Harmonization of global surface ocean pCO2 mapped products and their flux calculations; an improved estimate of the ocean carbon sink

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Abstract. Air-sea flux of carbon dioxide (CO2) is a critical component of the global carbon cycle and the climate system with the ocean removing about a quarter of the CO2 emitted into the atmosphere by human activities over the last decade. A common approach to estimate this net flux of CO2 across the air-sea interface is the use of surface ocean CO2 observations and the computation of the flux through a bulk parameterization approach. Yet, the details for how this is done in order to arrive at a global ocean CO2 uptake estimate varies greatly, unnecessarily enhancing the uncertainties. Here we reduce some of these uncertainties by harmonizing an ensemble of products that interpolate surface ocean CO2 observations to near global coverage. We propose a common methodology to fill in missing areas in the products and to calculate fluxes and present a new estimate of the net flux. The ensemble data product, SeaFlux (Gregor & Fay (2021), doi.org/10.5281/zenodo.4133802, https://github.com/luke-gregor/SeaFlux), accounts for the diversity of the underlying mapping methodologies. Utilizing six global observation-based mapping products (CMEMS-FFNN, CSIR-ML6, JENA-MLS, JMA-MLR, MPI-SOMFFN, NIES-FNN), the SeaFlux ensemble approach adjusts for methodological inconsistencies in flux calculations that can result in an average error of 15% in global mean flux estimates. We address differences in spatial coverage of the surface ocean CO2 between the mapping products which ultimately yields an increase in CO2 uptake of up to 19% for some products. Fluxes are calculated using three wind products (CCMPv2, ERA5, and JRA55). Application of an appropriately scaled gas exchange coefficient has a greater impact on the resulting flux than solely the choice of wind product. With these adjustments, we derive an improved ensemble of surface ocean pCO2 and air-sea carbon flux estimates. The SeaFlux ensemble suggests a
global mean uptake of CO₂ from the atmosphere of 1.92 +/− 0.35 PgC yr⁻¹. This work aims to support the community effort to perform model-data intercomparisons which will help to identify missing fluxes as we strive to close the global carbon budget.

1 Introduction

Surface ocean partial pressure of CO₂ (pCO₂) observations play a key role in constraining the global ocean carbon sink. This is because variations in surface ocean pCO₂ is the driving force governing the exchange of CO₂ across the air-sea interface, which is commonly described through a bulk formula (Garbe et al. 2014; Wanninkhof 2014):

\[ \text{Flux} = k_w \cdot sol \cdot (pCO_2 - pCO_2^{\text{atm}}) \cdot (1 - ice) \]  

(1)

where \( k_w \) is the gas transfer velocity, \( sol \) is the solubility of CO₂ in seawater, in units mol m⁻³ µatm⁻¹, \( pCO_2 \) is the partial pressure of surface ocean CO₂ in µatm, and \( pCO_2^{\text{atm}} \) in units of µatm represents the partial pressure of atmospheric CO₂ in the marine boundary layer. Finally, to account for the seasonal ice cover in high latitudes the fluxes are weighted by 1 minus the ice fraction (ice), i.e. the open ocean fraction.

With the increasing number of observations of pCO₂ available in each new release of the Surface Ocean Carbon Dioxide Atlas (SOCAT; Bakker et al. 2016) and the adoption of various pCO₂ mapping techniques, multiple observation-based estimates of the pCO₂ field are now publicly available and updated on an annual basis. Despite these advancements, the intercomparison of the products’ flux values is hindered (1) by different areal coverage and (2) by a lack of a systematic approach to calculate the sea-air CO₂ flux from pCO₂ (Table A1). These differences in flux calculations introduce uncertainty in comparisons between the products as well as with their comparisons to Global Ocean Biogeochemistry Models (GOBM). In this work, we harmonize these product’s flux estimates, specifically addressing three key differences between product methodologies. The resulting flux estimates can then be more meaningfully compared.

The first step addresses the variable spatial coverage of current pCO₂ products. Some of the current mapped products only cover roughly 90% of the ocean surface, missing coastal and high latitude regions. A newly released global pCO₂ climatology product (Landschützer et al. 2020b) includes coverage in the coastal and Arctic regions. We use this climatology to fill any missing areas in each individual product to create a consistent full global ocean coverage.

The second methodological step is the choice of flux parameterization, and appropriate scaling of wind speed data. Roobaert et al. (2018) present uncertainty in air-sea carbon flux induced by various parameterizations of the gas transfer velocity and
wind speed data products. Utilizing the MPI-SOMFFN pCO$_2$ product (Landschützer et al. 2020a) and a quadratic parameterization (Wanninkhof 1992) they find flux estimates that diverge by 12% depending on the choice of wind speed products. Additionally, they find regional discrepancies to be much more pronounced than global differences, specifically highlighting the equatorial Pacific, Southern Ocean, and North Atlantic as regions most impacted by the choice of wind product. Roobaert et al. (2018) stress that to minimize the uncertainties associated with the wind speed product chosen, the global coefficient of gas transfer must be individually calculated for each (Wanninkhof 1992, 2014). In this work, we assess the impact of wind speed product choice and scaling on six pCO$_2$ products’ calculated air-sea flux estimates. By applying a consistent flux calculation methodology to each pCO$_2$ product, we minimize the methodological divergence of fluxes within the ensemble.

