



A surface ocean $p\text{CO}_2$ product with improved representation of interannual variability using a vision transformer-based model

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Abstract. The ocean plays a crucial role in regulating the global carbon cycle and mitigating climate change. Spatial and temporal variations of ocean surface partial pressure of CO_2 ($sp\text{CO}_2$) influence the air–sea CO_2 flux through the difference between surface ocean and atmospheric $p\text{CO}_2$ ($\Delta p\text{CO}_2$), which is further modulated by surface wind speed and gas exchange velocity. However, constructing a global $sp\text{CO}_2$ data product that is able to resolve interannual and decadal variability remains a challenge due to the spatial sparsity and temporal discontinuity of observational data. This study presents an approach based on the Vision Transformer (ViT) model, combining high-quality observational data from the CO_2 Atlas (SOCAT) with multiple advanced global ocean biogeochemical models results to reconstruct a global monthly $sp\text{CO}_2$ dataset (SJTU-AViT) at 1° resolution from 1982 to 2023. The approach employs the self-attention mechanism of the ViT model to enhance the modeling of the spatial and temporal variations of $sp\text{CO}_2$, as well as incorporates physical-biogeochemical constraints from the derivative of $sp\text{CO}_2$ with respect to key controlling factors as additional features. The incorporation of advanced ocean biogeochemical models during the training process allows the ViT-based model to capture more accurate $sp\text{CO}_2$ variability in these data-sparse regions. Evaluations demonstrate that the new data product effectively captures $sp\text{CO}_2$ variability at both global and regional scales, showing good consistency with SOCAT observations, long-term ocean station data, and global atmospheric CO_2 trends. The reconstructed $sp\text{CO}_2$ demonstrates strong capability in reproducing $sp\text{CO}_2$ anomalies during El Niño–Southern Oscillation (ENSO) events, particularly in the eastern Pacific Ocean, where it shows a correlation of -0.81 with the Niño 3.4 index

and demonstrates high consistency with cruise data. Based on the SJTU-AViT dataset, the estimated global air–sea CO_2 flux patterns are consistent with known regional features such as strong uptake in the Southern Ocean and outgassing in the tropical Pacific. This study not only provides a new 42-year data product for advancing understanding of the ocean carbon cycle and global carbon budget assessments, but also introduces a new Transformer-based deep learning framework for Earth-system data reconstruction. The data product is publicly accessible at <https://doi.org/10.5281/zenodo.15331978> (Zhang et al., 2025) and will be updated regularly.

1 Introduction

Global warming is primarily driven by the continuous increase in atmospheric greenhouse gas concentrations, with carbon dioxide (CO_2) being the dominant contributor (Friedlingstein et al., 2023). The ocean, as one of the largest carbon sinks in the Earth system, absorbs approximately 25 % of anthropogenic CO_2 emissions ($\sim 2.80 \text{ Pg C yr}^{-1}$), playing a crucial role in regulating the global carbon cycle and climate change (Friedlingstein et al., 2023). However, the ocean's capacity to absorb CO_2 is not constant; rather, it is influenced by a complex interplay of atmospheric CO_2 concentration, ocean physical and biogeochemical processes, exhibiting significant spatiotemporal variability (Landschützer et al., 2016; Takahashi et al., 2002). Accurate estimation of oceanic CO_2 fluxes is therefore essential for understanding carbon cycle mechanisms and assessing the effectiveness of the ocean as a carbon sink.

Accurately quantifying air–sea CO_2 flux relies on precise estimates of sea surface CO_2 partial pressure ($sp\text{CO}_2$). While the surface ocean CO_2 atlas (SOCAT) database (Bakker et al., 2016) provides a valuable foundation, observational coverage remains sparse and uneven, particularly in high-latitude regions and during winter months when harsh sea conditions limit measurements (Mackay and Watson, 2021). Existing approaches for estimating $sp\text{CO}_2$ primarily fall into two categories: numerical biogeochemical modeling and data-driven methods. Traditional numerical biogeochemical models simulate $sp\text{CO}_2$ by parameterizing physical and biogeochemical processes (Kern et al., 2024; Roobaert et al., 2022). However, due to the highly nonlinear dynamics of the oceanic carbon cycle and regional heterogeneity, numerical biogeochemical models still exhibit considerable uncertainties in reconstructing the spatiotemporal distribution of $sp\text{CO}_2$ (Rödenbeck et al., 2015; Roobaert et al., 2022). Moreover, simplified parameterization of biogeochemical processes may lead to underestimation or overestimation of oceanic carbon uptake, ultimately affecting the accuracy of global carbon budget assessments (Resplandy et al., 2024).

To address these limitations, statistical interpolation and machine learning techniques have been increasingly employed to reconstruct $sp\text{CO}_2$ distributions based on available observations (Rödenbeck et al., 2015). Statistical interpolation methods, such as regression-based approaches (Rödenbeck et al., 2015), Bayesian techniques (Valsala et

al., 2021), and tree-based algorithms (Geurts et al., 2006), leverage the spatiotemporal correlation of $sp\text{CO}_2$ observations and have achieved moderate success in some regions (Gregor et al., 2019). However, these methods struggle with poor reconstruction accuracy in data-sparse regions and do not fully capture the complex ocean carbon biogeochemical processes effectively (Hauck et al., 2023). Consequently, machine learning approaches have gained prominence in recent years. In particular, feedforward neural networks (FFNNs) have demonstrated superior reconstruction accuracy and have become one of the most widely used tools for $sp\text{CO}_2$ and other ocean data estimation (Denvil-Sommer et al., 2019; Landschützer et al., 2013; Zeng et al., 2014). These methods yield root mean square errors (RMSE) of approximately $18 \mu\text{atm}$ in open ocean regions, aligning well with SOCAT observations (Gregor et al., 2019).

Despite recent advances, significant challenges remain in reconstructing $sp\text{CO}_2$, particularly in capturing its interannual and decadal variability, which plays a pivotal role in modulating oceanic carbon uptake. Previous machine learning (ML)-based interpolations of $p\text{CO}_2$ may overly smooths the spatial patterns and interannual variability, which represents a potential limitation in capturing these features fully. Accurate characterization of this variability remains a central issue in the ocean carbon field. Furthermore, the widely used FFNNs method may introduce discontinuities at cluster boundaries due to the discrete nature of data grouping, impacting the representation of $sp\text{CO}_2$ variability (Gregor et al., 2019). These discontinuities often require additional post-smoothing procedures, which may introduce artificial bias, thereby increasing reconstructed data uncertainty or suppressing real spatiotemporal variability (Gregor et al., 2019). More broadly, a persistent imbalance of approximately 1 Pg C yr^{-1} remains in the global carbon budget, reflecting unresolved discrepancies between estimated sources and sinks on the global scale. One plausible contributor to this imbalance is the inadequate characterization of the interannual variability in oceanic carbon uptake (Friedlingstein et al., 2023). Therefore, this study develops a novel reconstruction method to more accurately capture interannual dynamics, alleviate artificial spatial discontinuities, particularly across cluster boundaries, and ultimately contribute to close the global carbon budget (Rödenbeck et al., 2015).

Transformer architectures, originally developed for sequence modeling in natural language processing, have

demonstrated exceptional capabilities in capturing long-range dependencies and learning complex, nonlinear relationships across high-dimensional datasets. Their scalability and effectiveness in tasks such as machine translation, language understanding, and large language models (e.g., Chat-GPT) have established them as a cornerstone of modern artificial intelligence. Recently, these models have been extended to atmospheric science and oceanography, where they have shown promising performance in forecasting ocean states and extracting spatiotemporal patterns from large-scale environmental data. Given these advantages, Transformer-based frameworks offer considerable potential for data reconstruction in oceanography, where challenges such as sparse observations, multiscale variability, and strong spatiotemporal coupling demand flexible and powerful modeling approaches (Ji et al., 2025; Liu et al., 2024).

Against this backdrop, the image-based Vision Transformer (ViT) architecture, with its multi-head self-attention mechanism and high representational capacity, has emerged as a powerful tool for capturing the complex spatiotemporal features of oceanic environmental variables. This model is well-suited for reconstructing $sp\text{CO}_2$, as it can integrate diverse environmental drivers such as sea surface temperature (SST), salinity (SSS), chlorophyll concentration (Chl a), mixed layer depth (MLD), and atmospheric CO_2 concentration. To enhance the physical constraints of $sp\text{CO}_2$ reconstruction, this study incorporates ocean carbonate system sensitivities to key variables like SST, SSS, dissolved inorganic carbon (DIC), and total alkalinity (ALK) (Takahashi et al., 1993). In this context, multi-stage training strategies that combine simulated data from Earth system models and observational constraints have also proven effective in improving model robustness and accuracy. The $sp\text{CO}_2$ -based Shanghai Jiao Tong University aggregation Vision Transformer (SJTU-AViT) developed in this study effectively captures both spatial variations and interannual to decadal variability of ocean carbon dynamics at global scales. This contributes to enhancing our understanding of the temporal dynamics of oceanic carbon uptake and addressing imbalances in the global carbon budget.

2 Data and methods

2.1 Training data description

This study selects a range of input features for model training to comprehensively capture the dynamics of surface ocean $sp\text{CO}_2$ variability through sensitivity tests and other $sp\text{CO}_2$ data reconstruction studies (Denvil-Sommer et al., 2019; Landschützer et al., 2013; Zeng et al., 2014). The selected input features include SST, SSS, Chl a , MLD, and air CO_2 . Additionally, we introduce physical constraints based on the

relationship

$$\Delta sp\text{CO}_2 \approx \frac{\partial sp\text{CO}_2}{\partial \text{DIC}} \Delta \text{DIC} + \frac{\partial sp\text{CO}_2}{\partial \text{ALK}} \Delta \text{ALK} + \frac{\partial sp\text{CO}_2}{\partial \text{SST}} \Delta \text{SST} + \frac{\partial sp\text{CO}_2}{\partial \text{SSS}} \Delta \text{SSS} \quad (1)$$

that the sensitivities of CO_2 partial pressure to SSS, SST, DIC, and ALK ($\frac{\partial sp\text{CO}_2}{\partial \text{SSS}}$, $\frac{\partial sp\text{CO}_2}{\partial \text{SST}}$, $\frac{\partial sp\text{CO}_2}{\partial \text{DIC}}$, $\frac{\partial sp\text{CO}_2}{\partial \text{ALK}}$) are included as input features in the deep learning model to reinforce $sp\text{CO}_2$ physical-biogeochemical consistency (Takahashi et al., 1993). These parameters represent key physical, chemical, and biological factors influencing the distribution of $sp\text{CO}_2$ in the ocean. All the input features are interpolated into a uniform $1^\circ \times 1^\circ$ spatial resolution and monthly temporal resolution.

The input datasets consist of long-term time series and high-resolution spatial data, ensuring both temporal and spatial consistency across variables (Table 1). SST data were obtained from the NOAA Optimum Interpolation SST (OISST) (version v02r01) dataset, spanning from 1982 to 2023 with daily resolution and a spatial resolution of 0.25° (Reynolds et al., 2007; Huang et al., 2021). SSS data were sourced from the Hadley Centre EN.4.2.2 (c14) dataset, covering the period from 1982 to 2023 with daily resolution and a spatial resolution of 0.25° (Good et al., 2013). Chl a data were derived from the European Space Agency Climate Change Initiative (ESA CCI) Ocean Colour (version 5.0) dataset, spanning 1997 to 2022 with daily resolution and a spatial resolution of 4 km (Jackson et al., 2017). For periods prior to 1997 and for 2023, we employed a climatology computed from the 1997–2022 Chl a record to ensure full temporal coverage. Ocean MLD data were obtained from the World Ocean Circulation Experiment (WOCE) Global Data Version 3.0, providing monthly climatology with a spatial resolution of 2° (de Boyer Montégut et al., 2004). Atmospheric CO_2 mole fraction ($x\text{CO}_2$) data were sourced from the NOAA Earth System Research Laboratories (ESRL) marine boundary layer (MBL) CO_2 product, covering the period from 1982 to 2023 with about 8 d resolution and meridional spacing (Dlugokencky et al., 2019). In this study, the meridional band product was mapped onto the model's $1^\circ \times 1^\circ$ global grid using latitudinal interpolation and longitudinal replication, generating continuous 2D fields suitable for model simulations.

The monthly climatologies of $\frac{\partial sp\text{CO}_2}{\partial \text{SSS}}$, $\frac{\partial sp\text{CO}_2}{\partial \text{SST}}$, $\frac{\partial sp\text{CO}_2}{\partial \text{DIC}}$, $\frac{\partial sp\text{CO}_2}{\partial \text{ALK}}$ at a spatial resolution of 1° are included as additional input features, sourced from the ocean-driven global biogeochemical model simulations (Liao et al., 2020). These rate-of-change variables help to reflect the influences of temperature, salinity, alkalinity, and DIC on $sp\text{CO}_2$, thereby enriching the deep learning model's representation of the underlying biogeochemical processes. Additionally, $sp\text{CO}_2$ from the SOCAT database was used as the target variable for the model training and validation. The SOCAT dataset used in this study is version 2024 (Fig. S1 in the Supplement) which

Table 1. Summary of data sources and variable characteristics used in this study.

