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# [Ocean-driven interannual](https://www.frontiersin.org/articles/10.3389/fmars.2024.1272415/full) variability in atmospheric  $CO<sub>2</sub>$ quantifi[ed using OCO-2](https://www.frontiersin.org/articles/10.3389/fmars.2024.1272415/full) [observations and atmospheric](https://www.frontiersin.org/articles/10.3389/fmars.2024.1272415/full) [transport simulations](https://www.frontiersin.org/articles/10.3389/fmars.2024.1272415/full)

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Interannual variability (IAV) in the atmospheric  $CO<sub>2</sub>$  growth rate is caused by variation in the balance between uptake by land and ocean and accumulation of anthropogenic emissions in the atmosphere. While variations in terrestrial fluxes are thought to drive most of the observed atmospheric  $CO<sub>2</sub>$  IAV, the ability to characterize ocean impacts has been limited by the fact that most sites in the surface CO2 monitoring network are located on coasts or islands or within the continental interior. NASA's Orbiting Carbon-Observatory 2 (OCO-2) mission has observed the atmospheric total column carbon dioxide mole fraction  $(XCO<sub>2</sub>)$ from space since September 2014. With a near-global coverage, this dataset provides a first opportunity to directly observe IAV in atmospheric  $CO<sub>2</sub>$  over remote ocean regions. We assess the impact of ocean flux IAV on the OCO-2 record using atmospheric transport simulations with underlying gridded air-sea  $CO<sub>2</sub>$  fluxes from observation-based products. We use three observation-based products to bracket the likely range of ocean air-sea flux contributions to  $XCO<sub>2</sub>$ variability (over both land and ocean) within the GEOS-Chem atmospheric transport model. We find that the magnitude of  $XCO<sub>2</sub>$  IAV generated by the whole ocean is between 0.08-0.12 ppm throughout the world. Depending on location and flux product, between 20-80% of the IAV in the simulations is caused by IAV in air-sea  $CO<sub>2</sub>$  fluxes, with the remainder due to IAV in atmospheric winds, which modulate the atmospheric gradients that arise from climatological ocean fluxes. The Southern Hemisphere mid-latitudes and low-latitudes are the dominant ocean regions in generating the  $XCO<sub>2</sub>$  IAV globally. The simulation results based on all three flux products show that even within the Northern Hemisphere atmosphere, Southern Hemisphere ocean fluxes are the dominant source of variability in XCO<sub>2</sub>. Nevertheless, the small magnitude of the air-sea flux impacts on  $XCO<sub>2</sub>$  presents a substantial challenge for detection of oceandriven IAV from OCO-2. Although the IAV amplitude arising from ocean fluxes and transport is 20 to 50% of the total observed  $XCO<sub>2</sub>$  IAV amplitude of 0.4 to 1.6 ppm in the Southern Hemisphere and the tropics, ocean-driven IAV represents only 10% of the observed amplitude in the Northern Hemisphere. We find that for all three products, the simulated ocean-driven  $XCO<sub>2</sub>$  IAV is weakly anticorrelated with OCO-2 observations, although these correlations are not statistically significant (p>0.05), suggesting that even over ocean basins, terrestrial IAV obscures the ocean signal.

#### KEYWORDS

carbon cycle, OCO-2, interannual variability,  $CO<sub>2</sub>$ , ocean-atmosphere interaction

## 1 Introduction

The ocean regulates the uptake, storage, and build up of carbon in the atmosphere on annual to millennial timescales, helping mitigate climate change by significantly modulating the long-term trend in the atmospheric  $CO<sub>2</sub>$  growth rate. The ocean took up on average, 3.0 ± 0.4 PgC yr<sup>-1</sup> or 29% of the total anthropogenic CO<sub>2</sub> emissions for the decade beginning in 2011, and cumulatively has sequestered over 1/3 of fossil emissions since the industrial era [\(Le](#page-13-0) Quéré [et al., 2018](#page-13-0); [Friedlingstein et al., 2022](#page-13-0)). Although terrestrial ecosystems play the major role in modulating interannual fluctuations in the atmospheric  $CO<sub>2</sub>$  growth rate ([Keppel-Aleks](#page-13-0) [et al., 2014](#page-13-0)), when taking into account land-use change emissions to the atmosphere, which counteract the residual terrestrial sink, the ocean is the only long-term sink for anthropogenic carbon ([Ballantyne et al., 2012;](#page-13-0) [Crisp et al., 2022\)](#page-13-0).

Interannual variability (IAV) in the atmospheric  $CO<sub>2</sub>$  growth rate is superimposed on the long-term positive trend. The atmospheric  $CO<sub>2</sub>$  surface network shows a decadal-average growth rate of  $2.41 \pm 0.26$  ppm/y (mean  $\pm 2$  std dev) on an annual basis due to the impacts of internal climate variability during 2003–2016 [\(Buchwitz et al., 2018\)](#page-13-0). This IAV has been shown to reflect, primarily, variations in the rate of terrestrial  $CO<sub>2</sub>$  uptake due to climate stressors [\(Luo et al., 2022\)](#page-13-0) and disturbance [\(Keppel-Aleks et al., 2014](#page-13-0)), but also embodies IAV in net ocean carbon exchange and fossil fuel emissions ([Doney et al.,](#page-13-0) [2009;](#page-13-0) [Crisp et al., 2022](#page-13-0)). The global ocean carbon flux IAV is estimated at about 0.3 PgC/yr (equivalent to about 0.15 ppm  $CO<sub>2</sub>$ mixed into the global atmosphere), with the tropical Pacific Ocean which is modulated by El Niño-Southern Oscillation (ENSO), accounting for a large fraction of the variability ([Rödenbeck et al.,](#page-14-0) [2014](#page-14-0); [Bennington et al., 2022](#page-13-0)). However, the influence of key regions of ocean flux IAV on spatial patterns of atmospheric  $CO<sub>2</sub>$ IAV may be obscured unless local scale variations in atmospheric  $CO<sub>2</sub>$  are analyzed.

