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Estimating sea surface salinity in the northern Gulf of Mexico from satellite ocean color measurements

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ABSTRACT

Sea surface salinity (SSS) is an important parameter to characterize physical and biogeochemical processes, yet its remote estimation in coastal waters has been difficult because satellite sensors designed to "measure" SSS lack sufficient resolution and coverage, and higher-resolution ocean color measurements suffer from optical and biogeochemical complexity when used to estimate SSS. In the northern Gulf of Mexico (GOM), this challenge is addressed through modeling, validation, and extensive tests in contrasting environments. Specifically, using extensive SSS datasets collected by many groups spanning > 10 years and MODIS (Moderate Resolution Imaging Spectroradiometer) and SeaWiFS (Sea-Viewing Wide Field-of-View Sensor) estimated remote sensing reflectance (Rrs) at 412, 443, 488 (490), 555, and 667 (670) nm and sea surface temperature (SST), a multilayer perceptron neural network-based (MPNN) SSS model has been developed and validated with a spatial resolution of ~1 km. The MPNN was selected over many other empirical approaches such as principle component analysis (PCA), multi-nonlinear regression (MNR), decision tree, random forest, and supporting vector machines (SVMs) after extensive evaluations. The MPNN was trained by a back-propagation learning technique with Levenberg-Marquardt optimization and Bayesian regularization. The model showed an overall performance of root mean square error (RMSE) = 1.2, with coefficient of determination (R^2) = 0.86, mean bias (MB) = 0.0, and mean ratio (MR) = 1.0 for SSS ranging between ~1 and ~37 (N = 3640). Validation using an independent dataset showed a RMSE of 1.1, MB of 0.0, and MR of 1.0 for SSS ranging between ~27 and ~37 (N = 412). The model with its original parameterization has been tested in the Mississippi-Atchafalaya coastal region, Florida's Big Bend region, and in the offshore Mississippi River plume, with satisfactory performance obtained in each case. Comparison with concurrent Aquarius-derived SSS maps (110-km resolution) showed similar agreement in offshore waters as indicated above, but the new 1-km resolution SSS maps revealed more finer-scale features as well as salinity gradients in coastal waters. The sensitivity of the model to realistic model input errors in satellite-derived SST and Rrs was also thoroughly examined, with uncertainties in the model-derived SSS being always < 1 for SSS > 30. The extensive validation, evaluation, and sensitivity test all indicated the robustness of the MPNN model in estimating SSS in most, if not all, coastal waters and offshore plumes in the northern GOM. Thus, the model provided a basis for generating near real-time 1-km resolution SSS maps from satellite measurements. However, the model showed limitations when applied to regions with known algal blooms or upwelling as they both led to low Rrs in the blue bands that may be falsely recognized as caused by low SSS.

1. Introduction

1.1. Challenge in mapping sea surface salinity of coastal waters

Sea surface salinity (SSS) is an important parameter in understanding many physical and biogeochemical processes in coastal waters (Fennel et al., 2011; Xue et al., 2013). SSS data is used in support of studies examining the mixing between riverine freshwater and offshore oceanic water and changes in other water properties (Hu et al., 2004; Palacios et al., 2009; Devlin et al., 2015; Horner-Devine et al., 2015; Yang et al., 2015). Further, SSS is an important parameter in tracing the pathway of the riverine-delivered terrestrial substance (e.g. organic and inorganic carbon, nutrients) into the ocean, as well as examining the intensity of stratification and studying variations in water's optical properties, hypoxia, and algal blooms in coastal margins (Rabalais et al., 1996, 2002; Cannizzaro et al., 2013; Weisberg et al., 2014; O'Connor et al., 2016; Le et al., 2016).

However, obtaining SSS at synoptic scales with frequent coverage in

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coastal waters has proved difficult due to inadequate ship-based measurements (that lack of appropriate resolutions) or failures in satellite SSS measurement algorithms. The two existing satellite sensors, based on microwave remote sensing and designed to “measure” SSS from space, are the ESA SMOS (the Soil Moisture and Ocean Salinity) and NASA Aquarius/SAC-D. Yet the coarse spatial resolution (30–100 km) and low revisit frequency (3 days or more), along with the issue of land contamination, limit their use in observing the dynamic variations in SSS in coastal waters (Koblinsky et al., 2003; Lagerloef et al., 2008; Font et al., 2010; Kerr et al., 2010).

Recent advances in ocean color remote sensing have shown potentials in synoptic and frequent mapping of SSS (Wong et al., 2007; Ahn et al., 2008; Palacios et al., 2009; Marghany and Hashim, 2011; Urquhart et al., 2012; Bai et al., 2013; Geiger et al., 2013; Qing et al., 2013; Vandermeulen et al., 2014; Zhao et al., 2017). In these studies, SSS was modeled from apparent optical properties (AOPs) such as spectral remote sensing reflectance (Rrs, sr^{-1}), inherent optical properties (IOPs) such as absorption coefficient, or other satellite parameters such as Sea Surface Temperature (SST, °C) and chlorophyll-*a* concentrations (CHL, $mg\ m^{-3}$). Regardless of the method, the underlying principle is that colored dissolved organic matter (CDOM) is a good tracer of SSS in coastal oceans (Vodacek et al., 1997; Hu et al., 2003; Coble et al., 2004; Del Vecchio and Blough, 2004), and CDOM absorption coefficient (a_{CDOM}, m^{-1}) can be, at least in theory, estimated from ocean color measurements and then used to estimate SSS assuming conservative mixing for both (e.g., Siddorn et al., 2001; Johnson et al., 2003; Chen and Gardner, 2004; Hong et al., 2005; Guo et al., 2007; Bowers and Brett, 2008). Indeed, in river-dominated coastal regions, CDOM mainly comes from terrestrial inputs through river discharges and non-point source land runoff (Chester, 1990; Nelson et al., 2007). This plays a key role in determining the optical properties (especially Rrs) of coastal ocean waters. However, due to the distinct CDOM characteristics of each local river endmember and its seasonality, the relationship between a_{CDOM} and SSS may vary in space and time (Chen, 1999; Hu et al., 2003; Del Vecchio and Blough, 2004; Bowers and Brett, 2008; Bai et al., 2013; Geiger et al., 2013), making it impossible to apply a locally designed SSS algorithm to other regions. Adding to this difficulty are the uncertainties in the satellite-retrieved Rrs and a_{CDOM}; these uncertainties can cause a well-established, ship-based a_{CDOM} – SSS relationship to become unreliable. Such difficulties can be clearly seen from Fig. S1 in the supplemental materials for the northern Gulf of Mexico when satellite-derived a_{CDOM} was used to estimate SSS. Thus, in general, mapping SSS in coastal waters from space still represents a major challenge for the ocean color research community.