SeaFlux provides a more consistent approach specifically targeting the most commonly used pCO$_2$ data products to deliver an end product for consistent intercomparisons within assessment studies such as the Global Carbon Budget (Friedlingstein et al. 2020; Hauck et al. 2020). By first addressing differences in spatial coverage between the observation-based products we are able to better present a true global pCO$_2$ estimate for each product. This SeaFlux package also provides a means to normalize the gas transfer velocity to a consistent $^{14}$C inventory. By calculating fluxes using multiple scaled gas transfer velocities for different wind products, we present a methodologically consistent database of air-sea CO$_2$ fluxes. The SeaFlux package is an ensemble data product along with documented code allowing the community to reproduce consistent flux calculations from various data-based pCO$_2$ reconstructions.

2. Methods

The SeaFlux method is based on six observation-based pCO$_2$ products and spans years 1988-2018 (Table 1). These six include three neural network derived products (MPI-SOMFFN, CMEMS-FFNN, NIES-FNN), a mixed layer scheme product (JENA-MLS), a multiple linear regression (JMA-MLR), and a machine learning ensemble (CSIR-ML6). These select products are included as they have been regularly updated to extend their time period and incorporate additional data that comes with each annual release of the SOCAT database.

All of these methods provide full three-dimensional fields (latitude, longitude, time) of the sea surface partial pressure of CO$_2$ (pCO$_2$) and the air-sea CO$_2$ flux. In their original form each product may utilize different choices for the inputs to Equation 1 (Table A1). In this work recompute the fluxes using the following inputs to the bulk parameterization approach Equation 1: $k_w$ is the gas transfer velocity (further discussed in Sect. 2.3), sol is the solubility of CO$_2$ in seawater, in units mol m$^{-3}$ uatm$^{-1}$, calculated using the formulation by Weiss (1974), EN4 salinity (Good et al. 2013), Operational Sea Surface Temperature and Sea Ice Analysis (OSTIA) sea surface temperature (Good et al. 2020), and European Centre for Medium-Range Weather Forecasts (ECMWF) ERA5 sea level pressure (Hersbach et al. 2020); ice is the sea ice fraction from OSTIA
(Good et al. 2020); $p_{CO_2}$ is the partial pressure of oceanic $CO_2$ in $\mu atm$ for each observation-based product after filling as discussed in Sect. 2.1, and $p_{CO_2}^{atm}$ is the dry air mixing ratio of atmospheric $CO_2$ ($x_{CO_2}$) from the ESRL surface marine boundary layer $CO_2$ product available at https://www.esrl.noaa.gov/gmd/ccgg/mbl/data.php (Dlugokencky et al. 2017) multiplied by ERA5 sea level pressure (Hersbach et al. 2020) at monthly resolution, and applying the water vapor correction according to Dickson et al. (2007).

Flux is defined positive upward, i.e., $CO_2$ release from the ocean into the atmosphere is positive, and uptake by the ocean is negative. In the following sections we discuss the three steps that have the greatest impact on the inconsistencies between unadjusted flux calculations in the six $p_{CO_2}$ products and the approach that we utilize for the SeaFlux ensemble product.

2.1 Step 1: Area filling

Machine learning methods aim to maximize the utility of the existing in situ observations by extrapolation using various proxy variables for processes influencing changes in ocean $p_{CO_2}$. Extrapolation with these independently observed variables is possible due to the nonlinear relationship between $p_{CO_2}$ in the surface ocean and the proxies that drive these changes. However, not all of the proxy variables have complete global ocean coverage for all months, so the resulting $p_{CO_2}$ products are limited by the extent of the proxy variables (Figure 1). Additionally, in coastal regions there is the potential that different relationships of $p_{CO_2}$ are expected than in the open ocean, thus limiting the extrapolations. In contrast, the mixed layer scheme (utilized by the JENA-MLS product) does not suffer from such missing areas but does not distinguish between coastal and open ocean. While the area extent of the available air-sea flux estimates varies between products, there are consistent patterns; nearly all products cover the open ocean, whereas larger differences exist in the coverage of coastal regions, shelf seas, marginal seas and the Arctic Ocean.

To account for differing area coverage, past studies (Friedlingstein et al. 2019, 2020; Hauck et al. 2020) have adjusted simply by scaling based on the percent of the total ocean area covered by each observation-based product. This does not account for the fact that some areas have $CO_2$ flux densities that are higher or lower than the global average (Table 1,3). Thus, the magnitude of the adjustment by area-scaling is likely an underestimate (McKinley et al. 2020). One specific example is the northern high latitudes where coverage by the six products varies substantially. Similarly, three products provide estimates in marginal seas such as the Mediterranean while the other three products have no reported $p_{CO_2}$ values here. Shutler et al (2016) report that subtle differences in regional definitions can cause differences of >10% in the calculated net fluxes.

