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Remote estimation of surface pCO₂ on the West Florida Shelf

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ABSTRACT

Surface pCO₂ data from the West Florida Shelf (WFS) have been collected during 25 cruise surveys between 2003 and 2012. The data were scaled up using remote sensing measurements of surface water properties in order to provide a more nearly synoptic map of pCO₂ spatial distributions and describe their temporal variations. This investigation involved extensive tests of various model forms through parsimony and Principal Component Analysis, which led to the development of a multi-variable empirical surface pCO₂ model based on concurrent MODIS (Moderate Resolution Imaging Spectroradiometer) estimates of surface chlorophyll aconcentrations (CHL, mg m⁻³), diffuse light attenuation at 490 nm (Kd_Lee, m⁻¹), and sea surface temperature (SST, °C). Validation using an independent dataset showed a pCO₂ Root Mean Square Error (RMSE) of < 12 μatm and a 0.88 coefficient of determination (R²) for measured and model-predicted pCO₂ ranging from 300 to 550 uatm. The model was more sensitive to SST than to CHL and Kd Lee, with a 1 °C change in SST leading to a ~16 µatm change in the predicted pCO2. Application of the model to the entire WFS MODIS time series between 2002 and 2014 showed clear seasonality, with maxima (~450 µatm) in summer and minima (~350 µatm) in winter. The seasonality was positively correlated to SST (high in summer and low in winter) and negatively correlated to CHL and Kd_Lee (high in winter and low in summer). Inter-annual variations of pCO₂ were consistent with inter-annual variations of SST, CHL, and Kd_Lee. These results suggest that surface water pCO₂ of the WFS can be estimated, with known uncertainties, from remote sensing. However, while the general approach of empirical regression may work for waters from other areas of the Gulf of Mexico, model coefficients need to be empirically determined in a similar fashion.

1. Introduction

Atmospheric CO_2 has increased by 40% since the industrialization era (Sabine et al., 2004; Solomon et al., 2007). Correspondingly, oceanic uptake of CO_2 has resulted in ocean acidification and decreased surface water pH (by ~0.1 units) (Sun et al., 2012; Pachauri and Meyer, 2014), leading to ecological degradation and a decrease of marine biodiversity (Widdicombe and Spicer, 2008; Orr et al., 2005; Feely et al., 2012). Due to large spatial and temporal variations in surface water CO_2 partial pressure (pCO_2), the magnitude and even the sign of air/sea CO_2 fluxes can be highly variable (Takahashi et al., 2002, 2009, 2014; Sarma, 2003; Borges et al., 2005; Hofmann et al., 2011; Sarma et al., 2012; Chen et al., 2013; Wanninkhof et al., 2013). Accurate knowledge of surface pCO_2 distributions is therefore essential to quantify the ocean's role in carbon cycling.

A large number of studies have used field measurements to estimate air-sea CO₂ fluxes for both the open ocean and coastal sites (e.g., Takahashi et al., 2002, 2009, 2014; Tseng et al., 2011; Jiang et al.,

2008; Geilfus et al., 2012; Vandemark et al., 2011; Zhai et al., 2005). However, direct field observations are often limited in spatial and temporal coverage. While numerical models have also been used to estimate surface pCO₂ (e.g., Xue et al., 2014; Arruda et al., 2015), model results are strongly influenced by assumed initial conditions and can also be highly model-specific. In contrast, satellite remote sensing can provide frequent synoptic assessments of surface ocean properties, and in view of recent advances in surface pCO2 algorithm development (e.g., Ono et al., 2004; Sarma et al., 2006; Jamet et al., 2007; Telszewski et al., 2009; Hales et al., 2012; Nakaoka et al., 2013; Signorini et al., 2013; Bai et al., 2015), there is potential for the use of satellite remote sensing to augment direct field assessments of air/sea CO₂ fluxes. Nevertheless, except for two studies that focused on nearshore waters off the Mississippi River delta (Lohrenz and Cai, 2006; Lohrenz et al., 2010), such remote sensing approaches have rarely been applied to major ocean basins such as the Gulf of Mexico (GOM), a semi-enclosed sea of environmental and economic impor-

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Nomenclature		MODIS	Moderate Resolution Imaging Spectroradiometer
		MR	Mean Ratio
CDIAC	Carbon Dioxide Information Analysis Center	PCA	Principle Component Analysis
CHL	Chlorophyll-a Concentration	PCR	Principle Component Regression
GOM	Gulf of Mexico	RMSE	Root Mean Square Error
Kd_Lee	Diffuse light attenuation coefficient at 490 nm	SSS	Sea Surface Salinity
LC	Loop Current	SST	Sea Surface Temperature
MB	Mean Bias	USGS	U.S. Geological Survey
MLR	Multi-variate Linear Regression	WFS	West Florida Shelf
MNR	Multi-variate Nonlinear Regression		