The net flux of  $CO<sub>2</sub>$  between the atmosphere and the ocean is a function of (1) wind-driven gas exchange kinetic rates and (2) the difference of the partial pressure of  $CO<sub>2</sub>$  in the air and the ocean surface  $(\Delta p CO_2)$ , with the ocean component being far more regionally heterogeneous ([Wanninkhof and McGillis, 1999;](#page-14-0) [Garbe](#page-13-0) [et al., 2014](#page-13-0)). Local variations in oceanic  $pCO<sub>2</sub>$  are related to physical or biogeochemical processes including sub-surface water upwelling, which can enrich the surface water in  $CO<sub>2</sub>$ , temperature-driven solubility variations, alkalinity (which is closely related to salinity and controls the speciation of dissolved inorganic carbon), and phytoplankton photosynthesis and respiration [\(Doney et al., 2009;](#page-13-0) [Crisp et al., 2022](#page-13-0)). These variables are all affected by interannual climate variability [\(McKinley et al., 2020](#page-13-0)). Because the response of the global carbon cycle to climate fluctuations may provide insight into the long-term response to climate change, understanding the global and regional characteristics of ocean-driven atmosphere  $CO<sub>2</sub>$ IAV can help to improve our understanding of the climate–carbon cycle processes and our ability to project the fate of the ocean  $CO<sub>2</sub>$ sink in the future.

Although studies have suggested that ocean flux IAV may impart an observable impact on atmospheric  $CO<sub>2</sub>$  IAV [\(Crisp](#page-13-0) [et al., 2022\)](#page-13-0), gaps remain in quantifying the influence from the ocean since most atmospheric  $CO<sub>2</sub>$  observations are made on land and coasts, with fewer island and ship-based measurements in the remote open ocean. Early research deduced that the  $CO<sub>2</sub>$  flux variation over the ocean, especially the equatorial Pacific Ocean, is one of the main causes of the atmospheric  $CO<sub>2</sub>$  IAV ([Francey](#page-13-0) [et al., 1995\)](#page-13-0). Later studies based on inverse models, seawater system measurements, and air-sea  $CO<sub>2</sub>$  flux estimates ([Feely et al., 2002;](#page-13-0) [Rödenbeck et al., 2003\)](#page-14-0) suggested air-sea  $CO<sub>2</sub>$  flux is not the primary driver for interannual to seasonal variations in atmospheric CO<sub>2</sub>. [Nevison et al. \(2008\)](#page-14-0) used an atmospheric transport model with an underlying mechanistic ocean flux model to show that the amplitude of atmospheric IAV owing to ocean fluxes was around 10% of the IAV amplitude at northern hemisphere surface stations, and up to 50% of the observed IAV in the Southern Hemisphere. In neither hemisphere however, was the IAV owing to ocean fluxes highly correlated with the observations [\(Nevison et al., 2008\)](#page-14-0). Setting aside uncertainties within the atmosphere, there remain substantial uncertainties as to the magnitude of air-sea  $CO<sub>2</sub>$  flux variability itself based on ocean biogeochemical models ([Hauck et al., 2020;](#page-13-0) [Fay and McKinley,](#page-13-0) [2021](#page-13-0)), observation-based flux products ([McKinley et al., 2020;](#page-13-0) [Bennington et al., 2022;](#page-13-0) [Hauck et al., 2023\)](#page-13-0) and atmospheric CO<sub>2</sub> inverse models ([Peylin et al., 2013\)](#page-14-0).

Quantifying ocean-driven atmospheric  $CO<sub>2</sub>$  IAV remains challenging since direct observations of  $pCO<sub>2</sub>$  in surface waters and the corresponding difference with the atmosphere are sparse, and leading to large spatiotemporal gaps.  $CO<sub>2</sub>$  fluxes can be estimated/ calculated? from observation-based  $pCO<sub>2</sub>$  products. There are many such products available, each of which estimate near global 1°x1°, monthly  $pCO<sub>2</sub>$  fields from the sparse  $pCO<sub>2</sub>$  measurements available, using various techniques including statistical interpolation, linear and non-linear regressions, and machine learning-based methodologies ([Rödenbeck et al., 2015\)](#page-14-0). For all products, the  $CO<sub>2</sub>$  flux is then calculated from the interpolated  $pCO<sub>2</sub>$  fields [\(Fay et al., 2021](#page-13-0)). Here, we focus on only three representative data-based flux products ([Landschützer et al., 2014;](#page-13-0) [Rödenbeck et al., 2014](#page-14-0), [2016](#page-13-0), [Denvil-](#page-13-0)[Sommer et al., 2019](#page-13-0)) which are described in more detail below. Robust estimates of mean and seasonality can be derived from observation-based products [\(Fay and McKinley, 2021;](#page-13-0) [Gloege et al.,](#page-13-0) [2021](#page-13-0)), while significant uncertainties in terms of higher and lower frequency variability remain ([Rödenbeck et al., 2015](#page-14-0); [Hauck et al., 2020;](#page-13-0) [Bennington et al., 2022\)](#page-13-0).

New space-based observations of the column-integrated  $CO<sub>2</sub>$ mole fraction, XCO<sub>2</sub>, from NASA's Orbiting Carbon Observatory 2 (OCO-2) mission may provide a unique vantage to observe the atmospheric imprint of IAV in air-sea  $CO<sub>2</sub>$  fluxes. OCO-2 is NASA's first dedicated Earth remote sensing satellite to study atmospheric carbon dioxide from space [\(Eldering et al., 2017\)](#page-13-0). It was designed to collect space-based measurements of atmospheric CO2 with high precision and near-global coverage ([Crisp et al.,](#page-13-0) [2012,](#page-13-0) [2017](#page-13-0)). Compared to surface in-situ  $CO<sub>2</sub>$  observations, such as from the NOAA greenhouse gas network, which is mostly sited in coastal, island, and inland locations, OCO-2 can observe directly over the open ocean, which may improve the spatiotemporal attribution of ocean fluxes.