To address the inconsistent spatial coverage in products we utilize a newly released open and coastal merged climatology product (MPI-ULB-SOMFFN; Landschützer et al. 2020b) that is a blend of the coastal ocean SOMFFN mapping method (Laruelle et al. 2017) and the open ocean equivalent (MPI-SOMFFN; Landschützer et al. 2020a), but which now includes
missing coastal ocean regions, marginal seas and the full Arctic Ocean. For each observationally-based product, we fill missing grid cells with a scaled value based on this global-coverage climatology (Figure 2). The scaling accounts for year-to-year changes in pCO$_2$ in the missing areas (given that the extended MPI-ULB-SOMFFN product is a monthly climatology centered on year 2006) and is obtained as follows.

To extend the open and coastal merged monthly climatology (MPI-ULB-SOMFFN) to 1988-2018, we calculate a global scaling factor based on the product-based ensemble mean pCO$_2$ for regions which are covered consistently by all six pCO$_2$ products. We first mask all pCO$_2$ products to a common sea mask before taking an ensemble mean (pCO$_2^{ens}$). Next, we divide this ensemble mean by the MPI-ULB-SOMFFN climatology (pCO$_2^{clim}$) at monthly 1° by 1° resolution (Equation 2).

The monthly scaling factor ($sf_{pCO2}$) is calculated by taking the mean over the spatial dimensions.

$$sf_{pCO2} = \text{mean}_{x,y} \left( \frac{pCO_{2}^{ens}}{pCO_{2}^{clim}} \right)$$  \hspace{1cm} (2)

where $sf_{pCO2}$ is the one-dimensional scaling factor (time dimension), $pCO_{2}^{ens}$ is the ensemble mean of all pCO$_2$ products at three-dimension, monthly 1° by 1° resolution, $pCO_{2}^{clim}$ is the MPI-ULB-SOMFFN climatology, also at three-dimension but limited to just one climatological year. The $x$ and $y$ indicate that we take the area-weighted average over longitude ($x$) and latitude ($y$) resulting in the monthly scaling value. If a product mean is exactly equal to the climatology mean, the scaling factor is 1. Value ranges from 0.91 to 1.06 over the 31-year time period.

The one-dimensional scaling factor is then multiplied by the MPI-ULB-SOMFFN climatology for each spatial point resulting in a three-dimensional scaled filling map. These values are then used to fill in missing grid cells in each observation-based product.

Globally, the adjustments are all less than 20% of the total flux, with the mean adjustment for the six products at 9%. In the Northern Hemisphere however, the filling process can drive adjustments of up to 35% (Table 3). As expected, the observationally-based products with more complete spatial coverage tend to have smaller flux adjustments, however the impact on the final CO$_2$ flux depends on the ∆pCO$_2$ and wind speed of the areas being filled (Figures 2-3, Table 1,3). The only product that does not change during this adjustment process is the JENA-MLS mixed layer scheme-based product (Rödenbeck et al. 2013) which is produced with full spatial coverage and therefore needs no spatial filling.

Our approach is not without its own assumptions and limitations. We rely on a single estimate of the missing pCO$_2$ in coastal ocean regions, marginal seas, and the full Arctic Ocean, given that this is the only publicly available product currently
existing. Nevertheless, the fact that common missing areas along coastal regions and marginal seas are reconstructed using specific coastal observations provides a step forward from the linear-scaling approach currently used by the Global Carbon Budget (Friedlingstein et al. 2019, 2020). Further confidence is provided by previous research showing that climatological relevant signals, i.e. mean state and seasonality, are well reconstructed by the MPI-SOMFFN method (Gloege et al. 2021).

Furthermore, our scaled filling methodology assumes that pCO₂ in the missing ocean regions is increasing at the same rate as the common area of open-ocean pCO₂ used to calculate the scaling factor. Research from coastal ocean regions and shelf seas reveal that, in spite of a large spatial heterogeneity, this is a reasonable first order approximation (Laruelle et al. 2018). While our approach has a constant scaling factor for the missing ocean areas regardless of latitude we acknowledge that this could be improved with increased understanding.

### 2.2 Step 2: Wind product selection

Historical wind speed observations (including measurements from satellites and moored buoys) are aggregated and extrapolated through modeling and data assimilation systems to create global wind reanalyses. These reanalyses are required to compute air-sea gas exchange. Air-sea flux is commonly parameterized as a function of the gradient of CO₂ between the ocean and the atmosphere with wind speed modulating the rate of the gas exchange (Equation 1). Each of these wind reanalyses has strengths and weaknesses, specifically on regional and seasonal scales (Chaudhuri et al. 2014; Ramon et al. 2019) but all are considered reasonable options by the community (Roobaert et al. 2018). We use three wind reanalysis products for completeness: the Cross-Calibrated Multi-Platform v2 (CCMP2, Atlas et al. 2011), the Japanese 55-year Reanalysis (JRA-55, Kobayashi et al. 2015), and the European Centre for Medium-Range Weather Forecasts (ECMWF) ERA5 (Hersbach et al. 2020). The wind speed (U₁₀) is calculated at the native resolution of each wind product from the u- and v-components of wind. Details of each wind product are shown in Table A2.