With a surface area of 1.6 million km², the GOM encompasses the West Florida Shelf (WFS), Louisiana Shelf, Texas Shelf, Mexican Shelf, and the open Gulf (Robbins et al., 2009; Coble et al., 2010). As one of the most productive areas for fisheries in the world, it is essential habitat for numerous fish and wildlife species, and is likely to be strongly impacted by ocean acidification (Cai, et al., 2011; Wanninkhof et al., 2015). Thus, it is important to quantify the role of the GOM in modulating CO₂ flux (Takahashi et al., 2009). Based on field measurements, Takahashi et al. (2009) estimated the GOM as a CO2 source with a net flux of about 0.21 mol C/m²/year. However, with additional field observations, Robbins et al. (2014) reported that the GOM is a CO2 sink with a net flux near -0.19 mol C/m²/year. Using a 3-dimensional numerical model. Xue et al. (2014) estimated the GOM as a sink with a flux of -0.84 mol C/m²/year. Clearly, such discrepancies necessitate additional studies to better quantify CO₂ flux, and synoptic mapping of surface pCO₂ should play an important role. In particular, with continuous surface pCO2 collections in the GOM in recent years (see below for data sources), the application of satellite remote sensing can strongly contribute to a better understanding of surface pCO2 distributions and CO2 flux.

Within the GOM, of particular importance is the WFS between 24–31 °N and 80–85 °W (Fig. 1). The WFS is a broad carbonate-based shelf with a width of 220–275 km and a gentle slope, influenced by the Loop Current (LC) system as well as upwelling, river discharge, blooms of both harmful and non-harmful algae, summer and winter storms, and groundwater influx (Jolliff et al., 2003; Weisberg and He, 2003; Hu et al., 2005; Hu et al., 2006; Walsh et al., 2006; Benway and Coble,

2014). Although the GOM is typically characterized as being oligotrophic, the WFS is one of the most productive continental shelves in the United States, supporting numerous fisheries and diverse organisms (Saul et al., 2013; Chagaris et al., 2015). As one of the broadest continental shelves of United States (He and Weisberg, 2002), the WFS may play a big role in modulating $\rm CO_2$ flux in the GOM, and knowledge of synoptic surface $p\rm CO_2$ distributions as well as their temporal changes can help to quantify air-sea $\rm CO_2$ fluxes, biochemical and ocean acidification processes. However, despite significant efforts to collect surface $p\rm CO_2$ data through numerous ship surveys, and one study (Xue et al., 2014) to model $p\rm CO_2$ variability on the Louisiana Shelf and the GOM as a whole, little information is available for the WFS.

The objectives of this study are thus two-fold: (a) development of a remote sensing model to scale up ship-based surface $p\mathrm{CO}_2$ observations in order to take advantage of the more synoptic and frequent remote sensing observations for the WFS, and (b) application of the model to long-term remote sensing data to examine spatial-temporal distributions of surface $p\mathrm{CO}_2$ on the WFS. The present work is directed toward bridging knowledge gaps by providing, for the first time, monthly $p\mathrm{CO}_2$ distribution maps at medium resolution (1-km) and their temporal variations on the WFS.

2. Data and methods

2.1. A brief review of pCO2 remote sensing

While the details of different methods to estimate surface pCO₂

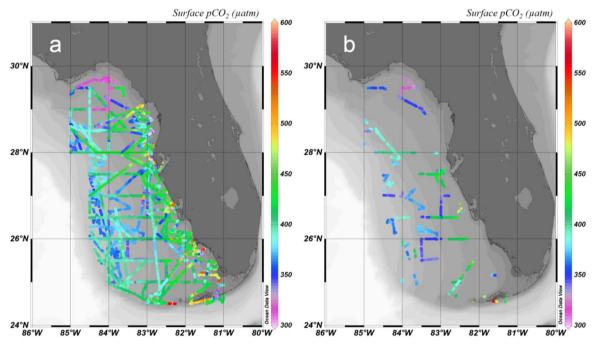


Fig. 1. (a) Spatial distributions of the field-measured pCO2 along the ship transects (Table 2). (b) The same field data where near-concurrent (±6 h) high-quality MODIS data exist.

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