-1}$) which incorporates uncertainty to some extent in the obtained R_{rs} at blue wavelengths. In addition, the *in situ* $R_{rs}(0^-)$ at blue wavelengths was very low ($\leq 0.002 sr^{-1}$). For some stations, in-water upwelling radiance near the sea surface was lower than the sensor detection limit, which resulted in larger uncertainty in R_{rs} values for $\lambda \leq 490nm$. In summary, the main source of the error for the closure in the blue range is likely caused by uncertainty in both *in situ* IOPs (especially, a_{t-w}) and R_{rs} in these the CDOM-rich dark waters.

The improvement in optical closure arising from the inclusion of inelastic scattering in the modeling was greatest in green wavelengths, resulting in an underestimation of only 1% vs. 14% (Table 9). Fluorescence in green wavelengths was dominated by f_{DOM} and these results are consistent with the findings of other studies (Tzortziou et al., 2006; Bausell and Kudela, 2021; Lefering et al., 2016a). Tzortziou et al. (2006) showed that inclusion of f_{DOM}

improved the closure in green by 2-5% in the Chesapeake Bay. In this environment, mineral particles are an important OSC, and the surface b_{bp} values in green reported by Tzortziou et al. (2006) were almost twice the magnitude of our b_{bp} (0.007 m^{-1} versus 0.015 m^{-1}). In another study, Lefering et al. (2016a) reported underestimation in L_w from HydroLight modeling in green wavelengths and suggested exclusion of f_{DOM} might be one of the reasons. While some of these studies suggested that the underestimation in green could be in part due to an erroneous scattering correction method for flow-tube meters such as AC-S, that is not applicable to the ICAM-based sensor used here.

The contribution of f_{DOM} to green R_{rs} reached $\sim 18\%$ in our study, which is higher than other closure studies, e.g. Tzortziou et al. (2006). This makes sense for this environment, as the Manicouagan nearshore waters are characterized by high CDOM and are relatively low in terms of particle load, resulting in dark waters (Araújo and Bélanger, 2022). These conditions increase the relative importance of CDOM fluorescence at the emission wavelengths (500 to 600 nm). We also considered if the large CDOM fluorescence contribution to modeled R_{rs} could be an artefact of the assumption of vertically-homogeneous a_{CDOM}/a_{t-w} ratio in the water column (0 to 4 m); this might be erroneous in the presence of strong stratification in the water column (Araújo and Bélanger, 2022). However, we assessed the impact of considering vertically homogeneous IOP data (see Supplementary Information Section S4) and found that stratification at greater depths had a negligible impact on optical closure at most stations. This is consistent with the shallow penetration depth in the study area that does not typically exceed $\sim 3.5 \text{ m}$ in the green-yellow bands (555-589 nm) (Fig. 34).

It is well known that SICF makes a critical contribution to $R_{rs}(0^-)$ in red wavelengths (see Babin et al. (1996) and references therein). Our results are consistent with the closure results observed in Tzortziou et al. (2006), which reported an underestimation of 30%-40% in 670-690 nm in simulated water-leaving radiance when ignoring SICF. In our results, the most substantial improvement from including SICF in the modeling was at 685 nm (Fig. 10b), although overestimation was observed at a few stations (Fig. S8 (b, d, i)). A possible

explanation could be mismatched $[chl]$ values in a stratified environment however, the same for CDOM had a negligible impact on the closure (See Section S4 in supplementary material). Uncertainty in fluorescence quantum yield may also be a factor, for both f_{DOM} and SICF. The default HydroLight quantum yield values were used in this study (Mobley, 1994; Hawes et al., 1992), but the values for f_{DOM} in particular compared to that of SICF are subject to high uncertainty due to a lack of published data. Moreover, The estimation of fluorescence quantum yields or more detailed measurement of $[chl]$ profiles was out of the scope of this work. Still, nevertheless, the results obtained give a good overall picture of the importance of considering inelastic processes in nearshore CDOM rich waters for remote sensing applications.

1.7 Conclusion

This study has assessed the criteria required to obtain good optical closure in CDOM-rich coastal waters. The study consisted of two *in situ* IOP packages (ASPH and HydroScat, AC-S and BB9), spectrophotometric determination of absorption coefficients and HydroLight simulations, where a number of challenges were identified to reach good optical closure in this water type.

In terms of IOPs, ASPH-derived a_{t-w} values were systematically lower than laboratory-measured spectrophotometric absorption but yielded good closure results. Potential explanations for this observation are fluorescence inside the ASPH integrating sphere or from very small particle (VSP) scattering leading to inaccuracies in the spectrophotometer CDOM absorption measurements followed by experimental uncertainty from βF and o in filter pad measured particulate absorption due to absence of concurrent absorption measurements with PSICAM. In particular, HydroLight simulations performed using bias-corrected a_{t-w} (aligned with the spectrophotometer) did not improve the optical closure, which implies the dual-beam spectrophotometer measurements may not be free of errors in our study. With respect to parti-

culate backscatter, b_{bp} , the HydroScat acquired values were almost half the magnitude of the BB9 values, the HydroScat data was spectrally smoother and almost flat, whereas the BB9 data were comparatively noisy. Various consistency checks, including correlation with SPM and the non-algal absorption coefficients, along with the overall pattern of the HydroScat and BB9 datasets, led to the conclusion the BB9 data were not sufficiently reliable for the current optical closure analysis. The BB9 data, together with the AC-S data, were therefore not further considered for the optical closure presented here (see Supplementary Material for AC-S and BB9 closure).

Overall, the best closure results were obtained from the ASPH and HydroScat data with incorporating inelastic scattering processes in the RT model simulations. Based on the HydroScat runs, we estimated the contribution of f_{DOM} to R_{rs} in the green was $\sim 18\%$, and SICF in the red of $\sim 20\%$. While most optical closure studies consider SICF, f_{DOM} is generally considered of secondary importance or negligible. Our results indicate that in CDOM-dominated coastal waters, the significance of CDOM fluorescence may need to be reviewed as an important component of remote sensing reflectance. However, especially for f_{DOM} , there is a general lack of knowledge of the possible range of the quantum yield, and the wavelength redistribution function, which determines the fluorescence spectral shape. These parameters, which are likely to vary dependent on specific materials present in the environment, undoubtedly propagate their own uncertainties to the modeled reflectance. Sensitivity analyses could be useful for quantifying this uncertainty. Ideally, methods for measuring quantum yields or full spectral functions for f_{DOM} could be further developed. We conclude that including CDOM inelastic scattering is important to obtain good optical closure in absorbing waters.

ARTICLE 2

A SEMI-ANALYTICAL BAYESIAN ERROR RETRIEVAL (S.A.B.E.R) ALGORITHM FOR THE INVERSION OF REMOTE SENSING REFLECTANCE IN OPTICALLY DEEP AND SHALLOW WATERS

Article submitted to **Limnology & Oceanography : Methods**

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2.1 ABSTRACT

The inverse problem in remote sensing of aquatic environment consists in retrieving optically significant constituents (OSC) from a spectral measurement of the reflectance (R_{rs}). OSC includes Chlorophyll-a concentration ($[chl]$), a proxy of phytoplankton biomass, absorption of coloured detrital matter (a_{dg}), a proxy of organic carbon and detrital matter, and particulate backscatter (b_{bp}), a proxy of total suspended particulate matter (SPM). In optically shallow waters, apart from OSCs, water depth (H) and benthic albedo (R_B) influence the R_{rs} spectral shape and magnitude. The *state-of-the-art* methods invert R_{rs} from a semi-analytical formulation of the problem using Gauss-Newton or gradient-descent-based optimization routines. However, these methods are inadequate to deal with the “*ill-posed*” nature of R_{rs} inversion, where multiple combinations of OSCs, H and R_B can produce almost identical R_{rs} spectra. Here a Bayesian probabilistic inversion scheme named S.A.B.E.R. is proposed and developed to simultaneously retrieve OSCs and H in optically complex waters following the Markov Chain Monte Carlo (MCMC) sampling approach. The model prior distribution (Prior) was fitted as *Log-Normal*, which was obtained from a comparison of three distributions in the Positive real domain ($\mathbb{R}^+$) and the model likelihood was fitted as *Gaussian*. The least ambiguous values were obtained from *Maximum-a-posterior* (MAP) estimates, which were associated with the highest MCMC sampled posterior probability density for each of the retrieved variables. This probabilistic approach was tested with both synthetic datasets and global *in situ* observations, and for both optically deep and shallow water cases. The model performance was compared to the quasi-analytical algorithm (QAA) in terms of mean uncertainty of OSC (SABER : 38.23% ; QAA : 48.86%) and to the Hyperspectral Optimization Process Exemplar model (HOPE) for H retrieval (SABER : 7.05% ; HOPE : 18.67%). Among the retrieved variables, the highest uncertainty was obtained for $[chl]$, whereas b_{bp} estimates had the least. The benefits and limitations of the MCMC-based inversion are finally discussed for its application to remote sensing of seawater constituents and bathymetry retrievals in optically complex waters.

2.2 RÉSUMÉ

Le problème inverse en télédétection de l'environnement aquatique consiste à extraire les constituants optiquement significatifs (OSC) à partir d'une mesure spectrale de la réflectance (R_{rs}). Les OSC incluent la concentration de chlorophylle-a ($[chl]$), indicateur de la biomasse phytoplanctonique, l'absorption de la matière détritique colorée, ou matière jaune, (a_{dg}), proxy du carbone organique et de la matière détritique, et la rétrodiffusion particulaire (b_{bp}), indicateur de la matière particulaire totale en suspension (MES). Dans les eaux peu profondes, en plus des OSC, la profondeur de l'eau (H) et l'albédo benthique (R_B) influencent la forme spectrale et l'amplitude du R_{rs} . Les méthodes actuelles (*state-of-the-art*) inversent le spectre de R_{rs} en utilisant une formulation semi-analytique du problème et des algorithmes d'optimisation de type Gauss-Newton ou à descente de gradient. Cependant, ces méthodes sont insuffisantes pour traiter la nature "*mal posée*" de l'inversion du R_{rs} , où de multiples combinaisons d'OSC, H et R_B peuvent produire des spectres R_{rs} presque identiques. Dans la présente étude, un schéma d'inversion probabiliste de type Bayésien, nommé S.A.B.E.R., est développé pour extraire simultanément les OSC et H dans des eaux optiquement complexes, suivant une approche d'échantillonnage par chaînes de Markov de Monte Carlo (MCMC). La distribution *a priori* du modèle a été ajustée sous forme de *Log-Normal*, obtenue par comparaison de trois distributions sur le domaine des réels positifs ($\mathbb{R}^+$), tandis que la vraisemblance du modèle a été ajustée comme une distribution *Gaussienne*. Les valeurs les moins ambiguës ont été obtenues à partir des estimations de *Maximum-a-posteriori* (MAP), associées aux densités de probabilité postérieures les plus élevées pour chacune des variables récupérées. Cette approche probabiliste a été testée à la fois avec des ensembles de données synthétiques et des observations globales *in situ*, pour des cas d'eaux optiquement profondes et peu profondes. Les résultats du modèle ont été comparées à ceux de l'algorithme quasi-analytique (QAA) en termes d'incertitude moyenne des OSC (SABER : 38,23% ; QAA : 48,86%) et au modèle *Hyperspectral Optimization Process Exemplar* (HOPE) pour l'estimation de H (SABER : 7,05% ; HOPE : 18,67%). Parmi les variables estimées, la plus forte incertitude a été

observée pour la $[chl]$, tandis que les estimations de b_{bp} étaient les plus robustes. Enfin, les avantages et les limites de l'inversion bayésienne basée sur MCMC sont discutés pour son application à la télédétection des constituants marins et l'estimation de la bathymétrie dans des eaux optiquement complexes et peu profonde.

2.3 Introduction

The spectral remote sensing reflectance, $R_{rs}(\lambda)$ [sr^{-1}], i.e. the ratio of water-leaving radiance (L_w) to downwelling irradiance (E_d), is an apparent optical property (AOP) on which we rely to quantify the optically significant constituents (OSCs) from remotely sensed multispectral or hyperspectral measurements. In the theory of aquatic radiative transfer (RT), the AOPs are primarily governed by the inherent optical properties (IOPs), i.e., spectral absorption $a(\lambda)$ [m^{-1}] and backscattering $b_b(\lambda)$ [m^{-1}] coefficients (Kirk, 1983; Mobley, 1994). The shape and magnitude of IOPs are found to have strong relationships with in-water OSCs, which are often quantified using water quality indicators, such as turbidity [NTU], and concentration of chlorophyll-a [chl] [mg m^{-3}] for phytoplankton biomass, total suspended solids (TSS; [mg L^{-1}]), suspended particulate matter (SPM; [mg L^{-1}]), or dissolved organic carbon (DOC) [$\mu\text{mol L}^{-1}$] (IOCCG, 2018). The IOPs of seawater constituents are additive and generally include absorption coefficients of phytoplankton ($a_{ph}(\lambda)$), chromophoric dissolved organic matter (CDOM) ($a_g(\lambda)$), detrital matter ($a_d(\lambda)$), and particulate backscattering coefficient ($b_{bp}(\lambda)$) (Bricaud et al., 1995, 1981; Siegel et al., 2002). In optically shallow waters, i.e., when sea bottom contribute to water-leaving radiance, water column depth ($H[m]$) and benthic reflectance (R_B [unitless]) have significant impacts on the magnitude and spectral shape of the R_{rs} apart from IOPs (Albert and Mobley, 2003).

In the last three decades, numerous studies have attempted to retrieve optically significant constituents along with water column depth and benthic composition in coastal and inland waters. The methods can be categorized as a mathematical “inversion” problem, that predicts the vector of OSCs and/or water depth and benthic composition (hereafter referred to as shallow variables or SV) variables from R_{rs} i.e., $f^{-1}(R_{rs}) = \phi_{var}$, where ϕ_{var} is a vector of retrieved variables : $\{[chl], a_{dg}(443), b_b(555), H, R_B\}^{\mathbb{R}^+}$. The underlying mathematical model for inversion are often based on semi-analytical (SA) approximations of the RT equations depicting the relationship between R_{rs} and IOPs (Gordon et al., 1988; Albert and Mobley, 2003; Hoge, 2003; Lee et al., 2006a; Dekker et al., 2011; Loisel et al., 2018). In

contrast, machine learning (ML) approach exploiting the intrinsic co-variance patterns between concurrent AOPs and IOPs for extensive *in situ* observations or simulated datasets have been proposed (Tanaka et al., 2004; Hieronymi et al., 2017; Smith et al., 2021; Pahlevan et al., 2022).

The state-of-the-art approach to perform the physics-based inversion of the SA equation is based on the Quasi Single Scattering Approximation (QSAA) of upwelling optical signal (Gordon et al., 1988). When the SA approach is applied to optically shallow water, R_{rs} is expressed as the sum of the contributions of the water column and bottom (zero in optically deep water), respectively (Lee et al., 1998a; Albert and Mobley, 2003). Diffused attenuation coefficients for downwelling and upwelling light fields (K_s) for both contributions are parameterized as functions of IOPs and viewing geometry. SA models have mostly been inverted following two approaches. First, spectrum matching technique based on Look-up tables (LUT) of R_{rs} spectra simulated using forward RT model for a large range of OSCs and SV (Hedley et al., 2009b; Mobley et al., 2005). Second, optimization techniques of an objective function (s_{obj}) is used, which denotes the residual error between the observed and modeled R_{rs} (Lee et al., 1998a; Maritorena et al., 2002; Brando et al., 2009; Werdell et al., 2019). A comprehensive overview of different applications of SA parameterized inversions can be found in Lee et al. (2006a), Dekker et al. (2011), and Werdell et al. (2018).

The majority of optimization-based inversion techniques are non-linear, i.e. optimized with derivative-based Levenberg-Marquardt or non-derivative-based Simplex Downhill methods (Dekker et al., 2011; Werdell et al., 2019). The first calculates the optimal set of variables by calculating the Jacobian matrix (first-order partial derivatives of a vector-valued function) for the objective function s_{obj} and tries to find the point of convergence where the change in the Hessian matrix (second-order partial derivatives of a vector-valued function, that gives the rate of change of the Jacobian) becomes flat. The simplex-based method does not attempt to approximate the gradient of s_{obj} . Instead, the objective function is evaluated at each vertex of a simplex defined by $N_\phi + 1$ points in a N_ϕ dimensional solution space,

where ϕ is symmetrical to ϕ_{var} , the vector of retrieved variables. The potential issue of using such nonlinear optimization schemes is attributed to the sensitivity of the inverse model to the initial magnitudes of each element of ϕ_{var} . In the case of a non-plausible initial vector used in mathematically “ill-posed”, in which multiple combinations of ϕ_{var} yield very similar R_{rs} (Defoin-Platel and Chami, 2007b), the solver might fail to reach the global minima/maxima associated with s_{obj} . Spectral matching LUT-based methods are also vulnerable to the “ill-posed” nature of inversion problem. The optimal vector of ϕ_{var} from the LUT is obtained by minimizing the Spectral dissimilarity of the modeled R_{rs} , which itself is ambiguous.

ML-based approaches encompassed various computational techniques and were applied to ocean colour inversion since the late 1990s. For example, Doerffer and Schiller (2007) used a Multi-Layer Perceptron (MLP) based Artificial Neural Network (ANN) trained on simulated datasets generated using Hydrolight (Mobley, 1994). More recently, Mixture Density Network (MDN), which can predict the probability distribution of the output space as a mixture of multi-modal Gaussian distributions, was found to perform better than MLP-based inversion (Smith et al., 2021). MDNs trained with global *in situ* R_{rs} and OSC variables are found to obtain better results compared to physics-based algorithms over multiple orders of magnitudes, for both the case of single variable retrieval (Smith et al., 2021; Jiang et al., 2023), or multiple variable retrievals (Pahlevan et al., 2022; O’Shea et al., 2023). For retrieval of SV, specifically H , supervised classification approach such as Support Vector Machine (SVM) has been used (Wang et al., 2018), while ensemble-based methods, i.e., Random Forest (RF) and XGBoost approaches were found to be more robust (Zhou et al., 2023). One possible concern for the ML models is the necessity of large volume of concurrent AOP-IOP data to train the model, which is essential for robust predictions. Also, categorical training might be necessary for different data sources of the WQ and SV to capture the water type variability for simultaneous retrievals (Pahlevan et al., 2022).

The quantification of uncertainties associated with ocean colour retrievals has become a priority in recent years (Mélin et al., 2016; Mélin, 2019). The sources of uncertainties are

numerous and complex, from IOP bio-optical models, acquisition uncertainty in input R_{rs} , noise from environmental interaction and the random error present in the inversion itself (Lee et al., 2006a; Jay et al., 2017b). In SA-based inversion, sensitivity analysis and noise perturbation methods have been used to estimate the sensor acquisition noise for dynamic atmospheric conditions and how it affects the IOPs retrieval (Roesler and Perry, 1995; Hoge and Lyon, 1996; Brando et al., 2009). Wang et al. (2005) assessed source and variable-specific uncertainty on a pixel-by-pixel approach by determining spectral shape filtering, which might fail to converge in case of a non-plausible spectral shape match. Cramer-Rao bounds (CRB) have also been used to assess uncertainty, which uses the Fisher information of model input (R_{rs} here) to calculate uncertainties (variance) for the retrieved variables (Jay et al., 2017b). Probabilistic Bayesian approaches (Jay and Guillaume, 2014; Erickson et al., 2020; Werther et al., 2022b) incorporate the probability distributions of ϕ_{var} to quantify uncertainty of the retrieved variable. These studies considered *Gaussian* joint probability of ϕ_{var} . However, The vector ϕ_{var} are physical quantities bound in positive real space, $\mathbb{R}^+ : \{0, \infty\}$, whereas the *Gaussian* distribution ranges in $\mathbb{R} : \{-\infty, \infty\}$. There is also an absence of a single probabilistic inversion approach, that can retrieve OSC and SV estimates and its associated uncertainty simultaneously.

The present study proposes a Bayesian inversion approach for SA models. We named this new approach SABER for “Semi-Analytical Bayesian Error Retrieval”. SABER uses $\mathbb{R}^+$ distribution(s) to model the *a priori* and a *Gaussian* error model (likelihood). SABER was developed to simultaneously retrieve the posterior distributions for both OSCs : $\{chl, a_{dg}(443), b_b(555)\}$ and SV : $\{H, R_B\}$. The optimal value from the posterior is obtained by selecting the value associated with the highest probability using the *Maximum-a-posterior* (MAP) approach (Rodgers, 2000; Tarantola, 2005). The associated parametric uncertainty of MAP estimates is obtained from the 95% Bayesian credible intervals (C.I.) of the posterior. SABER was tested on publicly available *in situ* and simulated datasets, and its performance was compared to popular inversion models (QAA by Lee et al. (2002) and HOPE by Lee et al. (1998b)).

2.4 Materials and Methods

2.4.1 Datasets

2.4.1.1 Optically deep waters

For the water column retrieval of OSC, *in situ* observations of $R_{rs}(0^+)$ along with $[chl]$, the sum of absorption coefficients of CDOM and detrital matter at 443 nm ($a_{dg}(443)$) and particulate backscattering coefficient at 555 nm ($b_{bp}(555)$) were compiled from publicly available datasets and synthetic benchmark data (Table 3). Two synthetic datasets were used for optically deep waters (IOCCG and LOISEL) based on Case-1 water type where the spectral IOPs were derived from their bio-optical relationships with $[chl]$ and/or a_ϕ (IOCCG, 2003; Loisel et al., 2023).

The *in situ* data (Table 3; Fig. 12c-e bins with black border) was assembled from two sources. First, Valente et al. (2022) curated several global merged datasets (V22). It contains $R_{rs}(0^+)$ data along with IOPs (a_ϕ , a_{dg} , b_{bp}) and OSC variables, i.e., $[chl]$, total suspended solids (TSS) (where available) from total 27 multi-project archives for time-period between 1997 and 2021. In this study, only the ones having collocated observations of $R_{rs}(0^+)$ with IOPs and OSC variables were used ($N = 1167$, observations from NOMAD, SEABASS, MERMAID, AERONET-OC) (Table 3). Second, Lehmann et al. (2023) compiled hyperspectral observations of $R_{rs}(0^+)$ from coastal and inland waters between 1990 and 2022 in a dataset named GLORIA. $R_{rs}(0^+)$ was least co-located with one observation of either $[chl]$, $a_g(440)$, TSS or Secchi depth. GLORIA does not include any observations for b_{bp} . The $R_{rs}(0^+)$ was filtered by using the “flag” metadata (data discarded if flag = 1) to discard redundant observations identified following the procedures mentioned in Table 3 in Lehmann et al. (2023). A further filter was applied using the “Water_type” metadata to select the CDOM-dominated and $[chl]$ +CDOM-dominated waters ($N = 5793$), where the a_d contribution would be negligible compared to a_g .

TABLE 3 – Summary of all the datasets used to develop the SABER model. Name column refers to the original dataset identifier, reference denotes the academic output documented the dataset. Number of obs refers to the number of complete (IOP-AOP) concurrent samples, Type refers to the mode of the data curation and lastly, a brief remark on each dataset is shown in Description.

Name	Reference	Number of obs.	Type	Description
IOCCG	IOCCG (2003)	500	Synthetic	Hydrolight simulations for optically deep water (no inelastic scattering) with
	Lee et al. (2006a)			calm sea states and sun zenith angle varying for 0°, 30° and 60°.
				The total absorption and backscattering were obtained as a four-component bio-optical model.
LOISEL	Loisel et al. (2023)	3320	Synthetic	Same configuration as IOCCG, but with a three-component bio-optical model with wider range of IOPs.
MERMAID	Valente et al. (2022)	159	<i>in situ</i>	Optically deep waters across the global ocean. Barker (2013a,b)
SEABASS	Valente et al. (2022)	96	<i>in situ</i>	Optically deep waters across the global ocean. Werdell et al. (2003)
NOMAD	Valente et al. (2022)	908	<i>in situ</i>	Optically deep waters across the global ocean (Werdell and Bailey, 2005).
AERONET-OC	Valente et al. (2022)	4	<i>in situ</i>	Optically deep waters in coastal ocean. Zibordi et al. (2009)
GLORIA	Lehmann et al. (2023)	5793	<i>in situ</i>	Hyperspectral reflectance from coastal and inland waters (optically deep filtered).
SHALLOW	This study	500	Synthetic	Optically shallow water simulations using Hydrolight. See section 2.4.1.2

It is important to mention that these filtered observations were used to determine the *a priori* distribution needed in the Bayesian inversion (See 2.4.2.4 and 2.5.2 on Prior). This selection facilitates capturing the inter-parametric covariance among the OSCs in a natural environment, which can be used to constrain the solution space of inversion for a more realistic retrieval (Pahlevan et al., 2022). All the R_{rs} data were interpolated to spectral domain between 400-700 nm with a 10 nm interval to ensure constant spectral resolution in the inversion.

2.4.1.2 Optically shallow water

A synthetic dataset of R_{rs} in the spectral domain between 400-700 nm with a 10 nm interval was generated to simulate a shallow coastal environment ($N = 500$) (Figure 37a). This dataset was produced through HydroLight simulations with a clear sky and calm sea state at sun zenith of 30° ignoring inelastic scattering. Variations in $[chl]$ spanned from 0.5 to 50 mg m^{-3} , while $a_{dg}(443)$ was constrained within 0.1 to 2 m^{-1} . $b_{bp}(555)$ ranged from 0.002 to 0.01 m^{-1} and the water column depth (H) extended from 0.5 to 10 meters. Each input combination of these OSCs and SV was sampled from a multi-variate *Log-Normal* (Campbell, 1995; Defoin-Platel and Chami, 2007b) and an uni-variate *Weibull* distribution, respectively. The sampling for the OSCs was constrained by the covariance pattern obtained from *in situ* observations stated in 2.4.1.1 to obtain realistic vectors of OSCs. The aerial fractions of R_B for three distinct benthic types (Rock, *Lithothamnium sp.*, and *Saccharina latissima*) were held constant at $\{0.50, 0.25, 0.25\}$, respectively. These particular spectra of R_B were derived from underwater radiometric measurements acquired in July 2022 at the south and southwest coasts of Anticosti Island ($\sim 49.3^\circ \text{N}$, 63.0°W), which is located in the Gulf of St. Lawrence in Canada. The benthic cover consisted of rock with dense patches of Kelp; among the different species of Kelps, *Saccharina latissima* was found to be dominant (Roy et al., 2023). Among other variants, *Lithothamnium sp.*, an encrusting algae was also observed. The spectral reflectance (R_B) of these benthic classes (Fig. 37b) was acquired using a handheld spectroradi-

diometer (Spectra Vista Corporation; SVC) deployed by a SCUBA diving team. To account for the acquisition uncertainty similar to *in situ* observations, a *Gaussian* noise ($\mu = 0$ and σ equivalent to 5% of the net standard deviation of the simulated dataset) was added with each simulated R_{rs} spectra before inversion.

2.4.2 The SABER model

The SABER model has two major components : 1. a parameterized forward radiative transfer model (see 2.4.2.1 for details), that relates the IOPs to AOPs ; 2. an inversion of the forward model based on Bayesian sampling, which is elaborated in 2.4.2.2.

2.4.2.1 Semi-analytical forward model formulation

The inversion model is based on the semi-analytic (SA) formulation of the oceanic radiative transfer proposed by Albert and Mobley (2003) (hereafter referred to as AM03) for both optically deep and shallow waters, which is briefly presented in this section. The generalized equation to sub-surface (0^-) R_{rs} can be expressed as :

$$R_{rs}(0^-, \lambda) = R_{rs,\infty} \cdot [1 - \exp\left\{-(K_d + \frac{K_{u,W}}{\cos \theta_v})H\right\}] + \left(\sum_{i=1}^n f_{a,i} \frac{1}{\pi} \cdot R_{B,i}\right) \cdot \exp\left\{-(K_d + \frac{K_{u,B}}{\cos \theta_v})H\right\} \quad (2.1)$$

Where, $R_{rs,\infty}$ is the contribution from the water column only (in optically deep waters, that is the only viable component), which can be expressed as :

$$R_{rs,\infty} = f^\uparrow(\omega_b, \theta_s, u, \theta_v) \cdot \omega_b \quad (2.2a)$$

$$= f^\uparrow(\omega_b) \cdot f^\uparrow(\theta_s) \cdot f^\uparrow(u) \cdot f^\uparrow(\theta_v) \cdot \omega_b \quad (2.2b)$$

$$= P_{rs,1} \cdot \left(1 + P_{rs,2} \cdot \omega_b + P_{rs,3} \cdot \omega_b^2 + P_{rs,4} \cdot \omega_b^3\right) \cdot \left(1 + P_{rs,5} \cdot \frac{1}{\cos \theta_s}\right) \cdot (1 + P_{rs,6} \cdot u) \cdot \left(1 + P_{rs,7} \cdot \frac{1}{\cos \theta_v}\right) \cdot \omega_b \quad (2.3)$$



Where, u is wind speed at surface, ω_b is the single-scattering albedo calculated as $\frac{b_b}{a+b_b}$ and $P_{rs,1-7}$ are parametric coefficients from AM03.

K_d , $K_{u,w}$ and $K_{u,B}$ are diffused attenuation coefficients for downwelling irradiance, upwelling light from the water column and bottom, respectively. These were parameterized following AM03 (assuming $K_{u,w} \equiv K_{u,B}$) as below :

$$K_d = \kappa_0 \cdot \frac{a + b_b}{\cos \theta_s}; K_u = (a + b_b) \cdot (1 + \omega_b)^{\kappa_i} \cdot \left(1 + \kappa_2 \frac{1}{\cos \theta_s}\right) \quad (2.4)$$

Where, κ_0 , κ_i and κ_2 are parametric coefficients and θ_s is solar zenith angle. In Eq. 2.1, the benthic reflectance is modeled as the areal fraction of R_B ($f_{a,i}$). Here we constrained it to three bottom types ($\sum_{i=1}^{n=3} f_{a,i} = 1$) and $\frac{1}{\pi}$ assuming Lambertian bottom type.

The non-water a and b_b values were calculated as the summation of OSC component-specific a and b_b as used in many other studies on inversion (Dekker et al., 2011).

$$a_t(\lambda) = a_w(\lambda) + a_\phi(\lambda) + a_{dg}(\lambda) \quad (2.5a)$$

$$b_{bt}(\lambda) = b_{bw}(\lambda) + b_{bp}(\lambda) \quad (2.5b)$$

a_t was parameterized as the following bio-optical parametrization of Eq. 2.5a as summation of absorption of pure water, phytoplankton (a_ϕ) and coloured detrital matter absorption (a_{dg}) :

$$a_t(\lambda) = a_w(\lambda) + \{(a_0(\lambda) + a_1(\lambda) \ln[a_\phi(443)]) \cdot a_\phi(443)\} + \{a_{dg}(443) \exp\{-S_{dg}(\lambda - 443)\}\} \quad (2.6)$$

Where, $a_\phi(443) = 0.06[chl]^{0.65}$, a_0 and a_1 are precomputed coefficients (Lee et al., 1998b). For a_{dg} , S_{dg} is the spectral slope calculated following Lee et al. (2002) in optically deep waters ; i.e., $S_{dg} = 0.015 + \left(\frac{0.002}{0.6 + R_{rs}(0^-, 443)/R_{rs}(0^-, 555)}\right)$. In the case of shallow water, a default value of 0.017 was used for S_{dg} .

The particulate backscatter was spectrally parameterized using the power-law model

used in SA inversion (Dekker et al., 2011),

$$b_{bp}(\lambda) = b_{bp}(555) \left(\frac{\lambda}{555} \right)^\eta \quad (2.7)$$

Where η is the spectral slope retrieved using the semi-empirical approach after Lee et al. (2002) in optically deep waters as : $\eta = -2.0 (1 - 1.2 \exp\{(-0.9 \cdot R_{rs}(0^-, 443)/R_{rs}(0^-, 555))\})$. In the case of shallow water, a default value of -0.50 was used.

The simulated sub-surface remote sensing reflectance was finally translated to the water-leaving $R_{rs}(0^+)$ following the air-water interaction formulation by Lee et al. (1998c), i.e., $R_{rs}(0^+) = \frac{0.518 \cdot R_{rs}(0^-)}{1 - 1.562 \cdot R_{rs}(0^-)}$.

2.4.2.2 Markov Chain Monte Carlo (MCMC) context

A probabilistic inversion approach was followed to retrieve the posterior distribution of ϕ_{var} using Markov Chain Monte Carlo (MCMC) sampling based on Bayes theorem. Numerically, the MCMC obtains a so-called *stationary distribution* approximating the conditional posterior distribution (also referred to as "target distribution" in MCMC) of ϕ_{var} for a given observation of R_{rs} . The posterior distribution, noted $\mathbb{P}(\phi_{var}|R_{rs})$ (onwards as $\mathbb{P}_{post}$) is theoretically expressed as :

$$\mathbb{P}_{post} = \mathbb{P}(\phi_{var}|R_{rs}) = \frac{\mathbb{P}(\phi_{var})\mathbb{P}(R_{rs}|\phi_{var})}{\mathbb{P}(R_{rs})} \quad (2.8)$$

Where, $\mathbb{P}(\phi_{var})$ is the multivariate probability density function (PDF) of ϕ_{var} denoting the Prior, $\mathbb{P}(R_{rs}|\phi_{var})$ is PDF of the likelihood of observing a specific R_{rs} if a constant set of ϕ_{var} is provided in the forward model multiple times. Essentially, the likelihood PDF addresses the PDF of the random error present in the forward model itself (Kaipio and Somersalo, 2005). $\mathbb{P}(R_{rs})$ is the marginal probability defined by a continuous PDF ; $\int \mathbb{P}(\phi_{var})\mathbb{P}(R_{rs}|\phi_{var})d\phi_{var}$ working as a normalization factor to ensure the $\mathbb{P}(\phi_{var}|R_{rs})$ has a closed form, i.e. [0, 1].