The research presented here leverages these two advances in carbon cycle data products to answer the following scientific questions: (1) What are the fingerprints of ocean carbon fluxes on IAV of atmospheric  $CO<sub>2</sub>$ , and from what regions are these imprints most prominent? (2) What differences emerge from different observation-based products, and how large are these differences compared to the IAV owing from atmospheric transport? (3) Is the IAV signal from ocean fluxes detectible in column  $CO<sub>2</sub>$  observed from the state-of-the-art OCO-2 satellite? To answer these questions, we run atmospheric transport simulations with underlying air-sea fluxes from several observation-based products. We use the output from these simulations to quantify the imprint of regional and global sea-air  $CO<sub>2</sub>$  fluxes on atmospheric  $CO<sub>2</sub>$  IAV. As a final step, we use OCO-2 observations of  $XCO<sub>2</sub>$  to contextualize the simulated ocean-driven  $XCO<sub>2</sub>$  variations.

## 2 Data and methods

## 2.1 Datasets

## 2.1.1 Observation-based products fluxes

Gridded air-sea CO<sub>2</sub> fluxes estimated from observation-based products for near-global surface ocean pCO<sub>2</sub> have been developed from the same sparse in situ  $pCO<sub>2</sub>$  data using a variety of interpolation/mapping methods ([Rödenbeck et al., 2015;](#page-14-0) [Fay](#page-13-0)

[et al., 2021](#page-13-0)). For each product, the sea-air  $CO<sub>2</sub>$  flux is calculated through gas exchange parameterization, using calculated values of the gas transfer velocity and the solubility of  $CO<sub>2</sub>$  in seawater for near-surface salinity and observed values of sea surface temperature and dry air mixing ratio of atmospheric  $CO<sub>2</sub>$ . We use the Global Carbon Budget (GCB; [Friedlingstein et al., 2022\)](#page-13-0) ocean fluxes from 2019 for three products that use different spatial interpolation methods and provide the best temporal and spatial coverage over the past 4 decades from 1982 to 2018, and then add a three year extension analysis based on the GCB 2022 products. We use the JENA product [\(Rödenbeck et al., 2014](#page-14-0)), which is obtained by fitting a simple data-driven diagnostic model of ocean mixed-layer biogeochemistry to surface-ocean  $CO<sub>2</sub>$  partial pressure data from the SOCAT database. Second, we use the Self-Organizing Map Feed-Forward Neural Network (SOMFFN) product, which is based on a combination of self-organizing maps [\(Landschützer et al.,](#page-13-0) [2013](#page-13-0), [2014](#page-13-0), [2016\)](#page-13-0). Finally, we use the Copernicus Environment Monitoring Service product (CMEMS; LSCE-FFNN-v1), which is a two-step neural network model for the reconstruction of surface ocean pCO<sub>2</sub> over the global ocean [\(Denvil-Sommer et al., 2019\)](#page-13-0). In these networks of models, the information travels forward in the neural network, through the input nodes then through the hidden layers (single or multiple), and finally through the output nodes. JENA has a resolution of about  $4^{\circ} \times 5^{\circ}$  spatially at daily time scale, while SOMFFN and CMEMS are reported at  $1^\circ \times 1^\circ$  on a monthly basis. For consistency among the three products, we averaged the JENA ocean fluxes to monthly mean. Each product covers the global ocean but excludes some coastal areas and/or the Arctic. When comparing the three observation-based products, we only include the flux regions that are in common among the three products. For example, when comparing JENA global  $XCO<sub>2</sub>$  with SOMFFN and CMEMS  $XCO<sub>2</sub>$ , we only sum tracers from the flux regions common to all three models. We omit the tracers from the Far North and Far South to ensure that differences do not arise due to spatial extent of the modeled fluxes.

We divide the ocean into 7 subregions (Figure 1) based on the oceanic biome regions proposed by [Fay et al. \(2014\)](#page-13-0) ([Supplementary Figure S1](#page-13-0)), defined by climatological criteria and analyze these flux products ([Supplementary Figure S2\)](#page-13-0) aggregated to the ocean subregions. [Supplementary Figure S2](#page-13-0) shows the annual trends of the global integrated fluxes based on the three ocean products. Oceanic biomes are classified from climatological sea surface temperature, spring/summer chlorophyll-a concentrations,



biome regions in [Fay et al., 2014](#page-13-0)

ice fraction, and maximum mixed layer depth [\(Fay et al., 2014\)](#page-13-0). The biome regions partition the surface ocean into regions of common biogeochemical function and are consistent with a variety of observational and modeling studies assessing air-sea  $CO<sub>2</sub>$  fluxes and primary productivity.

### 2.1.2 OCO-2 observations

We analyze IAV in dry air, column-average mole fraction  $XCO<sub>2</sub>$ inferred from OCO-2 satellite observations. The OCO-2 observatory was launched in July 2014 and has measured passive, reflected solar near-infrared  $CO<sub>2</sub>$  and  $O<sub>2</sub>$  absorption spectra using grating spectrometers since September 2014 [\(Eldering et al., 2017\)](#page-13-0). XCO<sub>2</sub> data are retrieved from the measured spectra using the Atmospheric CO2 Observations from Space (ACOS) optimal estimation algorithm, which is a full physics algorithm that solves for  $XCO<sub>2</sub>$  and other physical parameters, including surface pressure, surface albedo, temperature, and water vapor profile in its state vector (O'[Dell et al.,](#page-14-0) [2018](#page-14-0)). The satellite is in a polar and sun-synchronous orbit that repeats every 16 days, with three different observing modes of OCO-2, namely nadir (land only, views the ground directly below the spacecraft with insufficient signal to noise over the ocean), glint (ocean and land, views the spot with directly reflected sunlight resulting in a higher ocean signal), and target (sites of specific interest, primarily for validation) [\(Crisp et al., 2012,](#page-13-0) [2017\)](#page-13-0). We use the version 10 OCO-2 Level 2 biascorrected XCO<sub>2</sub> data product from 2014 September to 2022, (From Goddard Earth Sciences Data and Information Services Center Archive: [https://disc.gsfc.nasa.gov/datasets/OCO2\\_L2\\_Lite\\_FP\\_10r/](https://disc.gsfc.nasa.gov/datasets/OCO2_L2_Lite_FP_10r/summary) [summary](https://disc.gsfc.nasa.gov/datasets/OCO2_L2_Lite_FP_10r/summary)), which has been validated with collocated ground-based measurements from the Total Carbon Column Observing Network (TCCON). After filtering and bias correction, the OCO-2 XCO<sub>2</sub> retrievals agree well with TCCON in nadir, glint, and target observation modes, and generally have absolute median differences less than 0.4 ppm and RMS differences less than 1.5 ppm (O'[Dell et al.,](#page-14-0) [2012](#page-14-0); [Wunch et al., 2017](#page-14-0)).