### 2.3 Step 3: Calculation of gas exchange coefficient

We employ the quadratic windspeed dependence of the gas transfer velocity (Wanninkhof 1992) and calculate the piston velocity (kw) for each of the wind reanalysis products as

\[
kw = a \cdot \langle U^2 \rangle \cdot (Sc/660)^{-0.5}
\]

where the units of kw are in cm h⁻¹, Sc is the dimensionless Schmidt number, and \( \langle U^2 \rangle \) denotes the second moment of average 10-m height winds (m s⁻¹). We choose the quadratic dependence of the gas transfer velocity as it is widely accepted and used in the literature (Wanninkhof, 1992). Observational and modeling studies have often suggested that different
parametrizations could be more appropriate under specific conditions (Fairall et al. 2000; Nightingale et al. 2000; McGillis et al. 2001; Krakauer et al. 2006); however, recent direct carbon dioxide flux measurements made in the high latitude Southern Ocean confirm that even in this high wind environment, a quadratic parameterization fits the observations best (Butterworth & Miller 2016). Future updates of the SeaFlux product will include options for other parameterizations.

We calculate the square of the wind speed at the native resolution of each wind product and then average it to 1° by 1° monthly resolution (see Table A2). The order of this calculation is important as information is lost when resampling data to lower resolutions because of the concavity of the quadratic function. For example, if the second moment were calculated from time-averaged wind speeds, it would result in an underestimate of the gas transfer velocity (Sarmiento and Gruber 2006; Sweeney et al. 2007). The resulting second moment is equivalent to \( \langle U^2 \rangle = U_{\text{mean}}^2 + U_{\text{std}}^2 \) where \( U_{\text{mean}} \) and \( U_{\text{std}} \) are the temporal mean and standard deviation calculated from the native temporal resolution of \( U \).

In addition to the choice of wind parameterization, large differences in flux can result due to the scaling coefficient of gas transfer (\( a \)) that is applied when calculating the global mean piston velocity. This constant originates from the gas exchange process studies (Krakauer et al. 2006; Sweeney et al. 2007; Müller et al. 2008; Naegler 2009) which utilize observations of radiocarbon data from the GEOSecs and WOCE/JGOFS expeditions (Key et al. 2004). The \(^{14}\)C released from nuclear bomb testing (hence bomb-\(^{14}\)C) in the mid twentieth century has since been taken up by the ocean. The number of bomb-\(^{14}\)C atoms in the ocean, relative to the pre-bomb \(^{14}\)C, can thus be used as a constraint on the long-term rate of exchange of carbon between the atmosphere and the ocean. A probability distribution of wind speed is used to optimize the coefficient of gas transfer based on these observed natural and bomb \(^{14}\)C invasion rates. This coefficient must be individually calculated and is not consistent for each wind product. Further, the gas transfer velocity used by the different \( pCO_2 \) mapping products are not scaled to the same bomb-\(^{14}\)C estimate (Table A1). The range of the different bomb-\(^{14}\)C estimates is within the range of the uncertainty from the associated studies (Naegler, 2009), but the choice would introduce inconsistency that is easily addressed here.

We scale the gas transfer velocity to a bomb-\(^{14}\)C flux estimate of 16.5 cm hr\(^{-1}\) as recommended by Naegler (2009). The coefficient (\( a \)) is calculated for each wind product via a cost function which optimizes the coefficient of gas transfer

\[
a = k_w \cdot \langle U^2 \rangle^{-1} \cdot \left( \frac{Sc}{660} \right)^{0.5} \cdot (1 - ice)
\]

where parameters are as defined in Equation 3. The units of the coefficient \( a \) are \((\text{cm h}^{-1}) (\text{m s}^{-1})^{-2}\). Global winds from the wind speed products differ and therefore even with the same bomb-\(^{14}\)C observations the scaled coefficient (\( a \)) can have a
40% range (Wanninkhof 2014). By determining the optimal $a$ coefficient for each of the reanalysis winds, uncertainty in the global fluxes can be decreased. Our scaled coefficients (Table 2) correspond well with the estimate of Wanninkhof (2014) who uses the CCMP wind product to estimate $a$ as 0.251. Differences in the coefficient will also result from the time period considered and definition of global area and ice fraction applied in the calculation.