The *stationary distribution* is approximated using an "accept-rejection" approach in

MCMC (Hastings, 1970; Liang et al., 2010). We used the Delayed-Rejection & Adaptive Sampling (D-RAM) method to accept/reject states. It was used to ensure the efficient exploration of the variable space as well as to handle the high dimensionality in λ for *in situ* R_{rs} (Liang et al., 2010). The Delayed-rejection probability is calculated as :

$$D\{(\mathbf{x}'|\mathbf{x}) \cap (\mathbf{x}''|\mathbf{x})\} = \min \left\{ 1, \frac{\pi(\mathbf{x}')q(\mathbf{x}|\mathbf{x}')}{\pi(\mathbf{x})q(\mathbf{x}'|\mathbf{x})}, \frac{\pi(\mathbf{x}'')q(\mathbf{x}|\mathbf{x}'')}{\pi(\mathbf{x})q(\mathbf{x}''|\mathbf{x})} \right\} \quad (2.9)$$

Where x is the current state in a Markov chain, x' is the proposed state, and x'' is an alternative state proposed in D-RAM if x' is rejected. $D(\mathbf{x}'|\mathbf{x})$ is addressed as acceptance probability, whereas $D(\mathbf{x}''|\mathbf{x})$ is delayed-rejection specific probability. The acceptance criterion is defined by the ratio of the target distribution's probability at the candidate state $\{\pi(\mathbf{x}')q(\mathbf{x}|\mathbf{x}')\}$ and the current state $\{\pi(\mathbf{x})q(\mathbf{x}'|\mathbf{x})\}$, where $q(\cdot|\cdot)$ is the conditional PDF of the proposal distribution (See 2.4.2.3). $\pi(\mathbf{x})$ is the target posterior distribution, which can be approximated as $\mathbb{P}(\phi_{\text{var}})\mathbb{P}(R_{rs}|\phi_{\text{var}})$.

2.4.2.3 Proposal distribution and sampling

A multivariate *Gaussian* PDF with dimension $D = \dim(\phi_{\text{var}})$, mean vector $\bar{\mu}$ containing mean (μ) for each variable in ϕ_{var} and covariance matrix Σ was used to propose new sets of ϕ_{var} . For each newly proposed state (x^{t_n}) at time t_n , (n is the chain number), the $\bar{\mu}$ was supplied from the last accepted state of ϕ_{var} , whereas the Σ values at each state were estimated from sample space of the accepted states for the previous chains (1 to $n - 1$). To keep the random candidate states bound in $\mathbb{R}^+$, the probability of any occurrence of $x < 0$ was constrained to be zero resulting in the candidate state being rejected. A proposed state is either accepted or rejected for the next state in MCMC chains to reach the *stationary distribution*. In D-RAM MCMC, first a uniform random variable $U \sim \mathbb{U}(0, 1)$ is generated and the updated state $x^{(t_n+1)}$

is obtained as :

$$\mathbf{x}^{(t_n+1)} = \begin{cases} \mathbf{x}', & \text{if } U < D(\mathbf{x}'|\mathbf{x}) \\ \mathbf{x}'', & \text{if } U < D(\mathbf{x}''|\mathbf{x}) \\ \mathbf{x}, & \text{otherwise} \end{cases} \quad (2.10)$$

Where x' and x'' are states if the acceptance probability and delayed-rejection probability (Eq. 2.9) is higher than $\mathbb{U}(0, 1)$ respectively. x is the current state at time t_n in MCMC and it is retained as $x^{(t_n+1)}$ iff $U > \{D(x'|\mathbf{x}), D(x''|\mathbf{x})\}$.

2.4.2.4 Formulation of the Prior

The prior distribution $\mathbb{P}(\phi_{\text{var}})$ (also referred to as "Prior") was modeled as a multivariate PDF with dimension(d) = $\dim(\phi_{\text{var}})$, that particularly exist on the $\mathbb{R}^+$ domain, i.e. the population distribution does not contain any occurrence of negative values. Three probability distributions with positive support, i.e., *Weibull* ($\mathbb{W}$), *Log-Normal* ($\mathbb{L}$) and *Gamma* ($\mathbb{\Gamma}$) distributions were compared for *in situ* observations of $[chl]$, $a_{\text{dg}}(443)$ and $b_{\text{bp}}(555)$, separately. To select the optimal Prior distribution(s) for OSCs, each of the proposed distributions was fitted to the *in situ* data with its associated model parameters (e.g. μ (mean) and σ (standard deviation) for *Gaussian*). The model parameters for the proposed distributions were fitted by maximization of the analytical partial derivative of the likelihood function. Among each of the fitted distributions, the best fitting one was selected using statistical Goodness of Fit (GoF) tests described in 2.4.3.1.

The prior PDF of shallow water variables in ϕ_{var} , i.e., H and f_a were modelled using two fixed distributions. The prior of water column height H was modelled as *Weibull* distribution as it allowed for both asymmetrical distribution and tail-heaviness for support of extremes similar to distributions used for studies on mean sea level and wave height characterization (Leijala et al., 2018; Pellikka et al., 2018) . The f_a was assumed to be *Uniform* distribution varying between $[0, 1]$ and constrained to be the sum of $f_a = 1$. Finally, the multivariate log

prior PDF was obtained as :

$$\begin{aligned} \log \mathbb{P}(\phi_{\text{var}}) = & \log \mathbb{P}^*(x \in \phi_{\text{var}} \setminus \{f_a\}, \theta), \mathbb{P}^* : \mathbb{R}_{4D}^+ \rightarrow \mathbb{R}^+ \\ & + \log \mathbb{U}(x \in f_a), \quad \mathbb{U} : \mathbb{R}_D^+ \rightarrow [0, 1] \end{aligned} \quad (2.11)$$

Where $\mathbb{P}^*$ and $\mathbb{U}$ are the positive-real and uniform probability distribution(s) fitted to ϕ_{var} parameters, θ is the vector of model parameters for the fitted distribution(s).

TABLE 4 – Probability Density Function (PDF) and Cumulative Distribution Function (CDF) for Weibull, Log-normal, Gamma and Uniform distributions, along with the range of their associated model parameters (θ).

Distribution	PDF $f(x; \theta)$	CDF $F(x; \theta)$	Parameter (θ) range
Weibull ($\mathbb{W}$)	$\frac{k}{\lambda} \left(\frac{x}{\lambda}\right)^{k-1} e^{-(x/\lambda)^k}$	$1 - e^{-(x/\lambda)^k}$	$\lambda > 0, k > 0$
Log-normal ($\mathbb{L}$)	$\frac{1}{x\sigma\sqrt{2\pi}} e^{-\frac{(\ln x - \mu)^2}{2\sigma^2}}$	$\frac{1}{2} \left(1 + \operatorname{erf}\left(\frac{\ln x - \mu}{\sigma\sqrt{2}}\right)\right)$	$\mu \in \mathbb{R}, \sigma > 0$
Gamma (Γ)	$\frac{1}{\beta^\alpha \Gamma(\alpha)} x^{\alpha-1} e^{-x/\beta}$	$\frac{1}{\Gamma(\alpha)} \gamma(\alpha, x/\beta)$	$\alpha > 0, \beta > 0$
Uniform (f_a only)	$\frac{1}{b-a}$	$\frac{x-a}{b-a}$	$0 \leq a \leq b \leq 1$

erf (error function) : $\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$; Γ (Gamma function) : $\Gamma(x) = \int_0^\infty t^{x-1} e^{-t} dt$; t is the variable (i.e., variables in ϕ_{var}) under the integral for both erf and Γ functions.

2.4.2.5 Formulation of the Likelihood

The forward model likelihood $\mathbb{P}(R_{\text{rs}}|\phi_{\text{var}})$ was constructed as a linearly additive component in right-hand side of Eq. 2.1 and the corresponding PDF is set to be *Gaussian* with a known mean $\mu_{\mathbb{L}} = \mathbb{E}(x - \mu_{\mathbb{L}}) \approx 0$ (x is R_{rs}) and unknown population variance $\sigma_{\mathbb{L}}^2$. The *Gaussian* distribution was opted from addressing the linearized AM03 forward model random error for a sample $N = 10,000$ number of simulations (Fig. 38 in Annexe-II). The PDF mean, i.e., $\mu_{\mathbb{L}}$ was further considered as a random variable following *Gaussian* distribution. The $\sigma_{\mathbb{L}}^2$ was fitted by the *inverse Gamma* distribution, which is a conjugate prior for the va-

riance in a *Gaussian* distribution. As the $\sigma_{\mathbb{L}}^2$ is unknown, it was also estimated from inversion beside ϕ_{var} .

2.4.2.6 Estimation of uncertainty

The solution from MCMC for ϕ_{var} is not a vector of single point estimates, but a chain of states for ϕ_{var} explaining the posterior PDF $\mathbb{P}(\phi_{\text{var}}|R_{\text{rs}})$. In other words, it yields a probability distribution of possible values of each retrieved variable of ϕ_{var} . We obtained point-based estimates from Markov chains using the “*Maximum-a-posterior*” (MAP) approach, where we selected the vector of ϕ_{var} associated with the highest density magnitude for $\mathbb{P}(\phi_{\text{var}}|R_{\text{rs}})$. The MAP solution obtained optimal variables (θ_{MAP}) can numerically be presented as $\theta_{\text{MAP}} = \arg \max_{\phi_{\text{var}}} \mathbb{P}(\phi_{\text{var}}|R_{\text{rs}})$. The associated uncertainties were calculated using the 95% Bayesian Credible Intervals (BCI). The upper (UQ) and lower quantiles (LQ) of the BCI associated with θ_{MAP} can be calculated as :

$$\text{LQ} = F^{-1}\left(\frac{1-C}{2}\right); \text{UQ} = F^{-1}\left(1 - \frac{1-C}{2}\right) \quad (2.12)$$

Where, F^{-1} represents the inverse of the Cumulative Distribution Function (CDF), which gives the value of θ_{MAP} for a given probability.

2.4.3 Statistical metrics

2.4.3.1 Prior selection

The fitted probability distributions to OSCs in ϕ_{var} were evaluated using three approaches : **1.** descriptive statistics comprising mean, median, mode, minimum and maximum along with the 2nd - 4th order of the moments, i.e., variance, skewness and kurtosis, **2.** visually analyzing the histogram of fitted PDFs for proposed distribution ($\mathbb{P}^*$), quantile plots (QQ plot) and Cumulative Distribution Function (CDF) plots for each of the fitted

$\mathbb{P}^*$. **3.** The goodness of fit (GoF) tests for statistical significance performed with the widely used Kolmogorov–Smirnov (KS) test (Massey, 1951), the Cramer-von Mises (CM) criterion (Cramér, 1928) and the Anderson-Darling (AD) test (Anderson and Darling, 1952). These tests provide statistical significance (p -value) with the associated metric value (D) to assess the certainty of the proposed population distribution. The GoF information criterion consisted of Akaike Information Criterion (AIC) (Akaike, 1970) and Bayesian Information Criterion (BIC) (Schwarz, 1978). These metrics measure the trade-off between GoF and the associated model complexity.

2.4.3.2 Inversion assessment

The estimates retrieved by SABER were compared with those obtained using two established SA inversion algorithms for optically deep and shallow waters, respectively. Specifically, the Quasi Analytical Algorithm (QAA) (Lee et al., 2002) and the Hyperspectral Optimization Process Exemplar model (HOPE) (Lee et al., 1998c) were employed for the examination of OSCs and SV, respectively. The inter-comparison was carried out following commonly used statistical metrics used in single/multi-variable inversion studies : uncertainty (ϵ) and bias (β) (Pahlevan et al., 2022; Morley et al., 2018) :

$$\epsilon = (10^{\text{median}(|\log(\frac{e}{o})|)} - 1) \times 100 \quad (2.13a)$$

$$\beta = \text{sign}(M_R) \times (10^{|M_R|} - 1) \times 100 \quad (2.13b)$$

Where, M_R is median ratio : $\text{median}(\log(\frac{e}{o}))$. e is the actual value, o is the inversion retrieved value. Apart from these, the slope (m) of log-transformed linear regression and root mean squared log difference (RMSLD) were also calculated offering a robust evaluation.

2.5 Results

2.5.1 Optical variability of the datasets

A summary of the descriptive statistics of one sample vector (95% C.I.) of OSCs is presented in Table 5. $[chl]$ values ranged from 0.1 to $\sim 100 \text{ mg m}^{-3}$, ensuring a representation of all trophic state as defined by Carlson and Simpson (1996). Detrital absorption and particulate backscattering also vary within four orders of magnitudes, with average values of 0.64 and 0.0034 m^{-1} , respectively.

An Optical Water Type (OWT) classification (Spyrakos et al., 2018) was performed to assess the optical variability of the combined synthetic and *in situ* R_{rs} datasets. The classification was performed to assess the performance of SABER for inverting R_{rs} from different OWTs. 8 out of 21 OWTs of Spyrakos et al. (2018) were represented in our R_{rs} datasets (Fig. 12a). The proportion of synthetic versus *in situ* R_{rs} decreases from OWT 1 to OWT 8. OWT 1 is almost exclusively composed of synthetic data (mainly LOISEL), while OWT 8 is only represented by *in situ* spectra (GLORIA and NOMAD). OWTs 1-3 shows clear blue Case-I water with high reflectance at shorter wavelengths with decreasing magnitude towards red wavelengths, typical for ultra oligotrophic to oligotrophic conditions (Carlson and Simpson, 1996) (mean $[chl]$ of 0.03, 0.11 and 0.51 mg m^{-3}) with low detrital and CDOM absorption ($\leq 0.1 \text{ m}^{-1}$) and weak backscattering ($0.0007 - 0.0021 \text{ m}^{-1}$) due to low particle load. OWTs 4-5 represent common Case-II coastal waters with mesotrophic conditions (mean $[chl]$ of 1.65 and 4.45 mg m^{-3}). The magnitude of the R_{rs} in blue wavelengths for OWT 5 is lower than 4 indicating a higher absorption at blue, i.e., CDOM-rich characteristics (mean $a_{dg}(443)$ of 0.14 and 0.56 m^{-1}). OWT 6 and 7 show eutrophic inland waters (mainly from GLORIA) (mean $[chl]$ of 17.58 and 38.84 mg m^{-3}) with high phytoplankton bloom and organic matter presence making the signal in blue very low (mean $a_{dg}(443) > 0.85 \text{ m}^{-1}$). Lastly, OWT 8 represents hypertrophic water with mean $[chl]$ of 117 mg m^{-3} , resulting in the highest Sun-Induced Chlorophyll Fluorescence (SICF) peak among all OWTs.

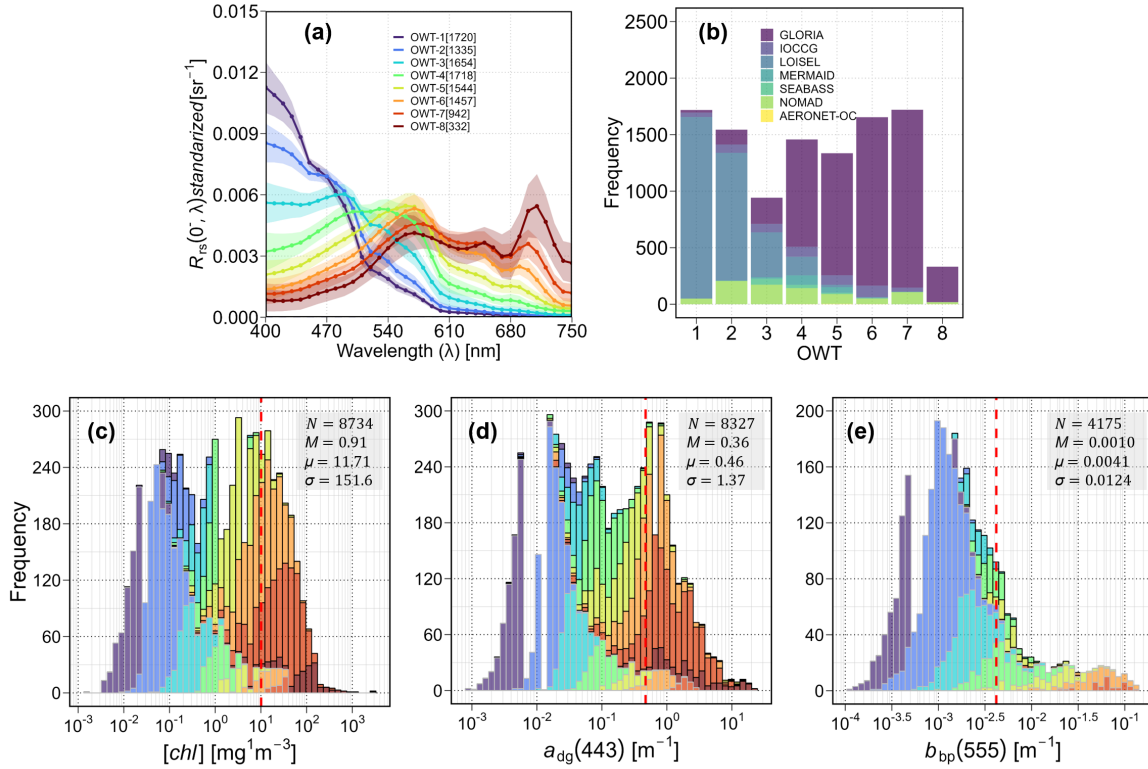


FIGURE 12 – (a) Standardized sub-surface (0^-) $R_{rs}(\lambda)$ for each Optical Water Type (OWT). The observations count for OWTs is in square braces beside legend entry of OWTs. (b) Count of data sources for OWTs. (c-e) Log-Normal distribution of $[chl]$, $a_{dg}(443)$ and $b_{bp}(555)$ for different OWTs. N = observations count; M = Median; μ = Mean (red dashed line), σ = Standard deviation.

2.5.2 Fitting the prior distribution

The measures of central tendencies of $[chl]$ indicate a non-Gaussian distribution, i.e., Mean > Median > Mode, indicating skewness in the observations (Table 5). Similarly, the skewness value > 1 denotes a long right tail with dispersion in the measures and very high kurtosis > 3 (Leptokurtic) points to a peaked distribution followed by a higher probability of extreme values on the further right tail. Among fitted distributions to $[chl]$, $\mathbb{L}$ (Log-normal) provided the best support for the values $< \sim 10 \text{ mg m}^{-3}$, however, for samples with higher concentrations, mostly belonging to eutrophic waters, the density of the fitted PDF

was slightly underestimated (Fig. 13a). Considering the GoF statistic, only $\mathbb{L}$ obtained D value lower than C_{val} among all three tests along with the lowest AIC and BIC making it the optimal choice to model the prior of $[chl]$ (Table 6).

$a_{\text{dg}}(443)$ observations varied between 0.003 to $\sim 5\text{m}^{-1}$, covering marine water to highly absorptive coastal conditions. The data followed a positively skewed distribution alike $[chl]$, but both the degree of skewness and kurtosis were relatively lower (Table 5), denoting a relatively flatter density peak with a lighter right tail. The $\mathbb{L}$ fitted the density peak around 0.2m^{-1} with greater support than $\mathbb{W}$ (Weibull) and Γ , but obtained relatively lower probability occurrence for higher values (Dispersion $> 0.8\text{m}^{-1}$ in Fig 13e). $a_{\text{dg}}(443)$ fitted density histogram and Q-Q plot (Fig 13b,e) interestingly showed features of bi-modality with two peaks at ~ 0.2 and $\sim 0.6\text{m}^{-1}$. Nevertheless, in the current study, we refrained from fitting the prior density as a mixture of two $\mathbb{L}$ or similar distributions due to a limited understanding of how the prior covariance structure changes with origin-specific $a_{\text{dg}}(443)$, and to keep the model complexity relatively low.

The prior for $b_{\text{bp}}(555)$ obtained the lowest skewness and kurtosis among the OSCs. It suggests a slightly skewed distribution, with a majority of values having a high likelihood of being located near the mean. Similarly, the central tendencies are relatively closer in magnitude to each other than $[chl]$ and $a_{\text{dg}}(443)$ (Table 5). The $\mathbb{L}$ obtained the best fit for the whole range of prior (Fig. 13c, Table 6) except values lower than $\sim 0.002\text{m}^{-1}$ (OWT 1-2). In this range, the left tail of the fitted $\mathbb{L}$ was heavier than the theoretical $\mathbb{L}$ distribution (Fig. 13f), i.e., the probability of observing $b_{\text{bp}}(555)$ values $\leq \sim 0.002$ was lower for the optimally fitted $\mathbb{L}$ than the same theoretical distribution. A similar case of the lighter left tail was also observed for $a_{\text{dg}}(443)$ fitted distributions for $\leq 0.06\text{m}^{-1}$, which correspond to the ultra-oligotrophic water type (OWT 1).

TABLE 5 – Descriptive statistics for the OSC data-set to model the prior distribution of deep water variables (x) in ϕ_{var} .

$x \in \phi_{\text{var}}$	Summary Statistics							
	Min	Max	sd ($\pm$)	Mean	Median	Mode	Skewness	Kurtosis
$[chl][\text{mg m}^{-3}]$	0.1	98.97	18.52	12.20	3.90	2.94	2.34	5.44
$a_{\text{dg}}(443)[\text{m}^{-1}]$	0.003	4.97	0.83	0.64	0.35	0.51	2.31	5.23
$b_{\text{bp}}(555)[\text{m}^{-1}]$	0.0007	0.01	0.0019	0.0034	0.0035	0.0030	0.93	0.66

TABLE 6 – Comparison of the Goodness of Fit statistics and information criterion for the fitted distributions to OSCs (x in table) in ϕ_{var} . The sample data used to fit the distributions and the corresponding units for each of x is the same as Table 5.

$x \in \phi_{\text{var}}$	Distribution	KS statistic	AD statistic	CV statistic	AIC	BIC
		($C_{\text{val}} = 0.138$)	($C_{\text{val}} = 2.492$)	($C_{\text{val}} = 0.461$)		
$[chl]$	Weibull	0.165 [#]	2.662 [#]	0.601 [#]	540	542
	Log-Normal	0.128	2.456	0.460	520	525
	Gamma	0.182 [#]	2.841 [#]	0.701 [#]	547	545
$a_{\text{dg}}(443)$	Weibull	0.117	2.24	0.372	48	147
	Log-Normal	0.009	1.27	0.202	45	97
	Gamma	0.104	1.56	0.257	48	101
$b_{\text{bp}}(555)$	Weibull	0.130	2.065	0.338	1052	1047
	Log-Normal	0.084	0.771	0.125	1038	1029
	Gamma	0.106	1.174	0.198	1048	1042

The theoretical distribution is rejected ([#]) for the sampled data if $D \geq C_{\text{val}}$. The significance level (α) associated with D and C_{val} is 0.05, i.e. 95% Confidence Interval.

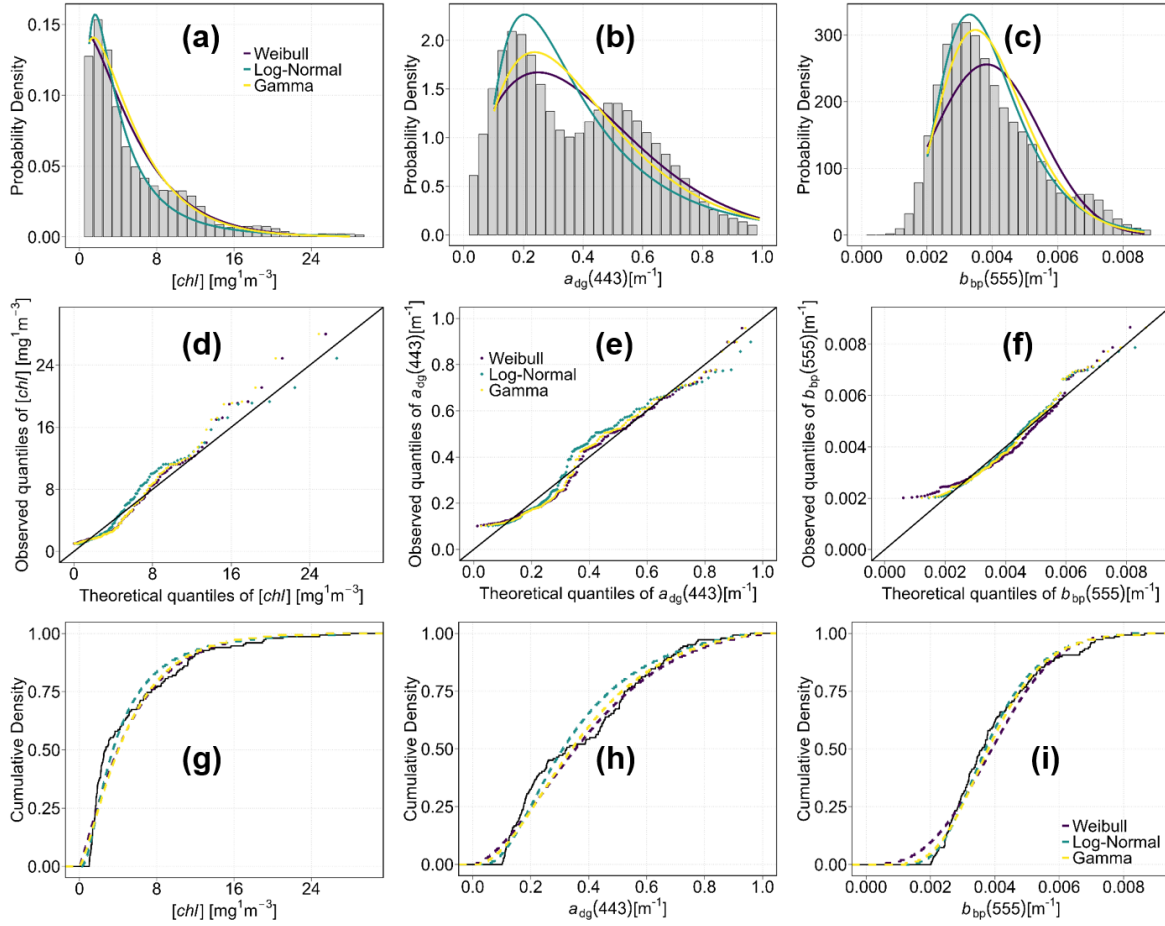


FIGURE 13 – Comparison of the Goodness of Fit among different positive support probability distributions (See Table 4) for a randomly drawn sample of OSCs in ϕ_{var} ; (a-c) shows the fit of the PDF of the proposed distributions on the observed density for $[chl]$, $a_{dg}(443)$ and $b_{bp}(555)$ respectively. (d-f) shows the fit of quantiles (QQ-plot) for the proposed distributions and (g-i) shows the fit of the cumulative densities (CDF plot).

2.5.3 Posterior inference from MCMC

In MCMC, the width and peakedness of the $\mathbb{P}_{post}$ for each retrieved variable serve as critical indicators of uncertainty. In the current study, we illustrate the degree of uncertainty for simultaneous retrieval of OSCs and SV using synthetic observation of R_{rs} following the simulation approach mentioned in 2.4.1.2. To illustrate this concept, we plot the $\mathbb{P}_{post}$ in Fig. 14 for one given inversion. Here, $\mathbb{P}_{post}$ were retrieved by inverting an R_{rs} spectrum simulated with

$[chl] = 4.87 \text{ mg m}^{-3}$, $a_{\text{dg}}(443) = 1.02 \text{ m}^{-1}$, $b_{\text{bp}}(555) = 0.007 \text{ m}^{-1}$ and $H = 2 \text{ m}$. $[chl]$ obtained the widest posterior distribution signifying the highest uncertainty among retrieved variables. It also captured a range of plausible values of $[chl]$ for the input R_{rs} , but with different magnitudes of probability densities quantifying the likelihood of the variable to be the true value. Conversely, $b_{\text{bp}}(555)$ showed the narrowest peaked distribution reflecting the highest degree of certainty, indicating a more constrained range of likely variable values. Similarly, the MAP estimates for each retrieved variable were obtained for the magnitude(s) with the highest probability peak in the $\mathbb{P}_{\text{post}}$.

The convergence of MCMC chains was assessed using trace plots. For each variable, three MCMC chains were sampled from a randomly chosen initial vector with values between $\{0, \infty\}$. We observed excellent mixing of the three chains (right-hand column in Fig. 14) after the transient *burn-in* phase in chain propagation. The auto-correlation also decayed rapidly in the *burn-in* (not shown) followed by an efficient exploration of parametric space in MCMC chains, i.e., the candidate state vector was not persistent to a specific value.

2.5.4 Inversion validation

2.5.4.1 Assessment of the optically deep water inversion

The *Maximum-a-posterior* (MAP) estimates of simultaneously retrieved OSCs, along with their 95% Bayesian Credible Intervals (BCI) obtained from MCMC chains, were validated against the actual data. Similarly, QAA retrieved estimates were assessed against the actual values, but the uncertainty (95% CI) was additionally obtained from diagonal solution of the inverted Hessian matrix associated with the QAA estimated OSCs in solution vector ϕ_{var} (See 5.1 in Annexe-II for details).

We found $[chl]$ retrievals had the highest uncertainty (ϵ) and bias (β) among the OSCs for both synthetic and *in situ* datasets (Table 7, Fig. 16a,b, Fig. 17a,b). The SABER

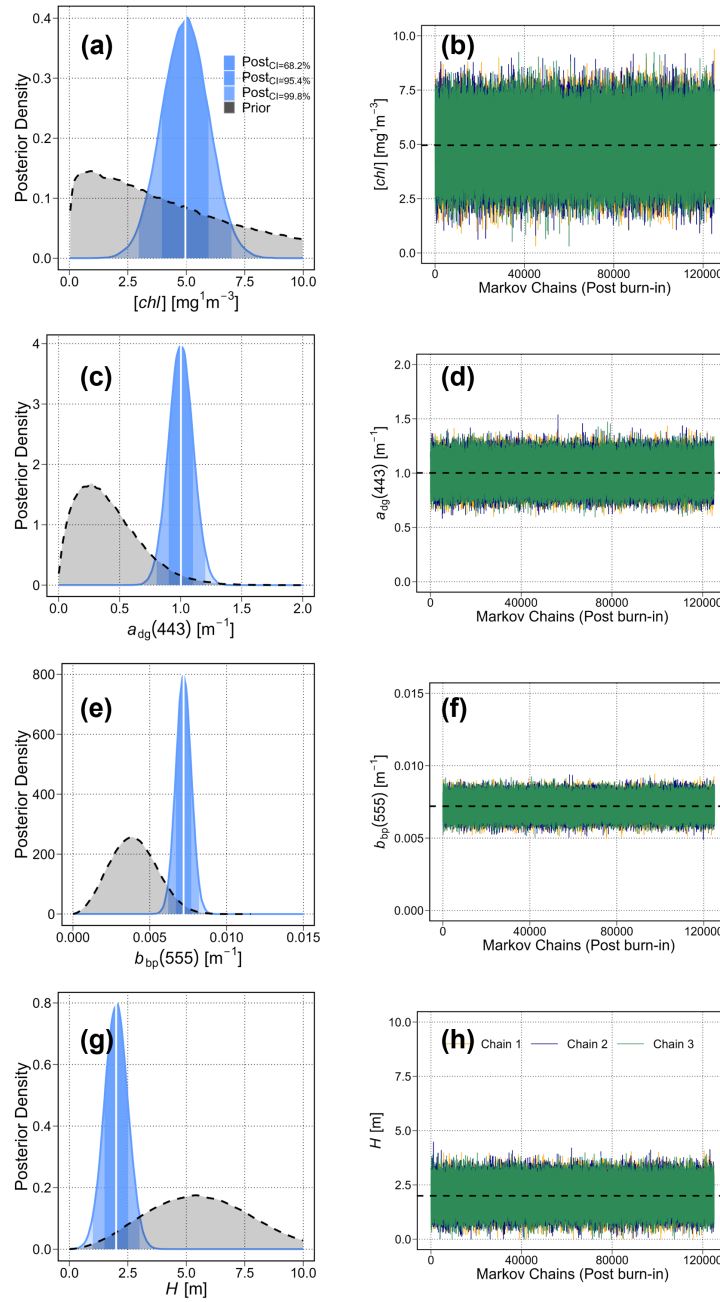


FIGURE 14 – SABER retrieved simultaneous posterior distributions (left) with different CI (1σ , 2σ and 2.5σ showed with decreasing saturation of fill colour blue), the MAP estimate (white vertical line) and the prior PDF (in grey) along with corresponding trace plots on right are shown for (a,b) $[chl]$, (c,d) $a_{dg}(443)$, (e,f) $b_{bp}(555)$ and (g,h) H .

estimated $[chl]$ for the synthetic dataset had both lower ϵ and β than QAA. Considering OWT-specific assessment, QAA estimates for OWT 1 ($[chl] < \sim 0.1 \text{ mg m}^{-3}$ in both synthetic and *in situ* data) were more accurate, (Fig. 15a,b). The parametric uncertainty ($p_\sigma \equiv 95\%$ CI) was higher for OWT 1 in SABER, possibly due to the absence of such low $[chl]$ values in the Prior distribution (see the Discussion for details). Note that the synthetic dataset is dominated by OWT1 (43%) followed by OWT2 (32%). Interestingly, a decreasing trend in ϵ for OWTs with increasing $[chl]$ (OWT 2-7) concentration was observed, whereas both β and p_σ obtained for QAA were consistently higher than for SABER. For the *in situ* data, SABER had an overall slightly better performance than QAA in terms of ϵ , β and m (Table 7). OWT-specific results had a similar trend as the synthetic retrievals, but for eutrophic and hypertrophic waters (OWT 7 and 8 for *in situ* data), QAA had slightly lower ϵ (SABER : 83.85%; QAA : 76.92%). Conversely, the β and m obtained for SABER for each OWT outperformed the QAA (Fig. 15b).