Variable	Units	Period	Resolution	Dataset	Reference
Atmospheric CO ₂ ($x\text{CO}_2$)	ppm	1982–2023	Meridional, monthly	ESRL MBL CO ₂ product	Dlugokencky et al. (2019)
Chlorophyll <i>a</i> (Chl <i>a</i>)	mg m ^{−3}	1997–2022	4 km, daily	ESA CCI Ocean Colour (Version 5.0)	Jackson et al. (2017)
Sea surface temperature (SST)	°C	1982–2023	0.25°, daily	NOAA OISST (Version v02r01)	Reynolds et al. (2007)
Sea surface salinity (SSS)	PSU	1982–2023	0.25°, daily	Hadley Center EN.4.2.2 (c14)	Good et al. (2013)
Ocean mixed layer depth (MLD)	m	12-month	2°, monthly climatology	WOCE Global Data Version 3.0	de Boyer Montégut et al. (2004)
SOCAT	µatm	1982–2023	1°, monthly	SOCAT version 2024 data products	Bakker et al. (2016)

is interpolated into the uniform $1^\circ \times 1^\circ$ spatial resolution and monthly temporal resolution (Bakker et al., 2016).

The Coupled Model Intercomparison Project Phase 6 (CMIP6) model results are downloaded from the Lawrence Livermore National Laboratory node database (<https://esgf31node.llnl.gov/projects/cmip6/>, last access: 27 February 2025, at the time of this study). We selected a subset of 7 ESMs based on the availability of download access through our cluster and the availability of environmental variables (see Sect. S2 for details). The biogeochemical model adopted in this study is from the Geophysical Fluid Dynamics Laboratory (GFDL). The model includes Modular Ocean Model version 6 (MOM6), sea ice simulator version 2, carbon ocean biogeochemistry, and lower trophics version 2 (COBALT v2), which is collectively referred to as MOM6-COBALT2 (Adcroft et al., 2019; Stock et al., 2020). The model performance is thoroughly assessed, and it reproduces well-observed physical and biogeochemical features in the global ocean (Stock et al., 2020). More detailed model evaluations and configurations, including spin-up, atmospheric forcing, and initial conditions, can be found in Liao et al. (2020, 2024).

2.2 Model architecture

The deep learning model employed in this study is a Vision Transformer (ViT, Fig. 1), originally proposed by Dosovitskiy et al. (2020) for capturing spatial dependencies in large-scale image-like datasets. The design of ViT tackled the key limitation of the CNN-like methods, which implies the translation-invariant property of learned kernels. This property failed to learn the remote connections across regions among multiple variables (Liu et al., 2024). The ViT model employs a self-attention mechanism to capture long-term connections and complex spatial and temporal patterns

(Nguyen et al., 2023), allowing it to dynamically adjust its receptive field and capture both localized details and large-scale variations. As a result, the model is able to provide a more comprehensive characterization of the relationships between $sp\text{CO}_2$ and oceanic variables across spatial scales.

The ViT-based framework for $sp\text{CO}_2$ reconstruction includes four main steps. The first is variable tokenization, a process that involves partitioning the input data into local regions. Each region is treated as an image patch for subsequent processing and feature extraction (Dosovitskiy et al., 2020). These input variables are standardized using variable-wise mean-variance normalization and formatted into a multi-channel input to ensure feature extraction occurs on a unified scale. Then, the ocean fields are segmented into fixed-size image patches. For example, the SST field (180×360) is divided into non-overlapping 6×6 grids on every patch, resulting in 30×60 patches. The data in each patch is then projected into a high-dimensional vector through a patch embedding layer, preserving critical spatial structures and providing a suitable input representation for the Transformer framework.

The second step is variable aggregation, where a cross-attention mechanism is employed to integrate information across multiple environmental input variables (Vaswani et al., 2017). Given that different variables influence $sp\text{CO}_2$ through distinct mechanisms, other methods like simple concatenation may obscure crucial dynamic relationships. The cross-attention mechanism enables the model to adaptively assign appropriate weights to different variables, emphasizing those that contribute most significantly to $sp\text{CO}_2$ variations (Jaegle et al., 2021). To further enhance its ability to capture spatiotemporal dynamics, the model incorporates position encoding and time encoding at this stage, ensuring temporal consistency in the input data and improving the

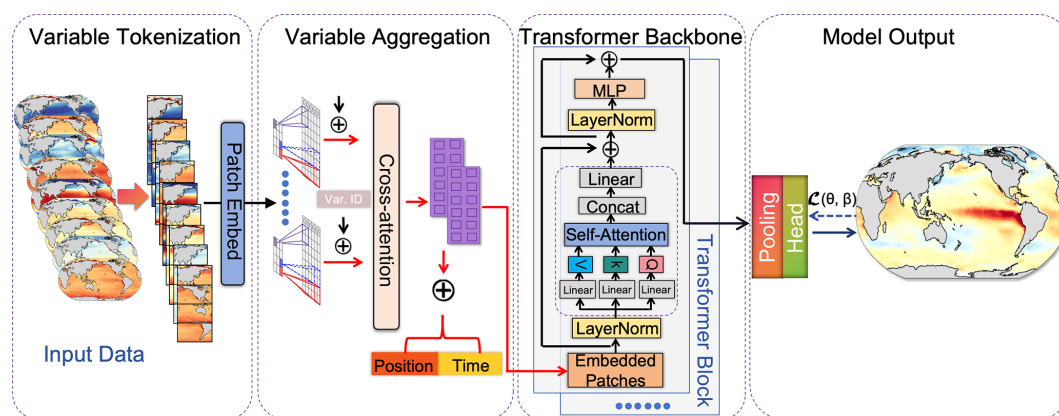


Figure 1. Schematic of the Vision Transformer (ViT)-based framework for $sp\text{CO}_2$ reconstruction. The framework includes four main steps. The first is variable tokenization, where the input oceanographic variables (e.g., SST, SSS, Chl a , MLD, and atmospheric CO_2) are divided into spatial patches and passed through a convolutional embedding layer. The second step is variable aggregation, where multiple variables are aggregated into one vector through the cross-attention mechanism. The third step is Transformer backbone, where the data are passed through stacked Transformer blocks that incorporate multi-head self-attention, layer normalization, and feedforward neural networks to capture complex spatiotemporal dependencies. The final step is model output, where a pooling head aggregates the learned representations and generates the $sp\text{CO}_2$ fields.

interpretability of ocean carbon cycle processes (Wu et al., 2021).

The third step is Transformer backbone, where the data are fed into a Transformer backbone composed of 10 stacked Transformer blocks. Each block integrates multi-head self-attention (16 heads), layer normalization (LayerNorm), and a feedforward neural network (MLP) (Dosovitskiy et al., 2020; Vaswani et al., 2017). The multi-head self-attention mechanism enables the model to learn long-range dependencies and capture complex spatial interactions by attending to multiple representation subspaces simultaneously – an essential feature for modeling the inherently spatiotemporal dynamics of oceanographic variables. To further enhance representation learning, linear transformation and concatenation operations (Linear & Concat) are employed across layers. These operations support deep feature fusion, enabling the network to integrate both fine-scale local variations and broader climate-driven signals.

The final step is the model output. This step incorporates a pooling head for dimensionality reduction, producing the global oceanic $sp\text{CO}_2$ fields as the output. The loss function is minimized by comparing the reconstructed values against observational datasets, ensuring both physical consistency and numerical accuracy. The ViT-based model contains approximately 115 million parameters and was trained in parallel on eight NVIDIA RTX 4090 GPUs for up to 200 epochs with early stopping (patience = 10); each training epoch required roughly 10 min.

To enhance model performance, we employ a multi-stage training strategy. First, we pre-train the ViT-based model using the 7 CMIP6 model results to learn a general relationship between $sp\text{CO}_2$ and the environmental variables (SST,

SSS, Chl a , MLD, and air CO_2). We then fine-tune the ViT-based model using data from the ocean-driven global ocean biogeochemical models (e.g., MOM6-COBALT) and further refine it with SOCAT observations to improve accuracy and applicability. The incorporation of the CMIP6 model and advanced ocean biogeochemical models enhances the $sp\text{CO}_2$ reconstruction by mitigating the data sparsity issue, particularly in regions with limited observations, such as the Indian Ocean and high-latitude areas. Through the use of transfer learning, the model can better leverage global climate data to fill gaps in observational coverage. The overall workflow of this multi-stage training strategy is summarized in Fig. 2, which also provides a schematic overview of the $sp\text{CO}_2$ reconstruction workflow based on the ViT framework. The figure clearly visualizes the main steps, from data preprocessing through model training to evaluation (see detailed description in Sect. S5.1).

2.3 Validation procedure and data

The SOCAT dataset was randomly divided into 80 % (277 528 samples) for training and 20 % (69 142 samples) for validation, using a fixed random seed (seed = 42) to ensure reproducibility. For the independent test at long-term stations, data from these stations were excluded, and the model was trained using the remaining SOCAT data. In the final results generation phase, the full SOCAT dataset was utilized to produce the $sp\text{CO}_2$ estimates. These estimates are subsequently used for analyses of climatological states, seasonal variations, and interannual changes in $sp\text{CO}_2$. For comparison with SOCAT, we used the monthly 1° gridded SOCAT product and evaluated our SJTU-AViT reconstruction on the same grid, without applying any additional spatial interpo-

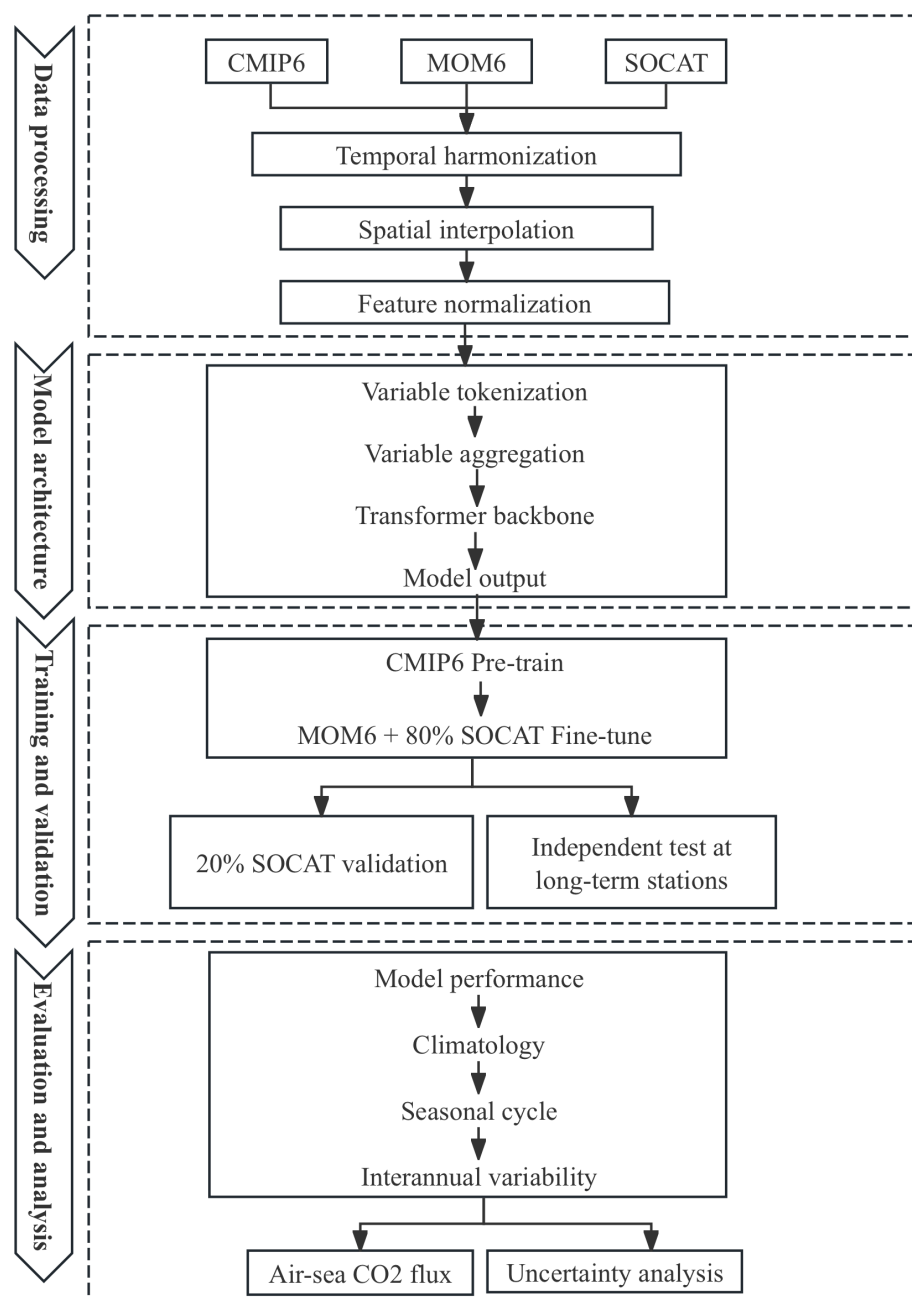


Figure 2. Workflow of the $sp\text{CO}_2$ reconstruction using the ViT-based framework. The workflow consists of four major stages: **(a)** data processing, where CMIP6, MOM6, and SOCAT inputs are temporally harmonized, spatially interpolated, and normalized; **(b)** model architecture, where variables are tokenized, aggregated into spatio-temporal embeddings, and processed by a Transformer backbone to predict monthly $sp\text{CO}_2$; **(c)** training and validation, involving CMIP6 pretraining, MOM6 and SOCAT fine-tuning, and evaluation against withheld SOCAT data and long-term stations; and **(d)** evaluation and analysis, where model performance metrics, climatology, seasonal cycles, and interannual variability are assessed, leading to downstream analyses such as air–sea CO_2 flux estimation and uncertainty analysis (see detailed description in Sect. S5.1).