1.2. Study region and objectives

The study region is the northern Gulf of Mexico (GOM) that receives discharge from numerous rivers. The Mississippi River provides the largest river discharge into northern GOM. Ranking as the world's 8th largest river in freshwater discharge and sediment delivery, the Mississippi River system drains 41% of the land in the United States (Milliman and Meade, 1983). About 70% of the river's flow drains through the lower Mississippi River into the GOM, with the remaining 30% delivered to the Atchafalaya basin, and finally into the GOM (U. S. Army Corps of Engineers, 2008) forming the Mississippi/Atchafalaya River system (MARS). In addition to the MARS, there are some smaller rivers along the coast of the northern GOM, such as Suwannee, Pensacola, and Apalachicola Rivers; these also play significant roles in affecting the coastal water properties (Mattraw and Elder, 1984; Averett et al., 1994; Murrell et al., 2002). With large seasonal loadings of freshwater, inorganic and organic matters, and nutrients, from the MARS and other rivers, the northern GOM maintains an active ecosystem with dynamic physical and biogeochemical processes. Here, SSS plays an important role in the physical mixing between the MARS and GOM open waters (Xue et al., 2013), the hypoxia phenomenon induced by intensified biological activities and vertical stratification (Wiseman et al., 1997; Rabalais et al., 2002), and the distribution and variation of the carbonate properties such as total alkalinity (TA) and surface partial pressure of CO_2 (pCO_2) (Yang et al., 2015; Chen et al., 2016).

Synoptic SSS estimation in the northern GOM has been attempted in several published studies. Using data from SMOS and Aquarius, Fournier et al. (2016) examined the seasonal and interannual variations of SSS in the GOM. However, the study was limited by the coarse spatial resolution (30–100 km) and lack of coverage in coastal waters as a result of sensor limitations. Based on total absorption coefficients at 486 and 551 nm derived from the SNPP-VIIRS (Suomi National Polar-orbiting Partnership satellite with the Visual Infrared Imaging Radiometer Suite) measurements and SSS measurements from several nearshore stations, Vandermeulen et al. (2014) developed a simple SSS model using linear regression between SSS and absorption difference. Due to the dynamics and complexity of the northern GOM, only 65% of the data tested with the model showed a SSS uncertainty of ≤ 2; one possibility for this result is that the relationship between absorption difference and SSS may change in space and time. Indeed, although linear relationships between SSS and a_{CDOM} have been developed on a regional basis (Blough et al., 1993; Ahn et al., 2008; Palacios et al., 2009; Bai et al., 2013), in the northern GOM the SSS-a_{CDOM} relationship appears to be different in several studies (Hu et al., 2003; Del Castillo and Miller, 2008; Lohrenz et al., 2010). Such discrepancies indicate that unlike SSS, CDOM may not follow conservative mixing, and both CDOM production from phytoplankton degradation (Nelson et al., 1998, 2010; Twardowski and Donaghay, 2001; Stedmon and Markager, 2005) and CDOM photochemical bleaching (Chen and Gardner, 2004) may contribute to the variations in the SSS-a_{CDOM} relationship (Del Vecchio and Blough, 2004). Consequently, to date there has been no reliable model to estimate SSS from ocean color measurements in this region.

Extensive SSS data have been collected from the northern GOM by numerous groups and agencies. Acknowledging the limitations of SMOS and Aquarius, lack of reliable ocean color-based SSS models, the unstable SSS-a_{CDOM} relationship in the northern GOM, and high uncertainties in satellite-derived a_{CDOM} (Hu et al., 2003; Le and Hu, 2013; Mannino et al., 2014), the goal of the present study is to address the challenge of mapping SSS from ocean color measurements over the optically complex northern GOM, with the following specific objectives:

1) Develop a relatively robust model to estimate SSS at 1-km resolution from ocean color measurements;
2) Quantify uncertainties in the estimated SSS through extensive evaluations under various oceanographic conditions (e.g., Mississippi-Atchafalaya coastal region, Florida's Big Bend, and Mississippi River plume) and through sensitivity studies;
3) Understand the limitations of this approach in order to determine its applicability to time-series data.

The paper is structured as follows. Field and satellite data are presented first, and optical characteristics of the waters with different SSS ranges are analyzed. Secondly, methods in developing SSS models are briefly reviewed. Finally, in the Results and Discussion sections, the trained SSS model is statistically validated and evaluated under different conditions, with model sensitivities to the model inputs analyzed and model limitations investigated.

2. Data and methods

2.1. Datasets

2.1.1. Field data

To assure enough spatial and temporal coverage under all possible oceanographic conditions and measurement scenarios, we compiled all publically available SSS data collected over the past 20 years in the