Performance of SABER and QAA for $a_{dg}(443)$ retrievals were different for the synthetic dataset; SABER obtained a higher ϵ (24.68 vs 17.65%), and also a greater β . For clear waters (OWT 1-3), the ϵ were within $\pm 10\%$ difference, β were within $\pm 5\%$, and strong linearity was found for both inversion approaches (Fig. 15a,c, Fig. 16c,d). In mildly eutrophic conditions (OWT 6) for both synthetic and *in situ* data, SABER had almost half the ϵ relative to QAA with almost null β . Conversely, for OWT 7 ($a_{dg}(443) > 1 \text{ m}^{-1}$), QAA performed better than SABER on synthetic data, but not for *in situ*. However, we should recall that the number of observations for OWT 7 represented only 2% of the synthetic dataset, which might have obtained large uncertainties for relatively smaller deviations in estimates. The inversion of *in situ* R_{rs} yielded much higher dispersion for $a_{dg}(443)$ compared to synthetic dataset (Fig. 17c,d). The ϵ , β and m for SABER applied to *in situ* were significantly better than QAA (Table 15) for $a_{dg}(443)$. SABER estimates were uniform across the OWTs for multiple orders of magnitude, with the lowest uncertainty for OWT 4 and 5. A negative β was consistent for all OWTs for both the algorithms, however, β for SABER was lower for each OWT (Fig. 15d). The marginal distribution of $a_{dg}(443)$ was adequately captured by SABER

TABLE 7 – Statistical assessment of the inversion retrieved variables from SABER and QAA (Lee et al., 2002) for OSCs in ϕ_{var} and for SV, it refers to HOPE (Lee et al., 1998c)).

Source	$x \in \phi_{\text{var}}$	ϵ (%)		β (%)		m		RMSLD	
		SABER	QAA	SABER	QAA	SABER	QAA	SABER	QAA
Synthetic	[chl]	64.09	97.79	48.90	89.17	0.90	0.94	0.26	0.35
	$a_{\text{dg}}(443)$	24.68	17.65	-1.05	0.39	0.96	1.02	0.04	0.05
	$b_{\text{bp}}(555)$	8.84	22.03	2.53	8.68	0.89	1.13	0.012	0.017
<i>in situ</i>	[chl]	70.32	74.93	7.81	9.66	1.10	1.35	0.91	1.00
	$a_{\text{dg}}(443)$	37.13	54.61	-5.09	-11.26	1.02	1.19	0.37	0.48
	$b_{\text{bp}}(555)$	22.07	26.50	8.43	9.53	0.98	1.07	0.0023	0.0031
		SABER	HOPE	SABER	HOPE	SABER	HOPE	SABER	HOPE
Shallow	[chl]	34.14	87.41	-14.04	31.46	0.75	-0.32	0.47	1.13
	$a_{\text{dg}}(443)$	6.27	19.47	2.37	7.44	0.87	1.24	0.079	0.45
	$b_{\text{bp}}(555)$	3.84	5.88	-0.09	3.19	1.18	-2.17	0.004	0.035
	H	7.05	18.67	1.80	-2.58	0.96	1.38	0.11	0.47

whereas, the same for QAA was heavily skewed (Fig. 17c,d).

The $b_{\text{bp}}(555)$ retrievals for the synthetic data from SABER had $\sim 13\%$ lower ϵ than QAA, and was less biased than QAA (β of 2.53% compared to 8.68%). $b_{\text{bp}}(555)$ retrieved with SABER for OWT 1 ($b_{\text{bp}}(555) < 0.0003\text{m}^{-1}$) was overestimated along with high p_{σ} width denoting higher parametric uncertainty in the low particle concentration range (Fig. 16e). It can be linked to the absence of $b_{\text{bp}}(555)$ with very low magnitude such as the values in OWT 1 in the prior formulation; a similar trend of overestimation for lower tail was observed for [chl]. For the other OWTs, SABER obtained much lower ϵ and β compared to QAA (Fig. 15a,c). The linearity of estimated $b_{\text{bp}}(555)$ was better (closer to unity) for SABER compared to QAA, which tended to gradually overestimate $b_{\text{bp}}(555)$ with increasing magnitude (Fig. 16e,f). For *in situ* data inversion, which are mainly available for OWT 2

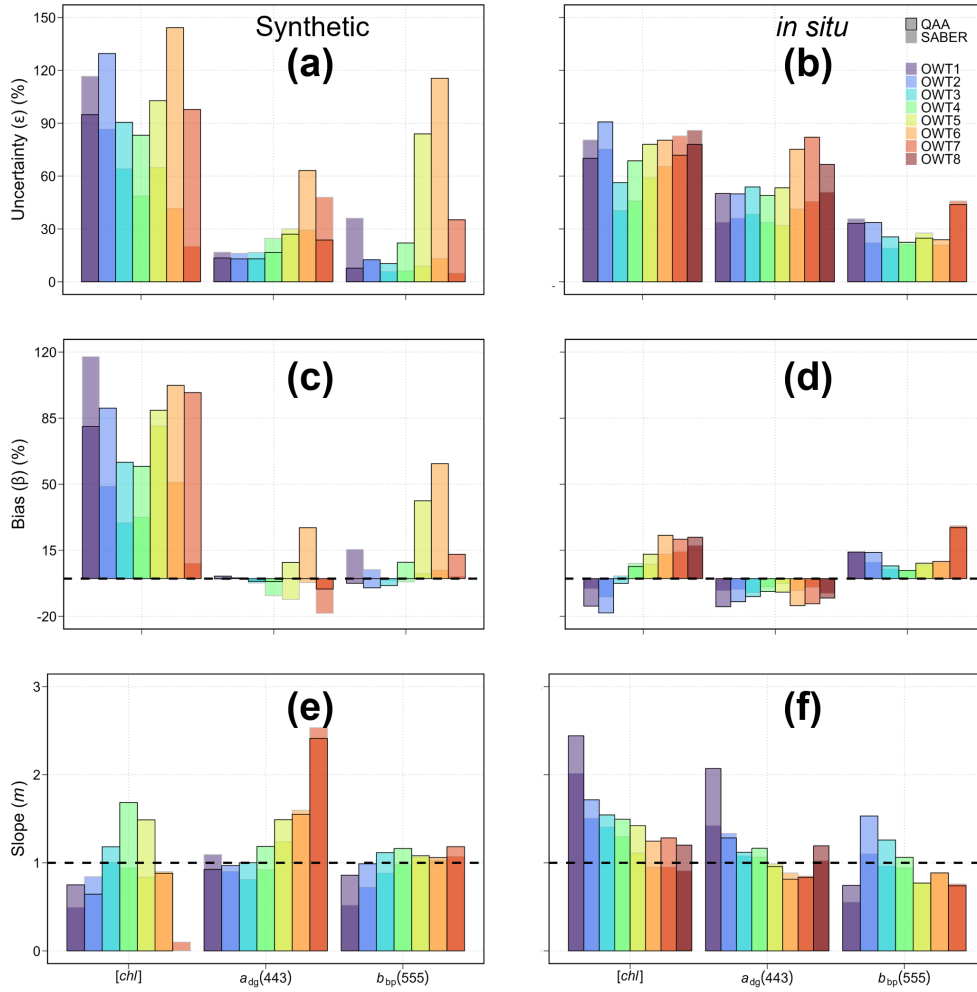


FIGURE 15 – Statistical inter-comparison of SABER and QAA in terms of **(a,b)** uncertainty, **(c,d)** bias and **(e,f)** slope (See section 2.4.3). The colour of each bin in the barplot is associated with its OWT group; the fill without border represents SABER, whereas QAA obtained results are shown bars margined with a black border.

to 4, SABER obtained lowest ϵ for OWT 2 followed by OWT 3 (22.07% and 18.96%), but similar performance in terms of ϵ , β and m for both SABER and QAA for the rest of the OWTs (Fig. 15b,d; Fig. 17e,f). It is important to mention that the *in situ* observation counts for OWT 5 to 7 were very small to obtain statistically significant results and might not impact the overall statistical results.

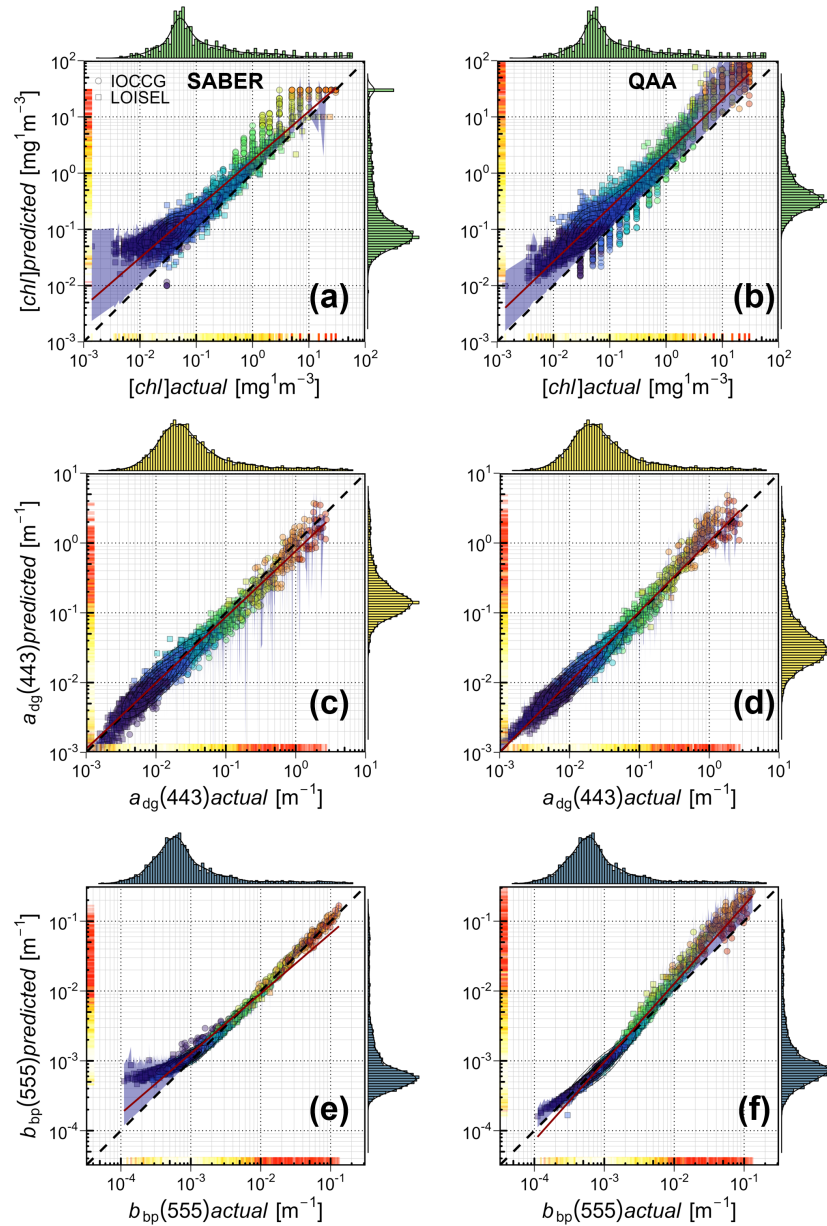


FIGURE 16 – Scatter plots showing the validation comparison between SABER and QAA for simultaneous OSC retrieval for the IOCCG and LOISEL synthetic datasets. In each plot, the points are colour-coded with their associated OWT. The black dashed line is the 1 :1 line, whereas the red line shows the obtained linear fit. The density overlaid histograms (densigram onwards) shows the marginal distribution for actual and inversion retrieved values. The blue-shaded region shows 95% CI as a measure of parametric uncertainty.

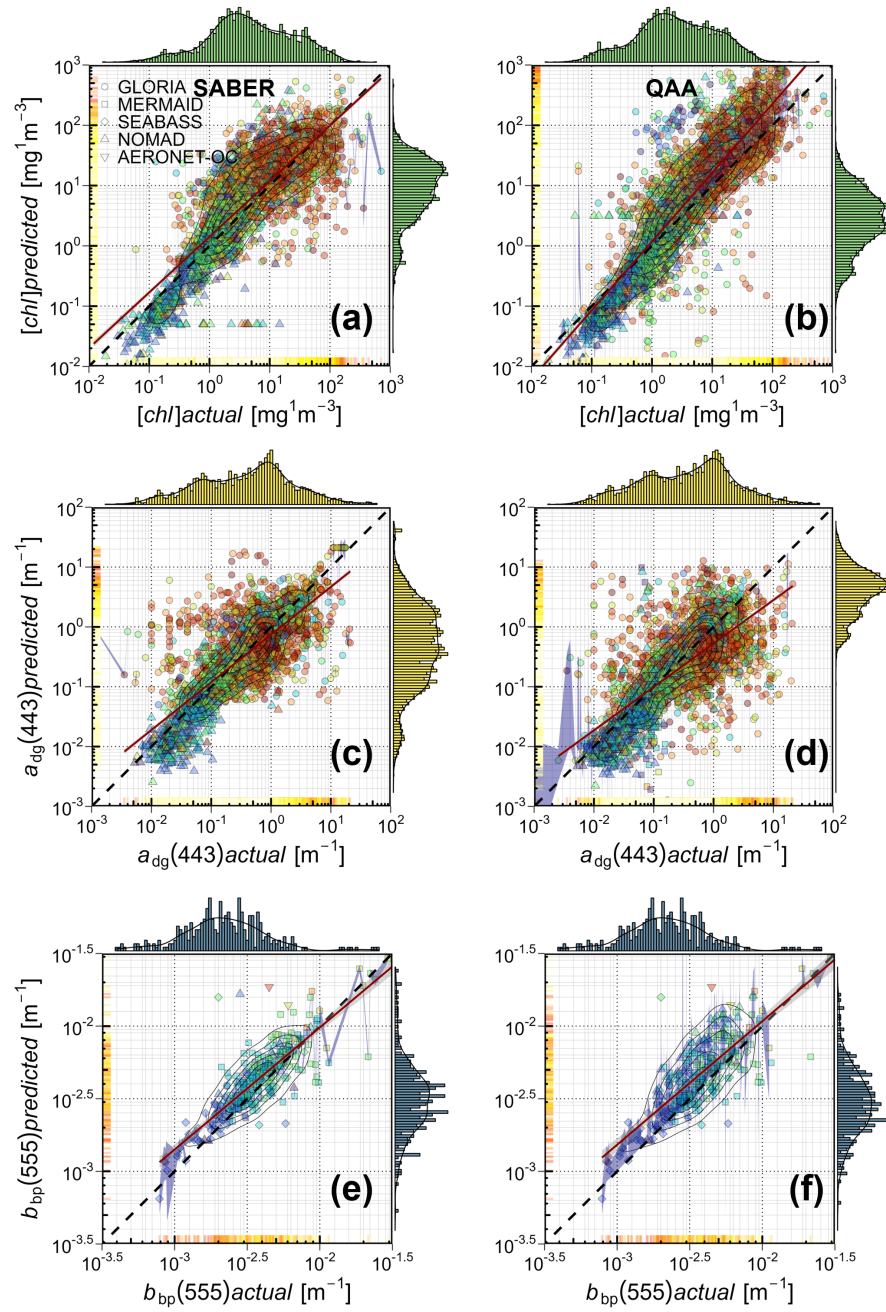


FIGURE 17 – Same as Fig. 16, but for the V22 and GLORIA *in situ* datasets.

2.5.4.2 Assessment of optically shallow water inversion

We apply SABER and HOPE to our synthetic optically shallow R_{rs} dataset, retrieving both the OSCs and SV. The simulated dataset was specifically designed to represent the near-shore coastal waters of the St Lawrence estuary and gulf, which are dark waters dominated by CDOM and low backscattering (Araújo and Bélanger, 2022; Mukherjee et al., 2023). We only assessed the H retrieval performance among the SVs, as the f_a was kept constant in the simulations for all R_{rs} . SABER obtained an ϵ of 7.1% for H retrieval, whereas HOPE error was more than 2 times higher (18.7%). The m associated with SABER was almost unity, but much higher for HOPE (1.38). For depths < 3 m, both approaches obtained similar results (Fig. 18). Conversely, for increasing depth, HOPE overestimated H and retrieved values were clustered around ~ 12 m (Fig. 18b). The p_σ for $H > 6$ m were also much higher than the same obtained with SABER. The HOPE inversion algorithm failed on 53 occasions when H ranged between 6-12 m, which was not the case for SABER. However, a slight saturation of retrieved H was also observed for the 9-12 m range for SABER.

We also compare the performance of SABER and HOPE to retrieve the water column IOPs in optically shallow waters. SABER outperformed HOPE in terms of both ϵ and β for all three OSCs (Table 7) in optically complex conditions where the number of variables in ϕ_{var} is higher than the optically deep cases illustrated in Section 2.5.4.1. HOPE was particularly poor for the retrieval of $[chl]$ and $b_{bp}(555)$ in terms of linearity with negative values for m . In contrast, statistical indicators for SABER were as good as, or even better, for optically deep waters. However, it is also worth mentioning that these results were obtained purely on a synthetic dataset of R_{rs} and the metrics might vary for R_{rs} obtained from *in situ* radiometric measurements, possibly from the uncertainty propagated from acquisition, sensor noise and protocol-based conversion of quantities.

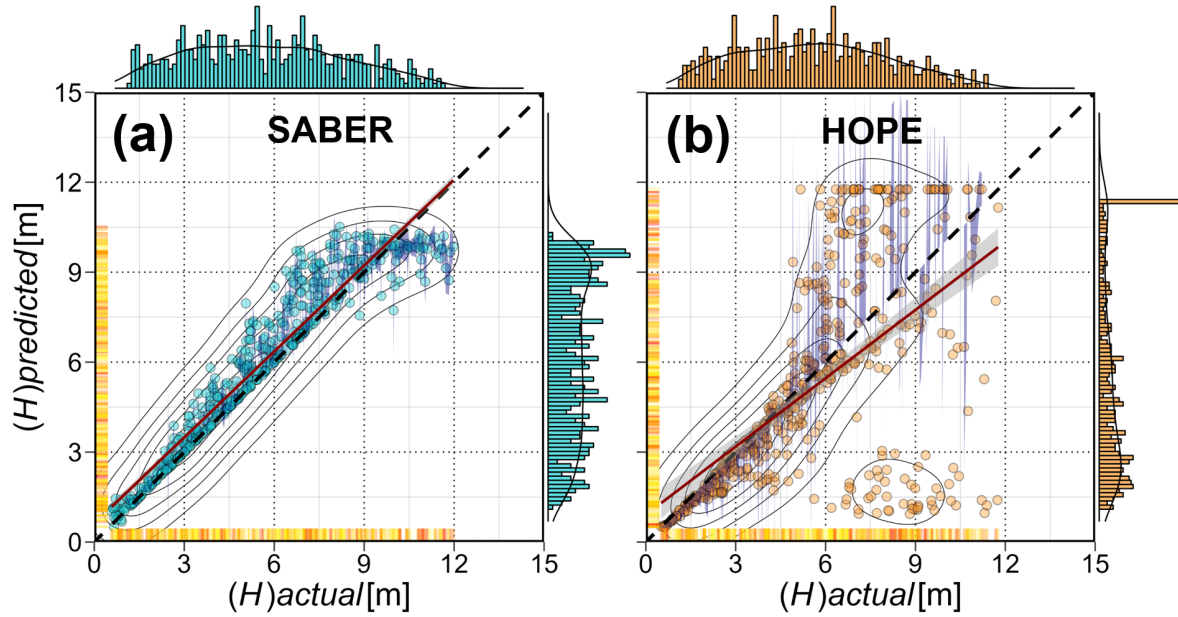


FIGURE 18 – Scatter plots showing the validation of shallow water variable; H for the synthetic shallow water dataset. **(a)** shows the validation of SABER retrieved H and **(b)** shows validation of H obtained from HOPE developed by (Lee et al., 1998c). The schematic of both the scatter plots is the same as the ones in Fig. 16 except for the absence of OWT classification, as it is not applicable for optically shallow water.

2.6 Discussion

2.6.1 Influence of Bayesian approach

We showed that MCMC has the potential to retrieve OSCs and SV such as H for multiple orders of magnitude variability on a global scale of observations. The major advantage of MCMC-based inversion over deterministic optimization-based approaches is its intrinsic quantification of parametric uncertainty obtained from the posterior distribution. In contrast, optimization methods need an additional step of uncertainty calculation, such as analytical Jacobian, CRB, etc. (Werther and Burggraaff, 2023; Jay et al., 2017b). For multi-variable retrieval, MCMC-based inversion can easily be constrained with the covariance present in *in situ* observations, which was found to improve the OSC retrieval accuracy in earlier studies

on *Gaussian* MDN inversion, especially for productive waters (Pahlevan et al., 2022; O’Shea et al., 2023). Similarly, the inclusion of the Prior informs the inversion with specific probability distribution of the population with optimal model parameters (θ). Previous studies on Bayesian inversion such as Erickson et al. (2020); Werther and Burggraaff (2023); Erickson et al. (2023) used *Gaussian* priors to linearize the forward model and to reduce model complexity. However, Rodgers (2000) reported natural variables cannot be accurately fitted using *Gaussian* distribution if the variances are not small compared to the central tendencies in data (e.g., $[chl]$). Hence, our approach of using $\mathbb{R}^+$ distributions for prior fits adequately for global observations of OSCs, especially for diverse natural waters.

Our MCMC approach also has its approximations and limitations. The $\mathbb{L}$ prior density of $[chl]$ was underestimated for the right tail due to the low numbers of observations for highly productive waters. Hence, the uncertainty was high for observations possibly occurring from small-scale phenomena, such as phytoplankton bloom or eutrophication (OWT 7-8). Pahlevan et al. (2022) reported similar results ($\epsilon > 80\%$) in $[chl]$ retrievals for highly eutrophic waters. The bi-modality for $a_{dg}(443)$ prior (Fig. 13b) can potentially be linked to different origins of the detrital matter, i.e. low magnitude marine CDOM at Case-I waters (OWT1-3) and higher values of CDOM at coastal and inland waters (OWT 5-8) affected by terrigenous runoff and riverine sources. Further study is needed to adequately incorporate the covariance of origin-specific $a_{dg}(443)$ with other OSCs for simultaneous retrievals.

2.6.2 Inversion performance

The highest uncertainty (ϵ) and bias (β) were associated with $[chl]$ values for the synthetic dataset (Table 7). $[chl]$ is derived from bio-optical relation with a_ϕ (Lee et al., 1998b), however, the spectral shape of a_ϕ is highly variable (Bricaud et al., 1995, 2004), and sensitive to the uncertainty in R_{rs} (O’Shea et al., 2023). In addition, when a_ϕ is small relative a_{dg} (Lee et al., 2006a), which is often the case in coastal and inland waters, more ambiguity is introduced in the bio-optical parametrization. Similarly, the posterior distribution of $[chl]$ shows

a larger width with a flatter peak indicating the propagated uncertainty (Fig. 14). Among different OWTs, SABER was most accurate for OWT 4 and 5 commonly found in coastal waters with R_{rs} peak in green wavelengths. The performance was comparatively poor for $[chl] < 1\text{mg m}^{-3}$ and $[chl] > 100\text{mg m}^{-3}$ (beyond the tails of the prior). Similar results have been shown in Pahlevan et al. (2022); Werther et al. (2022b) and lack of training data (prior in our study) in this range was identified as the primary cause.

The $a_{dg}(443)$ *in situ* estimates were most accurate for $0.1 \leq a_{dg}(443)\text{m}^{-1} \leq 1.0$. For values lower and higher than this range, we observed an overestimation and underestimation with SABER, respectively (Fig. 17c). A similar trend, but of a more severe degree, was found for QAA obtained $a_{dg}(443)$. This issue can be attributed to the sensitivity of spectral slope (S_{dg}) formulation used for both the algorithms. The spectral slope of detrital absorption (s_{dg}) strongly depends on the relative proportion of CDOM and nonalgal particles (NAP) (Babin, 2003), and the history of CDOM photobleaching (Fichot and Benner, 2012). Integration of the s_{dg} along with ϕ_{var} vector similar to Erickson et al. (2023); O'Shea et al. (2023) might improve the estimates, however, it can be considered as a next step in improving the current model. Another aspect, especially for high CDOM conditions, the Sun Induced CDOM Fluorescence (f_{DOM}) can contribute a large fraction (e.g., 20%) in the green wavelengths of R_{rs} (Mukherjee et al., 2023). Hence, a SA forward model for f_{DOM} might be necessary for improving the $a_{dg}(443)$ retrieval in highly absorptive CDOM-rich waters, a common situation in northern coastal and inland systems, such as the EGSL.

SABER outperformed QAA and HOPE in estimating $b_{bp}(555)$ and H , respectively. However, in the case of $b_{bp}(555)$ grouped in OWT 1 for synthetic data, SABER exhibited a higher error than QAA. This discrepancy is attributed to the loosely fit Prior for the lower tail and the absence very small $b_{bp}(555)$ ($< 0.0003\text{m}^{-1}$), values commonly present in clear case-I waters. H estimates closely aligned with observations, showing clustering only for values beyond 9m. This clustering, likely an artifact of inverting R_{rs} with an optical depth shallower than H , might be mitigated by constraining H priors with OSCs covariance. However,

the scarcity of globally available concurrent OSCs and H observations in optically shallow environments poses a challenge. That being said, the next chapter in this thesis quantified the different sources of uncertainty obtained from SABER retrieved OSCs and/or SV from *in situ* R_{rs} taken in contrasting optically shallow waters.

2.7 Conclusions

The quantification of uncertainty in inversion retrieved products has become one of the major recommendations in the ocean colour community (Lee et al., 2006a; Mélin, 2019). However, there is a scarcity of SA inversion models giving both the OSC/SV and their associated uncertainty. In this regards, we presented a Bayesian SA inversion model ; SABER that could simultaneously yield both the OSCs/SVs and their uncertainty estimate from the R_{rs} . Using publicly available *in situ* and synthetic datasets of R_{rs} across eight major optical water types (OWTs), OSCs and water depth from the OCRS community, SABER was compared with frequently used inversion methods, such as QAA for optically deep waters and HOPE for optically shallow waters. On comparison, SABER yielded more robust retrievals of OSCs and water depth (H) compared to QAA and HOPE, respectively. The highest uncertainty and BCI_{95} were observed for $[chl]$ retrieval, whereas the least was associated with $b_{bp}(555)$. In optically shallow water inversion, SABER retrieved OSCs were much more robust and had low uncertainty compared to the same obtained from HOPE. It indicated relatively stable inversion performance of SABER for optically complex shallow water, having a very high degree of ambiguity from the dynamic coastal processes. However, the free parameters, i.e., the spectral slopes (s_{dg} and γ) and benthic classes are kept fixed during the inversion. Hence, adequate knowledge of the IOPs and benthic composition for the study area is necessary prior to inversion. In case of absence of such priors, a sensitivity analysis for the model parameters might be necessary to improve the inversion performance. Lastly, as future improvement of SABER, it would be important to speed up the MCMC sampling time by potentially constructing likelihood LUTs for its application to airborne or satellite optical imagery.

ARTICLE 3

OCEAN COLOUR INVERSION AND ITS SOURCES OF UNCERTAINTY IN COASTAL SHALLOW WATERS

Article to be submitted to **Remote Sensing of Environment**

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3.1 ABSTRACT

In optical remote sensing (RS) of coastal and inland waters, radiative transfer (RT) theory links water-leaving remote sensing reflectance (R_{rs}) with Optically Significant Constituents (OSCs) and benthic properties. However, current RT inversion models do not simultaneously provide estimates and uncertainties for both OSCs and benthic properties. Additionally, uncertainty budgets quantifying propagated uncertainty in optically shallow, absorptive systems are lacking. This study addresses these gaps by evaluating a Bayesian inversion framework (S.A.B.E.R) for retrieving OSCs and benthic variables in the optically complex, CDOM-rich, shallow waters of the Manicouagan Peninsula (MP) in the Eastern St. Lawrence region. Using remote sensing reflectance spectra from multiple *in situ* sensors (HOCR, PSR, C-OPS), SABER corrected for inelastic scattering effects, reducing residual errors by 16% and 26% in blue-green and red wavelengths between *in situ* and reconstructed R_{rs} , respectively. However, the model encountered a “causality paradox” where key ancillary variables, such as chlorophyll concentration and detrital absorption, needed for inelastic scattering correction, were also outputs of the inversion. Further sensitivity analysis of SABER model parameters revealed that the detrital matter spectral slope (s_{dg}) and benthic substrate types, especially dark vegetation, significantly influenced retrieval uncertainty. Moreover, in the uncertainty budget, these two quantities explained $\sim 85\%$ of the propagated variance in SABER retrievals. Despite this, SABER successfully estimated benthic reflectance and abundance with high accuracy for bright substrates, but with relatively weaker performance for darker substrates, possibly due to the very low signal strength in these conditions. Overall, SABER’s ability to retrieve key water quality and benthic parameters in highly absorptive waters demonstrates its potential for advancing optical remote sensing techniques in shallow coastal environments. This work paves the way for future improvements, including integrating elastic and inelastic forward models in the course of inversion for more robust simultaneous retrieval of water column and benthic variables.

3.2 RÉSUMÉ

Dans le domaine de la télédétection optique (RS) des eaux côtières et intérieures, la théorie du transfert radiatif (RT) relie la réflectance de l'eau (R_{rs}) aux constituants optiquement significatifs (OSCs) et aux propriétés benthiques. Cependant, les modèles d'inversion RT actuels ne fournissent pas simultanément des estimations d'incertitudes pour les OSCs et les propriétés benthiques. De plus, il manque des bilans d'incertitude pour quantifier l'incertitude propagée dans les systèmes peu profonds et absorbants. Cette étude évalue l'algorithme d'inversion SABER qui s'appuie sur un cadre statistique bayésien pour l'estimation des OSCs et des variables benthiques dans les eaux complexes et riches en CDOM de la péninsule de Manicouagan (MP) dans l'estuaire du Saint-Laurent. SABER est appliqué aux spectres de réflectance de l'eau mesurés *in situ* (HOCR, PSR, C-OPS) et corrigés des processus de diffusion inélastique. Cette correction réduit les erreurs résiduelles de 16% et 26% dans les longueurs d'onde bleu-vert et rouge entre les mesures *in situ* et les R_{rs} estimés. Le modèle a rencontré un « paradoxe de causalité » où des variables clés, telles que la concentration en chlorophylle et l'absorption des matières jaunes, nécessaires pour la correction de la diffusion inélastique, font aussi parties des sorties du modèle d'inversion. Une analyse de sensibilité a montré que la pente spectrale des matières jaunes (s_{dg}) et les types de substrats benthiques, en particulier la végétation dense, influençaient l'incertitude des estimations. Ces deux quantités expliquaient environ 85% de la variance propagée. SABER a estimé la réflectance et l'abondance benthiques avec une grande précision pour les substrats clairs, mais a montré des performances plus faibles pour les substrats sombres, probablement en raison de la faible intensité du signal dans ces conditions. En conclusion, SABER montre son potentiel pour faire progresser les techniques de télédétection optique dans les environnements côtiers peu profonds et ouvre la voie à de futures améliorations, notamment l'intégration de modèles élastiques et inélastiques pour une estimation simultanée plus robuste des variables benthiques et de la colonne d'eau.

3.3 Introduction

Over the past two decades, substantial progress has been made in developing solutions to the shallow-water Radiative Transfer (RT) equation. The most widely applied technique across various Optical Water Types (OWTs) is the semi-analytical (SA) parametrization of the forward RT equation (Lee et al., 1998a; Albert and Mobley, 2003). In this approach, remote-sensing reflectance (R_{rs} [sr^{-1}]) is separated into contributions from the equivalent of infinite-depth water column ($R_{rs,\infty}$) and benthic reflectance (R_B) (Maritorena et al., 1994). The parameterized SA model in shallow water is optimized as an inverse problem to obtain estimates of Inherent Optical Properties (IOPs), i.e., spectral absorption $a(\lambda)$ [m^{-1}] and backscattering $b_b(\lambda)$ [m^{-1}] coefficients. The IOPs are further used to derive biogeochemical variables or the so-called Optically Significant Constituents (OSC), such as concentration of chlorophyll-a ($[chl]$; [mg m^{-3}]) for phytoplankton biomass, dissolved organic carbon, suspended particulate matter (SPM) concentration, etc. (Werther, 2022). Water column height ($H[m]$) and bottom reflectance (R_B [unitless]) are also derived when the propagating light reaches sea bottom (Dekker et al., 2011).