lation. Reconstructed values were masked where SOCAT is missing, and all skill metrics were computed only at grid-time points with valid SOCAT data. For the independent test at long-term stations, reconstructed values were extracted at the corresponding station locations using bilinear spatial in-

terpolation, which incorporates information from surrounding grid cells to provide smoother and more representative estimates, and skill metrics were subsequently computed to evaluate model performance. Detailed information for these stations, including their names, geographic locations, obser-

variation periods, number of samples, and data sources, is provided in Table S3, and their locations are shown in Fig. S2 to facilitate visual interpretation. Subsequently, the climatological mean, seasonal variations, and interannual changes are calculated at each grid point where data are available. The processed SJTU-AViT data are then compared with the corresponding SOCAT observations in the following sections.

In the training process, we adopt the latitude-weighted mean squared error (MSE) as the loss function to ensure that the model accommodates the spatial variability caused by the Earth's curvature. The latitude-weighted MSE effectively emphasizes the prediction accuracy in low-latitude regions, which occupy a larger proportion of the Earth's surface (Nguyen et al., 2023; Willard et al., 2024). The loss function is computed as follows:

$$\text{MSE} = \frac{1}{N} \frac{1}{H} \frac{1}{W} \sum_{t=1}^N \sum_{h=1}^H \sum_{w=1}^W \alpha(h) (y_{t,h,w} - y_{\text{obs},t,h,w})^2 \quad (2)$$

where N is the total number of time points in the dataset, H and W are the numbers of latitudinal and longitudinal grid points, respectively, and t , h , and w represent the time, latitude, and longitude indices, respectively. $y_{\text{obs},t,h,w}$ is the observed value, and $y_{t,h,w}$ is the predicted value. The term $\alpha(h)$ is the latitude weight.

In the validation process, we use multiple evaluation metrics, including mean bias error (MBE), mean absolute error (MAE), root mean square error (RMSE), and coefficient of determination (R^2). These metrics have been extensively used in reconstructed data assessments and climate model evaluations. It is computed as follows:

$$\text{MBE} = \frac{1}{n} \sum_{i=1}^n (y_{\text{rec},i} - y_{\text{obs},i}) \quad (3)$$

$$\text{MAE} = 1/n \sum_{i=1}^n |y_{\text{rec},i} - y_{\text{obs},i}| \quad (4)$$

$$\text{RMSE} = \sqrt{1/n \sum_{i=1}^n (y_{\text{rec},i} - y_{\text{obs},i})^2} \quad (5)$$

$$R^2 = 1 - \sum_{i=1}^n (y_{\text{obs},i} - y_{\text{rec},i})^2 / \sum_{i=1}^n (y_{\text{obs},i} - \overline{y_{\text{obs}}})^2 \quad (6)$$

where n represents the number of data samples, $y_{\text{rec},i}$ denotes the reconstructed values, while $y_{\text{obs},i}$ and $\overline{y_{\text{obs}}}$ represent the observed values and their mean, respectively.

To evaluate the performance of the deep learning model (ViT-base Model) adopted in this study, we selected eight global ocean $sp\text{CO}_2$ products (Table 2), nine independent observational stations (Fig. S2a), and SOCAT data. The chosen benchmark datasets include Jena-MLS, MPI-SOMFFN, OS-ETHZ-GRaCER, and five other data products (Table 2), which are widely used in the ocean carbon community. These data products cover periods from 1957 to 2023 at varying

spatial resolutions from 1 to 2.50° , with temporal resolutions ranging from daily to monthly. The nine stations span various periods and effectively capture the spatial and temporal variability of ocean $sp\text{CO}_2$. The diversity of the benchmark datasets provides a deeper understanding of the model's performance across different oceanic environments, thus further optimizing its predictive capabilities.

2.4 Air–sea CO_2 flux computation

We calculate the air–sea CO_2 flux ($F\text{CO}_2$, $\text{mol C m}^{-2} \text{ yr}^{-1}$) from the reconstructed $sp\text{CO}_2$ using a standard bulk parameterization (Wanninkhof, 2014), given by the equation:

$$F\text{CO}_2 = k_w \cdot K_0 \cdot (1 - f_{\text{ice}}) \cdot (sp\text{CO}_2 - ap\text{CO}_2) \quad (7)$$

Here, the flux ($F\text{CO}_2$) is considered positive when CO_2 is outgassed from the ocean and negative when CO_2 is absorbed by the ocean. The fluxes are adjusted to account for the ice-free area of each pixel, with the sea ice cover data (f_{ice}) taken from Rayner et al. (2003). The gas transfer velocity of CO_2 (k_w) is computed using the parameterization of Wanninkhof (2014), which assumes a quadratic dependence on wind speed. The Schmidt number (Sc) required in this formulation is calculated following the temperature-dependent empirical formula provided by Wanninkhof (2014). The wind speed data is sourced from ERA5, with a 6-hourly temporal resolution spanning 1982–2023 and a 1° spatial resolution. To ensure consistency with global radiocarbon-based constraints (Graven et al., 2012; Müller et al., 2008; Sweeney et al., 2007; Wanninkhof, 2014), the scaling factor is set as 0.251 (Wanninkhof, 2014), which equals about a global mean transfer velocity of 16 cm h^{-1} . The solubility of CO_2 in seawater (K_0) is calculated as a function of SST and SSS (Weiss, 1974). The partial pressure of atmospheric CO_2 ($ap\text{CO}_2$) is estimated using the mole fraction of CO_2 in dry air ($x\text{CO}_2$) from the ESRL MBL CO_2 product, with water vapor correction from Dickson et al. (2007).

2.5 ViT-based model uncertainty estimation

The uncertainty associated with our reconstructed $sp\text{CO}_2$ product was estimated using the method proposed by Landschützer et al. (2014, 2018). The uncertainty of estimated $sp\text{CO}_2$ for each grid cell was accumulated from the quadratic sum of four sources of uncertainties:

$$u_{sp\text{CO}_2} = \sqrt{u_{\text{obs}}^2 + u_{\text{grid}}^2 + u_{\text{algorithm}}^2 + u_{\text{inputs}}^2} \quad (8)$$

u_{obs} is the observational uncertainty inherited from observations. The SOCAT gridded product compiles the $p\text{CO}_2$ observations with WOCE flags A, B (uncertainty $< 2 \mu\text{atm}$), C, and D (uncertainty $< 5 \mu\text{atm}$). Adopting a conservative approach, we set the maximum value of u_{obs} to $5 \mu\text{atm}$. u_{grid} is calculated as the standard deviation of the samples used for gridding $sp\text{CO}_2$ in each grid cell (Roobaert et al., 2024a; Wu

Table 2. References for global $sp\text{CO}_2$ products used for comparison.

Dataset	Time range	Spatial resolution	Temporal resolution	Reference
Jena-MLS	1957–2023	$2.50^\circ \text{ lon} \times 2^\circ \text{ lat}$	daily	Rödenbeck et al. (2014)
MPI-SOMFFN	1982–2022	$1^\circ \times 1^\circ$	monthly	Landschützer et al. (2016)
OS-ETHZ-GRaCER	1982–2022	$1^\circ \times 1^\circ$	monthly	Gregor and Gruber (2021)
CMEMS-LSCE-FFNN	1985–2018	$1^\circ \times 1^\circ$	monthly	Chau et al. (2022)
CSIR-ML6	1985–2018	$1^\circ \times 1^\circ$	monthly	Gregor et al. (2019)
Watson	1985–2019	$1^\circ \times 1^\circ$	monthly	Watson et al. (2020)
NIES-NN	1980–2019	$1^\circ \times 1^\circ$	monthly	Zeng et al. (2014)
JMA-MLR	1985–2019	$1^\circ \times 1^\circ$	monthly	Iida et al. (2020)

et al., 2025). $u_{\text{algorithm}}$ is evaluated as the RMSE between the reconstructed and reference ocean model $sp\text{CO}_2$ field.

In addition to the three uncertainty sources previously mentioned, this study also considers the cumulative uncertainty introduced by input variables (u_{inputs}). The uncertainties associated with these variables are calculated through Monte Carlo simulations (Wu et al., 2025). For each input variable, white noise following a normal distribution ($N(0, u_{xi})$) is added, and $sp\text{CO}_2$ is recalculated using the perturbed inputs. By repeating 100 times, the uncertainty for each input variable is then determined by calculating the standard deviation of the differences between the original $sp\text{CO}_2$ and the $sp\text{CO}_2$ values obtained after adding noise. Detailed procedures for determining these input uncertainties are described in Sect. S1 in the Supplement.

3 Results

3.1 Evaluation of ViT-based model performance

The SJTU-AViT product demonstrated robust performance and high accuracy in capturing $sp\text{CO}_2$ variability (Fig. 3). In the training phase (Fig. 3a), the model achieved a high coefficient of determination ($R^2 = 0.86$), with low root mean square error (RMSE = 16.70 μatm), an MAE of 6.89 μatm , and minimal mean bias error (MBE = −0.36 μatm), based on over 277 528 (80 %) samples. In the validation phase (Fig. 3b), the model maintained robust performance, with an R^2 of 0.82 and an RMSE of 18.30 μatm , indicating strong generalization ability and no sign of overfitting. Most predicted values lie close to the 1 : 1 line, particularly within the climatologically common $sp\text{CO}_2$ range (300–420 μatm), as indicated by the high-density regions in Fig. 3. These results confirm the model’s ability to accurately reconstruct large-scale $sp\text{CO}_2$ patterns across diverse oceanic regimes. In addition, the sensitivity test indicates that the implementation of physical-biogeochemical constraints can significantly improve model performance, reducing the mean absolute error from 7.15 to 5.95 μatm .

Independent test with in-situ buoy observations (which were not used to train the model) (Fig. 4) indicates that

the model performs best in subtropical regions (e.g., HOT, BATS, CCE1, ESTOC, and Papa), accurately capturing both long-term trends (Fig. 4) and seasonal cycles (Fig. S3). At the HOT station, for instance, the model yields a minimal MBE of 0.31 μatm , a low RMSE of 8.65 μatm , and a high $R^2 = 0.86$, and similar performance is observed at other subtropical stations, indicating the model’s accuracy in data-rich, stable regions. In the equatorial Pacific Ocean, the model shows reasonable performance at the data-sparse TAO station in the Pacific Ocean, with a slight negative MBE (−7.02 μatm), an RMSE of 13.16 μatm , and an R^2 of 0.74, effectively capturing large-scale seasonal variability in equatorial upwelling-dominated environments (Fig. S3). Similarly, at the monsoon-influenced BOBOA station at the Bay of Bengal, where observations are also limited, the model captures overall variability with an MBE (−6.07 μatm), an RMSE of 10.48 μatm , and an R^2 of 0.65, indicating reasonable skill in capturing the overall variability driven by monsoonal forcing processes. In contrast, performance deteriorates at high-latitude stations and regions with strong dynamical variability. At the Irminger Sea and Iceland sites, the model exhibits large RMSE (35.24 and 21.82 μatm , respectively) and low correlations, with R^2 near zero. This suggests that the model has difficulty capturing rapid $sp\text{CO}_2$ fluctuations or processes that are not well represented by the available input features. This discrepancy is likely due to high-latitude processes such as seasonal sea-ice variability and freshwater inputs, which are not fully represented in the current observational constraints.