This scaling of the gas exchange coefficient ($a$) for each wind product is an essential, and an inconsistently applied step (Table A1), that has large implications for air-sea flux estimates (Figure 4). Without individual scaling, and instead utilizing a set value for the gas transfer coefficient ($a$) regardless of wind product, our results show that calculated global fluxes could be as high as 9% different depending on which $pCO_2$ and wind reanalysis product considered (Roobaert et al. 2018).

2.4 Further parameters for flux calculation

The remaining parameters of Equation 1 are the solubility of CO$_2$ in seawater ($sol$), the atmospheric partial pressure of CO$_2$ ($pCO_2^{atm}$), and the area weighting to account for sea ice cover. While the choices of products used for these parameters can also result in differences in flux estimates, the impacts are much smaller as compared with the parameters discussed above.

Atmospheric $pCO_2$ is calculated as the product of surface $xCO_2$ and sea level pressure corrected for the contribution of water vapor pressure. The choice of the sea level pressure product, or absence of the water vapor correction can have small, but not insignificant, impact on the calculated fluxes. Additionally, some products utilize the output of an atmospheric CO$_2$ inversion product (e.g. CarboScope, Rödenbeck et al. 2013; CAMS CO$_2$ inversion, Chevallier, 2013) which can introduce differences in the flux estimate outside of the sources related to a product’s surface ocean $pCO_2$ mapping method. Importantly, we do not advocate that our estimate of $pCO_2^{atm}$ is an improvement over other estimates thereof; rather we provide an estimate of $pCO_2^{atm}$ that has few assumptions and leads to a methodologically consistent estimate of $\Delta pCO_2$. We maintain the same philosophy in our estimates of solubility of CO$_2$ in seawater and sea-ice area weighting and therefore we do not elaborate on them here.

3. Results and Discussion

3.1 SeaFlux air-sea CO$_2$ flux calculation

Following Equation 1, CO$_2$ flux is calculated individually for each of the six observation-based products with each available wind product (CCMPv2, ERA5, JRA55) as discussed in Sect. 2.2 (Table 4). Since we account for spatial coverage differences via our filling method (Sect. 2.1), taking a global mean flux for each of the data products is now straightforward. Figure 4 shows the difference these wind products generate on the resulting global mean flux of the CSIR-ML6 product as
one example (other products in Figure A2). The three wind products show very consistent fluxes throughout the time series, however the importance of appropriate scaling of the gas exchange coefficient \((a)\) is evident by the significant differences between global mean fluxes calculated with unscaled and scaled \(a\) value (Figure 4). It is clear that the impact of applying the appropriate gas exchange coefficient through proper scaling has a larger impact on the resulting flux time series than solely the choice of wind product.

3.2 SeaFlux ensemble flux

By calculating each product’s flux using these consistent methods, we permit for a more accurate comparison of fluxes and increase confidence in the SeaFlux product ensemble mean flux estimate of \(-1.92 \pm 0.35\) PgC yr\(^{-1}\) (Table 4). Here, the stated uncertainty represents \(2\sigma\) as calculated from the 18 realizations of flux included in the SeaFlux ensemble (six pCO\(_2\) products and three wind products). This result is further strengthened by the use of multiple wind products which we consider to be independent estimates for the purpose of the uncertainty calculation. These flux values will be different from those produced by the observation-based pCO\(_2\) product’s original creator, both spatially and on the mean (Figure 5, Table A1, A3). However, by calculating fluxes using this standardized approach we have higher confidence in the uncertainties and in the ensemble mean of global fluxes.

3.3 Issues not addressed by SeaFlux

While the SeaFlux data set allows us to standardize much of the calculation of air-sea carbon flux, the community is still working towards consensus on other issues that impact this estimate. One source of uncertainty has been raised by Watson et al. (2020) who contend that a correction should be applied to pCO\(_2\) observations to account for the vertical temperature gradient between the ship water intake depth and the surface skin layer where gas exchange actually takes place. A further correction should be applied when calculating fluxes to account for the “cool skin” effect caused by evaporation (Woolf et al. 2016; Watson et al. 2020). Applying these corrections results in an increasing CO\(_2\) sink by up to 0.9 PgC yr\(^{-1}\) (Watson et al. 2020). Here, we do not take such corrections into account for two reasons. Firstly, the skin temperature correction to pCO\(_2\) needs to be applied directly to the measurements and not the final interpolated pCO\(_2\) from the data products. Hence, it is up to the developers of the SOCAT dataset and the developers of the pCO\(_2\) mapping products to decide on the inclusion of this correction. It would then be up to the developers of the data products to update their mapped products. Secondly, the cool skin correction would be equally applied to all methods and would not contribute to the inconsistencies that we are trying to address here. As the ocean carbon community moves towards consensus on such issues, the SeaFlux product will be updated to include revised protocols.