One of the first SA models for hyperspectral remote sensing of optically shallow water was introduced by Lee et al. (1999), i.e. the Hyperspectral optimization process exemplar model (HOPE). HOPE obtains the IOPs and benthic parameters using a predictor-corrector-based optimization scheme with only bright sand as the benthic type, which is mostly suitable for environments with a homogeneous benthic substrate cover. To address this issue, several studies have extended the approach of Lee et al. (1999) by incorporating more benthic types (up to $n = 13$ in some cases) using linear mixture models (LMM) and more advanced optimization techniques. For example, the Water colour simulator (WASI) by Gege and Albert (2006) formulated the R_B as an LMM of five benthic types (sand, silt, seagrass, mussel, macrophyte); the inversion is performed using a non-derivative-based simplex downhill method. Another approach, known as SAMBUCA (semi-analytical model for bathymetry, unmixing, and concentration assessment), introduced the Substrate Detectability Index (SDI)

to classify retrievals as true or quasi-optically shallow waters, enhancing depth (H) retrieval validation (Wettle and Brando, 2006; Brando et al., 2009). Look-up-table (LUT)-based approaches, such as Binary Space Partitioning (BSP) Tree, efficiently explored the parameter space iterating over a set of benthic reflectances in retrieving H (e.g., Hedley et al., 2009b). Further studies such as HOPE-LUT (Garcia et al., 2018) for hyperspectral images compared non-linear Update-Repeat LM and Latine Hypercube Sampling method to classify the scene as sand, non-sand and mixed pixels as an initial guess of benthic type. Each pixel is further inverted using BSP tree with the initial guess of benthic types (max of $n = 3$ from a set of 7) resulting in relatively high (74%) accuracy for the classified benthic type.

Apart from the deterministic approaches, probabilistic approaches were also formulated. Jay and Guillaume (2014) proposed a maximum likelihood-based objective function for the HOPE model, optimized for retrieving H and $[chl]$. This approach incorporates spatial pixel arrangement to capture variation in H values, employing a linear model to ensure robust performance under homogeneous IOP conditions. This method was further tuned with Bayesian “Maximum-a-Posteriori” (MAP) regularization, i.e., reduction in parameter search bounds using loss functions obtained from *a priori* knowledge of OSCs/IOPs and H by Jay and Guillaume (2016).

Despite advancements in optimization techniques and benthic modeling schemes, these methods overlook the uncertainty associated with the retrieved parameters. Quantifying uncertainty in ocean colour retrievals is essential for enhancing the reliability of derived variables (Mélin, 2019), particularly for R_B inversions, which are mathematically challenging due to the potential for multiple local minima in the solution space (e.g., Defoin-Platel and Chami, 2007a). The net uncertainty for a retrieved variable can be expressed as :

$$\sigma_{\text{total}} = \sqrt{\sigma_{\text{data}}^2 + \sigma_{\text{model}}^2 + \sigma_{\text{noise}}^2 + \sigma_{\text{inv}}^2} \quad (3.1)$$

σ_{data} denotes uncertainty in the R_{rs} occurred as a combined effect of conversion from radiometric quantities and binning the in water profiles (Mélin, 2019). Additionally, complex

computational models such as inversion often incorporate discretization in time or space for LUTs, along with various numerical approximations such as gradient approximation, which can introduce a numerical uncertainty denoted as σ_{model} . Sensor noise (σ_{noise}) consists of **(1)** spectrally flat noise, which represents wavelength-independent deviations in measured R_{rs} due to sensor degradation and/or miscalibration, and **(2)** spectrally dependent noise, known as sensor-environmental noise equivalent reflectance ($\text{NE}\Delta R_{\text{rs}}$), which accounts for uncertainties from atmospheric and air-water interface corrections (Brando and Dekker, 2003; Hedley et al., 2012). This spectrally dependent noise is typically obtained over a homogeneous deep-water region, and used to scale the retrieved parameters for a noise-robust estimate (Jay et al., 2017b; Garcia et al., 2020). However, this approach does not yield a bounded uncertainty estimate for retrieved IOPs or benthic variables.

Bootstrapping approaches were adopted to randomly perturb each R_{rs} observation with $\text{NE}\Delta R_{\text{rs}}$ for n times, and then retrieving the uncertainty for each estimate from the n retrievals. This approach cannot determine the uncertainty from the inversion (σ_{inv}), i.e., the bio-optical formulation of IOPs and existing spectral and surface roughness knowledge of possible benthic types. In this context, the Cramér-Rao bounds (CRB), which uses Fisher information from R_{rs} to calculate uncertainties for the retrieved variables, had been used to assess σ_{total} except σ_{data} (Jay et al., 2017a; Guillaume et al., 2023). While the CRB is effective for estimating the uncertainty of the estimator (i.e., the SA parameterization of forward radiative transfer), it relies on the assumption that the estimator is unbiased. Additionally, applying the CRB requires a separate step after parameter retrieval. Consequently, a coupled approach that retrieves both the parameter value and its associated uncertainty is needed for optically-shallow waters.

Finally, studies quantifying the uncertainty budget, specifically the relative contribution of each component in shallow water inversion, are sparse. Salama (2012) provided a comprehensive review of uncertainty quantification methods, comparing partial derivative techniques (e.g., chain rule and Taylor series expansion) and stochastic approaches (e.g., cross-entropy

maximization) in ocean colour RS using IOCCG 2003 and NOMAD benchmark datasets. They found that the inversion-related uncertainty component, σ_{inv} , contributed approximately 30% to OSC estimates in optically deep waters. However, the uncertainty arising from bio-optical IOP formulations or benthic class selection (components of σ_{inv}) in shallow waters remains largely unexamined.

In this chapter, we applied the new Bayesian inversion model (SABER) presented in Chapter 2 for the simultaneous retrieval of OSC parameters, specifically, chlorophyll-*a* concentration [*chl*] and absorption by coloured detrital matter a_{dg} , along with water depth (H) and benthic reflectance (R_{B}) from R_{rs} values measured in the CDOM-rich temperate coastal optically shallow waters of the St. Lawrence estuary. Here, significant CDOM absorption (a_{g}) diminishes the signal in the blue bands, with Sun-induced CDOM fluorescence (f_{DOM}) accounting for up to 20% of R_{rs} at 525-555 nm wavelengths (Chapter 1) (Mukherjee et al., 2023). To address this, we developed a SA model to estimate the fluorescence-equivalent R_{rs} and conducted a sensitivity analysis to refine the spectral slope parameters of detrital matter absorption (s_{dg}) and backscattering (γ), while optimizing the selection of benthic types across three classes. We also presented an uncertainty budget for SABER outputs, quantifying propagated uncertainties from σ_{inv} components through a probabilistic analysis of variance approach.

3.4 Materials and Methods

3.4.1 Study area

The field campaign is performed in the coastal waters of the Manicouagan Peninsula ($\sim 49^\circ\text{N}$, 68.3°W) at the lower estuary of St Lawrence (ESL) in Québec, Canada (Fig. 19). The sampling consisted of measurements for benthic depth from 0.5m up to $\sim 175\text{m}$, however, for the current study, only stations with a maximum depth of 10m were considered. This region is dominated by “green” waters type, with CDOM as the dominant absorbing

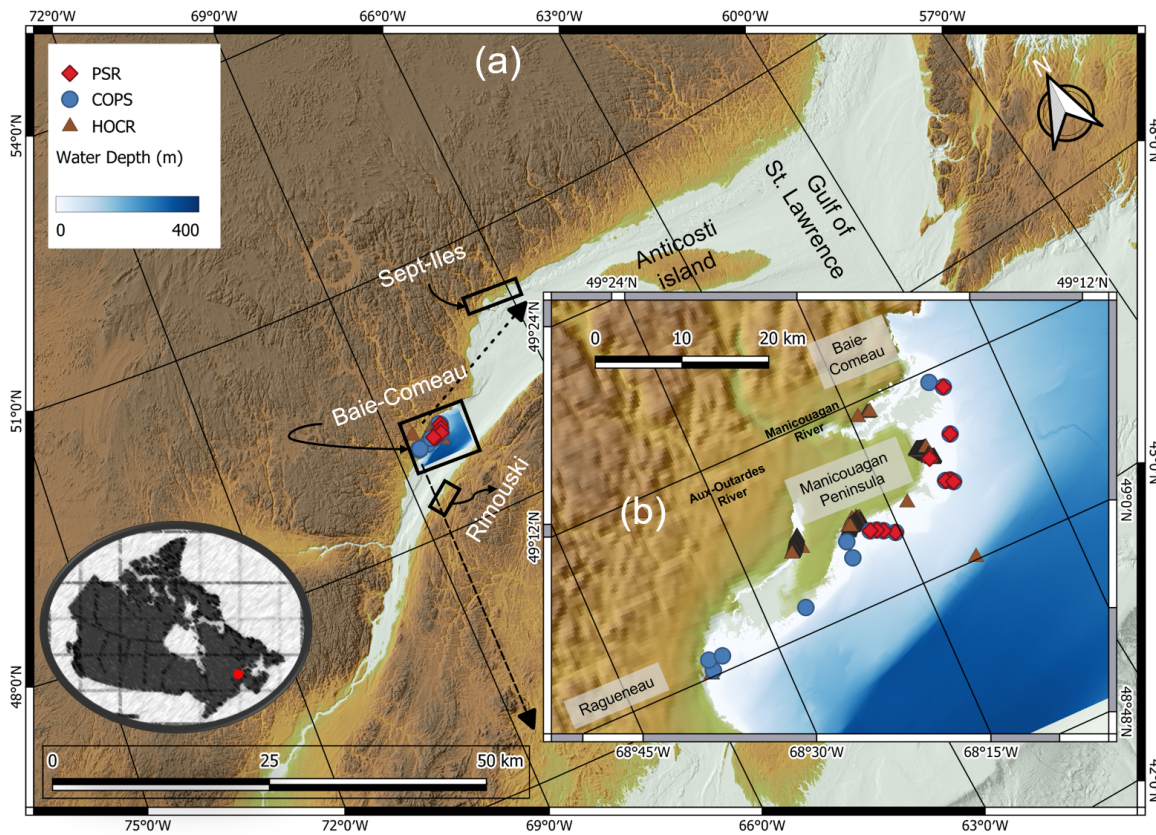


FIGURE 19 – Map of the study area for chapter three. (a) shows the geographical location of the study area in close proximity to the Gulf of Saint Lawrence in the Québec province in the east of Canada (the red dot in the encapsulated map of Canada). (b) The *in situ* sampling strategy for acquiring water depth (locations shown for HOCR, COPS), radiometric and biogeochemical (locations shown for HOCR, COPS, PSR) data in shallow coastal waters.

component (Mukherjee et al., 2023; Araújo and Bélanger, 2022). Further geographical and oceanographical details are presented in Section 1.4.1.

3.4.2 *In situ* datasets

3.4.2.1 Discrete sampling

The datasets used in this study were collected during a fieldwork campaign designed to evaluate the capabilities of the airborne Watersat Imaging Spectrometer Experiment (WISE) sensor for mapping benthic habitats and assessing water quality in optically complex and shallow waters. Two boats; the *Kildir* and *FJ Saucier* were used to collect radiometric measurements, IOPs and discrete water samples for biogeochemical determination. *Kildir* was set up with a profiler C-OPS (Biospherical) for multispectral radiometric measurement and IOPs were measured with an A-Sphere and Hydroscat-6 (HOBILabs), respectively. *FJ Saucier* was also equipped with a C-OPS, while IOPs were measured using a AC-S and BB9 (WETLabs) package. A detailed summary of the sampling strategy, field acquisition, data processing, and laboratory analysis for water samples specific to the WISE field campaign is given in Section 1.4.2.

3.4.2.2 Continuous sampling in shallow waters

In nearshore and very shallow waters (depth < 2 meters), a 12-foot zodiac was deployed to collect radiometric and acoustic data. A single-beam echo sounder (Hydroball) operating at 500 KHz was mounted for bathymetry measurements. The Hydroball frame was adapted to accommodate two hyperspectral in-water radiometers (HyperOCR, or HOCR; Satlantic) for measuring upwelling radiance at two depths below the sea surface : $z_1 = 0.15\text{m}$ and $z_2 = 0.30\text{m}$. Additionally, a third HOCR was mounted on a small mast on the Zodiac to continuously measure downwelling irradiance; $E_d(0^+)$ during transects. The water-leaving R_{rs} was then calculated as :

$$R_{rs}(0^+, \lambda) = \frac{L_w(\lambda)}{E_d(0^+, \lambda)} \quad (3.2a)$$

$$L_w(\lambda) = 0.54 \cdot L_u(0^-, \lambda) \quad (3.2b)$$

$$L_u(0^-, \lambda) = \frac{L_u(z_1, \lambda)}{e^{z_1 \cdot K_{L_u}(\lambda)}} \quad (3.2c)$$

$$K_{L_u}(\lambda) = \frac{\ln(L_u(z_1, \lambda)) - \ln(L_u(z_2, \lambda))}{z_2 - z_1} \quad (3.2d)$$

Finally, two GoPro cameras were mounted on the Hydroball frame to document the bottom type. This set up was deployed from August 18 to 25, totalizing 9500 meters of continuous transect of R_{rs} and H ($n = 1413$).

3.4.2.3 The "WISE experiment"

On August 25, 2019, a team of SCUBA divers, along with the vessels *Kildir*, *FJ Saucier*, and the zodiac, gathered near Pointe Lebel to conduct an experiment (hereafter referred to as EXPWISE) (Figs. 20 and 21). The objective of the experiment was to measure spectral benthic reflectance (R_B) using two distinct methods : the free-falling C-OPS instrument and the SVC HR-512i spectroradiometer operated by underwater divers (Fig. 20). A transect of approximately 40 meters, marked by two anchored buoys and located at a water depth of around 2.2 meters, was established for the experiment. The C-OPS was deployed along the 40-meter transect by a SCUBA diver, who brought the profiler to the sea surface before releasing it to obtain vertical profiles of downwelling irradiance (E_d), upwelling irradiance (E_u), and upwelling radiance (L_u). A total of ten vertical profiles were progressively carried out along the transect. To minimize turbulence and shadowing, the diver allowed the C-OPS to fall freely while quickly moving away from the profiler. R_B was calculated in two ways using E_u or L_u , and E_d (Fig. 20 b,c) at $H \approx 0.3m$ just above the bottom :

$$R_B^{E_u} = \frac{E_u^{H=0.3m}}{E_d^{H=0.3m}} \quad (3.3a)$$

$$R_B^{L_u} = \pi \cdot \frac{L_u^{H=0.3m}}{E_d^{H=0.3m}} \quad (3.3b)$$

The $R_B^{H=0.3}$ is extrapolated to the benthic floor using a non-linear extrapolation technique to account for the highly non-linear propagation of radiance in optically shallow water. At the location where the C-OPS made contact with the bottom, a hyperspectral benthic reflectance measurement of the seafloor was determined by a separate team of divers operating an HR-512i spectroradiometer (Spectral Vista Corporation, SVC) enclosed in an underwater housing (Fig. 20a). The SVC was used to collect hyperspectral radiance of the bottom target (L_t) and a calibrated reference spectralon panel (L_p ; 99% reflectance) at the height of approximately 0.2 meters from the seafloor. The instrument collects 512 radiances between 350 nm to 1050 nm at a 4° field-of-view (FOV). The benthic reflectance (R_B^{SVC}) was calculated as $R_B^{SVC} = L_t/L_p$. The SVC also captured RGB images of the bottom with an integrated camera at a native resolution of 640x480 pixels, whereas for C-OPS, a Hero 6 GoPro camera was mounted on the profiler frame to obtain underwater images (see below).

During the experiment, the *Kildir* was anchored a few meters south of the 40-m transect (Fig. 21), from which above-water $R_{rs}(0^+)$ was determined using a Spectral Evolution PSR-1100f (PSR) from the bow of the boat (Fig. 20d). The PSR with 3 nm spectral resolution and a 320–1100 nm range, was fitted with a bare fiber optic with a 25° FOV. Calibrated Spectralon panels served as reference targets to compute $R_{rs}(0^+)$ following Mobley (1999) similar to Harringmeyer et al. (2024). The viewing zenith angle (θ_v) was set to 40°, and the azimuth difference between solar and sensor planes ($\Delta\phi$) was maintained between 90–135° to reduce sun glint contamination (Mobley, 1999). Wind speed and sun-view geometry were recorded systematically for sky glint correction using the method in Zhang et al. (2017). Additionally, two C-OPS profiles were taken by the divers to obtain subsurface $R_{rs}(0^-)$ at the location where the PSR measurements were made.

3.4.3 SA parametrization of RT equation

The forward model to simulate R_{rs} can be divided into two parts, i.e. **(1)** R_{rs} equivalent to elastic scattering (R_{rs}^{el}) of the water and its OSCs and **(2)** R_{rs} equivalent to inelastic scattering (R_{rs}^{inel}) of OSCs. Then, the total R_{rs} is calculated as $R_{rs}^m = R_{rs}^{el} + R_{rs}^{inel}$. The parametrization for the R_{rs}^{el} component following Albert and Mobley (2003) model was presented in Section 2.4.2. We showed in Chapter-1 that the R_{rs}^{inel} contributed substantially to the green and red spectrum of water-leaving R_{rs} in MP coastal waters, hence, here we proposed an OSC seeded

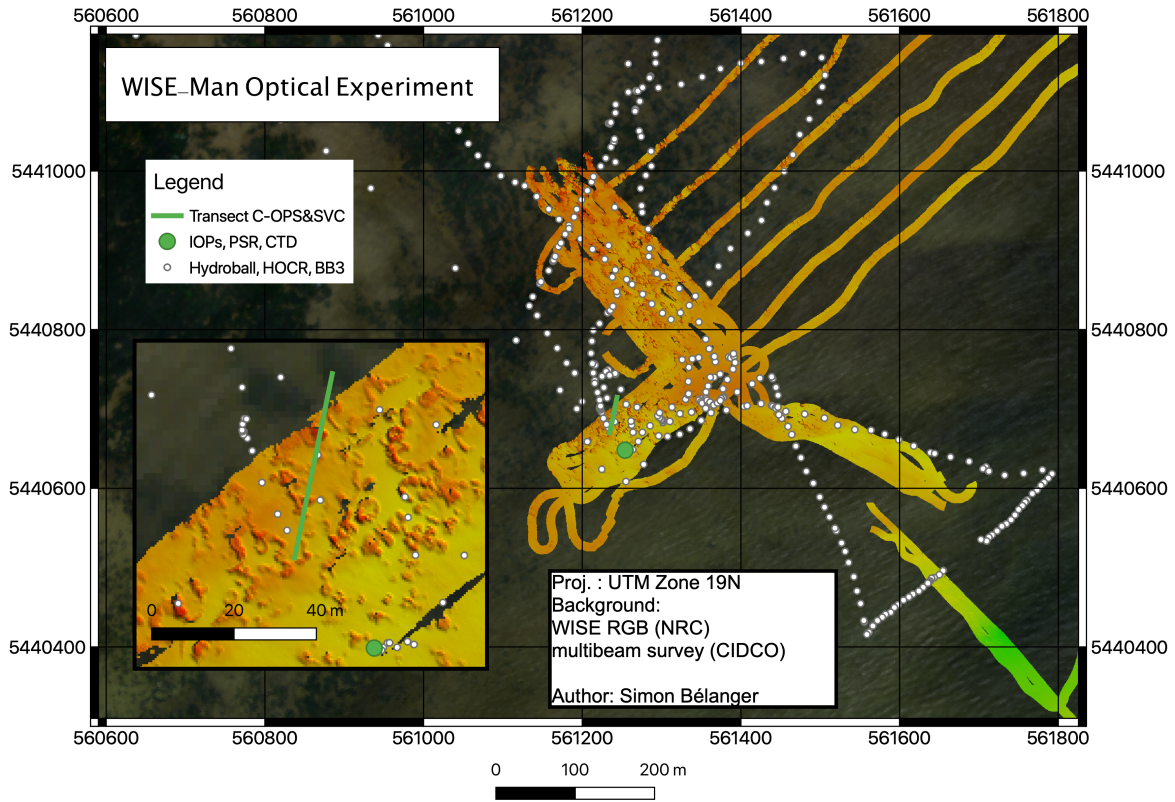


FIGURE 21 – Detailed map of the EXPWISE study area, showing the location of the 40-meter diver transect, the sampling station for IOPs and above-water R_{rs} from PSR, and the Zodiac measurement sites. The background includes a multibeam echosounder (MBES) bottom map (color-coded) highlighting eelgrass patches, overlaid with a true-color image from the WISE sensor.

model to estimate R_{rs}^{inel} , that we subtracted from the *in situ* R_{rs} prior to inversion input. R_{rs}^{inel} was obtained as a sum of remote sensing reflectance obtained from Sun-Induced Chlorophyll Fluorescence (SICF) and CDOM Fluorescence (f_{DOM}), i.e. $R_{rs}^{inel} = R_{rs}^{SICF} + R_{rs}^{f_{DOM}}$.

SICF affects the wavelengths between 670-730 nm λ with a peak at ~ 685 nm. The SICF equivalent radiance at the peak SICF emission wavelength, 685nm, i.e. $L_{\phi}(685)$ is calculated using measured $[chl]$ and $a_{dg}(443)$ values from discrete water samples :

$$L_{\phi}(685) = \frac{0.092[chl]}{(1 + 0.40a_{dg}(443) + 0.078[chl])} \quad (3.4)$$

The spectral shape of SICF is modelled as a summation of two Gaussian shapes with mean (μ) = 685, 730 [nm] and standard deviation (σ) = 25, 50 [nm] as the Full Wave Half Maximum (FWHM) of the Gaussian curve (Mobley, 1994) :

$$hc(\lambda) = \sqrt{\frac{4 \ln 2}{\pi}} \frac{1}{25} \exp \left[-4 \ln 2 \left(\frac{\lambda - 685}{25} \right)^2 \right] + \sqrt{\frac{4 \ln 2}{\pi}} \frac{1}{50} \exp \left[-4 \ln 2 \left(\frac{\lambda - 730}{50} \right)^2 \right] \quad (3.5)$$

The SICF equivalent radiance for $670 < \lambda[\text{nm}] < 730$ can be calculated as, $L_{\text{SICF}} = L_{\phi}(685) \cdot hc(\lambda)$. The SICF equivalent R_{rs} is calculated as, $R_{\text{rs}}^{\text{SICF}} = L_{\text{SICF}}/E_{\text{d}}(0^-)$, where, $E_{\text{d}}(0^-)$ is the sub-surface downwelling irradiance, calculated following Carder and Gregg (1990).

f_{DOM} affects λ between 310-600nm and the spectral shape can be modelled following a log-normal distribution (Lee et al., 1992). The f_{DOM} equivalent radiance, L_{fDOM} is calculated analytically by integrating a wavelength discretized source scatter function as

$$\beta_{\text{g}}(\psi, \lambda^*, \lambda) = b_{\text{g}}(\lambda^*) f_{\text{g}}(\lambda^*, \lambda) \beta_{\text{g}}(\psi) \quad (3.6)$$

Where, $b_{\text{g}}(\lambda^*)$ is loss of photon at excitation wavelength, λ^* which is equivalent to $a_{\text{g}}(\lambda^*)$. $f_{\text{g}}(\lambda^*, \lambda)$ is the wavelength redistribution function (WRF) calculated as, $f_{\text{g}}(\lambda^*, \lambda) = \eta_{\text{g}}(\lambda^*, \lambda) \frac{\lambda^*}{\lambda}$, where, $\eta_{\text{g}}(\lambda^*, \lambda)$ is the shape of quantum efficiency of f_{DOM} modelled as

$$\eta_{\text{g}}(\lambda^*, \lambda) = A_0(\lambda^*) \exp \left[- \left(\frac{\frac{1}{\lambda} - \frac{A_1}{\lambda^*} - B_1}{0.6 \left(\frac{A_2}{\lambda^*} + B_2 \right)} \right)^2 \right] \quad (3.7)$$

Where, $A_0(\lambda^*), A_1, A_2, B_1, B_2$ are coefficients given by Hawes et al. (1992), as implemented by Mobley (1994) in Hydrolight. The phase function for CDOM fluorescence is assumed isotropic, thus, $\beta_{\text{g}}(\psi)$ was set to $\frac{1}{4\pi}$. The L_{fDOM} is calculated as $\frac{1}{4\pi} \cdot \int b_{\text{g}}(\lambda^*) f_{\text{g}}(\lambda^*, \lambda)$. The f_{DOM} equivalent R_{rs} is calculated as, $R_{\text{rs}}^{\text{fDOM}} = L_{\text{fDOM}}/E_{\text{d}}(0^-)$. The $E_{\text{d}}(0^-)$ is calculated in the same approach used for $R_{\text{rs,SICF}}$.

Finally, we subtracted the estimated $R_{\text{rs}}^{\text{inel}}$ from the *in situ* R_{rs} to obtain the estimated $R_{\text{rs}}^{\text{el}}$. Note, the sensitivity analysis and further parameter retrievals were performed with the spec-

tral R_{rs}^{el} used as input. The effect of subtracting the R_{rs}^{inel} in course of inversion was assessed using R_{rs} reconstruction (Gege and Albert, 2006); inversion retrieved parameters (for both el and $el + inel$ spectrum) were input to the forward model shown in Eq. 2.1 to reconstruct the input R_{rs} . The residual error (Section 3.4.7) between the input *in situ* R_{rs} and reconstructed R_{rs} were analyzed.

3.4.4 Uncertainty estimation in SABER

SABER retrieves a vector (Y) of OSCs and benthic parameters and their uncertainties from subsurface R_{rs} (that has been prior corrected for Fluorescence following 3.4.3) as input. It employs the Bayesian inversion theory by combining a likelihood function with prior distributions for the OSCs and benthic variables, obtained from global and synthetic datasets. The prior is a complex multivariate distribution constructed with Log-Normal and Uniform distribution, i.e., $\mathbb{P}(Y) = \mathbb{P}_{\log\text{-normal}}(Y) \cdot \mathbb{P}_{\text{uniform}}(Y)$, and the likelihood, i.e., expectation value $\mathbb{E}[\cdot]$ of obtaining an R_{rs} (X) for observed OSCs and/or benthic parameter(s) (Y) ($\mathbb{E}[X|Y]$), is fitted by a Gaussian distribution (See section 2.4 for details). The probability of finding an estimate for Y is higher around the median of the Log-normal prior, but in a bounded domain of $[a, b]$, where a and b are the lower and upper limits for the Uniform distribution part in prior. The Y estimates are retrieved as $\mathbb{E}[\cdot]$ of OSCs and/or benthic parameter(s) for the observed R_{rs} , while its uncertainty is expressed as approximated posterior variance; $\text{Var}(Y|X)$, (referred as “retrieval uncertainty” onward) respectively :

$$\mathbb{E}[Y|X] = \int_a^b Y \cdot \mathbb{P}(Y|X) dY \quad (3.8a)$$

$$\text{Var}(Y|X) = \int_a^b (Y - \mathbb{E}[Y|X])^2 \cdot \mathbb{P}(Y|X) dY \quad (3.8b)$$

Finally, the 95% Bayesian Credible Intervals (BCI_{95}) and coefficient of variation (CV)

are obtained as :

$$BCI_{95} = \mathbb{E}[Y|X] \pm 1.96 \cdot \sqrt{\text{Var}(Y|X)} \quad (3.9a)$$

$$CV(\%) = \frac{\sqrt{\text{Var}(Y|X)}}{\mathbb{E}[Y|X]} \times 100 \quad (3.9b)$$

3.4.5 Sensitivity analysis

We conducted a One-at-a-Time (OAT) sensitivity analysis to evaluate how changes in specific free model parameters in SABER, namely the spectral slopes, i.e., s_{dg} and γ and the spectral benthic reflectance ($R_{\text{B}_{1, \dots, 3}}$), impact retrieval performance for $[chl]$, $a_{\text{dg}}(443)$ and H . Our OAT method systematically varied each free parameter across a defined range, while keeping others fixed, isolating each parameter's effect on the variance associated with the retrieved quantities, single at a time. Mathematically, for an inversion retrieved variable $Y \subset \phi_{\text{var}}$ (See 2.3 for ϕ_{var} definition) that depends on multiple free parameters $x_1, x_2, \dots, x_n$, the “sensitivity uncertainty” (σ) for a given free parameter x_i is calculated as :

$$\sigma_{x_i} = \frac{\Delta \text{Var}(Y_{x_i})}{Y_{\text{obs}}} \times 100(\%) \quad (3.10a)$$

$$\Delta \text{Var}(Y_{x_i}) = \sqrt{\text{Var}(Y(x_1, \dots, x_i + \Delta x_i, \dots, x_n))} - \sqrt{\text{Var}(Y(x_1, \dots, x_i, \dots, x_n))} \quad (3.10b)$$

We computed the variance $\text{Var}(\cdot)$ for each output Y (referred by “.” here) across a range of model parameters following Eq. 3.8b. Here, $\text{Var}(\cdot)$ captures the combined contributions of σ_{data}^2 and σ_{inv}^2 from Equation 3.1. Contributions from σ_{noise}^2 were assumed to be negligible, as the SABER model directly inverts sub-surface R_{rs} , while σ_{model}^2 was considered insignificant. Y_{obs} refers to *in situ* values against the retrieved $[chl]$, $a_{\text{dg}}(443)$ and H . The analysis considered all physically plausible combinations ($n = 90$) of s_{dg} and γ , varied over ranges of $\{0.002, 0.220\}$ and $\{0.2, 1.0\}$, respectively. For benthic reflectance R_{B} , we iterated over all

triplet combinations ($n = 20$) of five primary substrate types in the study area; i.e., Sand, Mud, Rock, eelgrass, Macroalgae, and Spartina to identify the optimal selection for the three benthic classes ($R_{B1,...,3}$).

3.4.6 Uncertainty budget

A global sensitivity analysis following the Sobol indices (SI) (Sobol, 2001) has been performed to quantify the contribution of different components in σ_{inv}^2 in the SABER obtained $Var\{.\}$ for each of the OSC and benthic parameters. The analysis is carried out using the global total SI (S_{Ti}), which quantifies how an individual component in σ_{inv}^2 such as s_{dg} , γ and $R_{B1,...,3}$ relatively contribute to the total variance obtained for each retrieval, each as a random variable denoting both explicit and cross interactions among the σ_{inv}^2 components. S_{Ti} is given as :

$$S_{Ti} = \frac{\text{Var}(\mathbb{E}(Y|\mathbf{X})) - \text{Var}(\mathbb{E}(Y|\mathbf{X}_{\sim i}))}{\text{Var}(Y)} \quad (3.11)$$

$\text{Var}(\mathbb{E}(Y|\mathbf{X}_{\sim i}))$ is the variance of the conditional expectation of model output (Y) given the parameter of interest in $x = \mathbf{X}_i$ in the parameter space $x_1, \dots, x_2, \dots, x_n$. Similarly, $\text{Var}(\mathbb{E}(Y|\mathbf{X}))$ is the variance of the conditional expectation of Y given all the parameters in $x_1, \dots, x_i, \dots, x_n$ are unconstrained. It is to be noted that S_{Ti} is always bound between $[0, 100](\%)$.

3.4.7 Validation metrics used

Several statistical metrics were used to assess the sensitivity analysis and SABER retrieved estimates of OSC and benthic variables. The absolute residual difference and % residual difference (δ_{var} and $\hat{\delta}_{var}(\%)$ in Eq. 3.12) were employed to assess the absolute and relative signed differences between quantities, respectively. SABER retrieved OSCs and benthic variables were validated against *in situ* observations using bias (β), the slope (m) of linear

regression and root mean squared log difference (RMSLD) formulated in Section 2.4.3.2 offering a robust evaluation (Pahlevan et al., 2022; Morley et al., 2018).

$$\delta_{\text{var}} = \hat{y}_i - y_i \quad (3.12a)$$

$$\hat{\delta}_{\text{var}}(\%) = \frac{\delta_{\text{var}}}{y_i} \times 100 \quad (3.12b)$$

In general, y_i is the observed or actual value, and $\hat{y}_i$ is the predicted value, i is a specific observation where n is the number of observations

3.5 Results

3.5.1 R_{rs} variability in optically shallow waters dominated by CDOM

The *in situ* water-leaving R_{rs} values exhibited signal peak at $\sim 550\text{-}580$ nm wavelengths with magnitude varying between 0.0005 and 0.005 sr^{-1} , denoting greenish to yellowish water types (Fig. 22a). The C-OPS-derived R_{rs} measurements ($n = 16$) covered 13 spectral channels, whereas the PSR ($n = 10$) and HOCR ($n = 469$) instruments provided >115 channels within the wavelength range of $400 < \lambda, [\text{nm}] < 750$. The water depth (H) associated with the spectrum spanned between $0.6\text{-}7.9$ m with a mean depth of 2.3 m. An inversely proportional relationship between R_{rs} magnitude and H can be observed in Fig. 22a, caused by the contribution of benthic substrate in very shallow waters. This contribution enhances the upwelling radiance from the water column, leading to an increase in signal strength in the green-red region of the spectrum.