We characterize IAV from OCO-2  $XCO<sub>2</sub>$  in [Guan et al. \(2023\).](#page-13-0) In that analysis, we determined optimal spatiotemporal scales for aggregating the observations to detect IAV variability in light of other sources of error. We evaluated IAV signals against the TCCON ground-truth network, confirming that the IAV inferred from OCO-2 is robust given the small magnitude of IAV compared to other sources of variance [\(Mitchell et al., 2023](#page-13-0)). Further, the OCO-2 IAV timeseries show similar zonal patterns of OCO-2 XCO2 IAV timeseries compared to GOSAT space-based observation and ground-based NOAA ESRL in situ data. The analysis by [Guan et al. \(2023\)](#page-13-0) validates that the OCO-2 satellite provides new capabilities for discerning atmospheric  $XCO<sub>2</sub>$  IAV.

## 2.2 Methods

## 2.2.1 GEOS-Chem simulations

We simulate atmospheric  $XCO<sub>2</sub>$  generated by ocean carbon fluxes using GEOS-Chem ([Bey et al., 2001\)](#page-13-0), an offline global chemical transport model driven by meteorological input from the Goddard Earth Observing System (GEOS) of the NASA Global Modeling and Assimilation Office (GMAO) and developed by an extensive global community of researchers. It has been widely used for gas flux inversion and source attribution studies, including for  $CO<sub>2</sub>$ ,  $CH<sub>4</sub>$  and  $CO$  (e.g., [Nassar et al., 2010](#page-14-0); [Fisher et al., 2017\)](#page-13-0). We use the version 12.0.0 of GEOS-Chem, released in Aug 2018.

To simulate atmospheric  $CO<sub>2</sub>$  fields from individual subregions, we modify the GEOS-Chem code base to tag the source regions and separately track different  $CO<sub>2</sub>$  tracers originating from each region ([Lin et al., 2020](#page-13-0)). This approach is possible since  $CO<sub>2</sub>$  is a passive tracer that is not involved in atmospheric chemical reactions. In the simulation, each  $CO<sub>2</sub>$  tracer corresponds to the influence of ocean  $CO<sub>2</sub>$  fluxes from one tagged region, and the simulation using the JENA product has two more tracers than SOMFFN and CMEMS since the JENA product has slightly larger data coverage in both the far North and the far South.

The meteorological inputs for GEOS-Chem come from the Modern-Era Retrospective analysis for Research and Applications, 80 Version 2 (MERRA2) reanalysis. We run simulations for 1982- 2021 at 2° latitude by 2.5° longitude resolution with 47 vertical levels up to 0.01 hPa on a hybrid eta (sigma-pressure) grid. The ocean flux products were rescaled to 2° latitude by 2.5° longitude resolution using the GEOS-Chem rescaling module. Convective transport in GEOS-Chem is simulated with a single-plume scheme ([Wu et al.,](#page-14-0) [2007](#page-14-0)) while boundary layer mixing in GEOS-Chem uses the nonlocal parameterization ([Lin and McElroy, 2010](#page-13-0)) which draws on the mixing depths, temperature, latent and sensible heat fluxes, and specific humidity. Although some bias in the vertical distribution of  $CO<sub>2</sub>$  has been shown in GEOS-Chem for northern high latitudes ([Schuh et al., 2019\)](#page-14-0), similar tagged transport runs have been shown to generally capture seasonal cycles in surface  $CO<sub>2</sub>$  as well as gradients between surface and mid-tropospheric  $CO<sub>2</sub>$  across a range of latitudes [\(Lin et al., 2020\)](#page-13-0). The model is initialized with a globally-uniform atmospheric  $CO<sub>2</sub>$  mole fraction equal to 350 ppm and allowed to spin-up for 3-years using cyclostationary ocean fluxes. Time-varying ocean fluxes are then applied beginning in 1982. We calculate  $XCO<sub>2</sub>$  in the GEOS-Chem runs by integrating the dry air mole fraction for the 47 model layers accounting for pressure differences with height. Because we are interested in isolating the impact of ocean-atmosphere  $CO<sub>2</sub>$  exchange, we do not simulate the imprint of either fossil or terrestrial biospheric CO<sub>2</sub> exchange on  $XCO<sub>2</sub>$ .

In a sensitivity study, we isolate the impact of atmospheric transport IAV, rather than air-sea flux IAV, on the resulting IAV in  $XCO<sub>2</sub>$ . For this analysis, we simulate  $XCO<sub>2</sub>$  from the seasonal climatology of air-sea  $CO<sub>2</sub>$  fluxes averaged over the 40-year period of the GEOS-Chem simulation, maintaining time-varying atmospheric transport from the MERRA2 reanalysis. Together with the baseline experiment using time-varying air-sea fluxes and timevarying transport, we can distinguish the effect of dynamical-driven variation, flux-driven variation, and the combination of both.