To compare these estimates of contemporary air-sea net flux (\(F_{\text{net}}\)) from surface ocean pCO\(_2\) with estimates of the anthropogenic carbon flux (\(F_{\text{ant}}\)) from interior data (Mikaloff Fletcher et al. 2006; DeVries 2014; Gruber et al. 2019), or from global ocean biogeochemical models (Friedlingstein et al. 2020; Hauck et al. 2020), it is necessary to account for the
outgassing of natural carbon which was supplied to the ocean by rivers as well as the non-steady state behavior of the natural carbon cycle (Hauck et al. 2020). Work is ongoing to quantify the lateral river carbon flux transported into the coastal and open oceans. Current estimates are 0.23 PgC yr\(^{-1}\) (Lacroix et al. 2020), 0.45 PgC yr\(^{-1}\) (Jacobsen et al. 2007), and 0.78 PgC yr\(^{-1}\) (Resplandy et al. 2018) with the regional distribution of these inputs remaining unclear (Aumont et al. 2001; Lacroix et al. 2020). Quantification of non-steady state behavior of the natural carbon cycle has only recently been proposed and significant uncertainty remains, with a magnitude range of 0.05-0.4 PgC/yr for 1994-207 (Gruber et al. 2019, McKinley et al. 2020). Similar to the “cool skin” correction suggested by Watson et al. (2020) discussed above, in this work we have not included a revision for this riverine input as it would not contribute to the inconsistencies between the different products for \(F_{\text{net}}\) itself, which is our focus.

4. Data Availability

Data (Gregor & Fay 2021) is available on Zenodo (https://doi.org/10.5281/zenodo.4133802) and the software used to generate this data is available on GitHub (https://github.com/luke-gregor/SeaFlux).

5. Conclusions

We introduce a standardized approach for flux calculations from observationally-based pCO\(_2\) products. The SeaFlux approach for flux calculations from available surface ocean pCO\(_2\) estimates enhances consistency and comparability for this ensemble of products. Specifically, we address the two largest sources of divergence, namely the differences in spatial coverage between the products, and the scaling of the gas transfer velocity for available wind speed products based on global \(^{14}\)C-based constraints. The area adjustment is the largest contributor to the methodological discrepancies, resulting in an increase in CO\(_2\) uptake of 0-20\% relative to the original, possibly incomplete coverage (depending on pCO\(_2\) product). The global scaling of the gas transfer velocity can change the CO\(_2\) flux on average by 6\% relative to non-standardized flux calculations. The impact of applying the appropriate gas exchange coefficient through proper scaling has a larger impact on the resulting flux time series than solely the choice of wind product. By accounting for these sources of differences, the global mean calculated air-sea carbon flux calculated from the six available products is adjusted by up to 24\%. The ensemble mean air-sea carbon flux is estimated to be \(-1.92 \pm 0.35\) PgC yr\(^{-1}\) with the uncertainty representing 2\(\sigma\) as calculated from the 18 realizations.

This work provides an ensemble data product of the sea-air CO\(_2\) flux based on observation-based pCO\(_2\) products. This ensemble product is meant to facilitate the use of the pCO\(_2\) observation-based ocean flux estimates in assessment studies of the global carbon cycle, such as the Global Carbon Budget or RECCAP-2. In addition to enhanced consistency, our area correction and the consistent scaling of gas exchange may help reduce the current carbon budget imbalance (Friedlingstein et al. 2019, 2020). Note that the original sea-air CO\(_2\) flux products still offer additional information important in other
applications, such as coverage over longer time periods, higher spatial or temporal resolution, or runs incorporating further auxiliary data sets or pCO₂ data (e.g., SOCCOM float data, Bushinsky et al. 2019).

Along with the ensemble of CO₂ flux fields, we also provide a public-use coding package allowing users to apply the presented standardized flux calculations to own data-based pCO₂ reconstructions.

Author Contributions

ARF and LG designed the experiment and LG developed the model code and performed the simulations with ARF focusing on analysis. ARF prepared the manuscript with contributions from all co-authors.

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Figure 1: Maps showing the fraction of observations available as a function of time for the six pCO$_2$ data products used in this study. The products are resampled to a monthly resolution if required and are for years 1988 to 2018.
Figure 2: Maps demonstrating the filling procedure used in this study using a snapshot of pCO$_2$ from May 2013. (a) map of unfilled CSIR-ML6 pCO$_2$. (b) the scaled pCO$_2$ climatology of Landschützer et al. (2020b) where the inlay shows the mean pCO$_2$ for the scaled climatology over time. (c) the CSIR-ML6 pCO$_2$ product (a) filled using the scaled climatology (b).
Figure 3: Mean flux (mol m$^{-2}$ yr$^{-1}$), 1988-2018, for CSIR-ML6 product. (a) map of mean calculated flux using the original pCO$_2$ product and 3 scaled wind products; (b) map of mean calculated flux using the filled pCO$_2$ product and 3 scaled wind products. Similar maps for all other products are available in Figure A3.
Figure 4: CSIR-ML6 product calculated air-sea CO$_2$ flux time series for various wind speed products; scaled (solid) and unscaled (dashed). Time series plots for all pCO$_2$ products and including 2 additional wind products (NCEP1 and NCEP2) are included in Figure A2.
Figure 5: Global flux timeseries from six observation-based products. Colored lines show fluxes calculated from the standardized approach presented here (spatial filling with flux calculated from three wind products and the average flux is then plotted here); black line shows the mean of six products. Shaded region shows spread of original flux calculations from product creators with the mean represented as a gray line.
Table 1: Global area coverage and mean pCO₂ for the six observation-based products. Unfilled area listed represents average area covered for 1988-2018 as this value changes monthly for many products (Figure A1). Change is defined as filled product – original product (i.e. a negative change implies the original product had a larger global/regional mean pCO₂ than the filled product).