The QWIP metric (Dierssen et al., 2022), which is designed to assess the quality of the $R_{\text{rs}}(0^+)$ in optically-deep waters, was applied to our data set. The majority of shallow observations (i.e., with $0 < H[\text{m}] < 3$) had a strong negative QWIP score (≤ -0.2) with the Apparent Visible Wavelength (AVW) shifting between $560\text{-}580$ nm (Fig. 22b). Negative QWIP scores are expected in optically-shallow waters with high peak in green, but low magnitude in

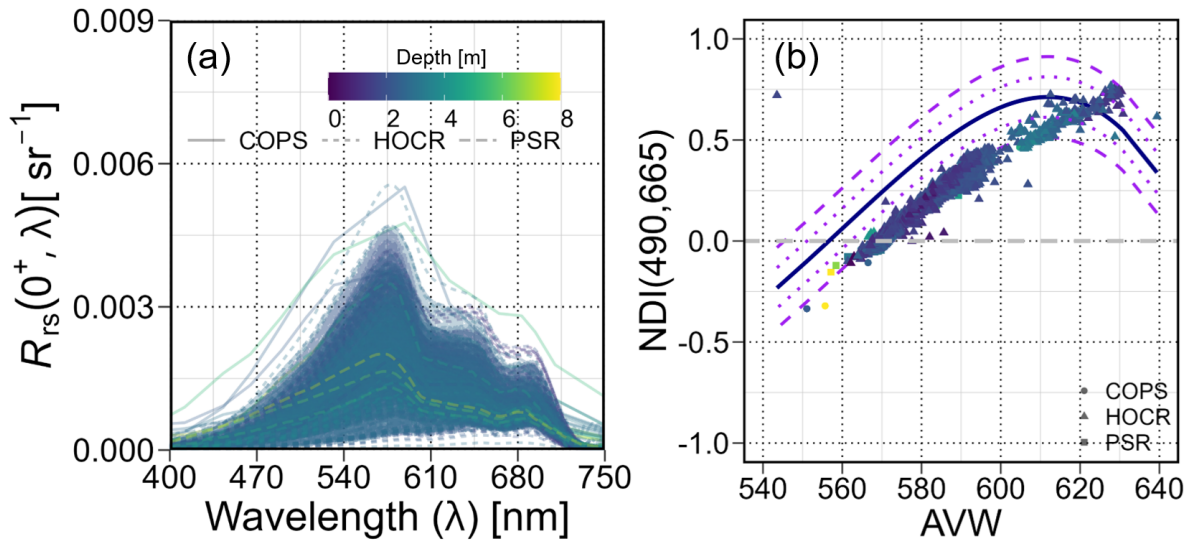


FIGURE 22 – (a) Spectral plots of water-leaving Remote-sensing reflectance; $R_{rs}(0^+, \lambda)$ derived from radiometric measurements from C-OPS, PSR and HO CR. The colour of each spectrum is mapped to the *in situ* water depth measured concurrently. (b) NDI values were obtained with 490 and 665 nm bands (Y-axis) plotted against AVW (X-axis); both derived for each R_{rs} spectrum shown in panel (a). The blue curve is the QWIP fitted line, whereas the dotted and dashed purple line(s) indicate the ± 0.1 and ± 0.2 ranges, respectively (See Dierssen et al. (2022) for details on QWIP). The colour of each point refers to the water depth alike panel (a).

red due to stronger water absorption suppressing the signal from the benthic floor (Dierssen et al., 2003). However, a few observations with a greater H value had AVW in the 560-570 nm range and the QWIP scores were between 0 and -0.2. The averaged penetration depth (z_{90}) in the area was estimated to be roughly 2.6 m at 555 nm λ (Mukherjee et al., 2023), hence R_{rs} observations with significantly higher H would have limited impact from the benthic floor. In line with this argument, the QWIP score exhibited a proportional relationship with H , increasing linearly with water depth, except for a few spectra.

The fluorescence-equivalent remote sensing reflectance, R_{rs}^{inel} , derived from Sun-Induced Chlorophyll Fluorescence (SICF) and f_{DOM} , was calculated for each concurrent lab measurement of chlorophyll concentration $[chl]$ and CDOM absorption coefficient $a_g(443)$. The values were then spectrally averaged to yield $\bar{R}_{rs}^{inel}$ and the elastic scattering-equivalent reflec-

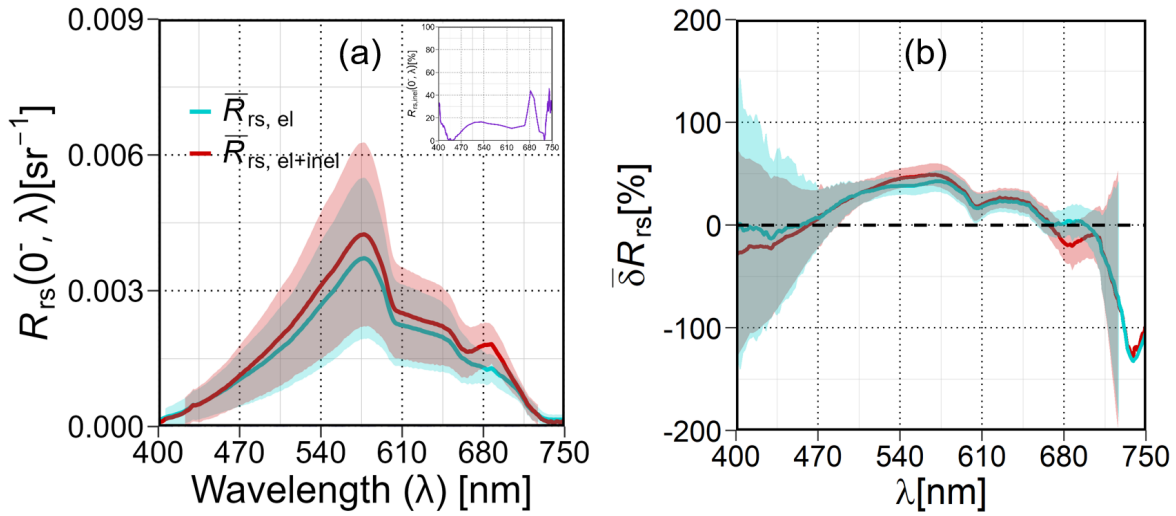


FIGURE 23 – (a) Spectral comparison between the mean sub-surface Remote-sensing reflectance with the inelastic scattering component present ($\bar{R}_{rs,el+inel}$ in red) and without it ($\bar{R}_{rs,el}$ in blue). The red and blue bands show the 95% Confidence Interval for each mean spectra. The inset panel on the top right shows the relative % contribution (purple line) for varying wavelength from $\bar{R}_{rs,inel}$ to the observed sub-surface Remote-sensing reflectance. (b) Mean % residual difference ($\bar{\delta R}_{rs}$) between input R_{rs} and reconstructed R_{rs} for *el* and *el + inel*, respectively. The colour scheme is the same as panel (a).

tance was obtained as $R_{rs,el} = R_{rs} - \bar{R}_{rs}^{inel}$. The mean $\bar{R}_{rs}^{inel}$ exhibited a 40% contribution at 400 nm, decreasing exponentially to near-zero by 440 nm (Fig. 23a). Two distinct shapes in $\bar{R}_{rs}^{inel}$ were evident across 470-600 nm and 670-710 nm, attributed to f_{DOM} and SICF, respectively, with mean contributions of $\sim 13\%$ and $\sim 22\%$ to the *in situ* R_{rs} (Fig. 23a). Moreover, the residual error percentage $\bar{\delta R}_{rs}$, calculated from reconstructed R_{rs} , demonstrated improved performance when R_{rs}^{el} was used as input to SABER. Specifically, remote sensing reflectance reconstructed with variables retrieved by SABER consistently exhibited mean residual errors that were 16% closer to zero in the 400–470 nm range compared to using $R_{rs}^{el+inel}$ as input for the inversion (Fig. 23b). The average residual error $\bar{\delta R}_{rs}$ was reduced by 13% across the 480-600 nm range and was nearly zero within the SICF range of 670-710 nm (Fig. 23b). Uncertainty in $\bar{\delta R}_{rs}$ was highest in the blue and red spectral regions and lowest in the green, closely aligned with the peak of R_{rs} as illustrated in Fig. 22a.

3.5.2 Uncertainty analysis of SABER model parameters

3.5.2.1 Uncertainty from spectral slopes

The sensitivity of the uncertainty (σ), derived from multiple SABER runs ($n = 500 \times 90$), where 500 observations of R_{rs} were randomly selected from the final dataset of the C-OPS, PSR, and HOCS sensors and each inverted 90 times for every combination of s_{dg} and γ , exhibited variations in both shape and magnitude across the retrieved variables. $[chl]$ had the highest range of σ (22%-211%) with multiple local minima in the uncertainty space (Fig. 24a). The uncertainties for $a_{dg}(443)$ and H retrievals were relatively lower, ranging from 0.79% to 26% and 0.26% to 40%, respectively and the σ spaces were much smoother with stricter minima (Fig. 24b,c).

The dispersion of the residual difference (δ_{var}) was also highest for $[chl]$ with a skewed distribution of the residuals, while the lowest residual difference was observed for $a_{dg}(443)$ retrievals (Fig. 24d), indicating that the retrieval of this variable is relatively insensitive to spectral shape of $a_{dg}(\lambda)$. The $\delta_{a_{dg}(443)}$ followed a strict Gaussian distribution with the central tendencies upon ~ 0 . A similar normality was observed for δ_H , but with a greater span and slight bi-modality centred upon the lower left quantiles (Fig. 24d). The optimal values of s_{dg} and γ were determined as $\{0.01403, 0.63\}$, obtained as the pairwise mean obtained from the observable σ minima for $[chl]$, $a_{dg}(443)$ and H found at $s_{dg} = \{0.0129, 0.0146, 0.0146\}$ and $\gamma = \{0.8, 0.6, 0.5\}$, respectively (Fig. 24 a,b,c).

3.5.2.2 Uncertainty from benthic classes

A total of 500×20 iterations, where 500 obs. of R_{rs} are inverted 20 times, i.e. for each triplet combination of benthic classes iterations and one constant set of spectral slope (see Section 3.5.2.1), were performed to assess the uncertainty propagated into retrieved estimates of $[chl]$, $a_{dg}(443)$ and H . The uncertainties associated with $[chl]$ and H were more sensitive

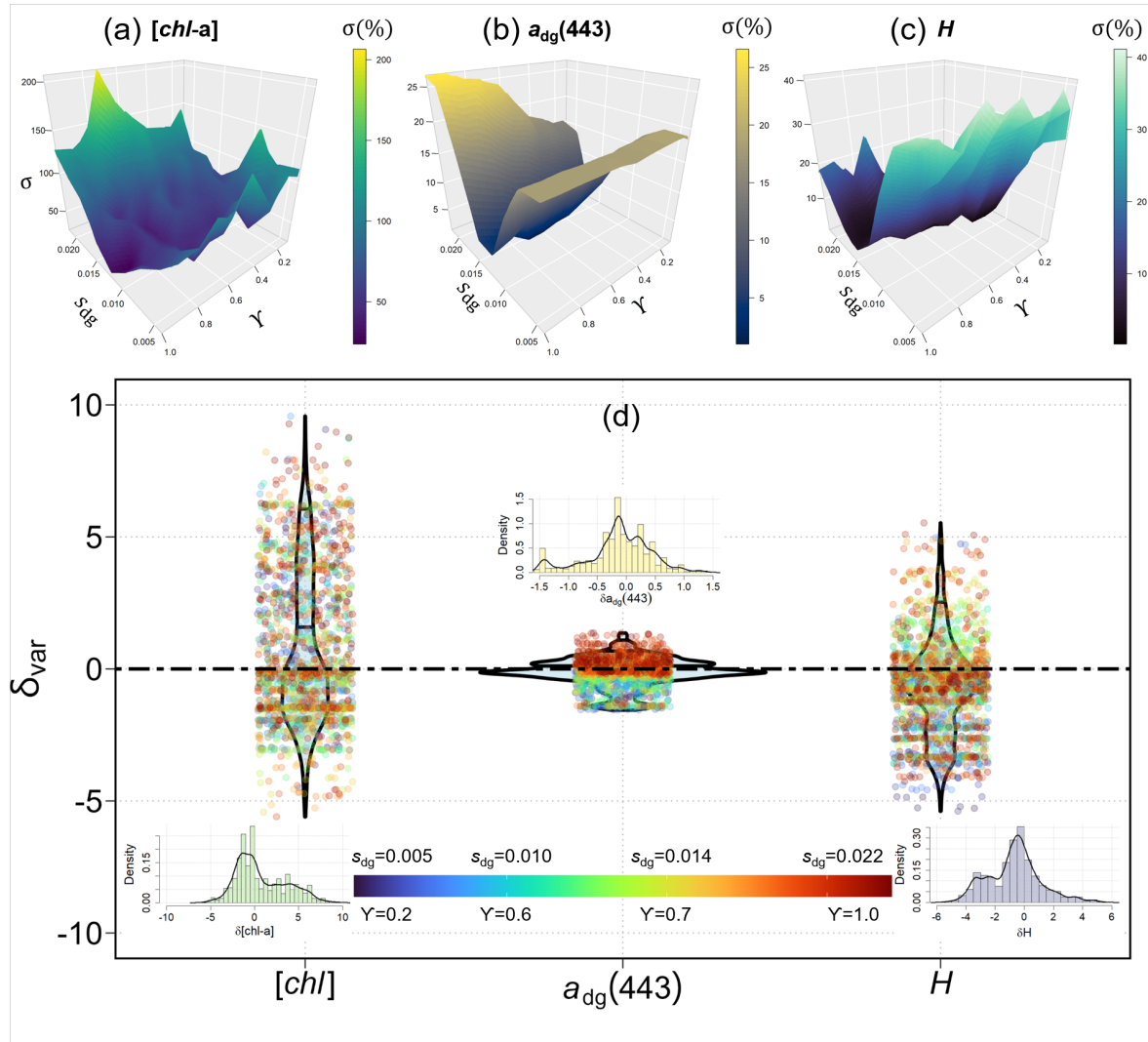


FIGURE 24 – Sensitivity analysis obtained uncertainty (σ) (Z-axis) surfaces shown against the vectors of s_{dg} (Y-axis) and γ (X-axis) for SABER retrieval of (a) $[chl - a]$, (b) $a_{dg}(443)$ and (c) H . (d) Violin plots showing the distribution of absolute residual difference (δ_{var}) obtained for each iteration in the sensitivity analysis. The overlaid points show the variability in δ_{var} magnitude over combinations of the slopes. The vertically aligned histograms show the central tendencies of the δ_{var} , where $var \subseteq \{[chl - a], a_{dg}(443), H\}$.

to the selection of benthic classes ($R_{B_{1,...,3}}$) than $a_{dg}(443)$. In particular, higher uncertainties are observed for benthic classes dominated by vegetation (Fig. 25). The σ increased from 30% to 50% and from 20% to 70% for $[chl]$ and H , respectively, when the vegetative fraction for $R_{B_{1,...,3}}$ were increased from 0% to 100% coverage (Fig. 25). In the case of $a_{dg}(443)$, the

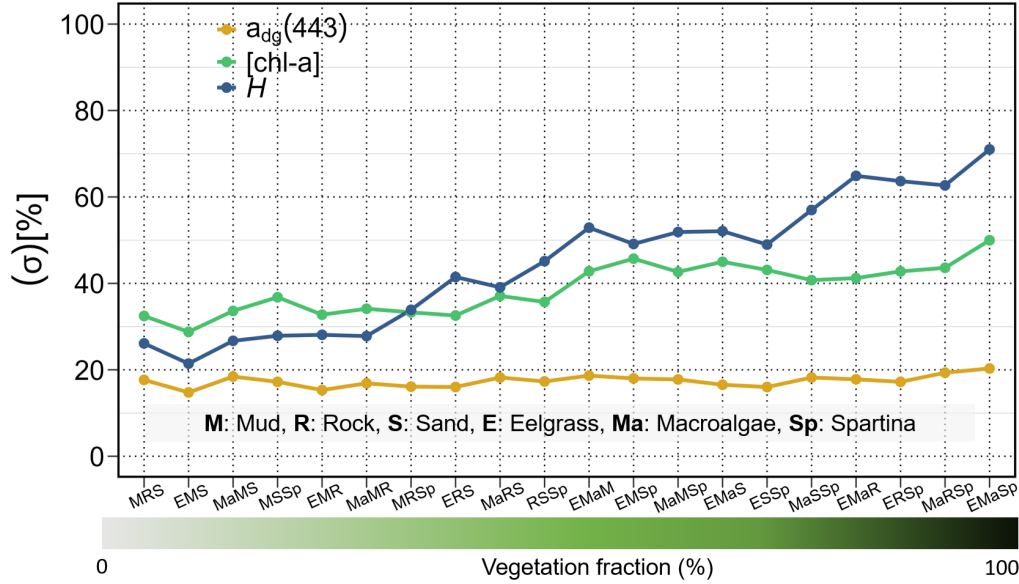


FIGURE 25 – Variation in sensitivity uncertainty (σ) for SABER retrieved $[chl - a]$, $a_{dg}(443)$ and H as a function of benthic class triplet combinations used in inversion. The benthic class combinations are arranged in order of increasing vegetation fraction, starting with non-vegetative combinations (e.g., Mud, Rock, and Sand, MRS) and ending with fully vegetative combinations (e.g., Eelgrass, Macroalgae, and Spartina, EMaSp) representing 100% bottom vegetation coverage.

σ varied between 14%-21% inferring a lower sensitivity towards benthic type selection. The lowest σ values indicating optimal benthic triplet for the dataset were found for combination of Eelgrass, Mud and Sand (EMS) for $[chl]$, $a_{dg}(443)$ and H .

3.5.3 SABER performance in optically shallow waters of the Manicouagan Peninsula

The SABER inversion model configured with the sensitivity analysis optimized spectral slope (0.01403, 0.63) and three benthic types (Sand, Mud, Eelgrass), was employed to invert shallow water datasets of R_{rs} measured using C-OPS, PSR and HOCR (each with their native acquisition spectral channel count) over the Manicouagan Peninsula. The *in situ* datasets used for validation included complete/partial observations in terms of OSCs, H , and R_B . We first illustrated the efficacy of the model in retrieving spectral R_B (as measured in-water using

C-OPS profiles and underwater SVC) from R_{rs} measured in-water using C-OPS or above-water using the PSR (the EXP-WISE dataset). The rest of the shallow water R_{rs} (WISE-Man data) was used to illustrate retrieval performance for $[chl]$, $a_{dg}(443)$ and H followed by an assessment of their uncertainties.

3.5.3.1 Retrieval of R_B from the EXP-WISE

The retrieved $R_B(\lambda)$ for ten R_{rs} obtained from C-OPS vertical profiles along a 40-meter transect showed good spectral agreement with the SVC-derived values, with a spectral correlation of $\rho = 0.92$. The BCI_{95} for the retrieved R_B showed a high dispersion with a mean CV of 106% across the wavelengths (Fig. 26). It indicated a low inter-class variability, i.e., the retrieval uncertainty was always high irrespective of the benthic substrate present. Nevertheless, the similarity in the spectral shape of the retrieved R_B was best for bright benthic substrates such as sand ($\rho = 0.985$, E :3%, M :16%, S :81% for profile 8). In contrast, it was worse for darker benthic types ($\rho = 0.83$), especially for absorptive vegetative substrates like the complete (Profile 3, $\rho = 0.59$, E :82%, M :10%, S :8%) and partial eelgrass patch (Profile 7, $\rho = 0.74$, E :64%, M :18%, S :18%) (Fig. 26). Subsequently, the measured R_B value for eelgrass was observed as extremely low ($< 1\%$) in blue and green wavelengths, probably making the retrieval more ambiguous. Both C-OPS and SVC were in agreement regarding this particular profile.

The spectral δ_{R_B} for profile 3 was almost 20 times higher than the mean of the non-vegetative (excluding profile 3 and 7) profiles (1530.09% vs 70.41%) in blue λ (Fig. 27 a,b). In green, it was 680.33% against 52.4% as the mean over the non-vegetative profiles. It is noteworthy, that the δ_{R_B} was also lowest in the green wavelength region (530-590 nm) for profile 3. In the red spectral range, the δ_{R_B} for profile 3 was 1605.71%, whereas for the rest of the profiles, the relative difference was obtained at 38.43%. Overall, the inversion estimated benthic reflectances had a trend of overestimation across the wavelengths, while the highest δ_{R_B} occurred in blue, followed by red and green spectral regions, respectively (Fig. 26, 27 a,b).

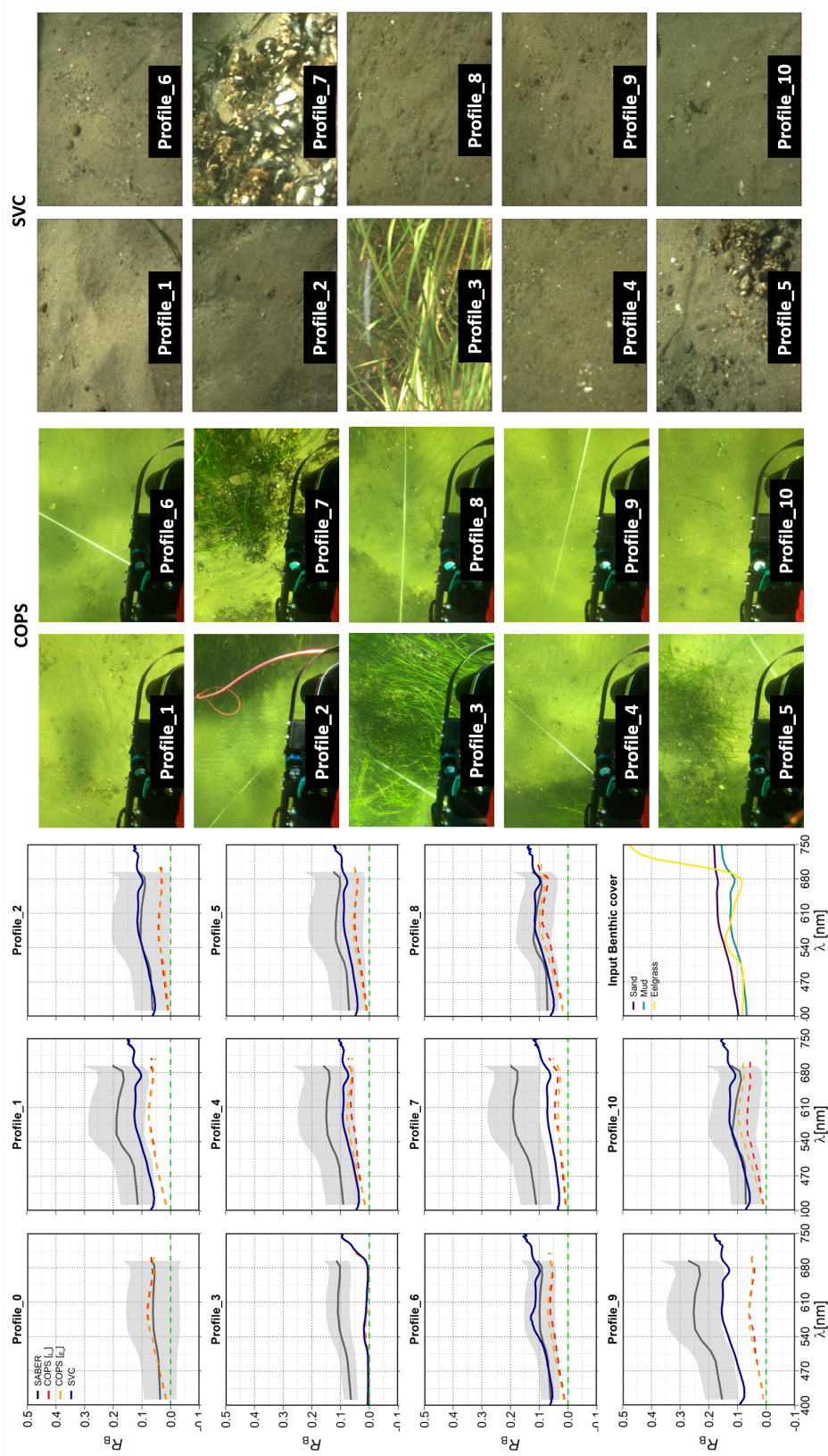


FIGURE 26 – Spectral comparison of SABER retrieved R_B (black solid line) with the *in situ* C-OPS (irradiance E_u in yellow dashed line, radiance L_u in red dashed line) and SVC (blue solid line) measured R_B for a total of 11 C-OPS profiles in EXP-WISE. The grey-shaded region shows the spectral BC_{I95} for each retrieval. RGB images acquired from SVC and C-OPS for each profile are shown horizontally to the spectral linear comparison plots.

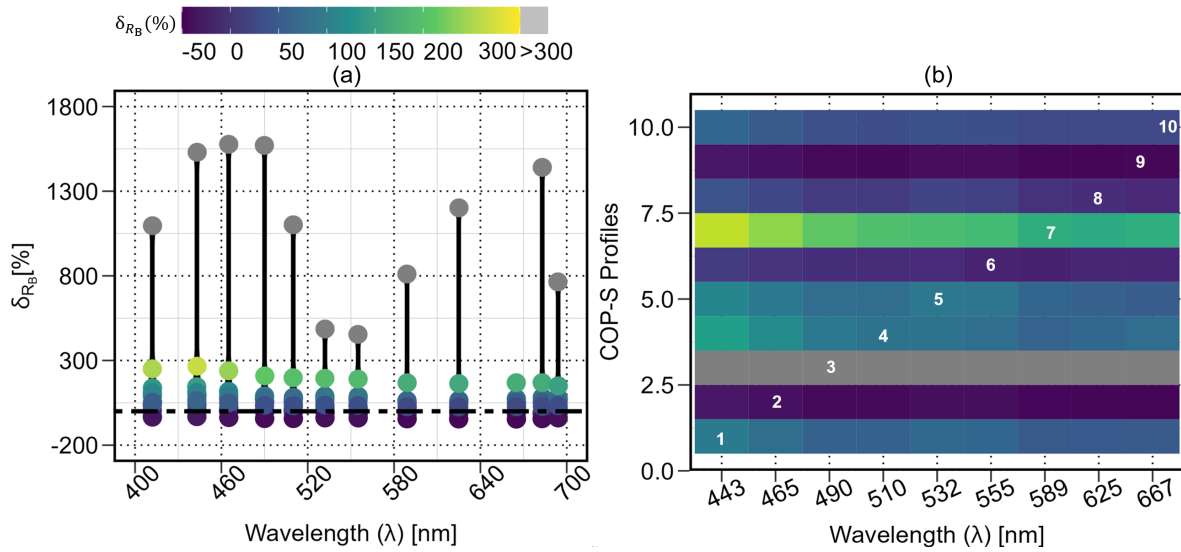


FIGURE 27 – (a) Profile-specific % residual difference (δ_{R_B} , Y-axis) for varying C-OPS wavelengths (X-axis). (b) Profile-wise (Y-axis) distribution of the same δ_{R_B} against the C-OPS wavelengths (X-axis). The diagonal white numbers indicate the profile number for each horizontal observation.

SABER was evaluated against six $R_{rs}(0^+)$ determined on the bow of the *Kildir* using the PSR-1100f and two vertical profiles of the C-OPS made during the experiment (Fig. 28a). The observations were made between 13 :35 and 15 :46 UTC during the ebb tide, which had peaked at 13 :45 UTC. The tide, as predicted from station 02840 from DFO, range varied between 2.24 meters at the beginning of the experiment and 1.95 meters at the end. The retrieved R_B spectrums showed high degree of consistency ; the R_B were spectrally very similar ($\rho = 0.99$) to each other ; the magnitude was also always $< 2\%$ residual difference from each other across all the wavelengths for both PSR and C-OPS (Fig. 28b). It indicated an almost constant presence of the same benthic classes for all the observations.

Conversely, for the OSCs and H , we observed variable estimates through a ~ 2 hrs steady acquisition. A big gradient between 14 :25 UTC and 15 :27 UTC was evident for all the retrieved parameters, whereas the gradient was relatively small between observations made within smaller intervals (Fig. 27c). $[chl]$ had highest mean retrieval uncertainty of 34%, followed by H (21%), $a_{dg}(443)$ (4.7%) and $b_{bp}(555)$ with 3.9% uncertainty, respectively (Fig.

28c). The coefficient of variation (CV) in estimated magnitude was also highest for $[chl]$, i.e., 32%. It was succeeded by H (19%), $b_{bp}(555)$ (9.8%) and $a_{dg}(443)$ (6.9%). Overall, noticeable inter-observation variability was observed for OSCs and H in the dynamic coastal water mass, whereas benthic reflectance remained nearly constant across these eight inverted observations.

3.5.3.2 WISE-Man

TABLE 8 – Statistical assessment and uncertainty quantification of the SABER based inversion retrieved variables from WISE-Man dataset. The CV of R_B is obtained as mean of $\sum_{i=1}^3 CV(f_{a_i} \cdot R_{B_i})$

Component	$X \in \phi_{\text{var}}$	CV (%)	β (%)	m	R^2	RMSLD
OSC	$[chl]$	46.02	12.80	0.92	0.87	0.18
	$a_{dg}(443)$	11.02	6.09	0.95	0.91	0.06
	$b_{bp}(555)$	8.65	-	-	-	-
Benthic	H	19.32	10.01	1.21	0.70	0.20
	R_B	131.72	-	-	-	-

A total of 495 observations of sub-surface R_{rs} (HOCR : 469, COPS : 16, PSR : 10) were inverted using the SABER model to obtain $[chl]$, $a_{dg}(443)$, $b_{bp}(555)$, H and the aerial fractions (f_{a_1} , f_{a_2} , f_{a_3}) corresponding to the benthic reflectances of Eelgrass, Mud and Sand. Rigorous validation exercise for $b_{bp}(555)$ and aerial fractions was not performed due to scarcity in field recorded observations. However, their retrieval uncertainty and relative contribution to the overall budget were assessed.

$[chl]$ had the highest retrieval uncertainty (CV = $\sim 46\%$) and bias ($\beta = \sim 13\%$) among OSCs variables, while the span of the BCI_{95} increased proportionately with increasing $[chl]$ magnitude (Fig. 29a). In sensor-specific terms, PSR derived R_{rs} obtained more accurate estimates, which can potentially be justified due to the greater spectral resolution of PSR (See

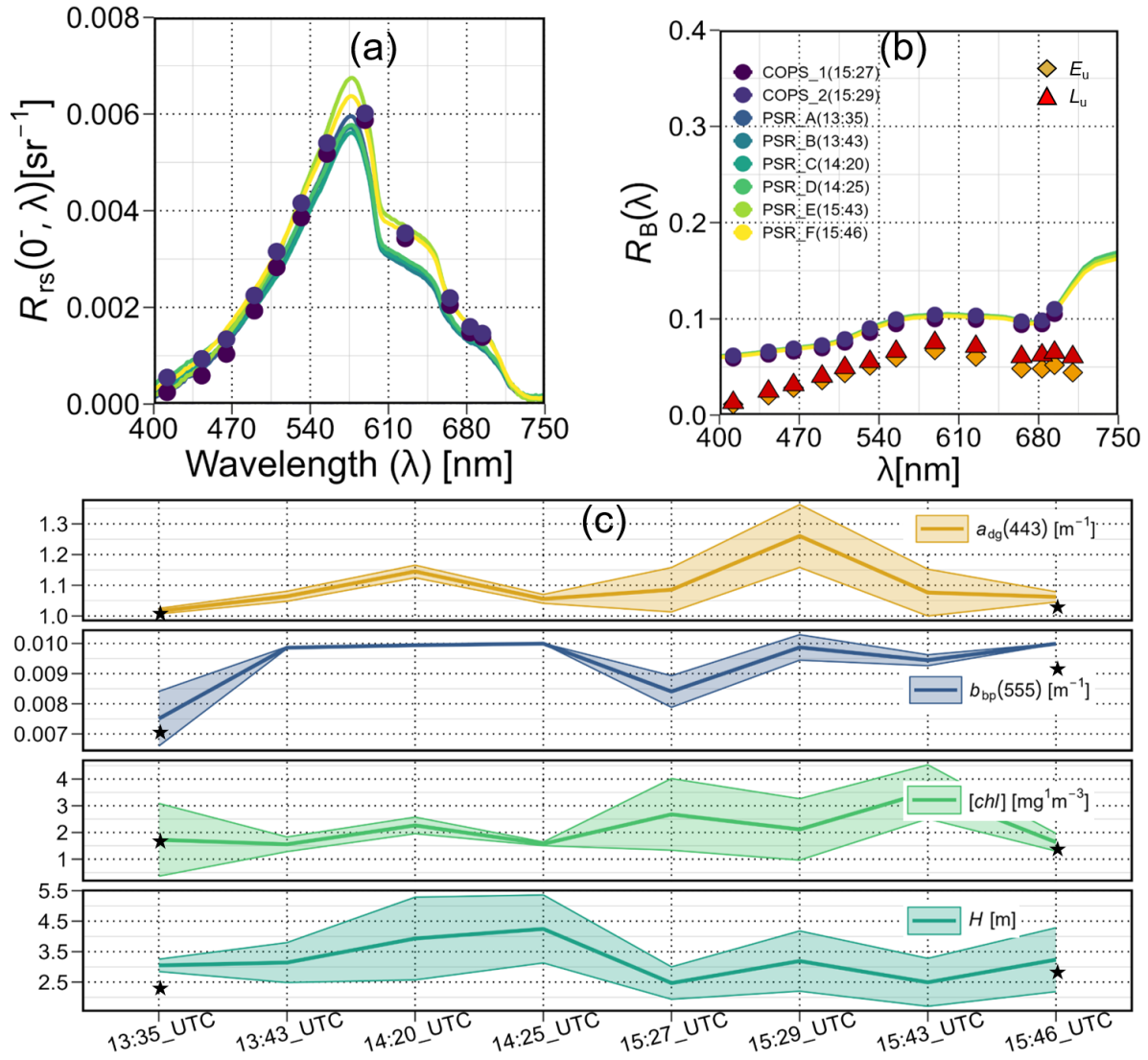


FIGURE 28 – (a) Spectral plots of sub-surface Remote-sensing reflectance; $R_{rs}(0^+, \lambda)$ derived from radiometric measurements from PSR and C-OPS. (b) Comparison of the C-OPS obtained R_B with the SABER retrieved spectral R_B obtained from each R_{rs} shown in (a) as input. The colour variation denotes C-OPS/PSR duplicates, followed by the measurement UTC-time in braces. (c) Temporal variation in retrieved $[chl]$, $a_{dg}(443)$, $b_{bp}(555)$ and H over a span of ~130 mins. The BCI_{95} for each retrieval is shown using a shaded band around the estimates. The star-shaped symbols for each subplot show the *in situ* values for the start and end of the experiment.