### 2.2.2 Timeseries analysis

We characterize spatiotemporal patterns of OCO-2 detected XCO2 by first aggregating OCO-2 observations to monthly averages on a 5° by 5° grid equatorward of 45° and to a 5° by 10° grid poleward of 45° from 2014.08 (August) to 2021, which overlaps with the simulation time period. Our analysis shows that averaging XCO<sub>2</sub> observations at these scales minimizes the effect of retrieval error and mitigates influences caused by missing measurements due to cloud cover in the tropics and weak winter sunlight in polar regions [\(Guan et al., 2023\)](#page-13-0). We similarly aggregate GEOS-Chem model output at this scale when compared to OCO-2. We use a consistent process to calculate IAV from the OCO-2 XCO<sub>2</sub> (Equation 1), and GEOS-Chem  $XCO<sub>2</sub>$  (Equation 2), but we note that we must account for an additional term in the multi-decadal GEOS-Chem simulations since curvature in the long-term atmospheric growth trend must be taken into account. The methodology is based on approaches used in [Keppel-Aleks et al.](#page-13-0) [\(2014\)](#page-13-0) and NOAA curve fitting methodology [\(Thoning et al., 1989\)](#page-14-0).

$$
IAVOCO-2(x, y, t)
$$
  
=  $Raw(x, y, t) - Trend(x, y, t) - Seasonal(x, y, m)$  (1)

$$
= Raw(x, y, t) - Trend(x, y, t) - Multi - Decadal(x, y, t)
$$

$$
- Seasonal(x, y, m)
$$
(2)

In these equations,  $(x,y)$  denotes a specific gridcell, t denotes a specific time, and m denotes a monthly average. We first fit a thirdorder polynomial to the Raw timeseries to calculate the trend at each location. For the GEOS-Chem simulation, since polynomial fitting does not fully capture the long-term trend over multiple decades, we apply a Fast Fourier Transform 10-year low-pass filter to remove decadal-scale variability. We calculate a mean seasonal cycle by taking the average value of all January, February, etc. data after removing the long-term trends. Finally, we remove the mean seasonal cycle from the detrended timeseries at each gridcell to obtain the IAV anomaly timeseries. We calculate the IAV amplitude as the standard deviation of the IAV anomaly timeseries. An identical method is used to calculate IAV from the gridded fluxes.

## 3 Results

 $IN_{GEOS-Chem}(x, y, t)$ 

[Figure 2](#page-5-0) shows the global distribution of air-sea  $CO<sub>2</sub>$  flux IAV amplitude (calculated as the standard deviation of IAV anomalies) over 40 years from 1982 to 2021 in the observation-based products. The three observation-based products show broadly similar magnitudes and spatial patterns in air-sea flux IAV in the Northern Hemisphere and Southern Hemisphere low to mid latitudes [\(Supplementary Figure S3\)](#page-13-0). The flux IAV amplitude is highest over the northern midlatitude ocean, Eastern Pacific, and Southern Ocean, with the largest inter-product differences in the northern hemisphere. In the Southern Hemisphere, the zonally integrated air-sea flux IAV is largest at 60°, around 0.6-0.7 mol m-2  $y^{-1}$ . The flux IAV decreases by almost a factor of three in the subtropical regions in both hemispheres to around 0.2 mol  $m^{-2}$  s<sup>-1</sup>. The large zonal IAV and the small zonal standard deviation around a latitude circle in the Southern Ocean, especially for SOMFFN and CMEMS (shading in [Figures 2D,](#page-5-0) F), is due to the fact that in the Northern Hemisphere, though there is larger flux IAV amplitude (solid blue line in [Figures 2D](#page-5-0)–F), there is also more variability from gridcell to gridcell (shaded blue area in [Figures 2D](#page-5-0)–F). Thus, the gridcell-level variability partially cancels when integrated around a latitude band, leading to a smaller northern ocean impact on atmospheric  $XCO<sub>2</sub>$ . Consequently, the Southern Hemisphere has a bigger imprint of atmospheric XCO<sub>2</sub> IAV, as we will show below.

The  $XCO<sub>2</sub>$  timeseries simulated from global air-sea fluxes (i.e., the sum of all tagged regions) shows IAV that ranges from +/-0.2 ppm for JENA ([Figure 3\)](#page-6-0) with smaller variations from +/-0.1 ppm for SOM-FFN and CMEMS. The IAV from the products is small compared with the OCO-2  $XCO<sub>2</sub>$  IAV ([Guan et al., 2023](#page-13-0)). Both spatially averaged timeseries ([Figure 3\)](#page-6-0) and maps of IAV ([Supplementary Figure S4](#page-13-0)) are notably different across the three observation-based flux products when propagated through an atmospheric transport model. The simulated XCO<sub>2</sub> from JENA is different compared to that derived from the other two observationbased flux products, due to differences especially in the Southern Hemisphere fluxes. We note, however, that  $XCO<sub>2</sub>$  simulated from any one flux product is generally coherent across latitude bands. The corresponding globally averaged  $XCO<sub>2</sub>$  IAV amplitude is about 0.11 ppm for JENA, but less than 0.07 ppm for SOMFFN and CMEMS ([Figures 4A](#page-7-0)–C). Each data product shows the oceandriven XCO<sub>2</sub> IAV amplitude largest over the tropical Pacific and the Southern Ocean. When the IAV amplitude is calculated for the period from September 2014 to 2021, the overlapping period between OCO-2 observations and observation-based products, the amplitude is similar for SOMFFN and JENA (around 0.12 ppm globally averaged), and similar for CMEMS (around 0.08 ppm). The difference in simulated IAV for a given observation-based product calculated across two different time periods suggests that the ocean may leave a larger imprint on  $XCO<sub>2</sub>$  IAV in recent years compared to historical averages.

