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Spatial-temporal bio-optical classification of dynamic semi-estuarine waters in western North America

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ABSTRACT

The use of standard ocean colour reflectance based algorithms to derive surface chlorophyll may have limited applicability for optically dynamic coastal waters due to the pre-defined coefficients based on global datasets. Reflectance based algorithms adjusted to regional optical water characteristics are a promising alternative. A class-based definition of optically diverse coastal waters was investigated as a first step towards the development of temporal and spatial constrained reflectance based algorithms for optically variable coastal waters.

A large set of bio-optical data were collected as part of five research cruises and bi-weekly trips aboard a ship of opportunity in the west coast of Canada, to assess the spatial and temporal variability of above-water reflectance in this contrasted coastal environment. To accomplish this, *in situ* biophysical and optical measurements were collected in conjunction with above-water hyperspectral remote sensing reflectance (R_{rs}) at 145 stations. The concentrations of measured biophysical data varied considerably; chlorophyll *a* (Chl*a*) (mean = 1.64, range: 0.10–7.20 μg l^{-1}), total suspended matter (TSM) (3.09, 0.82–20.69 mg l^{-1}), and absorption by chromophoric dissolved organic matter (CDOM) ($a_{cdom}(443nm)$) (0.525, 0.007–3.072 m^{-1}), thus representing the spatio-temporal variability of the Salish Sea. Optically, a similar large range was also found; particulate scattering ($b_p(650nm)$) (1.316, 0.250–7.450 m^{-1}), particulate backscattering ($b_{bp}(650nm)$) (0.022, 0.005–0.097 m^{-1}), total beam attenuation coefficient ($c_t(650)$) (1.675, 0.371–9.537 m^{-1}) and particulate absorption coefficient ($a_p(650nm)$) (0.345, 0.048–2.020 m^{-1}). An empirical orthogonal function (EOF) analysis revealed that R_{rs} variability was highly correlated to b_p (r = 0.90), b_{bp} (r = 0.82) and concentration of TSM (r = 0.80), which highlighted the dominant role of water turbidity in this region. Hierarchical clustering analysis was applied to the normalized R_{rs} spectra to define optical water classes. Class 1 was defined by the highest R_{rs} values, particularly above 570 nm, indicating more turbid waters; Class 2 was dominated by high Chl*a* and TSM concentrations, which is shown by high R_{rs} at 570 nm as well as fluorescence and absorption peaks; Class 3 shows strong fluorescence signatures accompanied by low TSM influence; and Class 4 is most representative of clear waters with a less defined absorption peak around 440 nm. By understanding the bio-optical factors which control the variability of the R_{rs} spectra this study aims to develop a sub-regional characterization of this coastal region aiming to improve bio-optical algorithms in this complex coastal area.

1. Introduction

Significant advances have been made in recent years in resolving Chl*a* concentrations in optically complex waters, called Case 2 (Morel and Prieur, 1977), by using regionally specific data to modify standard Chl*a* algorithms (e.g., Garcia et al., 2006; Komick et al., 2009; Le et al., 2013; Loisel et al., 2010; Lubac and Loisel, 2007; Werdell et al., 2009; Brewin et al., 2015; Loisel et al., 2017). These techniques are often based on an empirical relation between Chl*a* and remote sensing reflectance, $R_{rs}(\lambda)$, such as the ocean colour three-band algorithm for MODIS (OC3M), which capitalizes on the maximum band ratio of either $R_{rs}(443)$ or $R_{rs}(488)$ normalized to $R_{rs}(547)$ (O'Reilly, 2000), or through a semi-analytical approach that relates remote sensing reflectance below the air-water interface, $r_{rs}(\lambda)$, to the inherent optical properties (IOPs) of the water. For example, the standard semi-analytical

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Garver-Siegel-Maritorena version 1 (GSM01) (Gordon et al., 1988; Maritorena et al., 2002). However, both approaches consider pre-defined coefficients and/or assumptions that may have limited applicability for regional optically dynamic waters (Garcia et al., 2005; Komick et al., 2009; Lubac and Loisel, 2007; Mustapha et al., 2012; Vantrepotte et al., 2012; Loisel et al., 2017).

Specifically, for the coastal waters of western Canada, Komick et al. (2009) suggested that accuracy improvement of Chl*a* retrieval based on OC3M or GSM1 can be achieved by better addressing the local optical properties. With data limited to spring and summer conditions and only the Strait of Georgia, these waters have preliminarily been categorized into three spatially distinct water masses based on measured IOPs, including beam attenuation coefficient and absorption to scattering ratios (Loos and Costa, 2010). However, this classification is based on IOPs, and is spatially and temporally limited (i.e., it does not cover the full range of regional optical conditions). Studies from other regions have also shown the usefulness of apparent optical properties (AOPs), such as $R_{rs}(\lambda)$, to provide optical classification of surface waters (Lubac and Loisel, 2007; Vantrepotte et al., 2012; Moore et al., 2014; Mélin and Vantrepotte, 2015). Regardless of the optical property considered, these approaches have demonstrated the usefulness of developing a class-based simplification of optically diverse coastal waters for the development and success of class specific ocean colour algorithms (i.e., the improved retrieval accuracy is achieved when blending algorithms specifically designed for different optical classes) (Moore et al., 2014; Mélin and Vantrepotte, 2015; Jackson et al., 2017). Further, retrieval uncertainties can be defined according to the pre-defined optical water classes (Jackson et al., 2017).