Fig. 43 in Annexe-III). Nevertheless, the overall retrieval was linear (m) and precise (R^2) compared to the *in situ* observations (Table 8). $a_{dg}(443)$ estimates were more precise, the

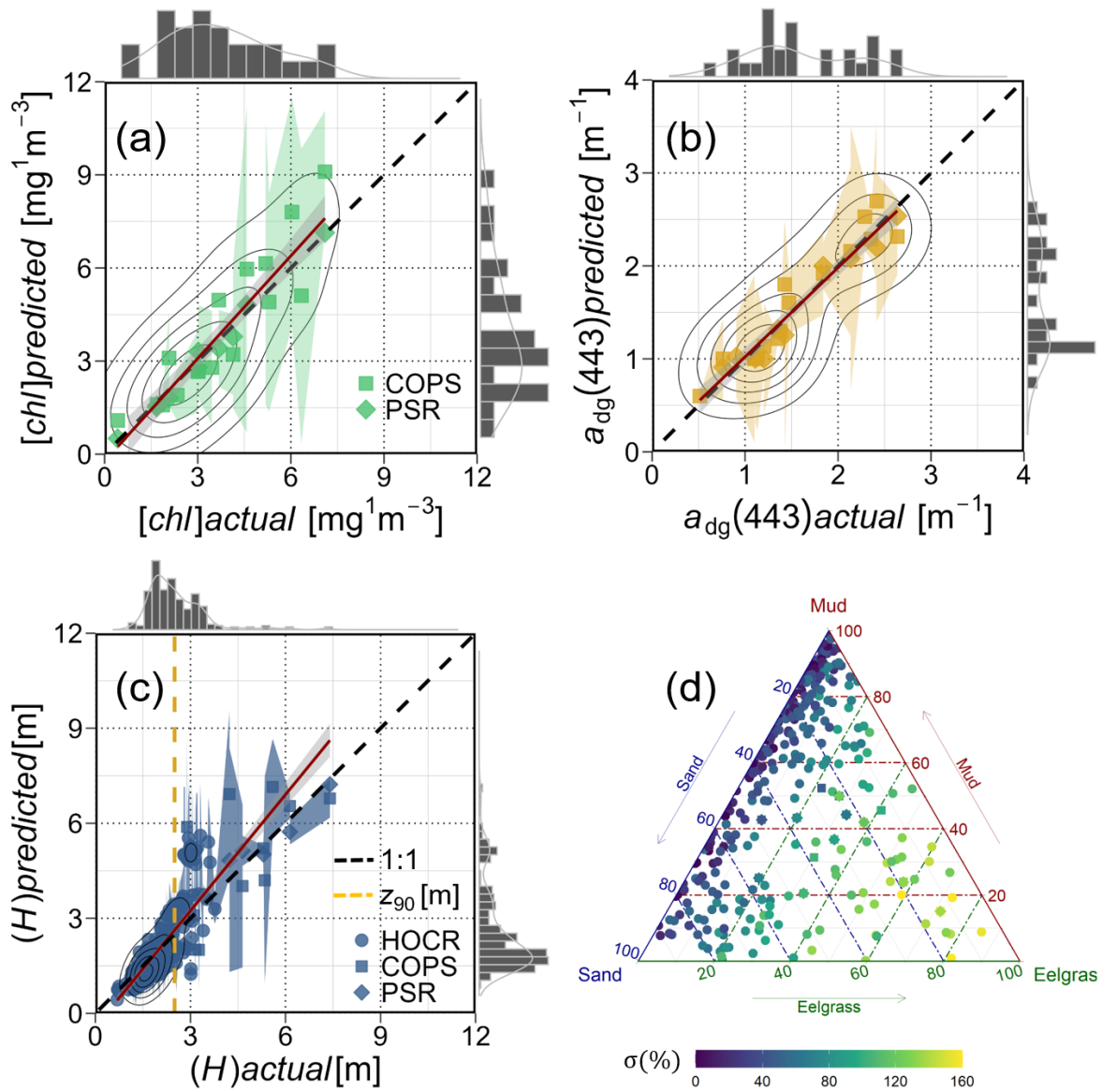


FIGURE 29 – (a) Scatter plot showing the validation between SABER retrieved $[chl]$ and *in situ* values, where available. The black dashed line is the 1 : 1 line, whereas the red line shows the obtained linear fit. The density overlaid histograms (densigram onwards) show the marginal distribution for actual and inversion retrieved values. The shaded region shows the BCI_{95} . (b) and (c) are the same as (a) but for $a_{dg}(443)$ and H retrievals. (d) ternary plot showing the benthic class abundance for the retrieved aerial fractions (0-100%). The colour for the points shows the associated coefficient of variation (CV).

associated CV was relatively lower than $[chl]$ with a better slope ($m = 0.95$). The RMSLD was one-third of the $[chl]$ estimate, indicating a more robust estimate for extreme magnitudes (Table 8).

The H estimates had 19.32% CV indicating a moderate uncertainty in the estimates. The BCI_{95} span had an increasing trend with increasing water depth made observations. Similarly, an overestimation trend is also observed for increasing magnitude of H , more prominent for observations with a physical depth well above the penetration depth ($H > z_{90}$) at 555 nm (Fig. 29c). HO-CR derived R_{rs} obtained more accurate estimates than PSR and C-OPS, nevertheless, majority of HO-CR observations had $H \leq z_{90}$, while C-OPS and PSR observations specific to WISE-Man dataset here were made at relatively deeper waters.

Among all the OSCs and benthic variables, R_B obtained the highest CV, indicating the presence of major uncertainty in the retrieval. In our analysis, we found that the variability in benthic composition differed substantially based on the relative proportions of Sand, Mud, and Eelgrass (Fig. 29d). The retrievals predominantly associated with sand-rich compositions had a lower CV ($< 40\%$), suggesting that sand-dominated scattering regions with higher reflectance may exhibit more stable or predictable conditions for inversion. In contrast, higher CV ($> 90\%$) values were observed for higher eelgrass fraction in R_B , indicating increased uncertainty in retrieved R_B for absorptive vegetative substrate presence.

3.5.4 Uncertainty budget

The uncertainty budget, representing the relative variance contributions from SABER model parameters, specifically s_{dg} (spectral slope of coloured detrital matter), γ (backscatter slope), and the three benthic reflectances $R_{B1..3}$ to the total inversion-derived variance, $Var(\cdot)$, was quantified using global Sobol analysis. We assumed the σ_{model}^2 contribution to be negligible ($< 1\%$) due to the SABER inversion method's avoidance of numerical approximations, such as gradient-based calculations. This approximation aligned with the uncertainty budget

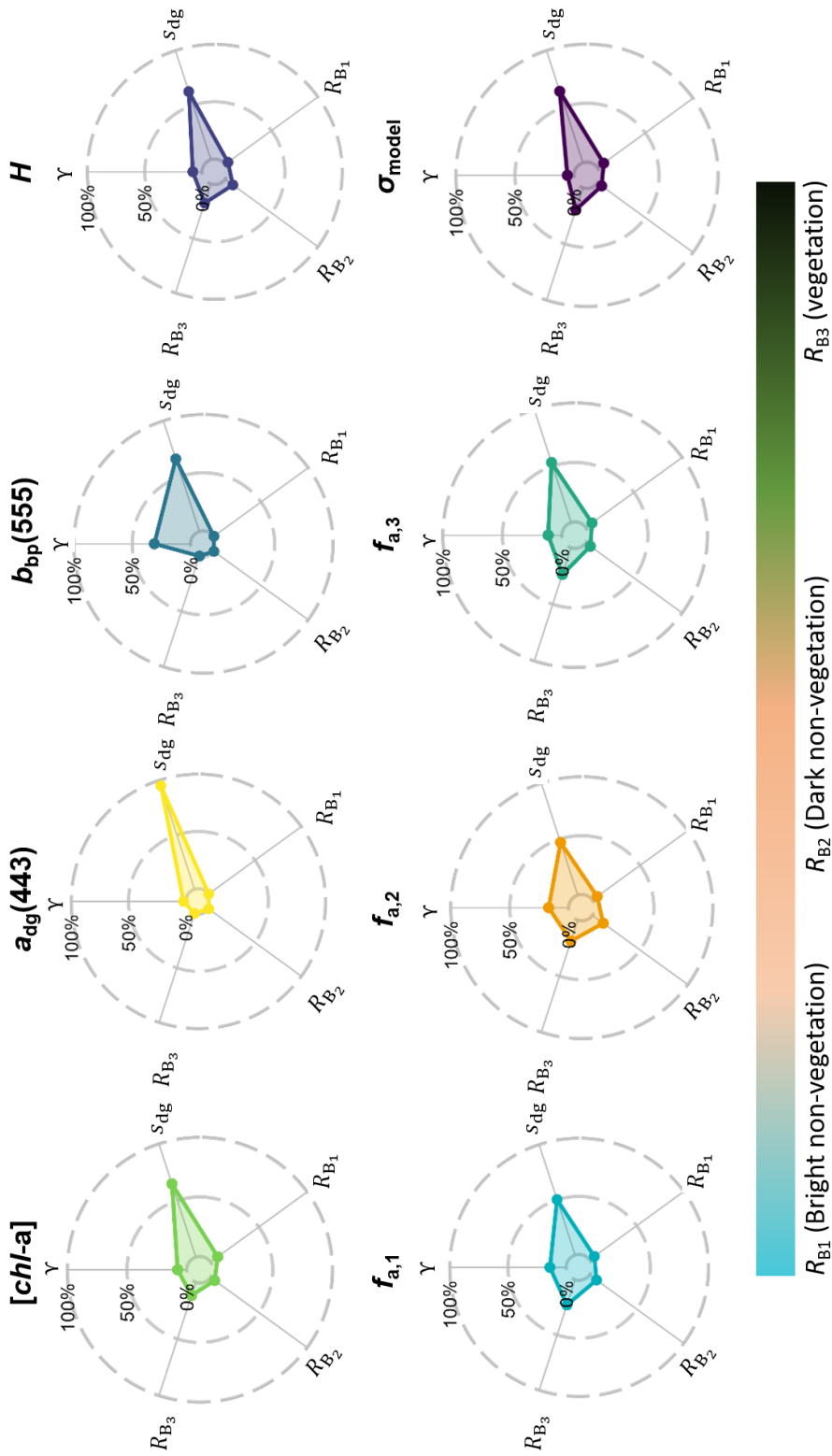


FIGURE 30 – Uncertainty budget for each SABER-retrieved OSCs and benthic variable across the entire R_{rs} dataset. Each radar plot illustrates the relative contributions to the total SABER-derived $Var()$ from the σ_{inv}^2 components : s_{dg} (spectral slope of coloured detrital matter), γ (backscatter slope), and benthic reflectances $R_{B_{1,3}}$. The three benthic reflectances are sorted in ascending order by brightness and vegetation type, with Sand (bright, non-vegetative), Mud (darker, non-vegetative), and Eelgrass (dark, vegetative).

for most of the retrieved variables, except $[chl]$ ($\sim 96\%$ of total variance).

The uncertainty budget showed the highest fraction of SABER-obtained variance was explained by the s_{dg} parameter, with a mean of 68.65% of the total variance considering all the retrieved OSCs and benthic variables (Fig. 30). It indicated the model's high sensitivity in perturbations of the s_{dg} , i.e., the log-likelihood for the variable we retrieved, e.g. $a_{dg}(443)$, was a strictly monotonic function of the continuous s_{dg} domain. In summary, the model will be highly accurate with an adequately approximated value of s_{dg} , conversely, the performance will worsen drastically for relatively small changes in the provided s_{dg} value. The highest variance by s_{dg} was propagated for $a_{dg}(443)$ (98.5%), whereas the lowest was obtained for the aerial fraction of Mud (48.9%). The other spectral slope γ had the most significant contribution for $b_{bp}(555)$ retrieval ($\sim 28\%$), followed by the aerial fraction (f_{a1}) for sand; a bright scattering benthic type. This could be linked to γ determining the spectral shape of backscatter, which can introduce uncertainties in presence of a strongly scattering benthic substrate, that contributes to the upwelling radiance giving a false sense of high particulate backscatter in the water column.

Among the pre-determined three benthic reflectances ($R_{B1..3}$), the dark vegetative substrate; eelgrass propagated highest uncertainty in SABER estimates, noticeably for H ($\sim 19\%$) and f_{a3} ($\sim 24\%$) (Fig. 30). Unlike sand, a dark benthic substrate like eelgrass absorbs radiation in the blue and green wavelengths, which potentially would yield an underestimation of the upwelling diffused attenuation coefficient mimicking optically deep waters. Overall, for an unconstrained shallow water inversion in the absorptive waters of MP, s_{dg} and R_{B3} contributed $\sim 69\%$ and $\sim 17\%$ of the total retrieval uncertainty, respectively for all the OSCs and benthic variables retrieved simultaneously.

3.6 Discussion

3.6.1 Evaluation of R_{rs} and its impact on inversion

The R_{rs} dataset was acquired using a combination of HOCR, PSR, and C-OPS sensors, each with distinct measurement principles. The shallow water R_{rs} spectra showed a peak magnitude in the 550-570 nm range ($\leq 6\%$ signal strength), with notable SICF peaks ($\leq 2.5\%$ signal strength) between 670-710 nm. This spectral profile was consistent with previous datasets from the ESL region (Araújo and Bélanger, 2022; Mabit et al., 2022; Mukherjee et al., 2023). Observations in waters shallower than 3 m had QWIP scores of ≤ -0.2 , indicating optically shallow conditions. This finding was justified compared with the penetration depth (z_{90}) being ~ 2.6 m in MP (Mukherjee et al., 2023), however, in cases where the benthic substrate was vegetative, the strong absorption of light in these waters diminished the expected response near the red-edge, resulting in lower QWIP scores, which was consistent with findings from Dierssen et al. (2022, 2003).

Our semi-analytical (SA) inelastic scattering model for f_{DOM} and SICF showed contributions of 13% and 22%, respectively, relative to the observed *in situ* sub-surface R_{rs} over 470-610 nm and 670-710 nm. The peak contributions were observed at 525 nm and 685 nm (18% and 39%), which align closely with the forward RT model estimates of fluorescence in these waters (21% and 31%) as reported in Chapter-1 and Mukherjee et al. (2023). Notably, we observed a shift in the effective emission range of f_{DOM} from 510-590 nm in Mukherjee et al. (2023) to 470-610 nm, potentially due to the use of a constant spectral shape for the f_{DOM} quantum efficiency across 310-600 nm (Hawes et al., 1992). This approximation may not fully account for conditions in the MP region, where high CDOM absorption in blue-green wavelengths could shift emissions toward the red (Mukherjee et al., 2023). Despite inherent uncertainties in parameterization, the residual % error between R_{el}^{el} and reconstructed R_{rs} from SABER obtained estimated were 16% and 26% more accurate in blue-green and red wavelengths, respectively, compared to the residual % error obtained with $R_{el+inel}^{el}$ as inversion

input. Subsequently, the linear agreement of the OSCs improved when SABER was input with inelastic scattering corrected R_{rs} (Fig. 41 in Annexe-III).

Nevertheless, our inelastic scattering model requires concurrent ancillary observations of $[chl]$ and $a_{dg}(443)$, which might not be always available to user. Also, SABER is built to retrieve these variables from R_{rs} , which itself needs to be corrected for inelastic scattering in absorptive waters, leading to a “casualty paradox”. Hence, in absence of $[chl]$ and $a_{dg}(443)$ observations, band ratio algorithms could be used as a trivial solution over deep water R_{rs} in close proximity to obtain rough estimates of the ancillary variables. As a more robust solution in course of future development, the SABER forward model for both elastic and inelastic component can be summed together and used as the forward model in inversion formulation. It would then yield optimal posterior distributions for OSCs and benthic variables, while retrieving the optimal R_{inel}^{el} simultaneously. However, this approach should be tested on Hyperspectral R_{rs} , due to the increasing number of unknowns (e.g. SICF quantum yield) and model complexity.

3.6.2 Uncertainty propagation in OSCs and benthic retrievals

Controlled perturbations of the inversion model components such as detrital matter’s spectral slope, backscatter slope, and benthic substrate types explain their respective uncertainty (σ) propagation for OSCs and benthic retrievals. The spectral slopes are reported to influence the shape and magnitude of the IOPs in water and also the benthic parameters in a shallow environment (McKinna et al., 2015; Salama, 2012). The benthic classes used for the inversion were sorted by the net brightness or signal-to-noise ratio in the seafloor, as several researches showed inversion uncertainty increases proportionally for a dark benthic type such as vegetation (Hedley et al., 2009b; Ackleson et al., 2018; Kutser et al., 2020).

$[chl]$ had the highest span of σ with multiple minima in the continuous parametric space, while $a_{dg}(443)$ had the smoothest surface with least range of σ (Fig. 24 a,b). This observation was in line with the $[chl]$ and $a_{dg}(443)$ posterior distribution having the highest and

lowest uncertainty (widest and narrowest span of BCI_{95}) obtained over the global datasets illustrated in Section 2.5.3 and 2.5.4.1. A non-normality was observed for the distribution of absolute residual difference attributed to inversion iterations over combinations of s_{dg} and γ (Fig. 24d) indicating the absence of latent factor(s) explaining the output variance for $[chl]$ retrieval. We used the model constant spectral shape for Phytoplankton absorption (See Section ??) instead of tuning with the mass normalized Phytoplankton absorption at the local scale. Similarly, Werther et al. (2022a) illustrated the retrieval uncertainty for $[chl]$ had major contributions from the phytoplankton structure and absorption for inland and productive waters. Pahlevan et al. (2022) also showed high validation uncertainties from multispectral R_{rs} for $[chl]$ estimates in coastal and inland waters. Interestingly, our uncertainty budget showed a 4% missing variance (Fig. 30), that cannot be explained by the model parameters, probably for assuming the Phytoplankton structure and abundance as constant. Nevertheless, SABER obtained highly accurate estimates of $[chl]$ for the current dataset, even for ones with high retrieval uncertainty (Table 8, Fig. 29a).

The $a_{dg}(443)$ retrievals were most accurate among the retrieved parameters (Table 8). Similar results were found in Garcia et al. (2014b), where retrieved detrital absorption had the lowest uncertainty among all. In the SABER inversion, s_{dg} , determining the spectral shape and magnitude for the detrital absorption in our CDOM-rich waters, had almost the entire contribution ($\sim 99\%$) relative to the total retrieval uncertainty. It should be noted that in Section 2.6.2, we discussed the need for a sensitivity test for spectral slopes to accurately estimate $a_{dg}(443)$ across coastal waters, while the current chapter addressed that need adequately.

SABER estimated water depth (H) values had higher uncertainty for observations made at greater depths. A similar increasing retrieval uncertainty for higher water depths was observed in the clearer waters at Heron Reef (Hedley et al., 2009b). SABER retrieved H were highly accurate within $\leq 3\text{m}$; a gradual overestimation was observed onward. Mukherjee et al. (2023) indicated the presence of freshwater lensing on the upper layers of water in MP from high riverine CDOM discharge, which restricted the light penetration after a few meters;

exactly at $z_{90} = 2.54\text{m}$ for 555 nm wavelength. Hence, SABER could not uniquely resolve the RT for $H > z_{90}$ (ambiguous case), while the uncertainty increased as further H strayed away from the $z_{90} = 2.54$ threshold. Zheng and DiGiacomo (2017) reported the majority of the inversion approaches for H estimation work well in clear waters, as seen in clear lagoons or reef areas (Hedley et al., 2009b; Klonowski, 2007; Ackleson, 2010; Garcia et al., 2015), however, the applicability of these approaches are limited in dark absorptive waters with low penetration depth. Despite this, SABER retrieved decently accurate estimates of H at shallow parts of MP, especially for observations with $H < z_{90}$ (Table 8, Fig. 29c).

Apart from s_{dg} being the primary source of uncertainty in H estimates, the benthic types contributed $\sim 30\%$ of the total uncertainty (Fig. 30). We observed an increasing trend of uncertainty being propagated with decreasing signal strength; i.e., darker benthic substrate ($R_{B_1} = 3\%$, $R_{B_2} = 8\%$, $R_{B_3} = 19\%$). We observed a similar nature in the propagation of sensitivity uncertainty for H in Section 3.5.2.2, when the R_B were varied from a bright scattering substrate to a darker absorptive cover such as eelgrass (Fig. 25). The low signal strength of eelgrass in the blue and green spectral region and its relatively small contribution in water-leaving R_{rs} resulted in a wider posterior distribution; i.e., higher uncertainty (See Section 2.5.3 for details on the shape of posterior distribution). Similar outcomes were observed in Ackleson et al. (2018), where the OSC estimates had a higher uncertainty, when coral or algae was present as benthic cover.

The retrieved spectral benthic reflectance $\left(R_B(\lambda) = \sum_{i=1}^3 f_{a_i} \cdot R_{B_i}(\lambda)\right)$ had the highest retrieval uncertainty among all the retrieved variables. The high absorption in MP waters diminishes the upwelling benthic signal making the relative contribution of the $R_B(\lambda)$ much smaller in the net R_{rs} , eventually increasing the uncertainty. The retrievals, when compared with the SVC-acquired benthic reflectance, had a greater spectral correlation (0.99) and lower residual % difference (24.13%) for bright substrate type, e.g., sand. Conversely, R_B estimates over vegetative substrate had poor spectral correlation (0.59) and very high residual % difference (989.33%). Similar results were shown in Garcia et al. (2014b, 2018); Hedley et al.

(2009a, 2012), i.e., the high uncertainty for benthic reflectance estimates increased substantially for darker substrate ($\pm 18.56\%$ to $\pm 1882.15\%$ in Garcia et al. (2014a)). Similarly, the propagated uncertainty from the eelgrass class was more than 2 times higher than Sand and Mud in SABER. Ackleson et al. (2018) stated the spectrally averaged signal from benthic vegetation such as Seagrass, is similar to the shape of the $R_{rs,\infty}$ in coastal waters. Therefore, at a shallow depth at MP, the net water leaving R_{rs} over eelgrass bottom was almost indistinguishable from $R_{rs,\infty}$, that resulted in obtaining poor estimate of the benthic reflectance.

Despite these challenges, SABER successfully provided a good approximation of the abundance of the benthic classes as well the spectral shape of the net R_B in the challenging dark coastal waters, probably for the first time in the EGSL region, at least to our knowledge. Werdell and Roesler (2010) assessed the spectral R_B in an absorptive environment ($z_{90} \approx 3\text{m}$), but could only provide valid estimates in the green wavelengths. Moreover, Werdell and Roesler (2010)'s approach was seeded with ancillary IOPS and H , whereas SABER retrieved all the OSCs and benthic variables simultaneously from the only input of R_{rs} . However, caution should be taken before the inversion in extreme waters with very high absorption or scattering, the model parameters, especially s_{dg} for absorptive waters, must be tuned. The Fluorescence equivalent R_{rs} must also be assessed and subtracted (if significant) prior to the inversion in CDOM-rich waters.

3.7 Conclusion

The SABER Bayesian inversion framework offered a reliable method for retrieving OSCs and benthic variables in challenging environments, such as the CDOM-rich shallow coastal waters of the Manicouagan Peninsula in the Eastern St. Lawrence region. These waters, characterized by high absorption, significant inelastic scattering from Sun Induced Fluorescence, and very shallow light penetration depth, pose unique difficulties for optical remote sensing. Despite these challenges, SABER demonstrated strong performance in estimating

water depth, spectral benthic reflectance, and concurrent OSCs in water column using only R_{rs} data, without requiring additional depth or IOP inputs. The corrections for inelastic scattering equivalent R_{rs} prior to inversion showed an improvement in the SABER estimates; the residual % error between the *in situ* and simulated R_{rs} with SABER estimates obtained from inelastic scattering corrected R_{rs} was 16% and 26% lower in blue-green and red channels, compared to the same obtained from uncorrected R_{rs} . However, a notable limitation in the inelastic scattering correction approach is the “causality paradox”, where ancillary variables like $[chl]$ and $a_{dg}(443)$ are required for inelastic scattering corrections but are themselves SABER outputs. Addressing this issue could involve integrating SABER’s elastic and inelastic forward models in course of inverting observations of R_{rs} , particularly for hyperspectral data, to optimize parameter retrievals simultaneously.

The analysis highlighted SABER’s sensitivity to certain parametrizations, especially the detrital matter spectral slope (s_{dg}) and pre-determined benthic reflectance classes (R_B) against which the aerial fractions are retrieved. During inversion in the CDOM-rich absorptive coastal waters of MP, s_{dg} propagated the highest mean uncertainty, i.e., $\sim 69\%$ for all the OSCs and benthic variables combined. The presence of darker benthic substrates, such as vegetation, also contributed significantly, i.e., $\sim 17\%$ to posterior uncertainties associated with SABER retrieved variables, while brighter substrates propagated relatively lower uncertainty. Subsequently, the SABER retrieved benthic reflectances had a greater spectral correlation with the *in situ* benthic reflectance compared to the ones retrieved over dark patches. Nevertheless, the model successfully resolved key OSCs and benthic parameters across various depths and substrates, even in highly absorptive waters.

In summary, SABER represents a significant step forward in advancing optical remote sensing for absorptive coastal environments with optically shallow regions. It provides valuable insights into benthic ecology and water quality while paving the way for more generalized approaches to RT based inversion in similarly complex aquatic systems.

GENERAL CONCLUSION

The major findings of this thesis has been achieved through using extensive *in situ* sets of AOPs, IOPs and BGC data, acquired on both global (for inversion algorithm development) and local (for application and validation of the inversion algorithm(s) in assessing the optical characteristics in CDOM-rich coastal waters) scales. However, the developed algorithms are solely based on the SA assumptions of radiative transfer, which can readily be aligned with space/air-borne RS optical data. Simultaneously, this study focused mainly on studying the optical characteristics of CDOM-rich absorptive coastal waters in the MP located in the ESL region, but as these results are drawn from physics-based simulations or SA inversions, the obtained results or inferences can be sought for other CDOM-rich coastal waters.

Broadly, this thesis has addressed the challenges associated with understanding and modeling the optical properties such as absorption, scattering etc. in shallow, absorptive coastal waters dominated by colored dissolved organic matter (CDOM), specifically in a temperate climate in the Northern hemisphere. By 1. integrating radiative transfer simulations for inelastic scattering, specifically for Sun Induced Fluorescence, 2. creating a robust inverse modeling approach to obtain water quality and benthic information in CDOM-rich waters and 3. assessing the major sources of uncertainty in the inversion retrieved estimates, this work has significantly contributed to improving the accuracy and interpretability of OCRS techniques in these optically complex environments.

In **Chapter-I**, the role of inelastic scattering processes, specifically Sun-Induced CDOM Fluorescence (f_{DOM}) and chlorophyll-a fluorescence (SICF) in shaping the remote-sensing reflectance (R_{rs}) spectra was thoroughly investigated through an extensive optical closure exercise. It was found from this exercise that f_{DOM} and SICF contribute up to substantially to the spectral signal in green and red regions. However, obtaining a good measure of IOPs and AOPs, that serves as the baseline of optical closure, was significantly challenging in the dark waters of Manicougnan Peninsula, even with a multi-frame approach as stated in Sec-

tion 1.4.2.1. The ASPH instrument measured absorption values had a spectrally dependent bias, caused from fluorescence inside the integrating sphere of the instrument in presence of monochromatic light. This limitation is not applied to the flow-tube based meters, i.e., AC-S. Unlike the HS6 VSF meter, the backscattering measured by the BB9 in the waters of MP were contaminated with spectrally independent noise and the values showed no correlation with bio-optical stressors such as SPM. The discretization between noise and measurand VSF for the BB9 sensor might not be adequately tuned for particles with low backscattering efficiency such as the ones with organic assemblage in the MP region (Araújo and Bélanger, 2022; Mabit et al., 2022) (Also see Gallegos et al. (2008)). The high absorption of CDOM in the blue wavelengths limited the C-OPS measured radiometric signals in the blue wavelengths to be extremely low, in some cases near to the sensor channel noise threshold. It eventually made the assessment of optical closure in the blue, specifically at < 490 nm, very critical. Hence, great care and preparation should be taken in course of collection and processing of *in situ* IOPs and AOPs.

A more in depth study of the wavelength redistribution function (WRF) of the Sun-induced CDOM fluorescence (f_{DOM}) would have been beneficial to understand the spectral contribution of f_{DOM} in the water-leaving R_{rs} . In this context, measurements of fluorescence excitation-emission matrix (EEM) or estimation of the apparent quantum yield (Zhu et al., 2020, 2024) can serve the purpose in fine tuning the WRF. Similarly, the backscatter fraction ($\tilde{B}$) in these waters is sensitive to the particulate backscattering efficiency, hence an accurate spectral measurement of $\tilde{B}$ would be beneficial.

Despite these challenges, this work served as the first step in understanding the relationship between IOPs and AOPs in MP or similar northern temperate coastal waters. The answers to the Research Questions associated to Chapter-I is stated below.

1. *What are the specific recommendations in measuring IOPs and radiometric measurements in CDOM-rich absorptive waters?*

In a CDOM-rich coastal environment, the *in situ* absorption should be measured with

flow-tube meters to avoid internal fluorescence and the laboratory spectrophotometry should ideally be performed in a PSICAM. The VSF meter should be well calibrated to account for very low backscattering values originated from organic substances, whereas the radiometers should be thresholded with the sensor noise value, i.e., any value below the threshold should be discarded and flagged.

2. *What is the relative contribution (%) of inelastic scattering in the water-leaving R_{rs} in CDOM-rich absorptive waters ?*

The Sun-Induced Fluorescence from CDOM obtained $\sim 18\%$ of the R_{rs} in the green spectral range, whereas the same from Chlorophyll resulted in $\sim 20\%$ in the red channels. The Raman scattering in coastal waters is very negligible, hence discarded.

In **Chapter-II**, the Semi Analytical Bayesian Error Retrieval (SABER) inversion model, introduced in this work, has been proposed as a robust OCS inversion framework for retrieving optically significant constituents (OSCs) and benthic variables (water depth and benthic composition) in optically complex waters for both optically deep and shallow cases. SABER, a Bayesian MCMC optimization based model performed at par or mostly better compared to conventional gradient-based optimization driven inversion approaches, such as QAA and HOPE for OSCs and benthic variables, respectively. The major advantage of SABER over traditional methods is that SABER explicitly provided uncertainty bounds (Bayesian Credible Intervals) for all retrieved variables, enabling more reliable and interpretable results.

One of the key components of SABER was the integration of global datasets representing eight distinct optical water types (OWTs). These datasets provided *a-priori* distributions of OSCs and benthic variable magnitudes, along with their cross-interactions (i.e., covariances). However, a bi-modality was observed for $a_{dg}(443)$ prior distributions, potentially caused from marine and coastal sources of the organic matter in the global dataset (See Table 3). The current version of SABER did not account for mixture of distributions for modeling

the *a-priori*, however, a sensitivity analysis on the mixture of several positive real distributions might improve the inversion estimates more. The retrieval performance for OSCs were relatively poor in extreme conditions, e.g., $[chl] < 0.5\text{mg m}^{-3}$ or $[chl] > 100\text{mg m}^{-3}$, however, a notable scarcity was also present in OSCs beyond the aforementioned range, that provided limited information on the shape of the *a-priori* distribution. Compilation of further *in situ* datasets for inland waters, e.g. GLORIA (See Lehmann et al. (2023)) with eutrophic coastal conditions or offshore waters, (See Loisel et al. (2023) curated dataset) with case-I characteristics would be beneficial in fitting the *a-priori* distribution at extreme observations.

The spectral slopes (s_{dg} and γ) embedded in the SABER SA formulation acts as model parameter, i.e., it determines the spectral shape of a_{dg} and b_{bp} . In optically deep waters, these slopes are derived from the R_{rs} (See Section ??), but for optically shallow case, these values are fixed. This assumption would propagate additional uncertainty to the retrieved variables, hence, a sensitivity test for the slope values conducted prior to the inversion for the given dataset would incorporate much lower uncertainty (See Chapter-III). Another approach in practice is to retrieve the spectral slopes along with the OSCs and/or benthic variables (Salama, 2012; Erickson et al., 2023; O'Shea et al., 2023), however, for a shallow water inversion, SABER retrieves 16 variables [estimates and uncertainty for each OSCs ($n = 3$), benthic variables ($n = 4$, population standard deviation ($n = 1$)]], adding the slopes would increase the variable vector size even more, resulting in a slower run-time.

