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Supporting Information for

A Spatially Explicit Uncertainty Analysis of the Air-Sea CO_2 Flux From Observations

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Introduction

This supplement presents further details on the development of the methods in order to better allow reproduction of the scientific method and justify the decisions made to quantify uncertainty in the SOM-FFN air-sea flux dataset. Additionally, it includes Figure S1, which provides the spatial spread of the available observations which drive our SOM-FFN data product.

Text S1.

In order to develop our overall equation, we combine two different sources of uncertainty: the systematic (i.e. μ) and random (i.e. σ) terms. To do this, we utilize statistical methods and incorporate based on the linear model (e.g. Peterson et al, 2001), where the two fundamental terms are combined in the form:

$$TE = |bias| + z^*\sigma$$

Where z represents how many standard deviations the value is away from the mean (Illowsky and Dean, 2013), and σ represents our uncertainty, in this case, the three independent sources of uncertainty which we combine in quadrature to calculate total sum. In our analysis, we use one standard deviation, so z=1. This leads to the equation 3 in the main text showing total error, although we always consider the error sources individually for the application of this analysis.

Our three independent sources of uncertainty include σ_{pco2}, σ_k, and σ_{wind} (See equation 3). (k) is the gas exchange transfer velocity of CO_2 normalized to a temperature of 20°C (for a sea surface salinity of 35). For σ_k, we selected four of the most commonly used parameterizations of k: Wanninkhof et al. 2014, Ho et al., 2006, Takahashi et al 2009, and Sweeney et al., 2007. Each of these are quadratic approaches with variations in their k-parameterization equations, further broken down and discussed in Roobeart et al., 2018. While there have been studies suggesting different parameterizations might be more appropriate under specific conditions such as high wind speeds, recent measurements imply quadratic parameterizations fit the observations best even at high-speed wind environments (Butterworth and Miller, 2016; Wanninkhof et al., 2014).

The dominant hydrodynamic factor that controls the turbulence at the air-sea interface and therefore is one of the key factors causing uncertainty in our k_w of the open ocean is wind stress (Sarmiento and Gruber, 2006). Therefore, our third σ is uncertainty stemming from choice of wind product. We selected from the most frequently used global wind products that covered our full time period of analysis, 1982-2022. This included three products: ERA 5 Global Reanalysis (Hersback et al., 2020), NCEP/DOE Reanalysis II (Kanamitsu et al., 2002), and NCEP-NCAR Reanalysis 1 (Kanlay et al., 1996). ERA5 is a reanalysis dataset that combines a weather model with observational satellite and ground data in order to provide gridded, hourly datasets. To ensure 1°x1° spatial resolution, we use cell aggregation to process it, since it has a finer spatial resolution (.25°x.25°). NCEP-NCAR 1 is a data assimilation, on a global T62 Gaussian grid. We use two-dimensional spine interpolation to translate to a continuous 1°x1° spatial field for both NCEP-NCAR 1 and NCEP/DOE Reanalysis II. NCEP/DOE Reanalysis II is based on NCEP-NCAR 1, with updated parameterizations for physical processes and fixed errors. Both products are unchanged for temporal resolution. Note that we do not tune the k_w to individual wind parameterizations, as we are calculating uncertainty based on the spread between our runs, not the actual mean transfer velocity.

Additional parameters that can be found in our flux equation (equations 1 and 2), such as fraction of sea ice, choice of SST product, atmospheric partial pressure of CO_2, or solubility of CO_2 in seawater can impact the flux, but on a global scale create negligible impacts than when compared with the parameters discussed above (Fay et al., 2021, Rooabert et al., 2019), and so were not included in this analysis.