In general, the evaluation confirms that the ViT-based method effectively generates essentially bias-free $sp\text{CO}_2$ fields with no signs of overfitting, achieving high accuracy in low latitudes and open oceans, while performance declines at high latitudes.

3.2 Evaluation of long-term climatology and annual means of $sp\text{CO}_2$

The reconstructed $sp\text{CO}_2$ product (SJTU-AViT) exhibits strong agreement with SOCAT observations in terms of long-term climatology, successfully capturing the large-scale spa-

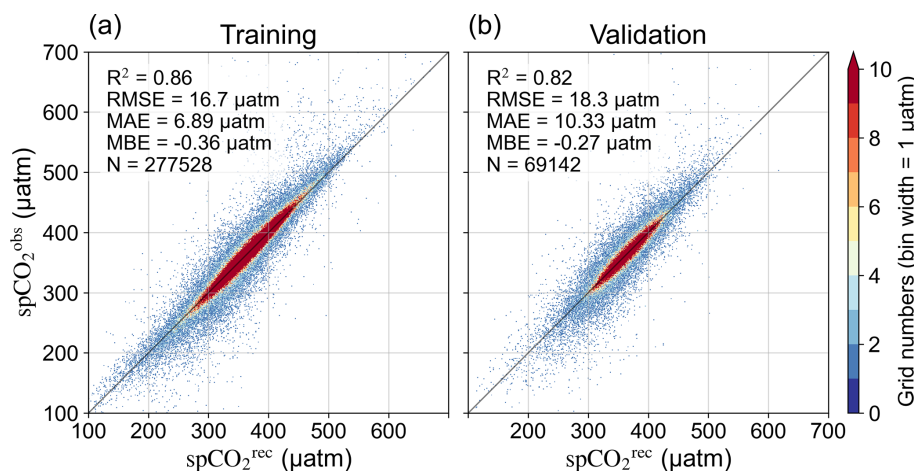


Figure 3. Performance evaluation of the ViT-based model for reconstructing the SJTU-AViT $sp\text{CO}_2$ product. Density scatter plots illustrate the comparison between model-reconstructed sea surface partial pressure of CO_2 ($sp\text{CO}_2^{\text{rec}}$) and in situ SOCAT observations ($sp\text{CO}_2^{\text{obs}}$) during (a) the training phase (using 80 % of the samples) and (b) the validation phase (using 20 % of the samples). Statistical metrics, including the coefficient of determination (R^2), root mean square error (RMSE), mean absolute error (MAE), mean bias error (MBE), and the number of samples (N), are provided to quantitatively assess model performance. The color bar indicates the number of data points within each bin, representing the density of observations. The $sp\text{CO}_2$ in SJTU-AViT is interpolated to match the SOCAT observation locations and times in the comparison.

tial distribution of $sp\text{CO}_2$ in the global ocean (Fig. 5a–c). This demonstrates strong consistency with previous climatology products (Landschützer et al., 2020; Takahashi et al., 2002). Elevated $sp\text{CO}_2$ values are prominent in the tropical oceans (e.g., equatorial Pacific Ocean) and coastal upwelling regions, driven by the upwelling of CO_2 -rich subsurface waters. In contrast, low $sp\text{CO}_2$ levels are predominantly observed in mid-latitude gyre areas (e.g., the North Pacific Ocean) which is driven by subduction processes. The relatively low $sp\text{CO}_2$ is present in the high-latitude regions, driven primarily by low temperature and a strong biological pump.

Compared with all SOCAT observation grid cells, the SJTU-AViT product exhibits good performance metrics in terms of long-term climatology, characterized by a low bias (MBE = $-0.21 \mu\text{atm}$, Fig. 5d), a low MAE of $5.95 \mu\text{atm}$, a low RMSE of $7.44 \mu\text{atm}$, and a notably high correlation coefficient ($R = 0.94$). The small averaged bias suggests that the model does not exhibit systematic over- or underestimation at the global scale, further validating its reliability in estimating the monthly and annual mean climatology of $sp\text{CO}_2$. However, despite the small overall bias, the spatial distribution of bias shows significant regional variation (Fig. 5d). The larger biases ($> 4 \mu\text{atm}$) are predominantly found in the coastal, tropical, and high-latitude oceans. The bias comparison between coastal and open oceans indicates the probability distribution function (pdf) for open ocean centers around $0.16 \mu\text{atm}$, with 90 % of the biases falling between -12 to $+10 \mu\text{atm}$ (Fig. 6b). Conversely, the pdf for coastal ocean (400 km distance from the coastline) bias centers around $-1.44 \mu\text{atm}$, with 90 % of the biases remain

within the range of -18 to $+14 \mu\text{atm}$ (Fig. 6c). The larger biases in the coastal ocean may stem from complex coastal physical-biogeochemical processes, such as terrestrial inputs, tidal mixing, and freshwater fluxes from rivers (Bauer et al., 2013; Cai et al., 2020; Roobaert et al., 2024b). These processes are often difficult to accurately capture in global-scale reconstruction models.

Comparison among different ocean basins (see basin boundary in Fig. S2b) indicate that $sp\text{CO}_2$ biases in high-latitude oceans, specifically the Arctic and Southern Oceans, are much larger than the biases in the low and middle latitudes of the Pacific, Atlantic, and Indian Oceans (Fig. 6). The bias of pdf line for the Arctic Ocean and Southern Ocean centers around -1.95 and $-0.64 \mu\text{atm}$, with 90 % of the biases falling within the range of -20 to $+16 \mu\text{atm}$ and -14 to $+12 \mu\text{atm}$ respectively (Fig. 6g and h). The biases in other ocean basins have a near-zero mean value and a narrow range of 90 % of the grid cells (-12 to $+10 \mu\text{atm}$, Fig. 6). The increased $sp\text{CO}_2$ uncertainty in the high-latitude oceans might be related to factors such as seasonal ice cover, intense local hydrological changes, and sparse observational data. The smaller bias in the low and middle latitudes of other ocean basins can be attributed to the relatively stable oceanic conditions and the availability of abundant observational data, which help improve the accuracy of model reconstruction in regions dominated by large-scale physical processes driving air–sea CO_2 exchange. Additionally, relatively large bias observed in the tropical ocean may stem from complex interannual variability associated with climate variability like El Niño–Southern Oscillation (ENSO) and Indian Ocean dipole (IOD). Despite these regional differences,

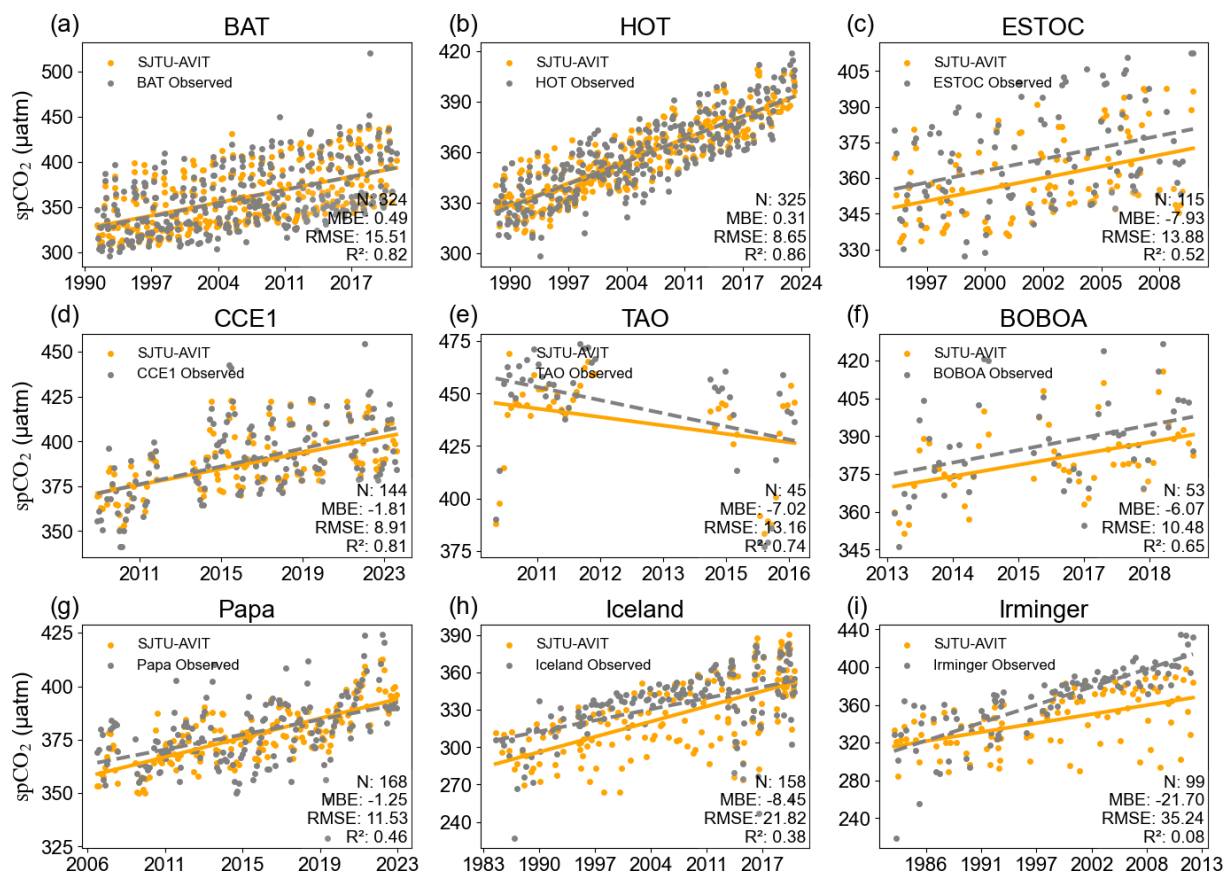


Figure 4. Independent test of $sp\text{CO}_2$ variability between SJTU-AViT and in situ observations at different stations. These in situ data are independent data and are not used to train the model. The station description and location refer to Sect. S2 and Fig. S2. The $sp\text{CO}_2$ in SJTU-AViT is interpolated to match the station locations and times in the comparison. For each panel, the number of samples (N), the mean bias error (MBE), root mean square error (RMSE), and correlation coefficient (R^2) between the reconstructed and observed $sp\text{CO}_2$ are displayed. The dashed and solid lines show the linear trend of SJTU-AViT and in situ data.

the low overall bias demonstrates the SJTU-AViT product's effectiveness in accurately capturing the spatial distribution of $sp\text{CO}_2$ on a global scale.

The distribution of temporal evolution of annual mean $sp\text{CO}_2$ (Fig. 7a) exhibits a clear rightward shift over time, indicating a long-term rise in $sp\text{CO}_2$. Specifically, the annual mean $sp\text{CO}_2$ rises from 330 to 400 μatm , with an estimated trend of $1.42 \mu\text{atm yr}^{-1}$. This trend is consistent with the long-term increase in global oceanic $sp\text{CO}_2$ driven by atmospheric CO_2 growth (Gruber et al., 2023; Landschützer et al., 2016), further validating the reliability of the reconstruction. In addition to this overall increase, the shape of the $sp\text{CO}_2$ frequency distribution varies across years (Fig. 7a). Notably, the pdf gradually broadens over time, suggesting enhanced spatial heterogeneity in surface ocean CO_2 concentrations under the combined influence of rising CO_2 levels and global warming. The distribution of reconstruction biases (Fig. 7b) centers around 0 with a narrow range ($< 30 \mu\text{atm}$), suggesting that the reconstruction data has no systematic offset. This further indicates that the features of shape variability across

years captured by SJTU-AViT data are trustworthy. In the early years (from the 1980s to the mid-1990s), the bias distribution is more dispersed with a notable skew toward negative values, implying that the model tended to underestimate surface CO_2 partial pressure during this period. As time progresses, the bias distribution becomes increasingly concentrated and more symmetric around zero. This shift reflects improved reconstruction accuracy as the spatial coverage of observational data increased (Fig. S4). However, we note that the absolute range of biases may increase in later years. This widening is likely due to a combination of factors, including the expansion of observational coverage to regions with more extreme or marginal conditions, which introduces a larger range of reconstructed values, as well as the enhanced seasonal and interannual variability that the model may not fully capture in some regions, leading to increased biases under local or extreme conditions. Overall, the temporal evolution of the bias distribution highlights both the influence of observational coverage and the challenges in capturing high-frequency or extreme variations.