In course of OCRS based inversion, the proposed probabilistic approach serves as an important step in quantifying uncertainties of OCRS derived variables, which had been one of the top priorities among OCRS product end-users (Mélin, 2019). The Research Questions associated with this chapter are answered below.

1. *Can SABER, a Bayesian probabilistic approach, using MCMC sampling, improve the retrieval accuracy of OSCs and benthic variables in optically shallow water compared to conventional inversion methods?*

SABER obtained OSCs had $\sim 10\%$ lower prediction uncertainty than of the QAA, whe-

reas for the water depth, SABER estimated values were $\sim 10.5\%$ more accurate than HOPE. Hence, the Bayesian probabilistic approach to solve the *ill-posed* OCRS inversion obtained less ambiguous and uncertain estimates than the gradient-based conventional approach.

2. Among Φ_{var} , which retrieved variables have the highest and lowest retrieval uncertainty and why?

[*chl*] values retrieved with SABER had the highest retrieval uncertainty (BCI_{95}), probably caused from the bio-optical formulation to derive [*chl*] values from $a_{\phi}(443)$. However, [*chl*] values in coastal waters can vary over 3 orders of magnitudes (Smith et al., 2021; Werther et al., 2022a; Werther, 2022), hence, a single parameterization might not be adequate for all the cases. The lowest uncertainty was associated with particulate backscatter values, specifically $b_{\text{bp}}(555)$, potentially from a lower sensitivity of the inversion relative to the γ .

3. Can SABER be applied to different Optical Water Types (OWTs) at a global scale of observations?

Yes, SABER has been extensively tested and validated on eight different OWTs encompassing offshore case-I oceanic water to case-II eutrophic waters for joint retrieval of OSCs.

In **Chapter-III**, an in-depth uncertainty analysis highlighted the dominant sources of uncertainty in OCRS inversion retrieved variables from R_{rs} measured over shallow, absorptive waters. The spectral slope parameter of detrital matter (s_{dg}) propagated the highest uncertainty i.e., it contributed a mean of almost 70% of the net uncertainty for the retrieved variables. It is important to mention this contribution in the net inversion uncertainty budget is specific to the fixed spectral slope values obtained from the sensitivity analysis stated in Section 3.5.2.1. For a different OWT, these values might not be completely accurate, so optimizing the spectral slopes prior to the uncertainty quantification is recommended.

The benthic variables retrieval over the absorptive waters emerged as a challenging task. The freshwater lensing in the surface layers of water (See (Araújo and Bélanger, 2022)) in the region severely limited the penetration depth of incident light, $< 3\text{m}$. Hence, water depths retrieved beyond this range might not be physically accurate and need to be flagged, which is absent in the SABER inversion method. Seeding the inversion with penetration depth in the region to limit the parameter bounds or estimation of the benthic detectability similar to the approach of Brando et al. (2009) can be beneficial in improving the metadata of the inversion. The benthic reflectances retrieved over bright targets, such as sand had significantly lower uncertainty than the same obtained over dark targets, such as patches of Eelgrass. The absorptive nature of vegetation in the blue-green range coupled with highly absorptive water mass made the SnR of the water-leaving signal very low, and the relative benthic contribution extremely small, which could not be resolved by SABER accurately. Existing literature on benthic vegetation mapping has been facing similar challenges as well, even with scattering-dominated OSCs presence (See Hedley et al. (2012); Garcia et al. (2014b); Kutser et al. (2020)).

Additionally, the study revealed the inversion explicitly lacks in existing fluorescence models, particularly for SICF and f_{DOM} , which contributes substantially in R_{rs} measured in CDOM-rich waters. An SA model for SICF and f_{DOM} has been proposed in this work, but it could not be readily integrated into the inversion process due to its limitations of generating estimates of $[chl]$ and $a_{\text{dg}}(443)$ necessary in the calculation. However, the need to account for fluorescence equivalent R_{rs} is intuitive to the findings of Chapter I, i.e., the forward model and this exercise underscored the need for improved SA parametrizations of the R_{rs} to further reduce retrieval uncertainties. The corresponding Research Questions are answered below.

1. *How uncertainty is propagated into SABER estimates from free model parameters such as the spectral slopes of detrital absorption and backscattering in the water column, as well as the benthic classes used?*

Uncertainty from the free model parameters, such as spectral slopes and the benthic classes are additive in nature, however, the net uncertainty followed a *Gaussian* distri-

bution. the uncertainty inflicted from spectral slopes was highest for $[chl]$ with skewed *Gaussian* distribution and multiple minima, whereas for other OSCs and benthic parameters, such as $a_{dg}(443)$ and H the uncertainty space strictly converged to a single minima. For the benthic classes, the lowest sensitivity uncertainty was obtained over the triplet of Eelgrass, Mud and Sand, specifically for the MP region. A trend of increasing uncertainty with increasing vegetation cover was also observed.

2. *What is the effect of correcting the input R_{rs} for inelastic scattering equivalent signal on the SABER retrieved quantities ?*

The subtraction of fluorescence equivalent R_{rs} from the observed R_{rs} improved the forward reconstruction error in green and red spectral regions compared to the reconstruction error obtained from inversion retrievals from uncorrected R_{rs} .

3. *What is the uncertainty budget for all the SABER retrieved Φ_{var} and which model parameter had the highest contribution ?*

For simultaneous retrieval of all the proposed OSCs and benthic variables in SABER, the uncertainty budget obtained for absorptive coastal waters in MP is; s_{dg} : 64%, γ : 6%, R_{B_1} : 8%, R_{B_2} : 4%, R_{B_3} : 17%. Among all the model parameters, s_{dg} had the highest contribution in the net uncertainty.

Through this work, several key contributions were made :

1. **Enhanced Optical Closure** : This study represents one of the first successful attempts to incorporate inelastic scattering processes comprehensively into radiative transfer models for CDOM-rich coastal waters, achieving improved forward modeling performance.
2. **Advanced Retrieval Framework** : The SABER model set a new standard for water quality and benthic parameter retrieval, offering a flexible, uncertainty-aware alternative to conventional algorithms.
3. **Quantitative Insights into Uncertainty Propagation** : By identifying and quantifying the sources of uncertainty, this thesis provided actionable insights for refining future

optical and radiative transfer models.

Looking ahead, this work highlights opportunities for further advancements. Refining fluorescence models, particularly SICF, could minimize residual uncertainties and improve both forward and inverse modeling. Expanding SABER's application to hyperspectral datasets and diverse environmental contexts would further validate its versatility and scalability. Finally, integrating these advancements into interdisciplinary studies could foster new applications in coastal ecosystem management and climate resilience planning.

In summary, this thesis has laid a solid foundation for more accurate and actionable remote sensing of optically complex coastal waters, addressing long-standing challenges in forward modeling, retrieval accuracy, and uncertainty quantification. These contributions will support future efforts to monitor, manage, and protect coastal ecosystems in an era of rapid environmental change.

ANNEXE I

CHAPTER 1: SUPPLEMENTARY MATERIALS

4.1 Scattering Correction for AC-S

We compared three scattering correction methods proposed by Zaneveld et al. (1994); Twardowski et al. (1999), Röttgers et al. (2013) and McKee et al. (2008, 2013), respectively. The first two methods are "self-contained" methods as no ancillary IOPs are necessary. The Zaneveld et al. (1994); Twardowski et al. (1999) method (SCR_{z99}) assumes a single λ independent value; b_{ua} representing the proportion of scattered light lost inside the $a(\lambda)$ flow tube of the AC-S, therefore to be subtracted from AC-S acquired T and S corrected absorption ($a_m(\lambda)$). The b_{ua} is calculated from NIR wavelengths as the correction assumes almost negligible absorption at NIR; i.e. $a_m(715)$ which is scaled by scattering ratio at λ versus at 715 nm;

$$a_n(\lambda) = a_m(\lambda) - a_m(715) \frac{c_m(\lambda) - a_m(\lambda)}{c_m(715) - a_m(715)} \quad (4.1)$$

Where $a_n(\lambda)$ is scatter-corrected absorption and $c_m(\lambda)$ is T and S corrected attenuation; both acquired from AC-S.

The Röttgers et al. (2013) scheme (SCR_{r13}) corrects the AC-S data using an empirical proportional method considering b_{ua} as λ dependent and proportionally varying with λ dependent scattering coefficient $b(\lambda)$ obtained as $c(\lambda) - a(\lambda)$ weighted by the difference between non-negligible T and S corrected absorption and true absorption, both at 715 nm. One potential issue with this scheme is use of scatter-uncorrected $c(\lambda)$ data which is tackled by a λ independent coefficient (ϵ_c) accounting for fraction of light scattered inside $c(\lambda)$ tube (b_{uc});

$$a_n(\lambda) = a_m(\lambda) - (a_m(715) - a(715)) \frac{(1/\epsilon_c) c_m(\lambda) - a_m(\lambda)}{(1/\epsilon_c) c_m(715) - a_m(715)} \quad (4.2)$$

Above, the ϵ_c value is set to 0.56 and the $a(715)$ is assumed as ICAM acquired true absorption is calculated as $a(715) = 0.212 * a_m(715)^{1.135}$.

McKee et al. (2008, 2013) proposed scattering correction methods (SCR_{m08} , SCR_{m13}) that could incorporate co-acquired *in situ* Volume Scattering Function (VSF) data in order

to perform the flow-tube scatter correction for both a and c tubes. The common approach for both SCR_{m08} and SCR_{m13} calculates the scattering errors for both the $a(\lambda)$ and $c(\lambda)$ tubes (b_{ua} & b_{uc} respectively) by using a Monte Carlo simulation given weighting function that describes the collection of angular scattering with ancillary use of relevant b_b data from the VSF;

$$a_n(\lambda) = a_m(\lambda) - f_a(\lambda)b_p(\lambda) \quad (4.3a)$$

$$c_n(\lambda) = c_m(\lambda) + f_c(\lambda)b_p(\lambda) \quad (4.3b)$$

Where, $b_p(\lambda)$ is the true particulate scattering coefficient calculated as;

$$b_p(\lambda) = \frac{b_m(\lambda)}{1 - f_a(\lambda) - f_c(\lambda)} \quad (4.4)$$

Here, $b_m = c_m(\lambda) - a_m(\lambda)$, $f_a(\lambda)$ is the fraction of scattered light not collected by the absorption sensor, and $f_c(\lambda)$ is the fraction of scattered light that is collected by the attenuation sensor. The $f_a(\lambda)$ and $f_c(\lambda)$ can theoretically be calculated as following two equations respectively.

$$f_a(\lambda) = 2\pi \int_0^\pi W_a(\psi) \tilde{\beta}_p(\lambda, \psi) \sin \psi d\psi \quad (4.5a)$$

$$f_c(\lambda) = 2\pi \int_0^{\psi_c} \tilde{\beta}_p(\lambda, \psi) \sin \psi d\psi \quad (4.5b)$$

Where $W_a(\psi)$ is a λ independent scattering weighing function describing the angular scattering collection efficiency of the absorption sensor in AC-S. $\tilde{\beta}_p(\lambda, \psi)$ is the λ dependent particulate scattering phase function and ψ_c is the maximum collection angle of the attenuation sensor.

For SCR_{m08} , Mckee et al. (2008) proposed two parameterizations using particulate backscatter fraction; $\tilde{B}(\lambda)$ to calculate $f_a(\lambda)$ and $f_c(\lambda)$ which are given as a 4th order polynomial and 3-parameter hyperbolic decay as shown in Eq. 4.6(a, b) respectively (λ is omitted

for brevity):

$$f_a = a_0 + a_1 \cdot \tilde{B} + a_2 \cdot \tilde{B}^2 + a_3 \cdot \tilde{B}^3 + a_4 \cdot \tilde{B}^4 \quad (4.6a)$$

$$f_c = \frac{6.809 \times 10^{-3}}{8.502 \times 10^{-3} + \tilde{B}} - 1.1918 \times 10^{-2} \quad (4.6b)$$

Where $a_0 - a_4$ are fixed coefficients from McKee et al. (2008).

For SCR_{m13} , a new variable r_w denoting the degradation of the a tube glass wall reflectivity (effective reflectance varying between 95% and 100%) is introduced which affects the $W_a(\psi)$ significantly for forward scattering angle between $0^\circ - 41.5^\circ$ McKee et al. (2013). The f_a in SCR_{m13} is fitted as a 6th order polynomial as:

$$f_a = a_0 + a_1 \cdot \tilde{B} + a_2 \cdot \tilde{B}^2 + a_3 \cdot \tilde{B}^3 + a_4 \cdot \tilde{B}^4 + a_5 \cdot \tilde{B}^5 + a_6 \cdot \tilde{B}^6 \quad (4.7)$$

Where $a_0 - a_6$ are coefficients from McKee et al. (2013) that are given in McKee et al. (2013) Table 1 for each proposed value of r_w between 0.95-1.0. The calculation of f_c in SCR_{m13} remains unchanged from SCR_{m08} .

Assessment of the influence of the scattering correction technique is performed as a part of checking the IOP consistency prior to the closure experiment. First, we have compared VSF-based methods, i.e. SCR_{m08} with SCR_{m13} for all r_w values proposed in McKee et al. (2013). The corresponding scatter corrected a_{t-w} values are validated against a_{t-w} obtained from *in lab* dual-beam spectrophotometry of discrete water samples. The validation metrics used are coefficient of determination (R^2) and Root Mean Square Error (RMSE). Figure 31 shows the validation of VSF-based SCR methods where SCR_{m08} obtained better statistical results than SCR_{m13} . However, there are a number of challenges associated with this scatter correction technique; firstly, the reference spectrophotometric absorption values are not as accurate as PSICAM obtained values due to error from flat baseline correction of a_{CDOM} and from uncertainty in path length amplification factor (βF) and scattering offset (o) for filter pad determined values of a_p . Moreover, the BB9 VSF used for both SCR_{m08} and SCR_{m13} are

potentially highly overestimated with very noisy spectral shape (Discussed in detail in Section 1.5.2.1 of the main manuscript), which also incorporates uncertainty in our selection of optimal VSF based scatter correction technique. Thus, even though SCR_{m08} was found to perform better, the associated uncertainty in 1. BB9 measured VSF and 2. in spectrophotometric absorption used as the validation reference makes this choice uncertain to some extent.

SCR_{m08} is further compared with methods of Twardowski et al. (1999) and Röttgers et al. (2013). We have performed HL simulation with a_{t-w} obtained with SCR_{m08} , SCR_{z99} and SCR_{r13} respectively along with subsequent b_{bp} and keeping the rest of the conditions constant. The simulated $R_{rs}(0^-, \lambda)$ from HL (Note, here inelastic scattering was not included) was compared with *in situ* $R_{rs}(0^-, \lambda)$ using spectral %-bias (given in Section 2.4 in main paper) as evaluation metric; the scatter correction (SCR) scheme generating consistently lowest spectral %-bias among the techniques was used to obtain a_{t-w} for the optical closure onward. Fig. 32a presents the SCR results for a single station (MAN-F22) for spectral representation of scatter correction on simulated R_{rs} . For MAN-F22, the SCR technique-specific spectral %-bias for HL simulated $R_{rs}(0^-, \lambda)$ showed high overestimation for SCR_{z99} and SCR_{r13} ; the mean spectral %-bias ($400 \leq \lambda \leq 700$) was reported +21.5%, and +21%, respectively. However, for SCR_{m08} , the mean spectral %-bias was reported to be significantly lower; +2.5 %. As per Bausell and Kudela (2021), the effect of SCR is most significant in "green-maxima" ($555 \leq \lambda(\text{nm}) \leq 560$) for HL simulated $R_{rs}(\lambda)$. In the current study, for all stations with successful AC-S deployment, the mean %-bias at "green-maxima" was found +41%, +34%, and +6% for SCR_{z99} , SCR_{r13} and SCR_{m08} , respectively (Fig.32b).

4.2 Optical Closure obtained with AC-S/BB9 package

The optical closure was performed for 9 stations with both elastic scattering components (HL_{el}) and elastic and inelastic scattering combined ($HL_{el+inel}$) where both AC-S and BB9 acquired data. $R_{rs}(0^-, \lambda)$ values were simulated with HL and it was compared to *in situ*

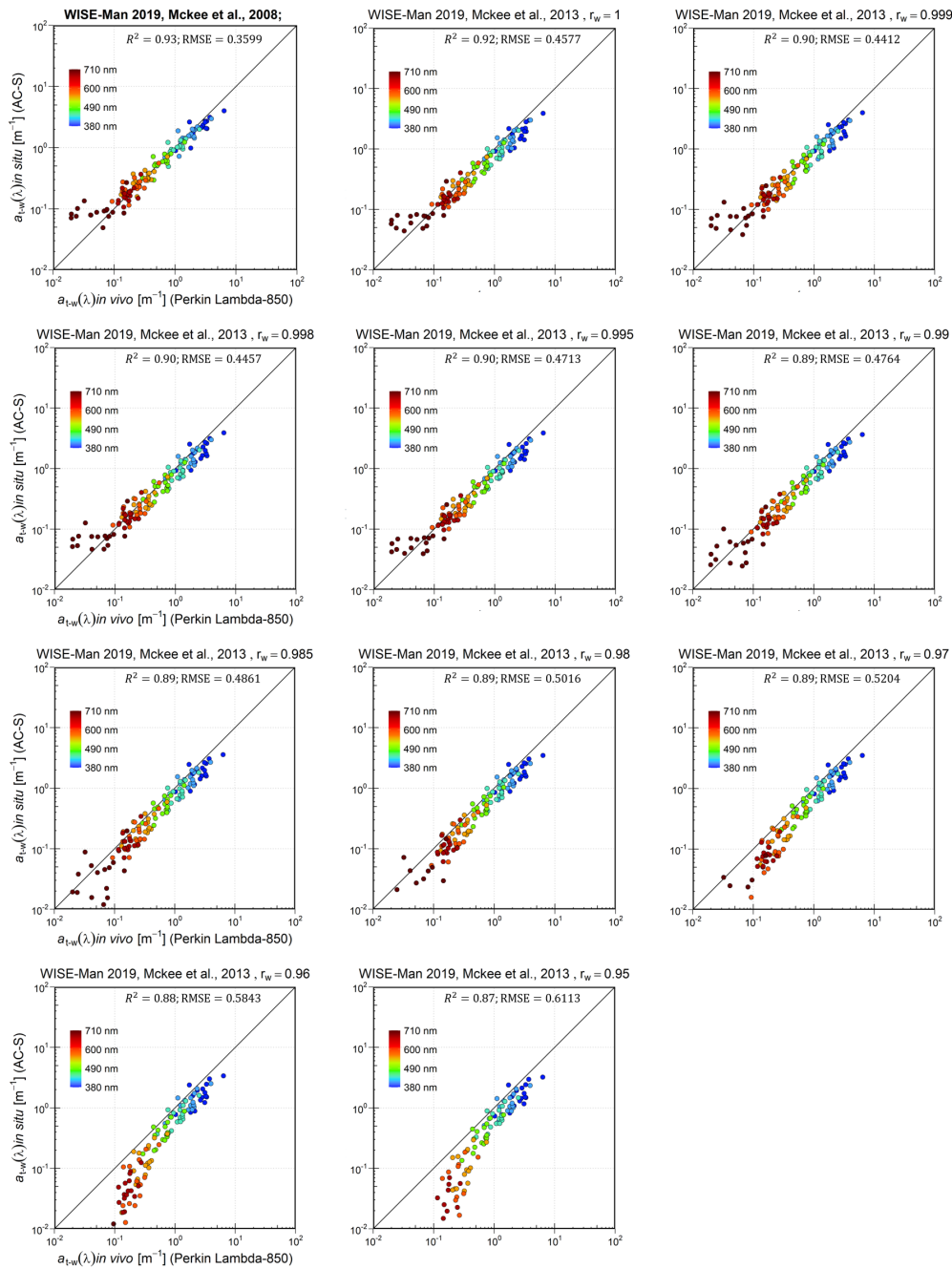


Figure 31 – Series of scatter-plots of Spectrophotometer obtained non-water absorption (X-axis) and AC-S obtained non-water absorption (Y-axis) on $\log_{10}$ scale. The AC-S data shown here are processed with SCR_{m08} for the plot in 1st row and 1st column, the rest are processed with SCR_{m13} for varying r_w values.

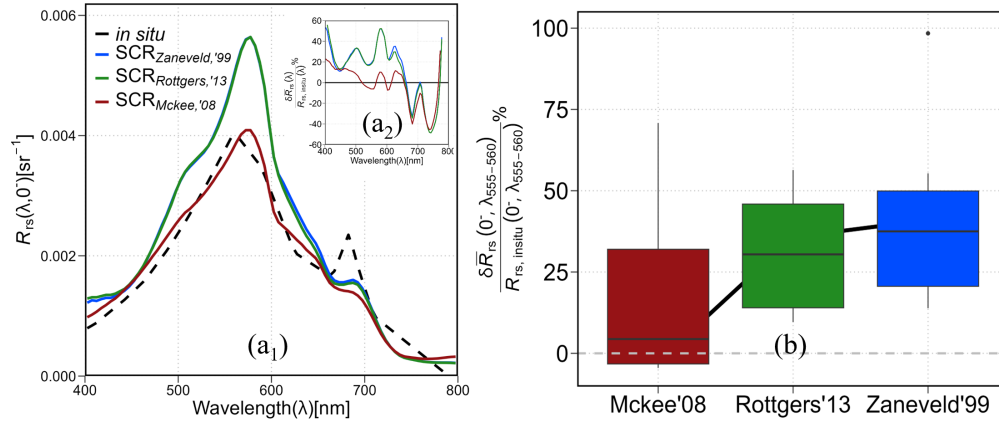


Figure 32 – (a₁.) Spectral plots of HL simulated $R_{rs}(0^-, \lambda)$ for station MAN-F22 with different SCR techniques to correct AC-S a_{t-w} data along with C-OPS acquired *in situ* $R_{rs}(0^-, \lambda)$ (dashed black line). (a₂.) The encapsulated plot inside shows the spectral %-bias between C-OPS acquired $R_{rs}(0^-, \lambda)$ and HL simulated $R_{rs}(0^-, \lambda)$ for each of SCR technique. (b.) Boxplot of %-bias at "green-maxima" for different SCR technique corrected AC-S data of all stations.

$R_{rs}(0^-, \lambda)$. The quality of HL obtained optical closure for AC-S/BB9 package is studied in three spectral groups, i.e. blue, green and red (Fig. 33). The statistical assessment of goodness of fit for both HL_{el} and $HL_{el+inel}$ is presented in Table 9. A constant overestimation can be seen in all the spectral groups for HL_{el} , i.e. %-bias of +34%, +27% and +12% for blue, green and red λ respectively. The addition of inelastic scattering in HL simulation increased the R^2 , however, it does neither correlate with accuracy (RGB RMS%E: 33% to 44%) nor with %-bias (RGB %-bias: +21% to +38%), eventually making the overestimation more severe than HL_{el} (Tab. 9).

For the WETLabs instrument-based optical closure, this overestimation in modelled $R_{rs}(0^-)$ might be caused by very high $b_{bp}(\lambda)$ values from the BB9 as discussed in Section 1.5.2.1. Relatively, the BB9 acquired potentially overestimated value of b_{bp} data is used to correct b_{ua} and b_{uc} for the scatter correction in *a* and *c*-tubes respectively, which can also not be σ corrected prior to VSF-based scatter correction. Mainly, the overestimated b_b might have increased the $R_{rs}(0^-)$ magnitude by an almost flat offset (See Fig.33). The addition of

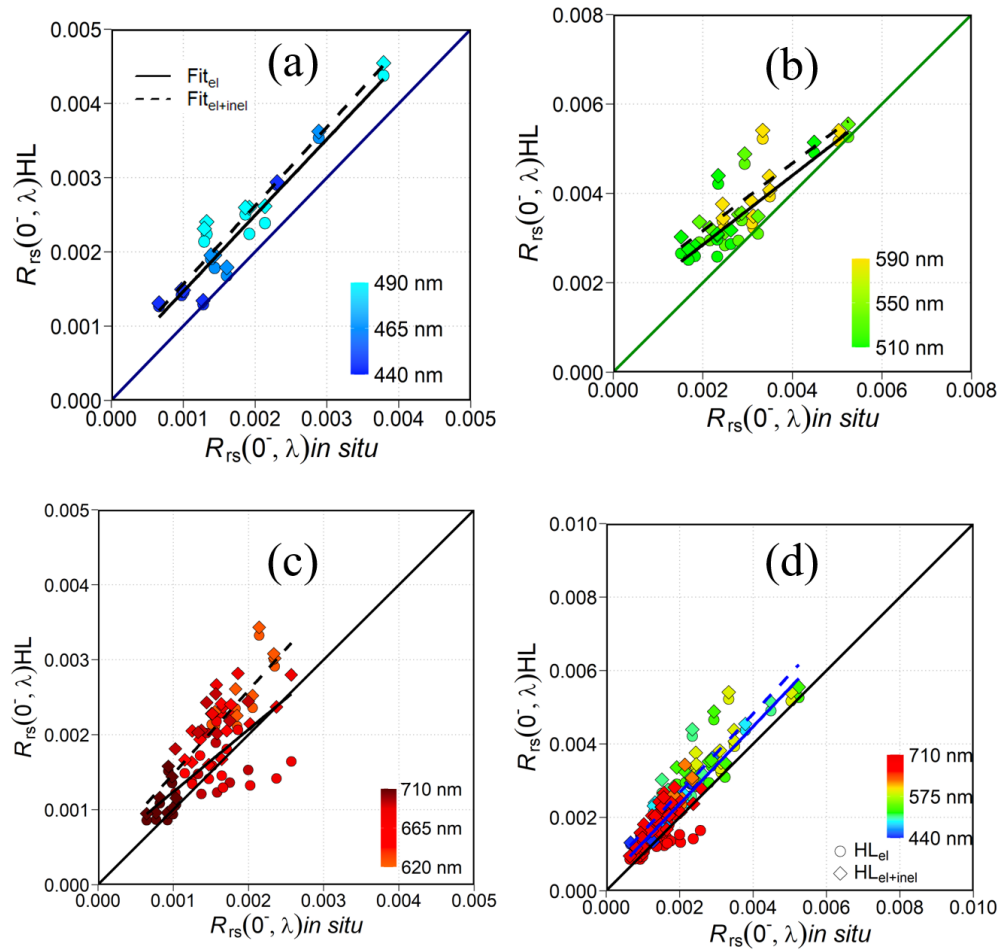


Figure 33 – Validation plots for HL optical closure obtained from AC-S and BB9 co-acquired IOPs for spectral groups, i.e. **(a)** Blue (440-490nm), **(b)** Green (510-590), **(c)** Red (620-710) and **(d)** RGB altogether (440-710). The solid-coloured diagonal line (slope; $m = 1$) in each plot is the 1:1 line. The black solid lines (Fit_{el}) show the linear fit between *in situ* $R_{\text{rs}}(0^-, \lambda)$ (X-axis) and HL simulated $R_{\text{rs}}(0^-, \lambda)$ (Y-axis) with elastic scattering (HL_{el}) whereas, the black dashed lines ($\text{Fit}_{\text{el+inel}}$) represent linear fit between *in situ* $R_{\text{rs}}(0^-, \lambda)$ (X-axis) and HL simulated $R_{\text{rs}}(0^-, \lambda)$ (Y-axis) with both elastic and inelastic scattering combined ($\text{HL}_{\text{el+inel}}$).

inelastic scattering parameters increased the RMS%E by $\sim 10\%$ in green wavelengths which is expected from HL simulations when the $a_{\text{t-w}}$ is CDOM driven. Summarizing these findings for ACS and BB9 acquired IOPs and to minimize input uncertainty in the closure, we decided to exclude the AC-S and BB9 obtained results of optical closure in the final quantification of

the contribution of inelastic scattering in the $R_{rs}(0^-)$.

Table 9 – Statistics on the goodness of fit between C-OPS acquired *in situ* $R_{rs}(0^-, \lambda)$ data and HL simulated $R_{rs}(0^-, \lambda)$ including elastic scattering for visible spectral domains (el) and the same but with both elastic and inelastic scattering (inel) respectively. The measured statistical metrics are the coefficient of determination (R^2), the slope of the linear fit (m), median absolute percentage error (MDAPE), root mean square percentage error (RMS%E) and %-bias. The R^2 and m are obtained with Major Axis regression of Type-II family.

λ	R^2		Slope (m)		MDAPE(%)		RMS%E		%Bias	
	el	inel	el	inel	el	inel	el	inel	el	inel
Blue	0.88	0.89	1.07	1.11	25	36	42	48	+34	+41
Green	0.67	0.69	0.93	0.78	17	29	36	46	+27	+38
Red	0.44	0.73	1.35	1.39	23	42	28	42	+12	+36
RGB	0.79	0.84	1.21	1.17	23	36	33	44	+21	+38

4.3 Impact of the vertical distribution of IOP and inelastic scattering inputs

The $\widehat{a}_{CDOM}(443)$ values (obtained following Eq. 3 in main paper) are observed to have a decreasing trend with depth (0-4 m) and higher values are mostly observed near the surface (Fig. 34). The surface ($z = 0^-$ m) $\widehat{a}_{CDOM}(443)$ (including both KD and SC) varied between 0.40 m^{-1} and 2.10 m^{-1} with median of 0.91 m^{-1} . It is worth to mention most of the highest values of $\widehat{a}_{CDOM}(443)$, i.e. $> 1.5 \text{ m}^{-1}$ were observed for stations visited with boat *Saucier* and the corresponding depths were on the shallower side; ≤ 20 m whereas for *Kildir* the depth of the visited stations on the higher side, i.e. ~ 30 -60 m and the estimated $\widehat{a}_{CDOM}(443)$ was lower than the other, i.e. $< 1.2 \text{ m}^{-1}$. In some shallower stations such as MAN-R05 (49.185° N, 68.011° W) and MAN-F0 (49.203° N, 68.082° W), a sharp decrease in $\widehat{a}_{CDOM}(443)$ is observed after the first couple of meters, which might be an effect of freshwater lensing in the stratified water column.

We also examined whether the vertical variability of IOPs has a significant impact on $R_{rs}(0^-, \lambda)$

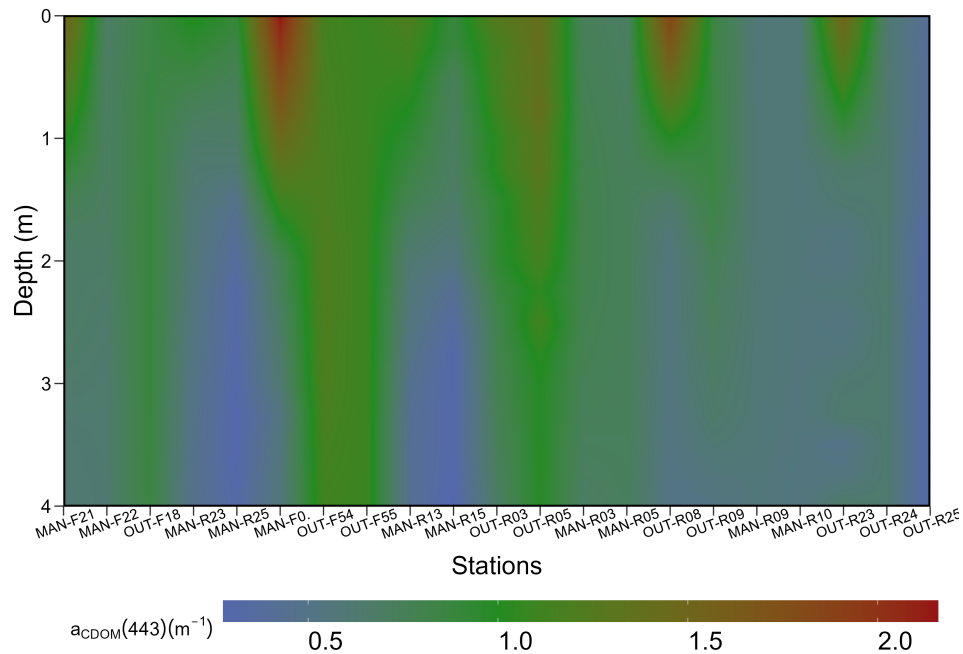


Figure 34 – Estimated depth (in meters) profile variability of $\widehat{a}_{\text{CDOM}}(443)$ among stations where *in situ* a_{t-w} was recorded. The station depth for all profiles is truncated at 4m.

