PCO2 in Inland Waters

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The traditional field-based measurements of carbon dioxide (pCO2) for inland waters are a snapshot of the conditions on a particular site, which might not adequately represent the pCO2 variation of the entire lake. However, these field measurements can be used in the pCO2 remote sensing modeling and verification. By focusing on inland waters (including lakes, reservoirs, rivers, and streams), this paper reviews the temporal and spatial variability of pCO2 based on published data. The results indicate the significant daily and seasonal variations in pCO2 in lakes.

pCO2 remote sensing

satellites

inland waters

CO2 flux

1. Introduction

Inland waters are an important component of the global carbon cycle. They function as active pipes to transport and transform a large quantity of naturally and anthropogenically derived carbon [1][2][3][4]. They serve as passive conduits from soil to sea and also divert carbon to the atmosphere and sediment sink. Carbon exchange occurs through the vertical interactions between inland waters and the atmosphere, often in the form of greenhouse gases (GHGs). The globally averaged surface temperature (combining land and ocean) has increased by approximately 1.0 °C (0.8–1.2 °C) above the pre-industrial levels ^[5]. Rising emission of natural and anthropogenic GHGs is highly likely to be the dominant cause of the observed warming since the mid-20th century ^[6]. Carbon dioxide (CO₂) in the atmosphere is the most important GHG because it can enhance the greenhouse effect, with a contribution rate of 60%. A global CO₂ emission survey on inland waters indicated that 95% of the 6708 streams and rivers have a median partial pressure of carbon dioxide (pCO_2) greater than the atmospheric value, and 7939 lakes and reservoirs are supersaturated [3]. The CO₂ flux released by inland waters is of the same order of magnitude as land-atmosphere and land-ocean net carbon exchanges. Hence, long-term monitoring of pCO2 and CO₂ emissions from inland waters is essential for quantifying and understanding how inland waters contribute to the global carbon cycle $[\underline{Z}][\underline{8}][\underline{9}]$.

The response of regional inland waters to global change has attracted the attention of the international research community [6]. Over the past decade, most of the research efforts have been on refining CO₂ flux estimation at the regional and global scales [3][10][11][12][13]. Nevertheless, the quantification of the pCO_2 in inland waters is also important for accurately estimating CO2 flux in the water-atmosphere interface and understanding the role of CO₂ in inland waters in the Earth's carbon budget. Some studies reported about the significant spatial and temporal variations of the pCO_2 in lakes and rivers $\frac{[13][14][15][16][17]}{16}$ and the strong influence of ambient environment and river discharge on the pCO_2 of inland waters [18][19][20]. However, the current pCO_2 data of inland waters

remain uncertain due to the large discrepancy of pCO_2 in the global inland waters. Moreover, the variation in CO₂ flux estimation to the atmosphere stems not only from the limited spatiotemporal data availability, but also from various methods in an un-unified pCO_2 estimation approach $\frac{12}{21}$. The common methods include the direct measurement of in situ pCO₂ using an air-flushing equilibrator connected to an infrared photoacoustic gas analyzer [23][24]; the underway pCO₂ system [25]; the underwater sensors, e.g., C-SenseTM, HydroCTM-CO₂, and Franatech CO₂-sensor $\frac{[25][26]}{25}$; calculation of pCO₂ based on in situ pH, total alkalinity, water temperature, and salinity values of inland waters [27]; and estimation of pCO_2 based on the dissolved CO_2 concentration in the water ^[28]. There is a lack of an effective and generalized method to characterize the spatial and temporal dynamics of pCO₂ in detail, particularly in some regions with a large freshwater surface area and regions sensitive to climate change ^{[28][29]}. According to climate model projections, extreme climatic events (e.g., rainfall and flood) would increase in some regions [30][31]. Some studies showed that intense rainfall events and floods could modify the water-atmosphere exchange of CO2 [32][33][34]. It is necessary to develop a common method to estimate pCO2, which covers long-term records and large spatial coverage, so that we could better illustrate the potential impact of such events on pCO₂ and accurately quantify CO₂ flux and the role of inland waters in the global carbon cycle. Over the past two decades, remote sensing of pCO₂ in the water environment has received much attention due to its unique advantages against the traditional field-based technologies [35]. In addition, this method has the ability to achieve the simultaneous observation and comparison of pCO₂ values in different waters and different times over the same location. The assessment of pCO_2 variations based on multi-source remote sensing data has contributed greatly to the accurate quantification of CO₂ flux in the atmosphere-water interface at high-spatiotemporal resolution in the ocean and coastal waters [36][37][38][39], while a similar attempt has also been conducted in the inland waters [11][13][40][41].