| Product | Area coverage (% global ocean) | Mean Global pCO₂ change (µatm) | Northern Hem pCO₂ change (µatm) | Southern Hem pCO₂ change (µatm) |
|---------|-------------------------------|--------------------------------|--------------------------------|--------------------------------|
| CMEMS-FFNN | 89%                           | -1.68                          | -4.35                           | 0.30                           |
| Denvil-Sommer et al. 2019 Chau et al. 2020 | | | | |
| CSIR-ML6 | 93%                           | -0.93                          | -2.15                           | 0.07                           |
| Gregor et al. 2019 | | | | |
| JENA-MLS | 100%                          | 0.00                           | 0.00                            | 0.00                           |
| Rödenbeck et al. 2013 | | | | |
| JMA-MLR | 85%                           | -0.69                          | -2.43                           | 0.77                           |
| Iida et al. 2020 | | | | |
| MPI-SOMFFN | 89%                           | -1.07                          | -2.62                           | 0.16                           |
| Landschützer et al. 2014 Landschützer et al. 2020a | | | | |
| NIES-FNN | 92%                           | -0.36                          | -1.95                           | 0.90                           |
| Zeng et al. 2014 | | | | |

Table 2: CSIR-ML6 product flux values Flux values are from filled product. All values are computed over the period 1988-2018

| Wind product | Scaled gas transfer coefficient (α) | Global flux mean (PgC yr⁻¹) | Mean flux difference: scaled – unscaled winds |
|--------------|-------------------------------------|-----------------------------|-----------------------------------------------|
| CCMP2        | 0.261                               | -1.77                       | -0.07                                         |
| ERA5         | 0.276                               | -1.78                       | -0.16                                         |
| JRA55        | 0.269                               | -1.83                       | -0.12                                         |

Table 3: Mean air-sea fluxes (PgC yr⁻¹), 1988-2018, using the mean of three wind products, calculated for the filled global area and the unfilled native “global” area for each pCO₂ product. The northern hemisphere (NH) and southern hemisphere (SH) fluxes (unfilled/filled) are included to highlight the imbalanced regional effect of the spatial filling process.

| Product     | Global Flux (unfilled/filled) | NH Flux (unfilled/filled) | SH Flux (unfilled/filled) |
|-------------|-------------------------------|---------------------------|---------------------------|
| CMEMS-FFNN  | -1.42/-1.79                   | -0.60/-0.92               | -0.82/-0.84               |
| CSIR-ML6    | -1.65/-1.80                   | -0.78/-0.93               | -0.87/-0.87               |
| JENA-MLS    | -1.94/-1.94                   | -1.00/-1.00               | -0.94/-0.94               |
| JMA-MLR     | -1.98/-2.23                   | -0.92/-1.16               | -1.06/-1.07               |
| MPI-SOMFFN  | -1.54/-1.77                   | -0.72/-0.94               | -0.82/-0.84               |
| NIES-FNN    | -1.96/-2.04                   | -0.81/-0.90               | -1.15/-1.14               |
Table 4: Mean fluxes (PgC yr\(^{-1}\)) for each observational pCO\(_2\) product over the period 1988-2018. Mean flux calculated from filled coverage pCO\(_2\) map and scaled gas exchange coefficient; global mean flux is for 3 wind products (CCMP2, ERA5, JRA55) and the average. Time series of the mean flux values for each product (right most column) are plotted in Figure 5.

| pCO\(_2\) mapping Product | CCMPv2 | ERA5 | JRA55 | Mean  |
|---------------------------|--------|------|-------|-------|
| CMEMS-FFNN                | -1.73  | -1.74| -1.79 | -1.75 |
| CSIR-ML6                  | -1.77  | -1.78| -1.83 | -1.79 |
| JENA-MLS                  | -1.89  | -1.90| -1.99 | -1.93 |
| JMA-MLR                   | -2.19  | -2.21| -2.26 | -2.22 |
| MPI-SOMFFN                | -1.75  | -1.76| -1.81 | -1.77 |
| NIES-FNN                  | -2.00  | -2.04| -2.07 | -2.04 |
| **MEAN**                  | -1.89  | -1.90| -1.96 | -1.92 |
Appendix A