The Southern Hemisphere oceanic regions are the dominant contributors to  $XCO<sub>2</sub>$  IAV across the three models. We calculated the XCO<sub>2</sub> IAV amplitude arising separately from each regional tracer, then determined the region that contributes the largest and second largest IAV amplitude to each global atmospheric gridcell (left-hand column of [Figure 5](#page-7-0) and [Supplementary Figures S5](#page-13-0)–7). Across all three models, the Southern Hemisphere low- and midlatitude regions are the primary contributors to IAV over 70-95% of the global area ([Table 1](#page-8-0)), including large swaths of the Northern Hemisphere for SOMFFN and CMEMS. In fact, the SOMFFN simulation shows that Northern Hemisphere ocean regions are not a dominant contributor to XCO<sub>2</sub> IAV even locally. In contrast, the XCO<sub>2</sub> IAV from the simulation with JENA and CMEMS fluxes show a modest contribution from the Northern Hemisphere, with the mid latitude region emerging as the dominant contributor to about 15% of the global area. The dominant region in each gridcell accounts for up to 60% of the atmospheric XCO<sub>2</sub> IAV amplitude for CMEMS [\(Figure 5F](#page-7-0)), and roughly 35-50% of the IAV amplitude for SOMFFN and JENA ([Figures 5B,](#page-7-0) [D\)](#page-7-0), suggesting more equable contributions from different regions. The second most-dominant contributors to atmospheric  $CO<sub>2</sub>$  IAV are similarly the Southern Hemisphere, or tropics or Northern Hemisphere mid-latitude across all three ocean-flux-GEOS-Chem simulations ([Table 2\)](#page-8-0).

<span id="page-5-0"></span>

FIGURE 2

Map of ocean flux IAV amplitude (A-C) and latitudinal profile of zonal mean flux IAV amplitude (D-F). More intense colors signify more IAV while lighter colors indicate lower IAV regions. The IAV amplitude is calculated from the standard deviation of the IAV timeseries. The zonal mean IAV is obtained by averaging the IAV timeseries for all longitudes within the specified latitude band, while the shading shows the standard deviation of the IAV timeseries among all longitudes, indicating the coherence of flux IAV around a latitude circle. (A, D) show results for SOMFFN; (B, E) show results for JENA and (C, F) show results for CMEMS (E, F) product.

Not all IAV in  $XCO<sub>2</sub>$  arises from IAV in local surface fluxes; IAV in patterns of atmospheric transport is also an important contributor to  $XCO<sub>2</sub>$  IAV. We calculate the relative contributions of ocean flux variability and IAV in atmospheric transport from GEOS-Chem simulations with climatological monthly-mean cyclostationary ocean  $CO<sub>2</sub>$  fluxes as surface boundary conditions. IAV in these simulations arises only from IAV in atmospheric transport acting on the spatial gradients in  $XCO<sub>2</sub>$  set up by the climatological annual cycle of ocean air-sea  $CO<sub>2</sub>$  exchange. All three products show nearly identical spatial patterns in the  $XCO<sub>2</sub>$ amplitude arising from cyclostationary air-sea  $CO<sub>2</sub>$  fluxes ([Figures 6A](#page-9-0)–C), suggesting that seasonal flux patterns result in similar atmospheric gradients [\(Landschtzer et al., 2023\)](#page-13-0) across the three models. The western Pacific warm pool is a hotspot for dynamics-driven variability, likely due to ENSO-driven changes

in atmospheric transport, and this region has an IAV amplitude of 0.07-0.08 ppm across all three simulations. Given the large variability in the magnitude of IAV among SOMFFN, JENA, and CMEMS [\(Figure 4\)](#page-7-0), the ratio of dynamics-driven variations to total IAV diverged among the ocean-flux-GEOS-Chem simulations ([Figures 6D](#page-9-0)–F). For SOMFFN and CMEMS, which showed smaller IAV when driven with interannually varying fluxes, transport contributes about 50% of IAV in the Southern Hemisphere subtropics and subpolar regions, and 50-80% of IAV in the tropics and high latitudes of both hemispheres. For JENA, which had high IAV in the full simulations [\(Figure 4B\)](#page-7-0), transport contributes less than 20% of total IAV except in the tropical Pacific, where it contributes 50%.

In the atmospheric transport simulations with cyclostationary fluxes, the Southern Hemisphere mid-latitude region is the

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dominant contributor to IAV for about 60% to 96% of the global area. Consistent across the three observation-based products, the second dominant contributor is the Southern Hemisphere lowlatitude region. These results suggest that IAV in transport interacts most strongly with atmospheric gradients set up by Southern Hemisphere fluxes. JENA and CMEMS show that the Northern Hemisphere mid latitude regions are also important contributors when run with cyclostationary fluxes, and are the dominant contributor to roughly 15% to 25% of the global area. [Figure 7](#page-10-0) shows that in the cyclostationary simulations, the influence of Northern and Southern Hemisphere regions are more localized to the originating hemisphere. Taken together with the results from the time-varying fluxes, these results suggest that IAV in the Southern Hemisphere fluxes is synergistic with IAV from atmospheric transport, whereas, in the Northern hemisphere, IAV in the fluxes counteracts the IAV due to transport alone.

The ocean-driven  $XCO<sub>2</sub>$  IAV simulated by the three observation-based products is largely unrelated to observed patterns of IAV as observed by OCO-2, which includes other sources of IAV. The OCO-2 IAV amplitude, which is of order 1 ppm for the 2014-2021 period, was an order of magnitude larger than that simulated from any of the three-ocean observation-based products which is of order 0.1ppm ([Figures 4](#page-7-0), [8](#page-11-0)). A possible explanation could be that the OCO-2 observations contain the imprint not only of ocean fluxes but also land and fossil emissions. The OCO-2  $XCO<sub>2</sub>$  IAV amplitude, calculated as the standard deviation of the IAV timeseries, suggests that  $XCO<sub>2</sub>$  interannual variability over ocean basins is smaller than that over continents (around 0.4 ppm vs 1.2 ppm; [Figure 8\)](#page-11-0), although this may be due to larger error variance due to complex topography and land surface albedo variations [\(Guan et al., 2023;](#page-13-0) [Mitchell et al., 2023](#page-13-0)). We calculate the correlation coefficient, slope, and fractional ratio

<span id="page-7-0"></span>

through the end of 2021) (bottom row) using (A, D) SOMFFN (B, E) JENA and (C, F) CMEMS ocean observation-based products as input surface CO<sub>2</sub> fluxes to GEOS-Chem atmospheric transport runs.



#### FIGURE 5

The most influential ocean subregions at different locations based on simulations from 1982 to 2021 with time-varying (A) SOMFFN, (C) JENA, and (E) CMEMS fluxes. The dominant tracer is identified by calculating the XCO<sub>2</sub> IAV amplitude for each gridcell caused by a single tracer and then ranking them. The fraction of the overall IAV amplitude accounted for by the dominant tracer is shown in the right-hand column for (B) SOMFFN, (D) JENA, and (F) CMEMS.