2. Remote Sensing of pCO₂

According to existing theoretical analysis and research results, pCO_2 in water surface cannot be directly derived from satellite radiance. It is mostly an indirect measurement that requires the estimation of other variables first. The remote sensing of pCO_2 in water surface requires some environmental variables related to the pCO_2 controlling processes as indicators (e.g., water surface temperature (T), water salinity (S), plankton concentration (Chla), colored dissolved organic matter (CDOM), mixed layer depth). There is also some directly remote sensing research of the dissolved CO_2 concentration or pCO_2 by developing the estimation model based on satellite imagery-derived products. At present, while remote sensing technology has been successfully applied for the estimation of pCO_2 in water surface, most of these studies focused on ocean and coastal waters.

2.1. Remote Sensing Estimating pCO₂ in Marine and Coastal Waters

Research on remote sensing of pCO_2 in sea and coastal waters has received much attention in recent years. It is useful for the accurate description of the spatial-temporal heterogeneity of sea-surface CO_2 flux and for quantifying the ocean's role in the global carbon cycle ^{[39][42][43]}. Moderate-Resolution Imaging Spectroradiometer (MODIS) imagery and MODIS-derived products are more commonly used in these pCO_2 remote sensing inversion processes ^{[38][43][44][45]}. Related studies using statistical approaches and machine learning techniques have been

conducted in many seas and coastal sites (Figure 1), e.g., the Gulf of Mexico [36][46][47], East China Sea [48][49], Caribbean Sea ^[43], Bering Sea ^[39], and West Florida Shelf ^[42]. In general, the empirical algorithms (e.g., linear or multiple regression relationships) and machine learning approaches can work reasonably well with good pCO_2 inversion results in the specified areas $\frac{[36][38][47]}{2}$. However, pCO_2 in the open ocean and coastal regions often exhibits a profound spatiotemporal heterogeneity and is controlled by multiple factors. Due to incomprehension of pCO₂ variability mechanisms, these empirical algorithms can only function reliably for areas with available in situ pCO_2 data. Thus, more complex semi-analysis algorithms, combined with the analysis of the main mechanisms causing pCO_2 variability, have been developed in different coastal waters and seas, such as the first implementation of a mechanistic semi-analytic algorithm (MeSAA) in the East China Sea [39][46][49]. A satellitebased semi-mechanistic model was developed for the river-dominated Louisiana Continental Shelf ^[50], while a nonlinear semi-empirical model with the self-organizing map (SOM) was implemented in the Pacific coast of central North America ^[51]. Nevertheless, the existing semi-analytical algorithms also have limited applicability in different regions, primarily because of the difficulty in parameterizing and standardizing the physicochemical and biological influence on pCO2 in sea and coastal waters. In the process of constructing the pCO2 remote sensing algorithm/model, it is important to choose and develop accurate quantitative expressions relating satellite-derived parameters based on controlling mechanistic analysis, which can assist to better implement remote sensing of pCO_2 in the similar oceanic conditions.



Figure 1. Locations of published works on remote sensing of the surface *p*CO₂ in sea and coastal waters.

According to a survey of literature, the net sea–air CO_2 flux of the global ocean is approximately 1.4 Pg y⁻¹ ^[52], and this value is subjected to large uncertainty. The air–sea CO_2 fluxes are different depending on the latitudinal and ecosystem diversity of the coastal ocean (particularly near-shore systems). The physical-biogeochemical distinction (including ocean-dominated margin and river-dominated ocean margin) has significant influence on the sources'/sinks' role of coastal waters ^[53]. In addition, the marginal seas at high and temperate latitudes often act as sinks of atmospheric CO_2 ; at subtropical and tropical regions, the marginal seas in these two climatic zones act as

sources of atmospheric CO_2 ^[54]. When integrating CO_2 fluxes in the coastal ocean at the global scale, the diversity, latitudes, and seasonal biological effect on ecosystems should be fully considered.