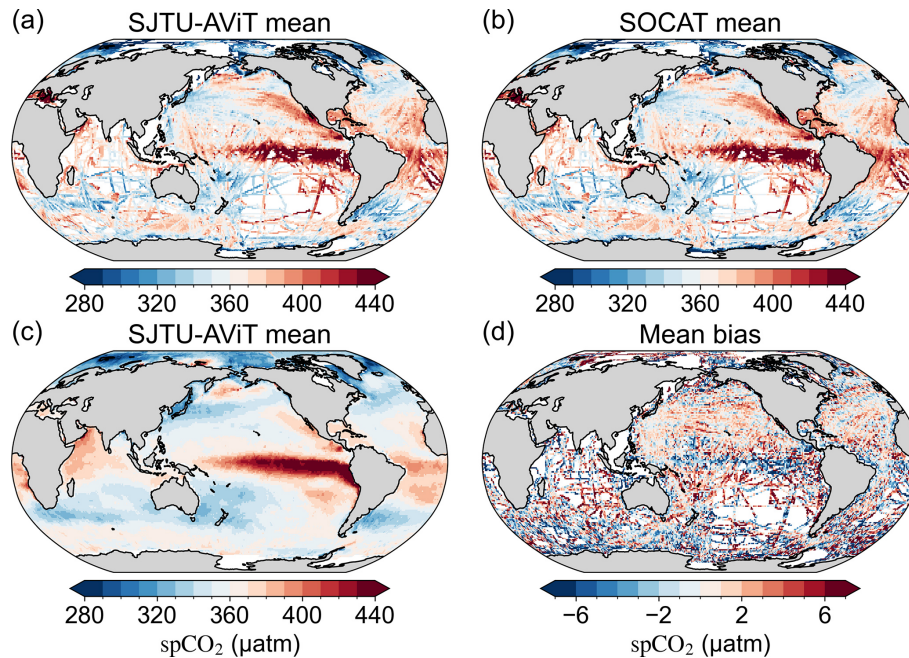


Figure 5. Comparison of long-term mean $sp\text{CO}_2$ between SJTU-AViT and SOCAT over 1982–2023. **(a)** Long-term mean $sp\text{CO}_2$ from SJTU-AViT on the SOCAT observation grid points. **(b)** Long-term mean $sp\text{CO}_2$ from SOCAT. **(c)** Long-term mean $sp\text{CO}_2$ from SJTU-AViT at all grid points. **(d)** Mean bias (SJTU-AViT minus SOCAT, panel a minus panel b) on SOCAT observation grid points. In panel a, SJTU-AViT values are first interpolated to match the spatial and temporal locations of SOCAT observations, after which the long-term mean is calculated at each grid point where data are available (see detailed computation in Sect. 2.3).

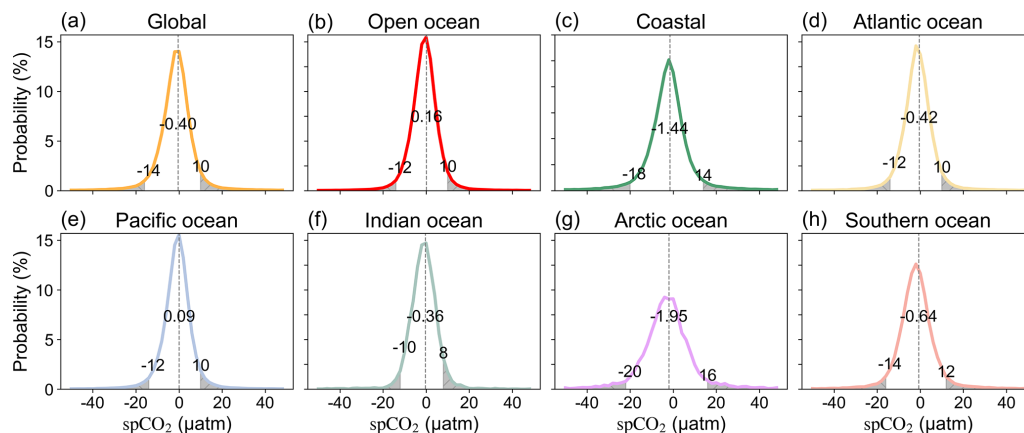


Figure 6. Bias probability density distributions of long-term mean $sp\text{CO}_2$ for the SJTU-AViT product compared to SOCAT data across different ocean regions. **(a)** Global ocean, **(b)** Open ocean, **(c)** Coastal ocean, and **(d–h)** individual ocean basins. Coastal ocean is defined as the region within 400 km from coastline. The spatial extents of the ocean basins are shown in Fig. S2. The vertical dashed line represents the mean $sp\text{CO}_2$ value for each region, with the 95 % and 5 % threshold points marked on either side of the mean. The values next to the dashed lines indicate the corresponding mean bias and the values at the two sides of dashed lines are 95 % and 5 % percentiles for each region. The $sp\text{CO}_2$ in SJTU-AViT is interpolated to match the SOCAT observation locations and times in the bias computation (see detailed computation in Sect. 2.3). The asymmetry in the percentiles is due to the asymmetric shape of the probability density function.

3.3 Evaluation of full $sp\text{CO}_2$ variability and seasonal cycle

The variability in $sp\text{CO}_2$ mainly includes the seasonal, interannual, and decadal variability. To evaluate the ability

of SJTU-AViT in reproducing this variability, we compute the overall standard deviation of $sp\text{CO}_2$ at each observational grid cell (Fig. 8a). The SJTU-AViT data product effectively reproduces the magnitude and spatial distribution of observed $sp\text{CO}_2$ variability from 1982 to 2023, as indicated

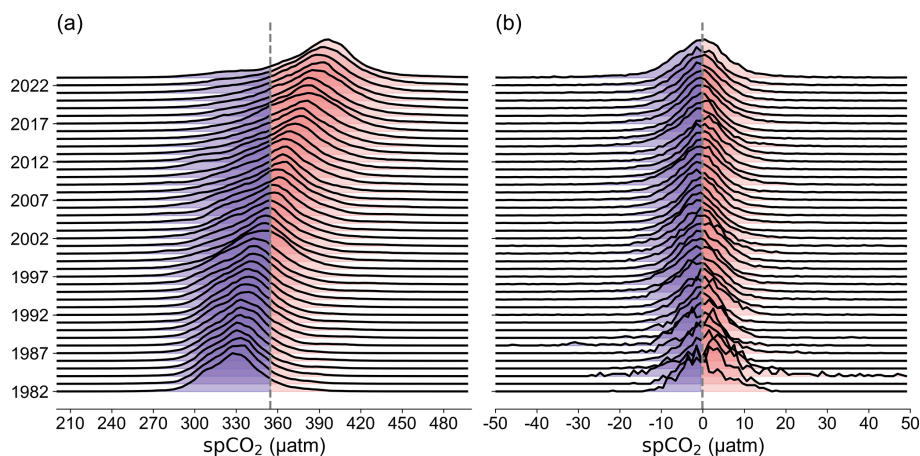


Figure 7. Probability density distributions of annual mean $sp\text{CO}_2$ from the SJTU-AViT and bias relative to SOCAT. **(a)** Probability density distribution of annual mean $sp\text{CO}_2$ from the SJTU-AViT; **(b)** bias probability density distribution of annual mean $sp\text{CO}_2$ between SJTU-AViT and SOCAT. The vertical dashed line indicates the mean $sp\text{CO}_2$ value and mean bias in panels a and b, respectively. The $sp\text{CO}_2$ in SJTU-AViT is interpolated to match the SOCAT observation locations and times in the bias computation (see detailed computation in Sect. 2.3).

by the consistent $sp\text{CO}_2$ standard deviation between SJTU-AViT and SOCAT data (Fig. 8a and b). The SOCAT observations (Fig. 8b) show that the strongest $sp\text{CO}_2$ variability ($\text{SD} > 30 \mu\text{atm}$) is concentrated in the tropical Pacific Ocean, the North Pacific Ocean (40° and 60° N), the North Atlantic Ocean (40° N), and parts of the South Pacific Ocean (30° S). The SJTU-AViT successfully reproduces these spatial features, exhibiting low bias across most regions (Fig. 8d). The ratio of SJTU-AViT vs SOCAT standard deviation ranges from 0.80–1.20 which indicates the SJTU-AViT data is able to capture the 80 %–120 % varied amplitude. The bias comparison shows that the deep learning model exhibits a mean bias in standard deviation of $-1.97 \mu\text{atm}$, indicating high reliability in capturing $sp\text{CO}_2$ variability (Fig. 8d). However, the standard deviation bias (Fig. 8d) reveals an overall underestimation of variability, with only 18.69 % of grid points showing a positive bias. This underestimation is particularly pronounced in high-latitude regions and is likely attributed to the smoothing effect of the machine learning model, which attenuates high-frequency variability, as well as the spatial inhomogeneity of observational data. In contrast, some overestimations are observed in regions with sparse data coverage, such as the Southern Ocean and the Indian Ocean (Fig. 8c).

The SJTU-AViT effectively captures the large-scale seasonal distribution and amplitude of $sp\text{CO}_2$, as shown in Figs. 9 and 10. Across the four climatological seasons – MAM (March–May), JJA (June–August), SON (September–November), and DJF (December–February) – the model reconstructs major spatial patterns that are broadly consistent with SOCAT observations. Notably, the model successfully reproduces persistently high $sp\text{CO}_2$ concentrations in the equatorial Pacific Ocean, primarily driven by continuous up-

welling of CO_2 -rich subsurface waters throughout the year. It also captures elevated $sp\text{CO}_2$ values in both the Atlantic and Pacific Oceans within the 5° – 30° N and 5° – 30° S latitudinal band during the respective summer and autumn seasons of each hemisphere, reflecting the combined effects of increased surface temperatures and seasonally weakened biological uptake. Furthermore, the model reasonably reproduces seasonal increases in $sp\text{CO}_2$ in the North Pacific and North Atlantic (40° – 60° N) during Northern Hemisphere winter and early spring. This suggests that the model has likely captured underlying mechanisms, such as the deepening of the winter mixed layer and the entrainment of DIC-rich subsurface waters, which drive seasonal variations in surface ocean $p\text{CO}_2$ (Keppler et al., 2020). Conversely, a pronounced seasonal decrease in $sp\text{CO}_2$ is simulated in the high-latitude Southern Ocean (south of 60° S) during the same period, indicating that the model may also have learned the influence of cooling-driven solubility changes and biological activity on ocean $p\text{CO}_2$. These spatial and seasonal patterns demonstrate the model's capacity to incorporate key physical and biogeochemical processes regulating $sp\text{CO}_2$ variability.

Bias analysis in Fig. 9i–l reveals seasonal model–observation discrepancies through the mean absolute error distribution. Larger errors (MAE exceeding $10 \mu\text{atm}$) are observed in mid- to high-latitude regions during JJA and SON, particularly in the North Pacific Ocean, North Atlantic Ocean, and coastal zones. These discrepancies are likely linked to complex biological processes (e.g., seasonal blooms, net community production), which are not well captured using data-driven approaches. In contrast, lower mean absolute errors are found in subtropical gyres during DJF and MAM, with MAE values typically below $6 \mu\text{atm}$, where

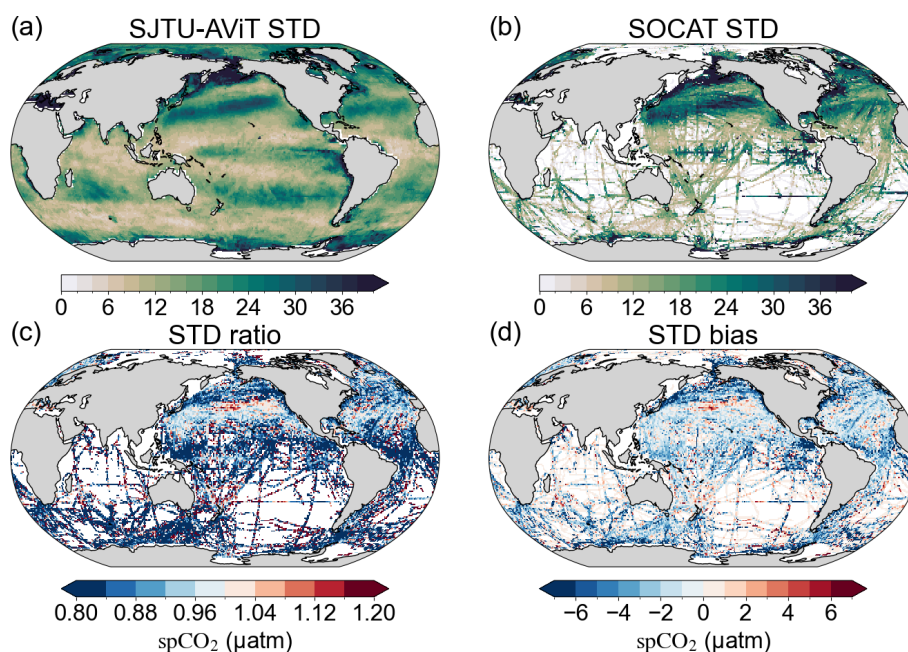


Figure 8. Comparison of spCO_2 standard deviation from 1982–2023 between SJTU-AViT and SOCAT. (a) Standard deviation of spCO_2 from the SJTU-AViT reconstruction. (b) Standard deviation of spCO_2 from SOCAT data. (c) Standard deviation ratio, representing the ratio of SJTU-AViT to SOCAT standard deviation (SJTU-AViT divided by SOCAT). (d) Standard deviation bias, showing the difference between the SJTU-AViT and SOCAT standard deviations (SJTU-AViT minus SOCAT). The standard deviation (SD) is quantified as the standard deviation of residuals after removing long-term trends. In the panels (c) and (d), the SJTU-AViT values are interpolated to match the spatial and temporal locations of SOCAT observations (see detailed computation in Sect. 2.3).