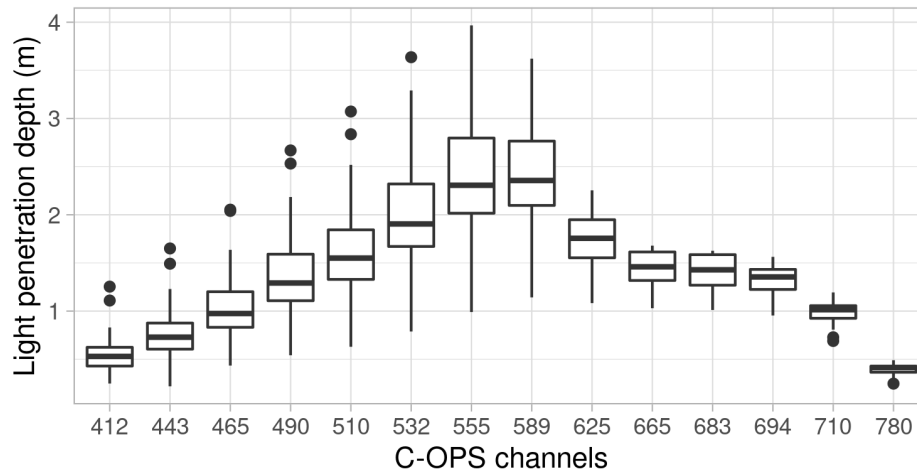


Figure 35 – Box-plot of measured penetration depth (in meters) Gordon and McCluney (1975) using the C-OPS at deep stations.

in our stratified environment. For this, HL simulations were performed using both the full-depth IOPs profiles available and vertically constant IOPs values obtained as mean for the

first 4 meters. In general, $R_{rs}(0^-, \lambda)$ obtained assuming vertically homogeneous water column yielded similar values compared to $R_{rs}(0^-, \lambda)$ obtained using the full depth IOP profiles (i.e., differences $< 2\%$, not shown). This result was in line with the thin penetration depth measured with the C-OPS (Fig. 35) Gordon and McCluney (1975). The penetration depth was less than 4.0 meters, with an average of 2.42 meters at 555 and 589 nm.

4.4 Closure results by station

The spectral comparison of HL simulated $R_{rs}(0^-, \lambda)$ (for each of the 12 stations with ASPH/HS6 IOPs as input) with the same derived from COP-S is shown in Fig. 36. These simulations showed the inclusion of inelastic scattering, i.e. f_{DOM} and SICF, improved the agreement with *in situ* $R_{rs}(0^-, \lambda)$ at all stations except at OUT-R03 (Fig. 36d).

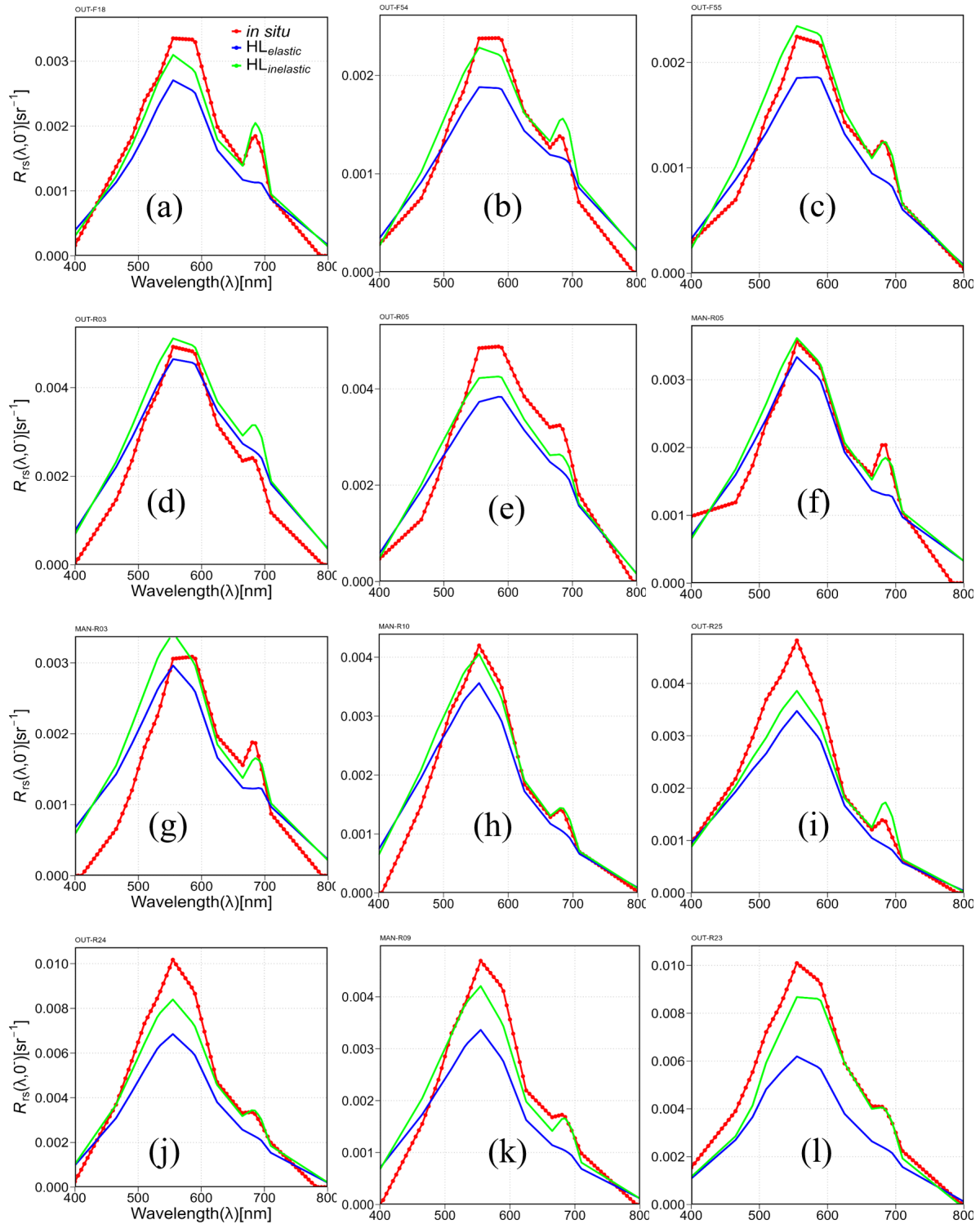


Figure 36 – Spectral comparison of station-wise optical closure obtained from HL for ASPH/HS6 IOPs with C-OPS derived $in situ$ $R_{rs}(0^-, \lambda)$. The red line shows the C-OPS acquired $R_{rs}(0^-, \lambda)$ where the overlaying red solid circles denote C-OPS $R_{rs}(0^-, \lambda)$ resampled to HL simulation wavelengths. The blue line denotes HL simulated $R_{rs}(0^-, \lambda)$ for elastic scattering (HL_{el}) whereas the green line shows the same but for both elastic and inelastic scattering combined ($HL_{el+inel}$).

ANNEXE II

CHAPTER 2: SUPPLEMENTARY MATERIALS

5.1 Calculation of uncertainty for gradient-based retrievals

In the context of gradient-based optimization for shallow water inversion, uncertainty in retrieved parameters can be estimated using the Jacobian matrix to propagate uncertainties in observed reflectance. Below, the mathematical formulation and derivations are provided.

The forward model $f(\theta)$ relates the observed reflectance $\mathbf{R}_{rs}^{\text{obs}}$ to the independent parameter vector θ :

$$\mathbf{R} = f(\theta) \quad (5.1a)$$

$$\theta = [\text{IOPs}, H, R_B] \quad (5.1b)$$

Here, $\mathbf{R} \in \mathbb{R}^n$ (R_{rs} is noted as R here for ease in mathematical notations further here) represents the modeled reflectance, and $\theta \in \mathbb{R}^p$ represents the parameters to be retrieved, including OSCs and inherent optical properties (IOPs), water depth H , and bottom reflectance R_B . Now, the Jacobian matrix $\mathbf{J}$ quantifies the sensitivity of the modeled reflectance $\mathbf{R}$ to changes in the parameters θ :

$$\mathbf{J} = \frac{\partial \mathbf{R}}{\partial \theta}, \quad (5.2a)$$

$$J_{ij} = \frac{\partial R_i}{\partial \theta_j} \quad (5.2b)$$

where J_{ij} is the partial derivative of the modeled reflectance R_i at wavelength λ_i with respect to the parameter θ_j . Uncertainty in the observed reflectance $\mathbf{R}_{\text{obs}}$ is represented by the covariance matrix $\mathbf{S}_R$:

$$\mathbf{S}_R = \begin{bmatrix} \sigma_{R_1}^2 & \text{Cov}(R_1, R_2) & \cdots & \text{Cov}(R_1, R_n) \\ \text{Cov}(R_2, R_1) & \sigma_{R_2}^2 & \cdots & \text{Cov}(R_2, R_n) \\ \vdots & \vdots & \ddots & \vdots \\ \text{Cov}(R_n, R_1) & \text{Cov}(R_n, R_2) & \cdots & \sigma_{R_n}^2 \end{bmatrix} \quad (5.3)$$

where $\sigma_{R_i}^2$ is the variance of R_{obs} at wavelength λ_i , and $\text{Cov}(R_i, R_j)$ is the covariance between

R_{obs} at wavelengths λ_i and λ_j . If errors are independent, $\mathbf{S}_R$ is diagonal. Now, the covariance matrix for the retrieved parameters θ is computed as:

$$\mathbf{S}_\theta = (\mathbf{J}^T \mathbf{S}_R^{-1} \mathbf{J})^{-1} \quad (5.4)$$

where $\mathbf{J}^T$ is the transpose of the Jacobian matrix, and $\mathbf{S}_R^{-1}$ is the inverse of the reflectance covariance matrix. The diagonal elements of $\mathbf{S}_\theta$ represent the variances of the retrieved parameters θ . The standard deviations (uncertainties) are given by:

$$\sigma_{\theta_j} = \sqrt{\mathbf{S}_\theta[j, j]} \quad (5.5)$$

where $\mathbf{S}_\theta[j, j]$ is the j -th diagonal element of $\mathbf{S}_\theta$. This allows the uncertainties in θ to be directly computed from the propagated uncertainties in $\mathbf{R}_{\text{obs}}$.

5.2 Supplemental Figures relevant to development of SABER

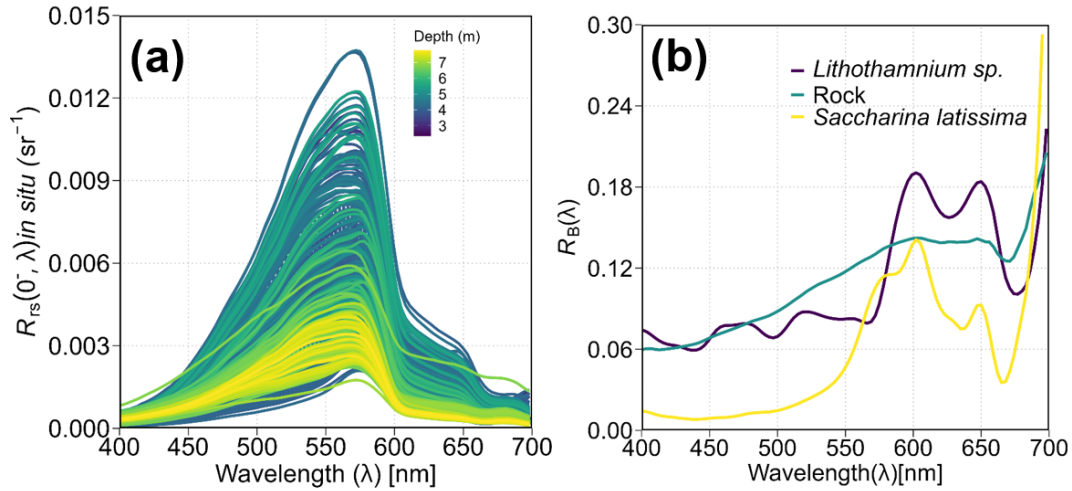


Figure 37 – (a) Synthetic dataset of $R_{rs}(0^-, \lambda)$ simulated following the approach in Section 2.4.1.2. (b) The *in situ* spectral benthic reflectance (R_B) of the three coastal benthic substrates used in simulation to obtain (a).

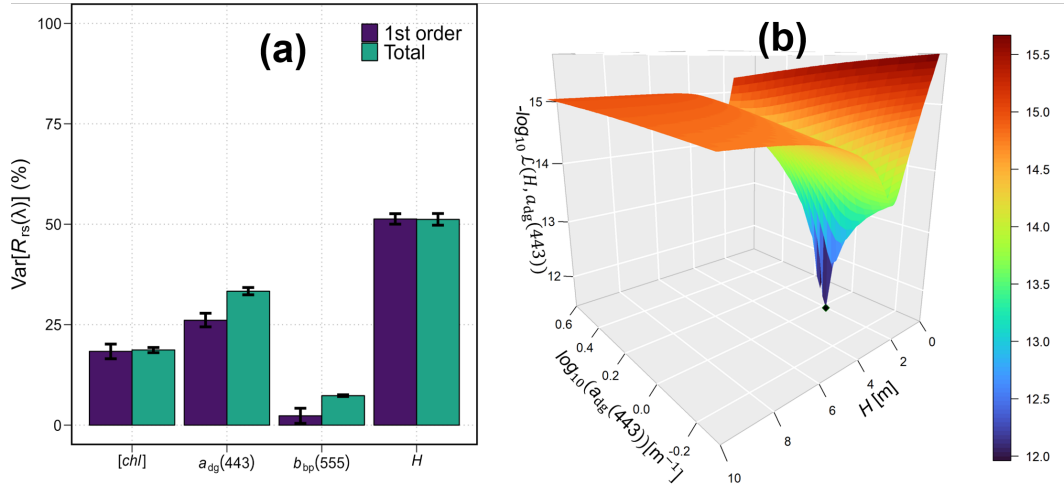


Figure 38 – (b) The likelihood ($\mathcal{L}$) surface as a function of $a_{dg}(443)$ and H (for $n = 10,000$ observations), i.e., the variables in θ explaining the highest % of variance in the obtained R_{rs} as per Sobol sensitivity analysis shown in (a). The green diamond shape shows the actual solution for θ ; i.e., $\{a_{dg}(443) = 1.02 \text{ m}^{-1}, H = 2 \text{ m}\}$. The $\mathcal{L}$ and $a_{dg}(443)$ are in $\log_{10}$ scale for a better illustration of how the likelihood surface is controlled by ϕ_{var} over a large variability in magnitude.

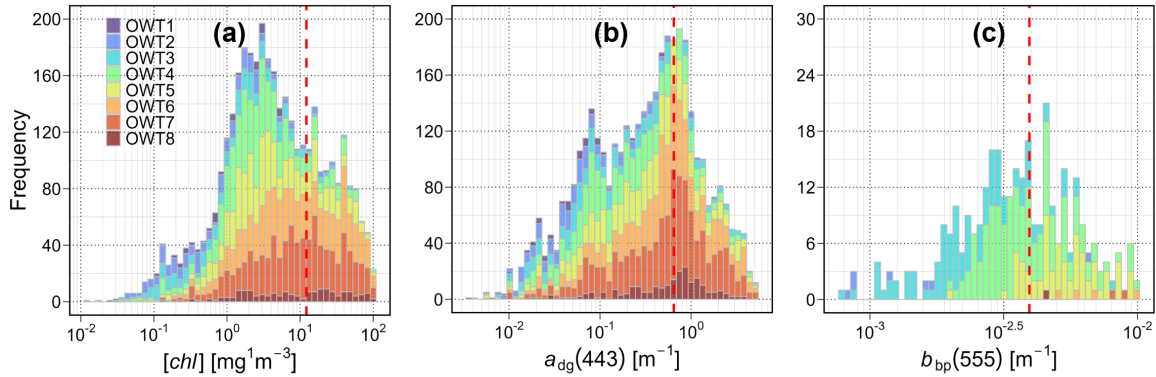


Figure 39 – (a-c) Log-Normal distribution of $[chl]$, $a_{dg}(443)$ and $b_{bp}(555)$ used to model the *a-priori* distributions encompassing eight OWTs. The red dashed line in each histogram shows the corresponding mean.

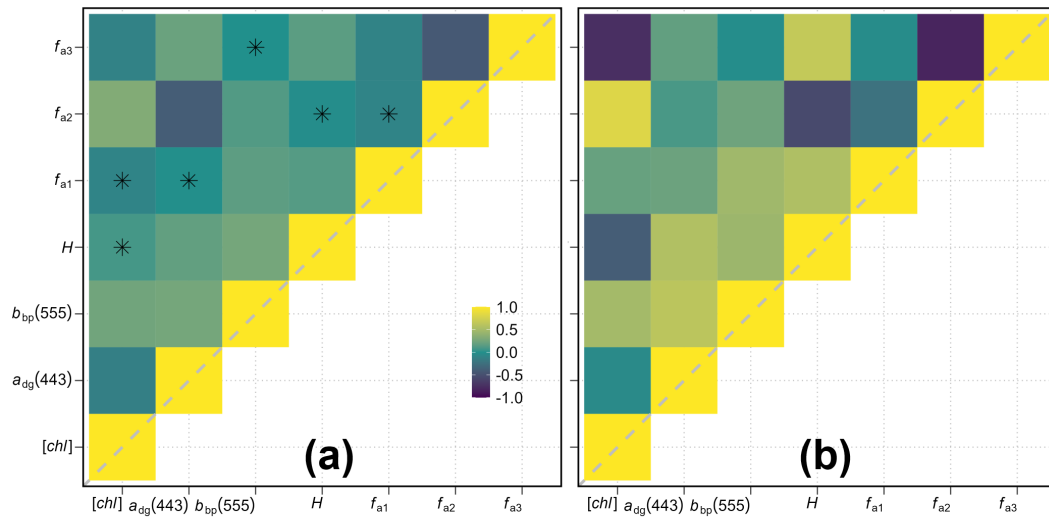


Figure 40 – **a)** Correlation matrix between different variables in θ obtained from the a -priori fit of parameters for a specific inversion. The asterisk marked ones are not statistically significant at an α -level of 0.05. **a)** Correlation matrix same as (a), but obtained from the Posterior distribution (post *burn-in*).

ANNEXE III

CHAPTER 3: SUPPLEMENTARY MATERIALS

6.1 Impact of inelastic scattering correction of R_{rs} on inversion

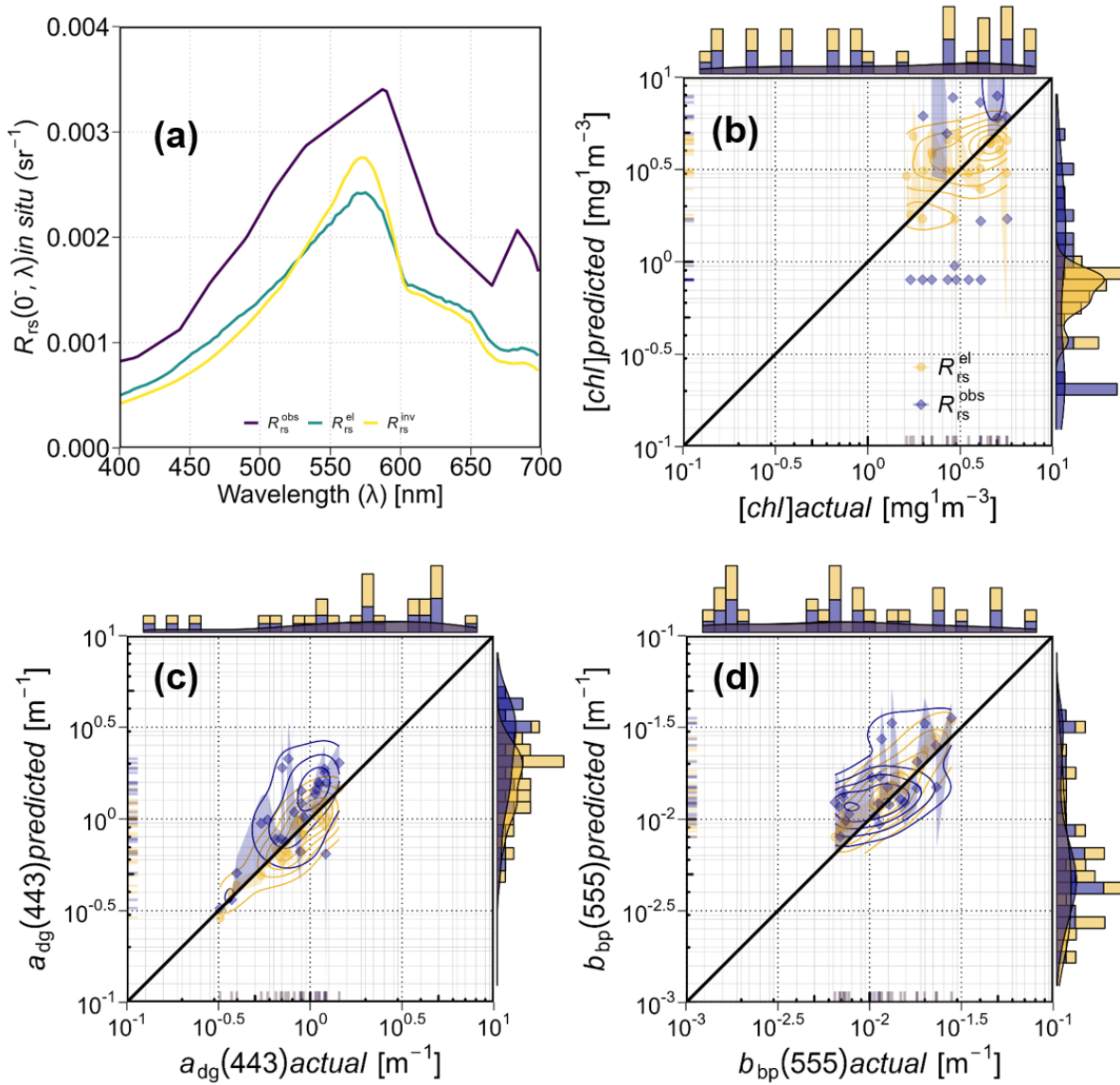


Figure 41 – **(a)** Spectral comparison of *in situ* R_{rs} derived from C-OPS (Purple) with inelastic scattering corrected R_{rs} (cyan) and reconstructed R_{rs} (yellow) with the SABER forward model with inversion retrieved variables from the inelastic scattering corrected R_{rs} shown. **(b-d)** Validation scatter-plots for $[chl]$, $a_{\text{dg}}(443)$ and $b_{\text{bp}}(555)$ from inverting *in situ* and inelastic scattering corrected R_{rs} , respectively.

6.2 Inter-comparison of spectral resolution of R_{rs} on inversion

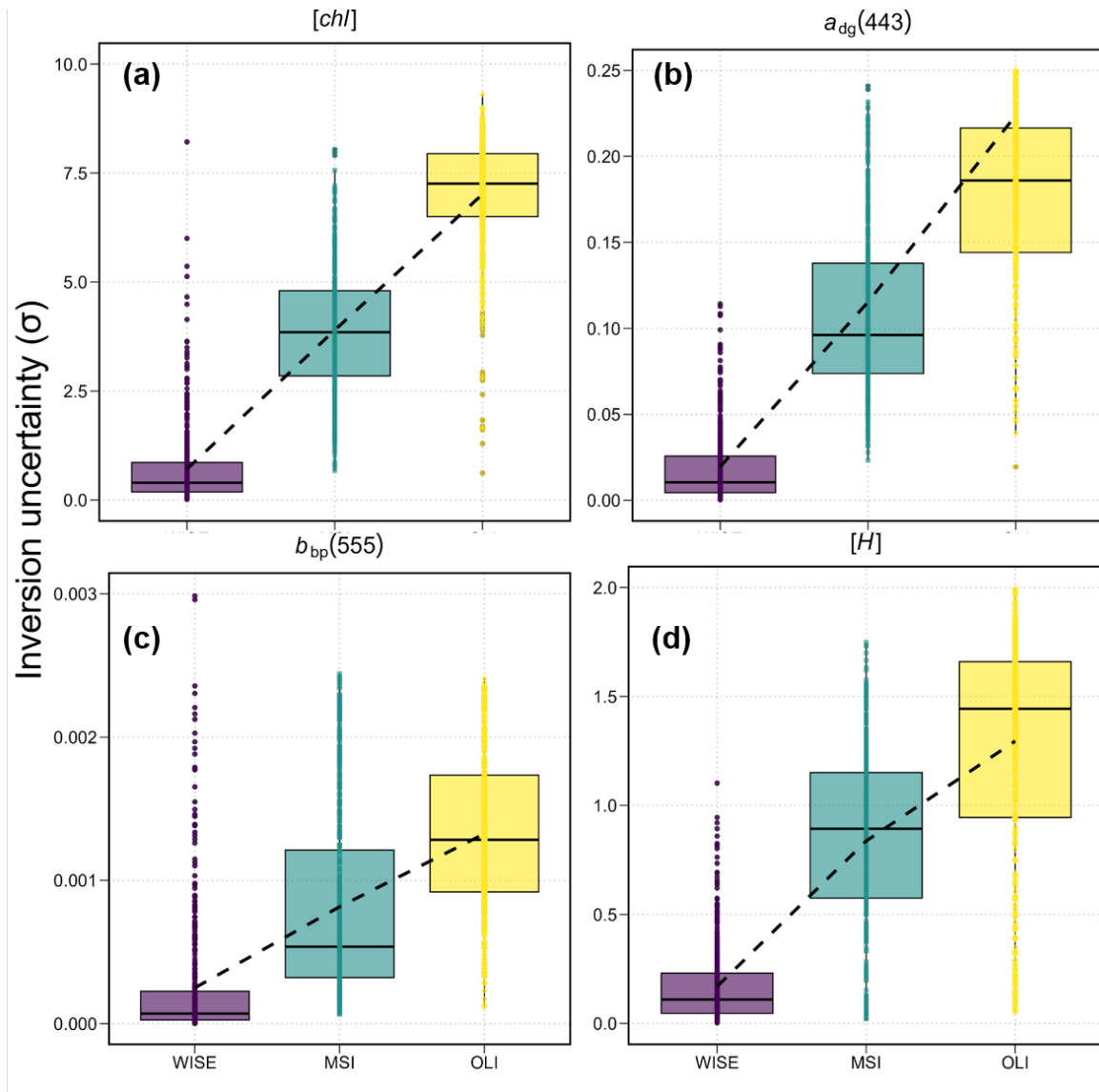


Figure 42 – **a)** Box-plot showing variation in the inversion retrieved uncertainty associated with SABER retrieved $[chl]$ estimates as a function of different sensory Spectral response Function (SRF) convolved R_{rs} . A strictly increasing trend in uncertainty is observed when the R_{rs} is convolved to sensors with a few number of bands (MSI: $N = 6$, OLI: $N = 4$), compared to the hyperspectral sensor WISE ($N = 88$). **(b-d)** same as a, but for $a_{dg}(443)$, $b_{bp}(555)$ and H , concurrently retrieved with $[chl]$ from inverting $N = 5000$ observations of HL simulated R_{rs} , depicting the aquatic optical conditions of EGSL.

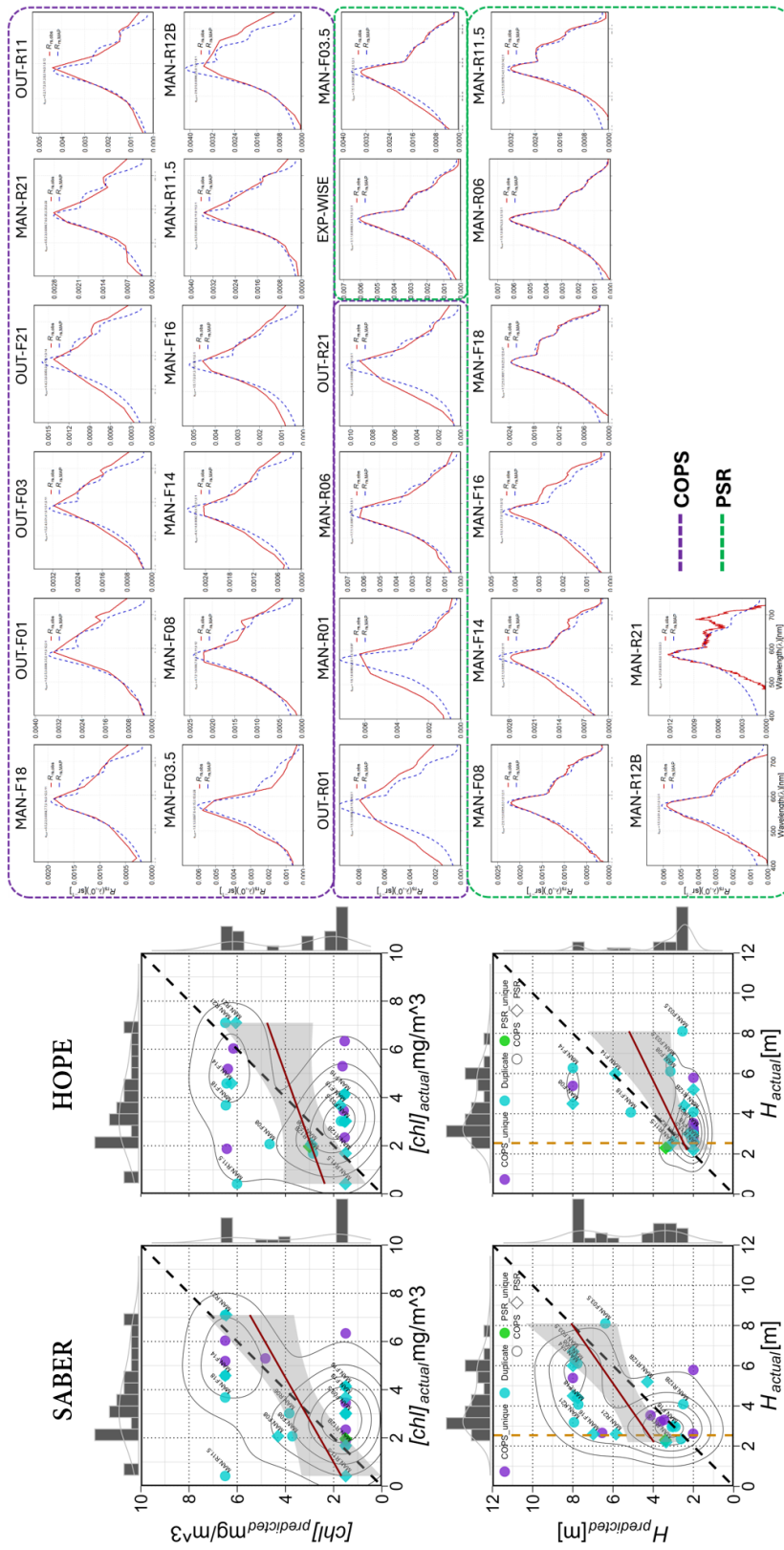


Figure 43 – On the left side, retrieval performance between SABER and HOPE is compared for $[chl]$ and H . The input R_{rs} source is expressed using the colours of the points, i.e., the purple points are C-OPS derived unique observations, whereas the green ones are PSR exclusive observations. The blue points denote the common observations between C-OPS and PSR. The right-sided spectral plot shows comparison of input R_{rs} (Blue dashed line) derived from C-OPS and PSR sensors and the reconstructed R_{rs} (Red solid line) with SABER retrieved parameters.

6.3 Application of SABER on Satellite RS image

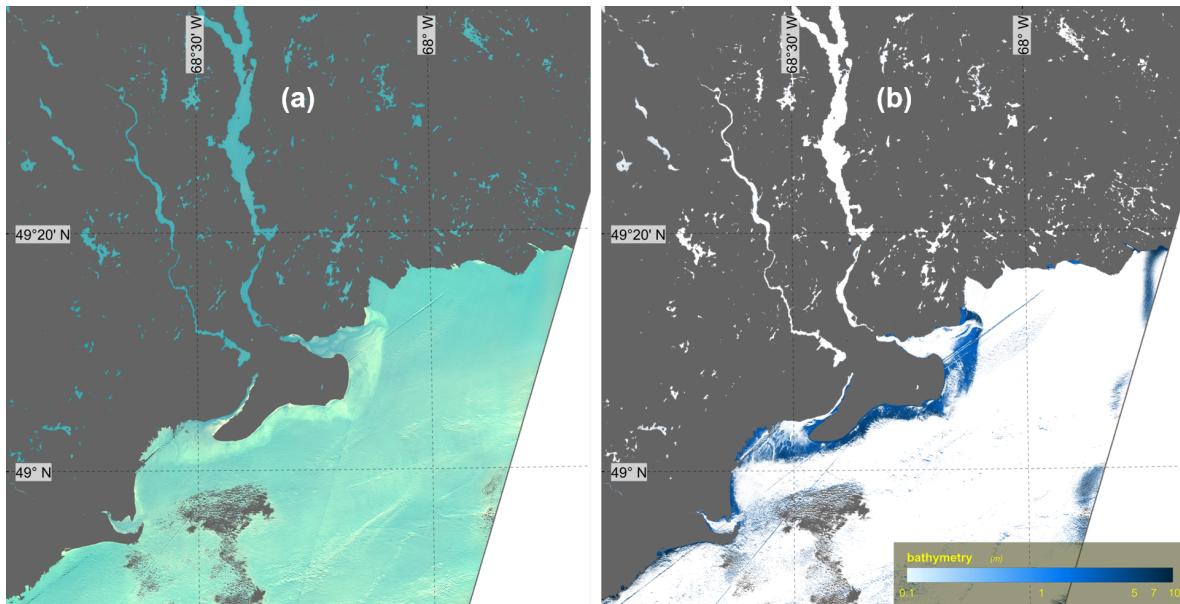


Figure 44 – **(a)** Map of $R_{rs}(559)$ derived from Sentinel 2 MSI sensor acquired radiance (Atmospheric correction following Singh and Shanmugam (2014)) over MP on 26th August 2019. **(b)** SABER retrieved water depth (H) map from the Sentinel 2 MSI sensor derived R_{rs} for 6 bands in 400-750 nm wavelength region.

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