The objective of this study is to characterize the spatio-temporal bio-optical diversity of the surface coastal waters of the Salish Sea, a dynamic semi-estuarine system located on the west coast of Canada and the United States, and group waters with similar optical traits as a first step towards defining a sub-regional reflectance-based inversion model for retrieving Chl*a*. We implicitly assume that waters with similar optical water constituents possess a similar $R_{rs}(\lambda)$ spectral signature, and thus demonstrate a spatial and/or temporal component based on the hydrodynamics and biogeochemistry of the region. To accomplish this, we use a large database of *in situ* observations combined with data using radiative transfer simulation from Hydrolight modeling, and apply an empirical orthogonal analysis to understand the drivers of $R_{rs}(\lambda)$ variability followed by a hierarchical clustering analysis to classify these data into distinct classes. This research contributes to the body of literature that in the recent years has demonstrated the importance of optical water classification for improving the accuracy of reflectance-based retrievals of surface chlorophyll *a* concentrations (Lubac and Loisel, 2007; Vantrepotte et al., 2012; Mélin and Vantrepotte, 2015; Loisel et al., 2017; Jackson et al., 2017).

2. Methods

2.1. Study area

The study area is the Salish Sea, which includes the estuarine system of the Strait of Georgia, Puget Sound, and the Juan de Fuca Strait on the west coast of North America. The Strait of Georgia, located between Vancouver Island and mainland British Columbia on the Pacific continental shelf of North America (Fig. 1), is the largest partially enclosed sea in the region, extending over 200 km in length and reaching depths beyond 350 m within its central region (Masson and Peña, 2009). Connections to the Pacific Ocean are through the Juan de Fuca Strait in the south, and the Johnstone Strait in the north. The region is highly productive and heavily influenced by terrestrial runoff from the Fraser River (Johannessen et al., 2003), which drives an estuarine circulation that is subject to wind and tidal mixing (Li et al., 2000; Sutherland et al., 2011). The outflow of the Fraser River typically peaks with a freshet in June, where flow can often be several times greater (average discharge 7391 m^3s^{-1}) than that of low winter values (1734 m^3s^{-1}) (Environmental Canada, 2014; Masson, 2002). The Skagit and Snohomish river systems dominate in Puget Sound, with freshwater influx peaking around June (maximum ~ 7000 m^3s^{-1}) (Sutherland et al., 2011; USGS, 2015). Because the northern Johnstone Strait is constricted by narrow channels, most of the estuarine exchange flows through the Juan de Fuca Strait in the south (Masson, 2002).

Biogeochemically, the Salish Sea is largely dynamic, both spatially and temporally. Phytoplankton abundance in the region has been shown to vary with the influence of the Fraser River plume, tidal mixing, wind speed strength, and cloud cover (Allen and Wolfe, 2013; Collins et al., 2009), with a maximum diatom bloom in the spring typically followed by a smaller fall bloom (Allen and Wolfe, 2013; Costa et al., 2014; Masson and Peña, 2009). A strong growth of diatoms occurs as light becomes less limited due to decreasing cloud cover and a near-surface vertical stratification, due to the significant freshwater flux, confining phytoplankton to a shallow well-lit surface layer (Masson and Peña, 2009). Chl*a* concentrations have been found to range from <1.00 $\mu g\ l^{-1}$ in the winter to >10.00 $\mu g\ l^{-1}$ during early spring (Harrison et al., 1983; Li et al., 2000; Masson and Peña, 2009).

Optically, the Salish Sea is also largely dynamic as a result of the biogeochemistry variability. Specifically, in the Strait of Georgia, the optical variability has been shown to correlate with the discharge of the Fraser River during the spring and summer time (Loos and Costa, 2010). At this period of the year, high loads of fine inorganic particles are discharged (Johannessen et al., 2006), resulting in high, wavelength independent, particulate scattering in these waters (Loos and Costa, 2010). Away from direct river influenced waters, an estuarine circulation exists for much of the region where absorption and scattering show spectral dependence. In these waters, total absorption was shown to be equally influenced by CDOM and particles (Loos and Costa, 2010). In northern waters, CDOM has been shown to dominate total absorption ($a_{cdom}(411) = 0.18{-}1.58\ m^{-1}$) and significantly contributed to attenuation of light as these waters are less influenced by the Fraser River plume (Loos and Costa, 2010).

2.2. Dataset

In situ data were collected for analysis of water biogeochemical and optical properties. In addition, above water optical data was measured or modeled using radiative transfer modeling for stations in which data could not be acquired. An empirical orthogonal function analysis was applied to the above water remote sensing reflectance ($R_{rs}(\lambda)$) data, along with a correlation analysis with the biogeochemical and optical data, to understand the drivers of $R_{rs}(\lambda)$ variability. Finally, a hierarchical clustering analysis was applied to group the $R_{rs}(\lambda)$ data into distinct classes.

In situ data were collected during five research cruises (September, October, March, June and July in 2012 and 2013), aboard the Canadian Coast Guard (CCG) *W.E. Ricker*, and bi-weekly trips, aboard a ship of opportunity BC Ferry *Queen of Alberni*, from Duke Point, Nanaimo, to Tsawwassen, Vancouver, during the same time period. The route of the research cruises followed a consistent pattern, thus guaranteeing that the sample stations were approximately at the same location. Measurements were acquired between 11 a.m. and 2 p.m. to mimic time of most ocean colour satellite acquisition and optimized sun illumination conditions. Water