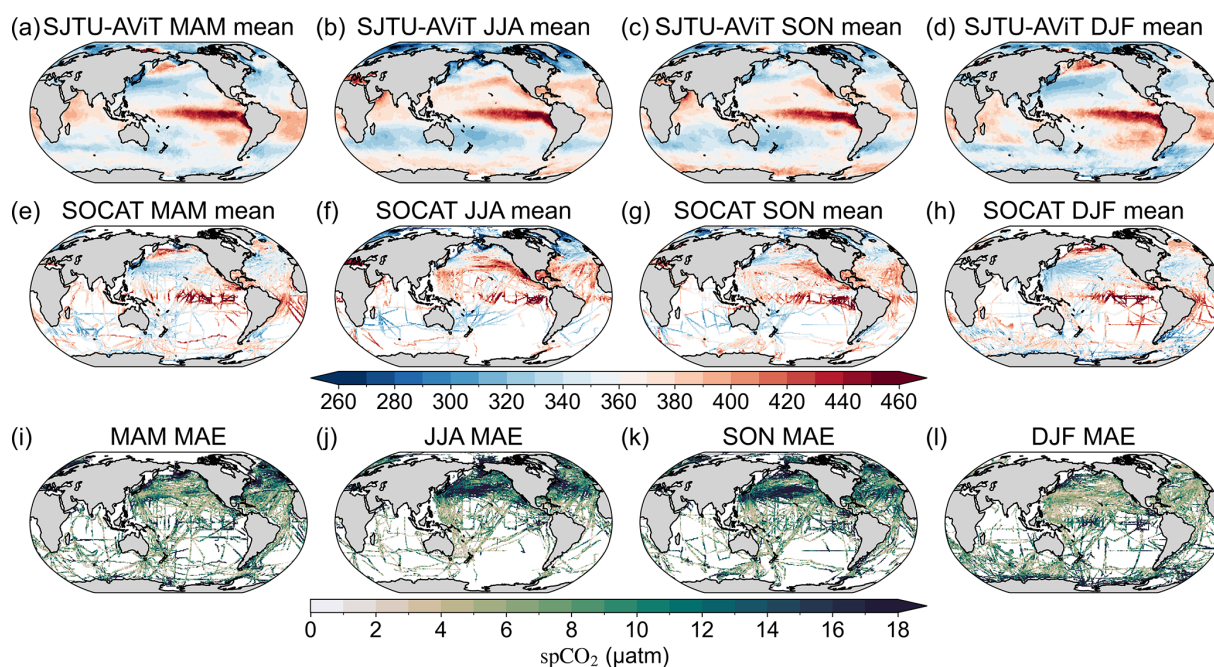


Figure 9. Comparison of seasonal spCO_2 means and mean absolute errors between SJTU-AViT and SOCAT. (a–d) Seasonal mean spCO_2 from the SJTU-AViT reconstruction for MAM (March–May), JJA (June–August), SON (September–November), and DJF (December–February). (e–h) Seasonal mean spCO_2 from SOCAT data. (i–l) Mean absolute error (MAE) of spCO_2 between SJTU-AViT and SOCAT for each season. The spCO_2 in SJTU-AViT is interpolated to match the SOCAT observation locations and times in the MAE computation (see detailed computation in Sect. 2.3).

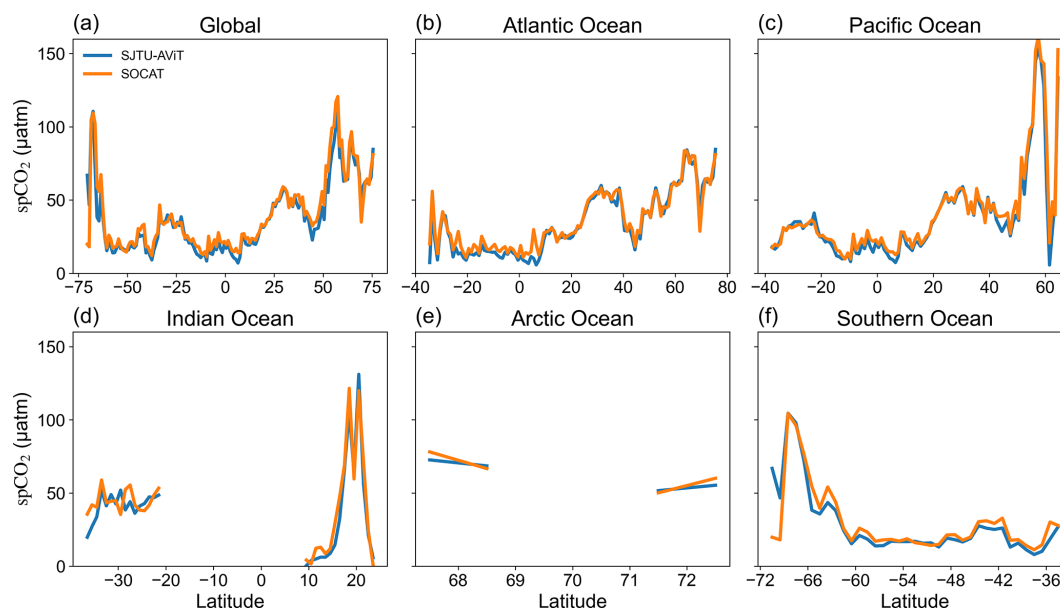


Figure 10. Comparison of meridional seasonal amplitude of $sp\text{CO}_2$ between SJTU-AViT and SOCAT across different ocean regions from 1982–2023. The seasonal amplitude is defined as the absolute value of the difference between winter (December–February) and summer (June–August) means, subsequently averaged zonally. The spatial extents of the ocean basins are shown in Fig. S2. The $sp\text{CO}_2$ in SJTU-AViT is interpolated to match the SOCAT observation locations and times in the comparison (see detailed computation in Sect. 2.3).

variability is predominantly governed by physical drivers like SST and MLD, which are more effectively resolved by the model. Despite the pronounced interannual influence of ENSO events on $sp\text{CO}_2$ variability in equatorial regions, the model consistently achieves low reconstruction bias across different seasons, indicating that SJTU-AViT effectively captures ENSO-related interannual anomalies in $sp\text{CO}_2$. Additionally, the reduced observation density may contribute to the high bias of seasonal variability in the Southern Ocean and parts of the Indian Ocean.

Figure 10 further supports the model's performance in reproducing seasonal $sp\text{CO}_2$ amplitude. Zonally averaged seasonal amplitudes across the global ocean and individual ocean basins show a high degree of agreement between SJTU-AViT and SOCAT, particularly in the Atlantic and Pacific Oceans. The model captures the amplitude peaks in the Northern Hemisphere around 40–60° N and in the Southern Hemisphere near 50° S, aligning with regions of pronounced seasonal forcing. However, deviations are observed in the Arctic Ocean, where limited data coverage likely leads to an underestimation of seasonal amplitude. Similarly, in the Southern Ocean, the model slightly overestimates seasonal amplitude in some latitudes, which may stem from the smoothing nature of machine learning algorithms and the scarcity of high-frequency, high-latitude measurements.

To evaluate the accuracy of the SJTU-AViT in capturing the seasonal phasing of $sp\text{CO}_2$, we compared it against SOCAT climatology (Figs. S16–S18). Climatological seasonal cycles were evaluated for the global ocean and five ma-

ior basins, separately for the Northern and Southern Hemispheres. The SJTU-AViT closely reproduces the timing of seasonal maxima and minima in $sp\text{CO}_2$, generally aligning with SOCAT observations. Global maps of phase differences show that most regions deviate by less than ± 1 month, with only $\sim 5\%$ of grid points exceeding this range. These results demonstrate that the reconstruction data reliably captures the observed seasonal phasing.

The bias of standard deviation in each season remains relatively low and spatially coherent across all four climatological seasons, providing further evidence of the model's robustness in representing both the magnitude and spatial distribution of seasonal $sp\text{CO}_2$ variability (Fig. S5). Overall, the SJTU-AViT product exhibits strong skill in reconstructing seasonal $sp\text{CO}_2$ patterns, amplitudes and phases globally. The remaining biases highlight the need for improved observational coverage in polar and biologically dynamic regions, and for enhanced model formulations that better account for nonlinear biological and physical interactions driving seasonal CO_2 variability.

3.4 Evaluation of $sp\text{CO}_2$ variability on timescales longer than 1 year

This section evaluates $sp\text{CO}_2$ variability on timescales longer than one year. Specifically, the variability is quantified as the standard deviation of residuals after removing both long-term trends and seasonal cycles. For the SOCAT data, calculating the residual standard deviation is challenging due to the gap in the observation record. Therefore, we

use the long-term trend and seasonal amplitude derived from the SJTU-AViT data to compute the residual for the SOCAT data. While this variability encompasses both interannual and decadal variability, the signal shown here is predominantly driven by interannual fluctuations due to the limited temporal range of the data, spanning only 42 years. Therefore, for simplicity, we refer to it as interannual variability throughout this study. A comprehensive assessment of the global spatial distribution of this variability is presented in Fig. 11.

Figure 11a and b compare the interannual variability of $sp\text{CO}_2$ derived from the SJTU-AViT model and SOCAT observations. The model accurately captures the spatial patterns of interannual variability, showing strong structural agreement with the observational dataset. High variability is well reproduced in key regions such as the equatorial Pacific Ocean (15°N – 15°S , 120 – 280°E), the subpolar gyres of the North Pacific and North Atlantic (30 – 60°N), and the high latitudes of the Southern Ocean (south of 60°S). The variability in these areas is probably related to the interannual change of wind stress, upwelling, and mixed layers. To evaluate the model's performance in reproducing variability amplitude, Fig. 11c shows the bias in interannual standard deviation relative to SOCAT. On a global scale, the bias is generally small ($-2.66\text{ }\mu\text{atm}$) but tends toward slight underestimation. The most pronounced underestimations ($> 6\text{ }\mu\text{atm}$) appear in the high-latitude North Pacific, North Atlantic, and Southern Ocean, where high-frequency variability is often suppressed by machine learning models due to their inherent smoothing.

Figure 11d presents the interannual standard deviation from SJTU-AViT, while Fig. 11e shows the ensemble mean of standard deviation in each existing $sp\text{CO}_2$ products as a reference. Notably, SJTU-AViT reveals stronger variability in most global oceans – especially the Southern Ocean, tropical Pacific, and North Atlantic subtropical gyre (Figs. 11f and S6). Considering the SJTU-AViT still underestimates the interannual variability compared to SOCAT, the Fig. 11 comparison suggests the ViT-based model better retains ocean–climate variability signals rather than excessively smoothing them. The improved performance of SJTU-AViT in capturing interannual amplitude is likely due to the multi-head self-attention mechanism, high representational capacity, and the transfer learning approach applied using CMIP6 and ocean-driven biogeochemical model results. This helps the model better capture the interaction between ocean $p\text{CO}_2$ and interannual variability modes, leading to more accurate estimations of $sp\text{CO}_2$ fluctuations on the interannual timescale.

We further assessed the performance of the SJTU-AViT product in the equatorial Pacific Ocean, where interannual variability of $sp\text{CO}_2$ is the strongest in the global ocean. The SJTU-AViT dataset demonstrates clear and spatially coherent $sp\text{CO}_2$ anomaly patterns associated with ENSO events (Figs. 12 and S7). In terms of spatial distribution, SJTU-AViT reproduces a significant decline in $sp\text{CO}_2$ over the eastern Pacific Ocean during El Niño and a pronounced

increase during La Niña. These strong comparisons between different phases of ENSO are consistent with well-established physical-biogeochemical mechanisms of ENSO-driven carbon variability through changes in upwelling, SST, precipitation, and biology (Liao et al., 2020; Sun et al., 2025). Due to the limited availability of long-term observational data, we compare the SJTU-AViT with the composite mean of multiple available $sp\text{CO}_2$ data products. The spatial patterns of anomalies in SJTU-AViT are broadly consistent with those in the multi-model ensemble. Notably, the SJTU-AViT provides finer spatial detail, particularly in the nearshore eastern Pacific Ocean, where sharp gradients and coastal processes are more pronounced.