<span id="page-8-0"></span>TABLE 1 The percentage of global area or global gridcells for which each ocean flux region is the dominant driver of IAV in simulations with timevarying ocean fluxes and time-varying atmospheric transport.

between simulated XCO<sub>2</sub> IAV and OCO-2 XCO<sub>2</sub> IAV [\(Figure 9,](#page-11-0) [Supplementary Figure S8](#page-13-0)) at the gridscale to explore where the imprint of the ocean might be detectible. Over most of the planet, the observed  $XCO<sub>2</sub>$  IAV is only weakly correlated with the  $XCO<sub>2</sub>$ IAV simulated from ocean fluxes, with many regions showing a slight negative correlation. These correlations are generally not statistically significant, with p>0.05. Simulations from the three different flux products show different meridional patterns of correlation, with JENA simulations showing slight positive correlations within the tropics and CMEMS showing slight positive correlations in the Southern Hemisphere, although we note these relationships are not statistically significant. Across all

regions, the slope between the observed and simulated  $XCO<sub>2</sub>$  IAV is less than 0.2 units? [\(Figures 9D](#page-11-0)–F), consistent with the magnitude of the observed IAV being dominated by terrestrial signals. The maps of correlations and slopes suggest that detecting ocean IAV directly from space-based measurements is challenging given other sources of variability. Disentangling these multiple impacts to differentiate between plausible ocean flux products, such as the three analyzed here, will require a combination of observations and modeling.

Previous analysis of OCO-2 observations over the tropical Pacific suggested that space-based observations can detect an ocean-driven decrease in XCO<sub>2</sub>, potentially as large as 0.5 ppm,





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The ocean XCO<sub>2</sub> IAV amplitude from transport-only simulations based on (A) SOMFFN, (B) JENA, and (C) CMEMS. The ratio of total IAV generated by transport alone for (D) SOMFFN, (E) JENA, and (F) CMEMS

during the initial phases of the strong 2015 El Niño ([Chatterjee](#page-13-0) [et al., 2017\)](#page-13-0). Our simulations show that atmospheric  $XCO<sub>2</sub>$ decreases over the Nino 3.4 region during the strong 1997-1998 El Niño (by about 0.3 ppm), but show a weaker decrease (about 0.1ppm) during 2015-2016 El Niño. The decrease in the atmospheric  $XCO<sub>2</sub>$  IAV timeseries corresponds to the reduced ocean outgassing over the Niño 3.4 region (up to 1.5 mol/m<sup>2</sup>/y) ([Figure 10](#page-12-0)), which is roughly similar between the two El Niño periods and leads to similar decreases in the tropical  $XCO<sub>2</sub>$  tracer ([Supplementary Figure S9](#page-13-0)). During the strong 1997-98 El Niño, however, a temporary reduction in Northern Hemisphere  $CO<sub>2</sub>$ outgassing also reduced  $XCO<sub>2</sub>$  over the Niño.4 region, amplifying the apparent response [\(Supplementary Figure S9](#page-13-0)). As expected,  $XCO<sub>2</sub>$  anomalies during the two El Niño events are mainly driven by changes in the air-sea  $CO<sub>2</sub>$  flux rather than changes in the atmospheric circulation ([Supplementary Figure S10](#page-13-0)). However, these flux-driven anomalies are small (less than +/- 0.03 ppm). Our simulations suggest that even during strong El Niño events, detecting the direct atmospheric imprint of changes in ocean outgassing within the tropics will be challenging given the small direct signal predicted from all three observational flux products, compounding variability from other ocean and terrestrial regions, and retrieval uncertainties in  $XCO<sub>2</sub>$ .

## 4 Discussion

We simulate ocean-driven IAV in atmospheric  $CO<sub>2</sub>$  based on three estimates of air-sea  $CO<sub>2</sub>$  fluxes from interpolated observationbased products. Although these observation-based products all use the same ocean  $pCO<sub>2</sub>$  data to estimate gridded fluxes and show largely similar spatial patterns offlux IAV, they result in very different estimates of atmospheric  $XCO<sub>2</sub>$  IAV over the 40 year period from 1982-2021 ([Figures 3,](#page-6-0) [4A](#page-7-0)–C). The inter-model spread was much reduced when looking at the four years from 2014-2021 overlapping with OCO-2 observations ([Figures 4D](#page-7-0)–F). Our results largely corroborate the results from [Nevison et al. \(2008\),](#page-14-0) who showed a small imprint for the ocean on atmospheric  $CO<sub>2</sub>$  IAV. Our results show that even in the remote Southern Ocean, which shows large IAV in the fluxes, the atmospheric IAV signature imparted by the ocean is small.

Further, our simulations show that up to 80 percent of the IAV of the IAV in atmospheric  $XCO<sub>2</sub>$  results from IAV in atmospheric transport acting on atmospheric gradients derived from cyclostationary ocean fluxes (Figure 6), not from IAV in the ocean fluxes themselves. The three observation-based products showed a very similar pattern of transport-induced IAV, with the dominant spatial contributors (SH low-lat and SH mid-lat) showing

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high consistency among the three data products [\(Table 1](#page-8-0)). This is somewhat expected, since the MERRA/GEOS-Chem atmospheric transport patterns were common among all three simulations, but also requires that the three observation-based products provide similar mean spatial seasonal patterns in oceanic  $CO<sub>2</sub>$  fluxes ([Supplementary Figure S11](#page-13-0)).

Our study shows that atmospheric  $XCO<sub>2</sub>$  IAV is affected most strongly by air-sea  $CO<sub>2</sub>$  fluxes in the Southern Hemisphere (Figure 7), although the observation-based products show tradeoffs between the Southern Hemisphere low- and midlatitude regions in terms of which region dominates. In the simulations with time-varying air-sea fluxes, the Southern Hemisphere, and to a lesser extent the tropics, dominate oceandriven XCO<sub>2</sub> IAV even in the Northern Hemisphere. This pattern generally holds in the simulations with cyclostationary fluxes, although the Northern Hemisphere regions have a relatively larger contribution.