2.2. Remote Sensing of pCO₂ and CO₂ Fluxes for Inland Waters

Typically, inland waters are characterized by the supersaturated, dissolved CO₂ concentrations. However, there are huge differences in optical properties, physicochemical environments, trophic status, and circulation of materials between inland waters and ocean/coastal waters [11][13][40][41]. Some effective remote sensing algorithms and models for pCO₂ in ocean/coastal waters cannot be used directly for that in inland waters. Considering the influencing factors and mechanisms of surface pCO₂ in inland waters, some remote sensing algorithms for pCO₂ in inland waters have been developed based on the relationship between pCO2 and the retrieved water biogeochemical and optical parameters, e.g., chromophoric dissolved organic matter (CDOM) optical property, algal productivity, and water surface temperature [41]. Earlier studies demonstrated that the temporal and spatial distributions of pCO_2 in inland waters often exhibited high heterogeneity, which resulted in a large uncertainty in lake CO_2 flux calculations. Satellite observations of pCO_2 in inland waters could achieve a relatively high frequency and continuous, large-scale, and long-term data compared to field surveys. There are growing studies in this area in recent years despite a small number of published works. Combining with a high-resolution (25-m resolution), stream network map based on remote sensing, a Random Forest model was applied to predict the stream pCO_2 with an average of 1134 µatm (range: 154–8174 µatm) in Denmark, Sweden, and Finland ^[55]. Estimations of inland waters' CO₂ emissions have been realized in relation to terrestrial net primary production, which can be obtained from a global data set based on remote sensing, such as in a temperate stream network [56] and in boreal lakes [13]. More recently, optical indicators generated from satellite-derived variables have been utilized to estimate pCO2 indirectly in some rivers and lakes based on the strong relationship between them, such as CDOM optical properties used in the Lower Amazon River [31] and a turbidity index used in the Swedish lakes Mälaren and Tämnaren [30]. Nevertheless, the direct application of the long-term satellite products to estimate pCO₂ or dissolve CO₂ in inland waters is still in its infancy. The long-term series mapping of dissolved CO₂ pattern based on the remote sensing technology was conducted in Lake Taihu, China, which developed a dissolved CO₂ estimation model based on MODIS-derived products. It was applied to perform the spatiotemporal distribution analysis of dissolved CO₂ concentrations from 2003 to 2018 ^[22]. MERIS products have also been used to estimate lake pCO_2 [40].

When using long-term remote sensing imagery to directly estimate the CO₂ concentration or pCO₂ in waters or retrieving pCO₂ in water from some relevant environmental remote sensing indicators based on stable relationship ^{[38][41][50]}, it should be noted that the retrieved CO₂ concentration or pCO₂ values are the instantaneous value at the satellite transit time. The previous studies showed some pronounced changes in the CO₂ concentration over a day and seasons ^{[15][22][57]}. To achieve the transformation of retrieved pCO₂ values from an instant to hours/days, some researchers have established the relationship between instantaneous lake CO₂ concentration/pCO₂ at the regular satellite flyover and the daily/weekly mean value ^{[15][22][58]} by using the satellite estimation results to extrapolate the daily/weekly CO₂ mean values. In addition, combined with the in situ measured values of the diurnal pCO₂ variation and seasonal pCO₂ variation in a lake, we could realize the conversion of the daily value to

the seasonal mean value of the lake's CO_2 through cross verification between different sensors with different time resolutions. More observations and additional efforts would be needed to achieve them in the further studies.

In fact, researchers have a full understanding of biogeochemical mechanism of CO_2 generation and consumption in inland waters. Most of the determining and influence factors of pCO_2 or dissolved CO_2 in different inland waters have been elucidated. Some of these factors can be derived from satellite data, e.g., lake surface temperature, chlorophyll-a concentration, latitude, dissolved organic carbon (DOC), and solar radiation absorption. Therefore, in principle, it is possible to identify the spatiotemporal distribution of pCO_2 in a specific lake or river using the satellite-derived variables and realize the long-term estimations. However, the accuracy and universality of the prediction models should be developed and evaluated as a priority in the large-scale estimation. Nevertheless, it is known that the relationships in the prediction models can vary among different lakes and lake regions, which is the current challenge of the pCO_2 remote sensing in inland waters ^{[22][40][41][58][59][49][50][60][61]}. Due to the great influence of outside source input, the geochemical processes of inland lakes can show strong spatial heterogeneity, and the influence factors of the pCO_2 in surface water are often coupled together. This leads to the unstable, non-universal relationship between pCO_2 and its indicators among different lakes and lake regions and the large uncertainties from such extrapolations. Consequently, the development of the inverse models based on dissolved biogeochemical processes and the machine learning algorithm based on lots of measurement data may have better applicability over longer periods and across larger spatial scales.

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