The consistency between the SJTU-AViT product and these data products is further confirmed by the temporal correlation between $sp\text{CO}_2$ anomalies and the Niño 3.4 SST index. The SJTU-AViT shows a correlation of -0.81 and the multiple data products range from -0.40 to -0.78 (Fig. S7), indicating that the SJTU-AViT model captures the temporal evolution of ENSO-related variability in the carbon system. The latitudinal comparison also indicates a strong agreement between SJTU-AViT results, data product, and SOCAT observations during both El Niño and La Niña periods (Fig. 13).

These results indicate that the SJTU-AViT model reliably reconstructs the spatial patterns of interannual and decadal $sp\text{CO}_2$ variability at SOCAT observation sites and across the global ocean. Its ability to capture variability in line with key physical indicators such as SST and MLD demonstrates its robustness in physically consistent reconstructions. Nevertheless, regional discrepancies highlight the need for further refinement, particularly in under-observed areas and regions where non-physical factors may dominate reconstructed variability.

3.5 Evaluation of the air–sea CO_2 fluxes

The air–sea CO_2 flux based on SJTU-AViT $sp\text{CO}_2$ reproduces consistent known features with multiple data products (Gregor et al., 2019; Landschützer et al., 2016; Takahashi et al., 2009). Elevated $F\text{CO}_2$ is observed along the equator, particularly in the eastern equatorial Pacific, associated with the upwelling of carbon-rich waters. In contrast, mid-to-high latitudes act as net CO_2 sinks (Fig. 14a). This substantial carbon sequestration is primarily driven by the enhanced solubility of CO_2 in cold waters, deep water mixing, transport processes, and the biological carbon pump (DeVries et al., 2017; Gregor et al., 2018; Sarmiento et al., 2004; Takahashi et al., 2009). While SJTU-AViT effectively reproduces the overall spatial patterns and mechanisms of air–sea CO_2 flux, Fig. 6 indicates that negative $sp\text{CO}_2$ biases remain in certain high-latitude regions. The negative bias, likely associated with underrepresented high-latitude processes such as seasonal sea-ice variability and freshwater inputs, can lead to an overestimation of global ocean CO_2 uptake through the

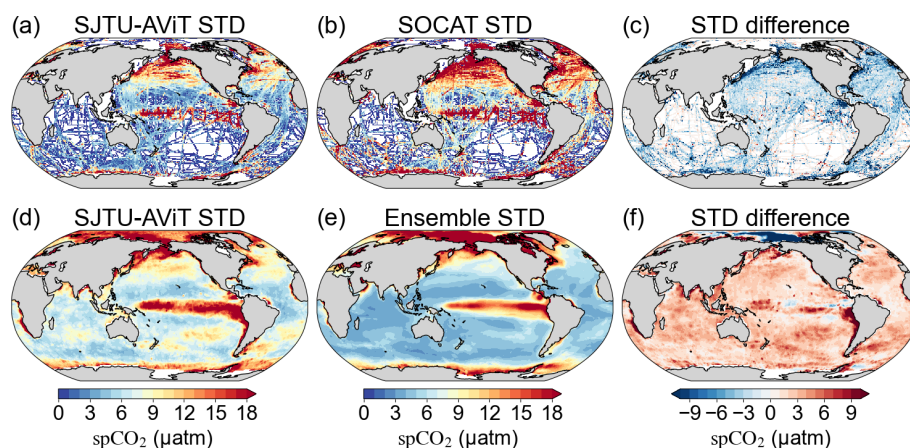


Figure 11. Comparison of $sp\text{CO}_2$ standard deviations on timescales longer than one year between SJTU-AViT, SOCAT, and multiple data products. (a) Standard deviation of $sp\text{CO}_2$ from the SJTU-AViT at SOCAT observation grid points. (b) Standard deviation of $sp\text{CO}_2$ from SOCAT data. (c) Standard deviation bias between SJTU-AViT and SOCAT – panel (a) minus panel (b). (d) Standard deviation of $sp\text{CO}_2$ from the SJTU-AViT. (e) Ensemble mean standard deviation from multiple existing $sp\text{CO}_2$ data products. (f) Standard deviation difference between the SJTU-AViT and the ensemble mean standard deviation – panel (d) minus panel (e). The standard deviation (SD) is quantified as the standard deviation of residuals after removing both long-term trends and seasonal cycles, representing the variability on timescales longer than one year. The $sp\text{CO}_2$ in SJTU-AViT is interpolated to match the SOCAT observation locations and times in the panel (a)–(c) comparison (see detailed computation in Sect. 2.3).

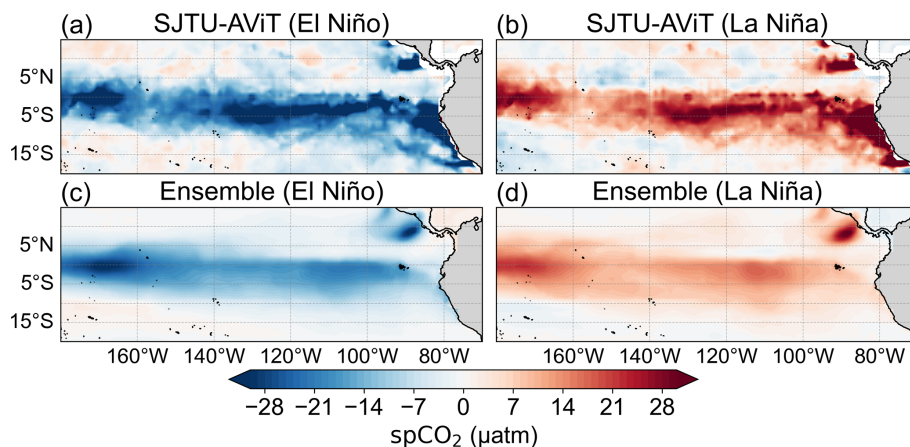


Figure 12. Comparison of $sp\text{CO}_2$ anomalies during El Niño and La Niña events between SJTU-AViT and multiple data products. Panels (a) and (b) show the composite mean $sp\text{CO}_2$ anomalies during eight El Niño and seven La Niña events, respectively, as reconstructed by the SJTU-AViT product. Panels (c) and (d) display the corresponding composite mean anomalies from the ensemble mean of eight $sp\text{CO}_2$ data products. The eight El Niños and seven La Niñas are indicated in Sects. S2 and S3. The $sp\text{CO}_2$ anomalies are defined as residuals after removing both long-term trends and seasonal cycles.

bulk equation and should be considered when interpreting the absolute flux magnitude.

The time series of global air–sea CO_2 flux (Fig. 14b) shows a strengthening oceanic carbon sink over the past four decades, from $-1.40 \text{ Pg C yr}^{-1}$ in the early 1980s to $-2.60 \text{ Pg C yr}^{-1}$ in the 2010s. Notably, the SJTU-AViT reconstruction is consistently maintained within the ± 2 SD (standard deviation) envelope of existing multi-product ensemble estimates and exhibits strong agreement with other $F\text{CO}_2$ products. Interannual and decadal variability are ev-

ident, such as a temporary weakening of the sink from the late 1990s to the early 21st century, reflecting the modulation of global carbon sink strength by external forcing and climate variability (DeVries, 2022; McKinley et al., 2020). In particular, the significant weakening of the carbon sink during the 1997–1998 strong El Niño event is effectively reproduced, without exhibiting the abrupt discontinuities or artificial jumps.

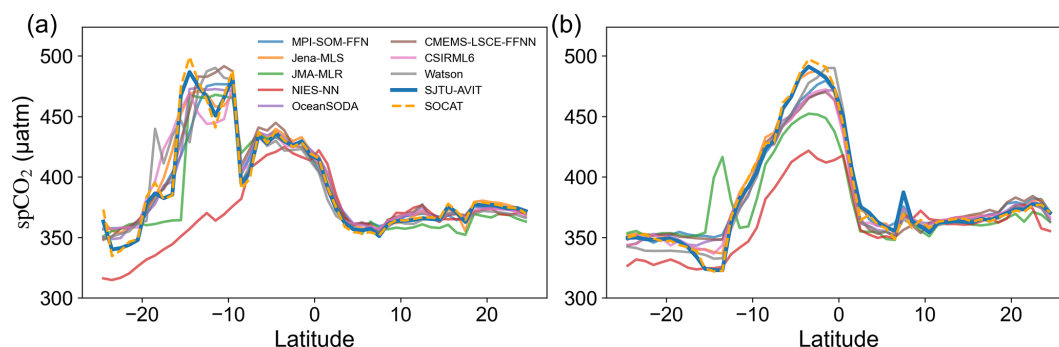


Figure 13. Comparison of meridional $sp\text{CO}_2$ between SJTU-AViT, SOCAT, and multiple data products during (a) El Niño and (b) La Niña events. The selected El Niño events are 1997–1998 and 2002–2003, while the La Niña events are 1995–1996 and 1998–1999. These events are selected due to the availability of several cruise datasets during these periods. The cruise data are distributed over 240–280° E, which are shown in Fig. S8. The $sp\text{CO}_2$ in all data products is interpolated to match the SOCAT observation locations and times in the comparison.

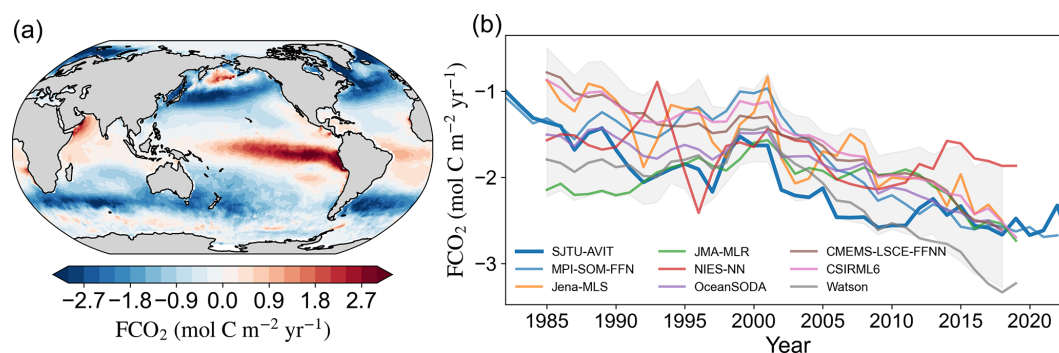


Figure 14. Spatial and temporal characteristics of air–sea CO_2 flux (FCO_2 , $\text{mol C m}^{-2} \text{yr}^{-1}$); (a) spatial distribution of the long-term annual mean FCO_2 ; (b) comparison of time series of yearly global integrated CO_2 flux between SJTU-AViT and multiple data products. Colored lines represent individual products, with SJTU-AViT highlighted in bold. The shaded area indicates the ± 2 SD (standard deviation) range, centered on the ensemble mean. Negative = ocean uptake (sink), Positive = release to the atmosphere (source).

3.6 Evaluation of the uncertainty of reconstructed $sp\text{CO}_2$

The global uncertainty associated with the reconstructed $sp\text{CO}_2$ is estimated to evaluate the reliability of the data product. The estimated global mean uncertainty is $11.05 \mu\text{atm}$, with the dominant contribution arising from the algorithm uncertainty ($u_{\text{algorithm}}$), which reaches $7.39 \mu\text{atm}$. This value was obtained through error propagation and reflects the cumulative impact of both systematic and random errors introduced throughout the reconstruction procedure. Given the conservative nature of our uncertainty estimation, this magnitude is considered reasonable. Specifically, to ensure a conservative approach, the observational uncertainty (u_{obs}) for each SOCAT data point was uniformly set to $5 \mu\text{atm}$, following established practices. The gridding process applied to SOCAT data (u_{grid}) resulted in an uncertainty of $6.34 \mu\text{atm}$. The contribution from uncertainties in the input variables (u_{inputs}) is comparatively minor, also estimated at $1.50 \mu\text{atm}$.

Regionally, the estimated uncertainties of reconstructed $sp\text{CO}_2$ exhibit moderate spatial variability across the major ocean basins. Among the five RECCAP2-defined open ocean regions, the Indian Ocean shows the lowest mean uncertainty at $8.62 \mu\text{atm}$, followed by the Pacific Ocean ($10.10 \mu\text{atm}$) and the Atlantic Ocean ($10.28 \mu\text{atm}$). Higher uncertainty levels are observed in the Southern Ocean ($11.64 \mu\text{atm}$) and the Arctic Ocean ($12.45 \mu\text{atm}$), consistent with sparser observational coverage, enhanced seasonal variability, and more complex air–sea interactions in these regions. These regional patterns suggest that while the global uncertainty level remains controlled, localized differences – particularly in high-latitude oceans – should be considered when interpreting the product in regional carbon budget assessments.