Given the small signature of ocean fluxes on atmospheric  $XCO<sub>2</sub>$ IAV, attributing ocean-induced IAV based on space-based observations will be challenging. [Mitchell et al. \(2023\)](#page-13-0) provide a

detailed assessment of time and space scales of variation in OCO-2 XCO2 over North American land and coastal ocean using a geostatistical approach. They identify synoptic scale variations as contributing up to 2 ppm<sup>2</sup> variance, mesoscale transport, and correlated error as contributing up to 1  $ppm<sup>2</sup>$  variance, and random noise as up to 1 ppm. Given that our simulations suggest the imprint of ocean IAV is less than 0.1 ppm, these results suggest that directly observing ocean IAV is not possible with the current technology for space-based remote sensing of atmospheric  $CO<sub>2</sub>$ . Rather, XCO<sub>2</sub> observations will require precision better than 0.1 ppm, or 0.025% on a ~400 ppm background to detect and attribute ocean-driven variation.

Furthermore, because transport is an important contributor to the patterns of atmospheric  $CO<sub>2</sub>$  IAV, using methods such as atmospheric inversions to back out ocean fluxes in an optimal estimation framework requires fidelity in atmospheric transport modeling [\(Schuh et al., 2019](#page-14-0)). Here, patterns of atmospheric transport-induced IAV from cyclostationary air-sea  $CO<sub>2</sub>$  fluxes ([Figure 6\)](#page-9-0) are similar because all flux products were transported through the same GEOS-Chem transport model. The choice of a

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different transport model would likely result in different spatial patterns, albeit with a similarly small magnitude compared to the IAV amplitude of the observations.

During the four years from 2014-2021 overlapping with OCO-2 observations, all three observation-based flux products show a multi-year

decrease in the net ocean flux. There is low correspondence between the simulated  $XCO<sub>2</sub>$  IAV driven by ocean fluxes with total IAV detected from OCO-2. We hypothesize that multi-decadal variability in air-sea  $CO<sub>2</sub>$  fluxes may be more detectable in atmospheric  $XCO<sub>2</sub>$  than the yearto-year variability presented here, but testing this hypothesis requires ongoing space-based observations of  $XCO<sub>2</sub>$ .

Our results temper the optimistic results from [Chatterjee et al.](#page-13-0) [\(2017\)](#page-13-0), who showed that a large ocean flux signal could be discerned from space-based  $XCO<sub>2</sub>$  data. Our study shows that the Southern Hemisphere oceans were the largest ocean-driven  $XCO<sub>2</sub>$  IAV in our simulations ([Figure 4\)](#page-7-0), and that tropical Pacific that was most sensitive to IAV in atmospheric transport [\(Figure 6](#page-9-0)).

Nevertheless, all three ocean products we analyze suggest a smaller XCO2 IAV than what was observed for the 2015-16 El Niño. These results suggest that flux anomalies associated with changing modes in ocean oscillations in other basins may impart smaller variations in the atmosphere that are difficult to detect using OCO-2 or a similar satellite.

# 5 Conclusions

We evaluate the imprint that air-sea  $CO<sub>2</sub>$  fluxes from the whole ocean and different oceanic subregions leave on the atmospheric  $XCO<sub>2</sub>$  interannual variation. We simulate ocean-driven  $XCO<sub>2</sub>$  using



(A–C) The correlation coefficient between simulated ocean XCO<sub>2</sub> IAV and OCO-2 IAV for (A) SOMFFN, (B) JENA, and (C) CMEMS data products. (D-F) The ratio of IAV amplitude between simulated oceanic XCO<sub>2</sub> IAV and OCO-2 XCO<sub>2</sub> IAV, for (D) SOMFFN, (E) JENA, (F) CMEMS

<span id="page-12-0"></span>

the GEOS-Chem atmospheric transport model and air-sea  $CO<sub>2</sub>$ fluxes estimated from observation-based surface  $pCO<sub>2</sub>$  products and compare against the observed total XCO<sub>2</sub> IAV based on OCO-2 column-mean  $CO<sub>2</sub>$  observation from late 2014 to 2022. The oceandriven IAV amplitude (standard deviation) in atmospheric XCO<sub>2</sub> caused by air-sea  $CO<sub>2</sub>$  exchange and IAV in atmospheric transport is generally between 0.08 and 0.12 ppm. While this magnitude is up to  $40\%$  of the total IAV in OCO-2 XCO<sub>2</sub> over the tropical and subtropical ocean basins, it is well below random noise in individual OCO-2 soundings and systematic errors in the satellite observations themselves. These results indicate that direct observation of air-sea  $CO<sub>2</sub>$  flux variations from total column  $XCO<sub>2</sub>$ would be very challenging with current space-based sensors.

# Data availability statement

The raw data supporting the conclusions of this article will be made available by the authors, without undue reservation.

# Author contributions

YG: Conceptualization, Data curation, Formal analysis, Investigation, Methodology, Software, Visualization, Writing – original draft, Writing – review & editing. GM: Conceptualization, Funding acquisition, Methodology, Project administration, Resources, Supervision, Validation, Writing – review & editing. AF: Conceptualization, Data curation, Methodology, Resources, Software, Writing – review & editing. SD: Conceptualization, Funding acquisition, Methodology, Project administration, Resources, Supervision, Writing – review & editing, Validation. GK: Conceptualization, Funding acquisition, Methodology, Project administration, Resources, Supervision, Validation, Writing – original draft, Writing – review & editing.

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# <span id="page-13-0"></span>Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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# Supplementary material

The Supplementary Material for this article can be found online at: [https://www.frontiersin.org/articles/10.3389/fmars.2024.1272415/](https://www.frontiersin.org/articles/10.3389/fmars.2024.1272415/full#supplementary-material) [full#supplementary-material](https://www.frontiersin.org/articles/10.3389/fmars.2024.1272415/full#supplementary-material)

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