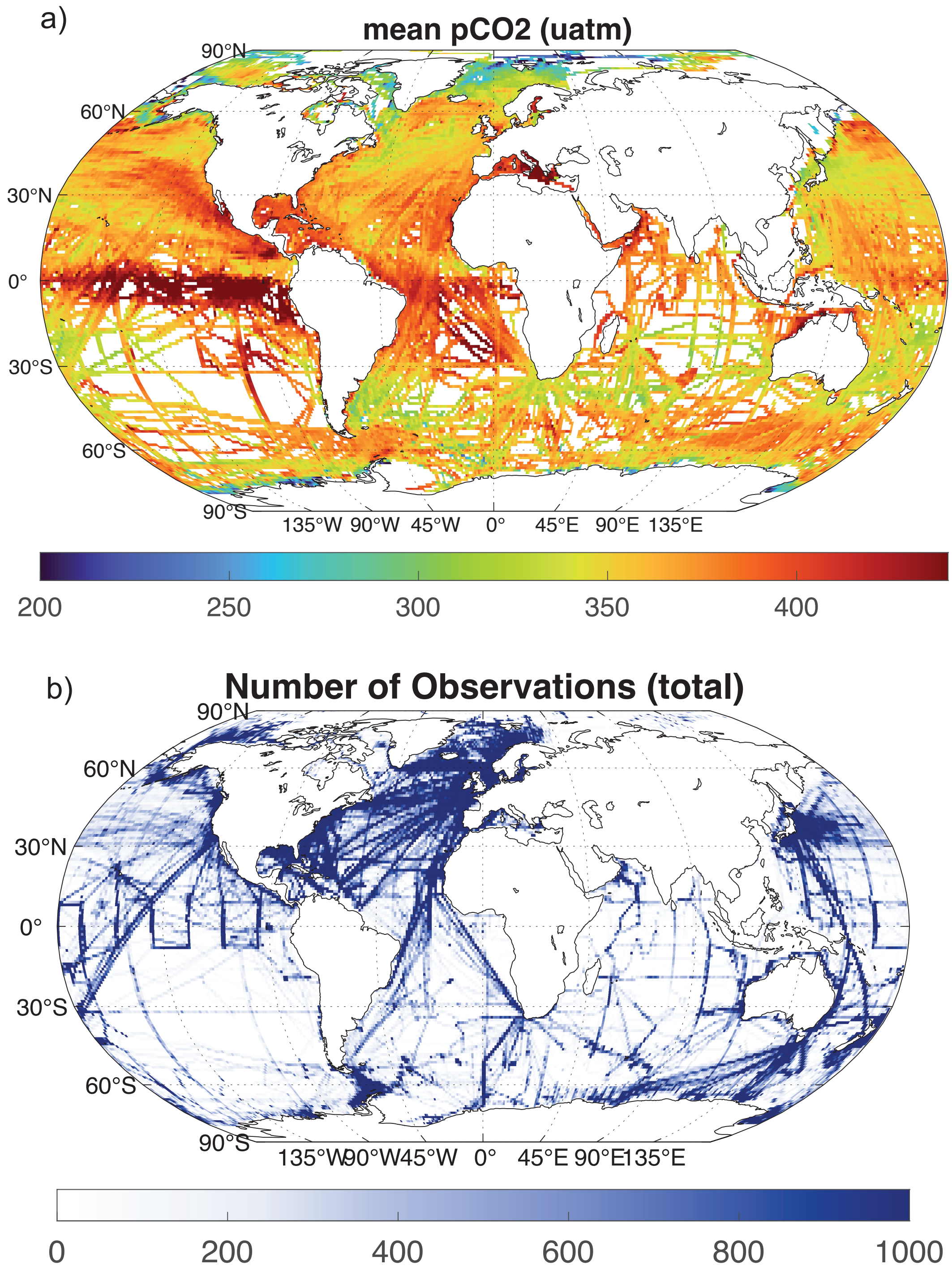

Figure S1. Surface Ocean CO2 Atlas (SOCAT) observations averaged over time from 1982-2022. (a) shows averaged pCO2 (uatm). (b) displays numbers of observations at each gridpoint. These figures incorporate data generously provided by the contributors and investigators who are a part of SOCAT (Bakker et al., 2016).

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