Table A1: Summary of parameters used to calculate flux

| pCO₂ mapping Product | Wind speed product | Scaling of gas transfer value | Atmos surf pressure | Gas exchange Parameterization |
|----------------------|-------------------|------------------------------|---------------------|-----------------------------|
| This study           | Calculated for three and final result is an average of the resulting fluxes: ERA5, JRA55, CCMP2 | Scaled to 16.5 cm/hr  | ERA5 Hersbach et al (2020) | Quadratic Wanninkhof (1992) |
| CMEMS-FFNN           | ERA5 Hersbach et al (2020) | Scaled to 16.0 cm/hr  | CAMS inversion Chevallier (2013) | Quadratic Wanninkhof (1992) |
| CSIR-ML6 Gregor et al. 2019 | ERA5 Hersbach et al (2020) | Scaled to 16.0 cm/hr  | ERA5 Hersbach et al (2020) | Quadratic Wanninkhof (1992) |
| JENA-MLS Rödenbeck et al. 2013 | NCEP1 Kalnay et al (1996) | Scaled to 16.5 cm/hr  | NCEP1 Kalnay et al (1996) | Quadratic Wanninkhof (1992) |
| JMA-MLR Iida et al. 2020 | JRA55 Kobayashi et al. (2015) | Scaled to 16.5 cm/hr  | JRA55 Kobayashi et al. (2015) | Quadratic Wanninkhof (1992) |
| MPI-SOMFFN Landschützer et al. 2020a | ERA5 Hersbach et al (2020) | Scaled to 16.0 cm/hr  | NCEP1 Kalnay et al. (1996) | Quadratic Wanninkhof (1992) |
| NIES-FNN Zeng et al. 2015 | NCEP1 Kalnay et al. (1996) | Utilized $a = 0.26$ Takahashi et al. (2009) | NCEP1 Kalnay et al. (1996) | Quadratic Wanninkhof (1992) |
Table A2: Summary of wind products used in this study. Note that the date range starts for the first full year of data. We do not use NCEP1/2 in the main body of our study. Time units are in hours and space in degrees. Mean wind speed is given for the ice-free ocean.

| Product name                        | Resolution | Date range     | Mean speed (m s\(^{-1}\)) | Scaling (\(a\)) | Reference               |
|-------------------------------------|------------|----------------|-----------------------------|------------------|-------------------------|
| Cross-Calibrated Multi-Platform v2  | 6          | 0.25 1988-present | 7.7                         | 0.261            | Atlas et al. (2011)     |
| ECMWF Reanalysis 5th Generation     | 1          | 0.25 1979-present | 7.5                         | 0.276            | Hersbach et al. (2020)  |
| Japanese 55-year Reanalysis         | 3          | 0.50 1958-present | 7.6                         | 0.269            | Kobayashi et al. (2015) |
| NCEP-NCAR reanalysis 1             | 6          | 2.50 1948-present | 7.2                         | 0.293            | Kalnay et al. (1996)    |
| NCEP-NCAR reanalysis 2             | 6          | 2.50 1979-present | 8.3                         | 0.219            | Kanamitsu et al. (2002) |
Table A3: Mean fluxes, PgC yr\(^{-1}\), 1988-2018 for each observational pCO\(_2\) product. Mean flux calculated from unfilled (filled) coverage pCO\(_2\) map and unscaled (scaled) gas exchange coefficient; calculated for 3 wind products (CCMP2, ERA5, JRA55) with the average shown here. Percent change is calculated as the difference between the unfilled/unscaled and filled/scaled as a fraction of the filled/scaled; does not indicate an error in the product’s flux but is a representation of the impact the filling and scaling can have on the end flux estimate. The mean flux as reported in the original pCO\(_2\) product is included for comparison (Figure 5).

| pCO\(_2\) mapping Product | Unfilled, unscaled | Filled, scaled | % change | Original product |
|----------------------------|--------------------|---------------|----------|------------------|
| CMEMS-FFNN                 | -1.33              | -1.76         | 24%      | -1.70            |
| CSIR-ML6                   | -1.54              | -1.80         | 14%      | -1.51            |
| JENA-MLS                   | -1.81              | -1.94         | 6%       | -1.91            |
| JMA-MLR                    | -1.85              | -2.22         | 17%      | -1.59            |
| MPI-SOMFFN                 | -1.45              | -1.78         | 19%      | -1.47            |
| NIES-FNN                   | -1.84              | -2.04         | 10%      | -2.01            |
Figure A1: Time series showing the fraction of area covered by observations as a function of time (monthly) for the six pCO$_2$ data products used in this study.
Figure A2: Air-sea CO$_2$ flux time series (PgC yr$^{-1}$) calculated using five wind speed products (CCMPv2, ERA5, JRA55, NCEP1, NCEP2); scaled (solid) and unscaled (dashed).
Figure A3: Mean flux (mol m$^{-2}$ yr$^{-1}$), 1988-2018. Left hand column: map of mean calculated flux using the unfilled pCO$_2$ product and 3 scaled wind products. Right hand column: map of mean calculated flux using the filled pCO$_2$ product and 3 scaled wind products.