4 Discussion

In this study, we present a new reconstructed data product of $sp\text{CO}_2$ (SJTU-AViT) with improved interannual variability using the ViT-based deep learning model. The ViT-based deep learning model integrates the Vision Transformer

(ViT) architecture with physics-informed constraints and assimilates outputs from advanced ocean biogeochemical models, including CMIP6 models and ocean-driven biogeochemical model (MOM6-COBALT2). This integration enables a more precise extraction of the complex relationships between oceanic environmental variables and $sp\text{CO}_2$. The SJTU-AViT product effectively captures key spatiotemporal patterns and reconstructs improved interannual $sp\text{CO}_2$ variability.

In addition, we evaluated the contributions of CMIP6 pre-training, MOM6 fine-tuning, SOCAT observations, and MOM6-derived physical-biogeochemical constraints within the SJTU-AViT framework. CMIP6 pre-training substantially improved model initialization and skill, reducing validation RMSE by $\sim 56.57\%$ versus random initialization by supplying large-scale structure and low-frequency variability. MOM6 fine-tuning further stabilized the model – especially in observation-sparse regions – lowering RMSE by $\sim 39.36\%$ and enforcing physically plausible relationships. Including SOCAT during fine-tuning was critical for local and regional accuracy, reducing RMSE by $\sim 72.31\%$ through high-quality pointwise constraints. Sensitivity tests indicate the reconstruction is largely robust to the specific choice of CMIP6 pre-training subsets, provided multiple models are used to capture diverse large-scale patterns. Finally, adding MOM6-derived physical constraints improved overall performance (MAE from 7.15 to 5.95 μatm) and reduced seasonal RMSE by 1.36%–8.49%, with the largest gains in high-latitude and data-sparse regions. Collectively, these results confirm that CMIP6 pre-training followed by MOM6- and SOCAT-constrained fine-tuning with physically informed constraints yields a robust, reliable, and physically consistent reconstruction of $sp\text{CO}_2$ across spatial and temporal scales.

Despite the strong performance of SJTU-AViT, several challenges remain. A key issue is to understand and reconcile the discrepancy among different reconstruction products, particularly when considering the influence of specific climate modes such as the Indian Ocean Dipole (IOD). As illustrated in Fig. 15, during positive IOD events, nine distinct $sp\text{CO}_2$ data products exhibit divergent composite anomaly patterns across the Indian Ocean (see IOD definition in Sect. S2). The SJTU-AViT results indicate an increase in $sp\text{CO}_2$ in the western Indian Ocean basin and a decrease in the eastern basin (Valsala et al., 2020). The other data products present divergent or even opposite spatial patterns, raising fundamental questions about which data product most accurately reflects reality in the data-limited region. The scarcity of in situ observations in the Indian Ocean exacerbates the difficulty in determining the most reliable $sp\text{CO}_2$ distribution (Valsala et al., 2021). These uncertainties underscore the urgent need to enhance observational efforts, particularly in regions where data products exhibit significant divergence (Rödenbeck et al., 2015). Future work should focus on expanding observation networks and lever-

aging autonomous platforms such as biogeochemical Argo floats (Claustre et al., 2020; Williams et al., 2017) to provide crucial validation data.

Decadal variability presents more significant challenges, with larger biases that require increased attention. Current reconstruction methods primarily capture these climate modes (e.g., Pacific Decadal Oscillation, PDO) implicitly and do not explicitly incorporate relevant indices in the machine learning model training. While increasing observational coverage is essential, it may not quickly resolve the issues related to decadal variability. A more effective solution may lie in improving the reconstruction methods themselves, particularly through the integration of physics-informed approaches. For instance, implementing physical-biogeochemical constraints, such as incorporating $sp\text{CO}_2$ sensitivity to SST, SSS, DIC, and Alk, can significantly improve model performance, reducing the mean absolute error from 7.15 to 5.95 μatm . Future research should focus more on exploring physics-informed machine learning approaches that integrate climate indices as explicit inputs to enhance model interpretability and predictive capability (Reichstein et al., 2019; Willard et al., 2020).

While ViT-based models effectively learn spatial patterns from observational data, they remain susceptible to inherent biases in training data (Dosovitskiy et al., 2020). Systematic biases in SOCAT observations or oceanic variables (e.g., temperature and salinity) may propagate through the reconstruction process, impacting regional carbon cycle estimates (Takahashi et al., 2009). To address this, uncertainty quantification techniques such as Bayesian deep learning or ensemble learning could be incorporated to assess confidence intervals in reconstructed $sp\text{CO}_2$ and improve anomaly detection capabilities (Gal and Ghahramani, 2016; Lakshminarayanan et al., 2016). It should be noted that the climatological MLD used in this study cannot capture interannual or monthly variability, which may slightly underestimate local or short-term impacts on $sp\text{CO}_2$. Nevertheless, it provides adequate physical constraints for reconstructing long-term and large-scale spatiotemporal patterns. Future work will explore incorporating high-quality time-varying MLD data as it becomes available to improve model fidelity at regional and seasonal scales.

Furthermore, existing $sp\text{CO}_2$ reconstruction approaches predominantly rely on physical environmental variables while largely neglecting biological processes. In high-productivity regions such as the North Atlantic, Southern Ocean, and Arctic Ocean, biological processes play a crucial role in regulating CO_2 exchange, with phytoplankton photosynthesis significantly lowering $sp\text{CO}_2$ (Bates and Mathis, 2009; Boyce et al., 2010; Takahashi et al., 2009). However, Chl *a* only partially represents biological influences and is subject to considerable uncertainties in high-latitude regions, particularly in ice-covered areas (Arrigo et al., 2008). To better account for biological processes, future efforts should incorporate additional biogeochemical variables such as net

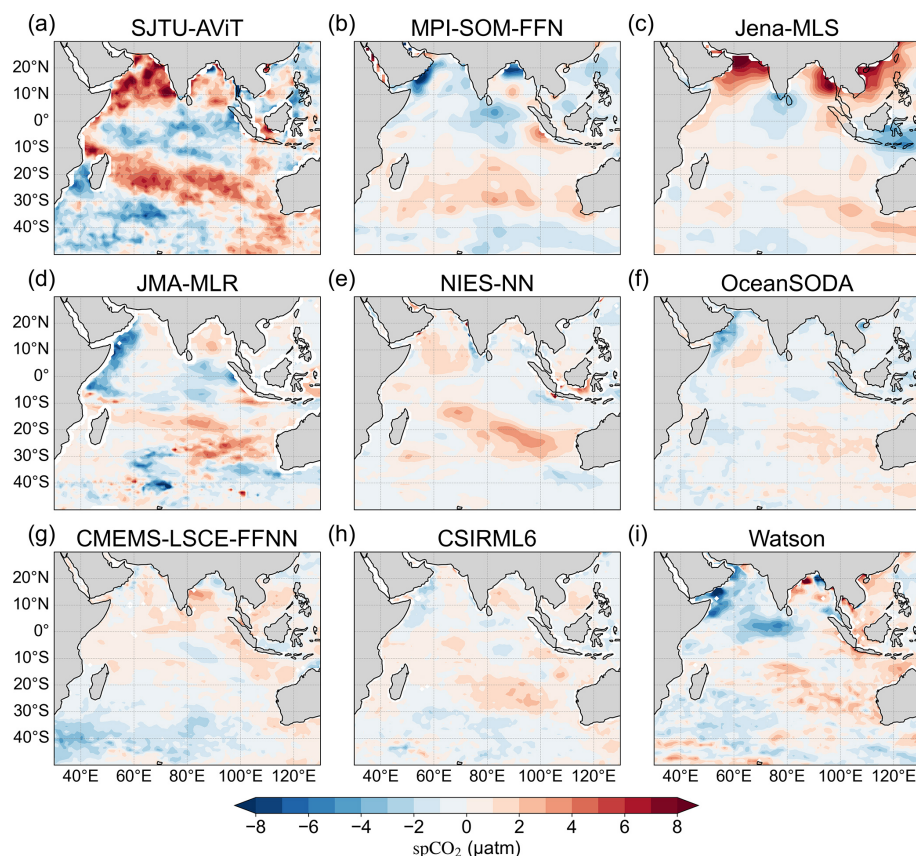


Figure 15. Spatial patterns of $sp\text{CO}_2$ anomalies during positive IOD in the Indian Ocean between SJTU-AViT and multiple data products. The $sp\text{CO}_2$ anomaly is the composite mean of eight positive IOD events (detailed IOD events are shown in Sects. S2 and S3). For each IOD event, the anomalies are averaged over the months of September, October, and November.

community production (NCP) (Arrigo and Dijken, 2011; Behrenfeld et al., 2006) and phytoplankton community structure, alongside bio-optical remote sensing techniques, to enhance reconstruction accuracy and the physical coherence of carbon cycle interpretations.

The generalization capability of machine learning models is contingent on the completeness and representativeness of training data, leading to substantial uncertainties in data-sparse regions (Gloege et al., 2021). This is particularly evident in high-latitude oceans, where $sp\text{CO}_2$ is modulated by sea ice cover, biological carbon pumps, and deep-water upwelling – processes that cannot be fully inferred from surface environmental variables alone (Mongwe et al., 2018). Since current models primarily rely on surface observations, their ability to capture vertical carbon transport and subsurface processes remains limited. Future studies should integrate three-dimensional ocean state variables (e.g., dissolved inorganic carbon and alkalinity) (Fennel et al., 2023; Wang et al., 2024; Zhou and Zhang, 2023) and incorporate physical conservation constraints (e.g., mass balance and chemical equilibrium) to enhance the physical robustness of machine learning models (Leal et al., 2020; Wang and Gupta, 2024).

Additionally, applying data assimilation techniques or coupling machine learning with physics-based biogeochemical models could further improve reconstruction accuracy (Arcucci et al., 2021; Brajard et al., 2021; Chen et al., 2023).

In summary, high-resolution $sp\text{CO}_2$ reconstruction is critical for understanding global ocean carbon sink variability. While the ViT-based approach offers an innovative solution, key challenges remain regarding dataset discrepancies, climate variability impacts, data uncertainties, and the omission of physical and biological processes. Existing reconstruction data product must be interpreted with caution when assessing regional carbon fluxes. As ocean acidification and climate change continue to alter marine carbon dynamics, improving our ability to reconstruct historical $sp\text{CO}_2$ trends is essential for predicting the future ocean carbon uptake. Advancing $sp\text{CO}_2$ reconstruction toward higher accuracy and reliability will require multi-source data integration, explainable machine learning, and robust uncertainty quantification techniques. Furthermore, this study highlights the critical synergy between observational programs and machine learning-based modeling approaches in achieving more precise global carbon assessments.

5 Data availability

The reconstructed $sp\text{CO}_2$ and $f\text{CO}_2$ datasets are publicly available as a NetCDF file at <https://doi.org/10.5281/zenodo.15331978> (Zhang et al., 2025) and will be updated regularly. The input datasets used for the reconstruction are also publicly accessible. The SST and SIC datasets were obtained from the NOAA OISST product (<https://www.ncei.noaa.gov/products/optimum-interpolation-sst>, last access: 20 February 2025). Chl a data were derived from the ESA CCI Ocean Colour project (<https://climate.esa.int/en/projects/ocean-colour/>, last access: 20 February 2025). $x\text{CO}_2$ data were sourced from the ESRL MBL CO_2 product (<https://gml.noaa.gov/ccgg/mbl/data.php>, last access: 20 February 2025). Wind speed and sea level pressure data were retrieved from the ERA5 reanalysis provided by the Medium-Range Weather Forecasts (ECMWF) (<https://doi.org/10.24381/cds.f17050d7>, Hersbach et al., 2023).

6 Conclusions

This study presents a novel global data product of $sp\text{CO}_2$ reconstructed by a ViT-based deep learning model at a 1° spatial resolution for the period 1982–2023. By integrating multi-source observational data, biogeochemical ocean model results, and physics-informed constraints, the reconstructed data product demonstrates strong accuracy and spatial coherence across diverse oceanic regions, with a particular improvement in capturing interannual variability.

The model performs robustly during both the training and independent validation phases, with high accuracy ($R^2 = 0.86$ in training, $R^2 = 0.82$ in validation) and low bias (RMSE of $16.70 \mu\text{atm}$ in training). The implementation of physical-biogeochemical constraints can significantly improve model performance, reducing the mean absolute error from 7.15 to $5.95 \mu\text{atm}$. The reconstructed data product shows strong agreement with SOCAT observations and accurately reproduces long-term climatological and annual mean $sp\text{CO}_2$, with a low global mean bias of $-0.21 \mu\text{atm}$, a low mean absolute error of $5.95 \mu\text{atm}$, and a high correlation coefficient ($R = 0.94$). However, biases were found in coastal and high-latitude oceans, suggesting the need for further refinement in these areas.

The evaluation of seasonality reveals that the SJTU-AViT model effectively captures both seasonal patterns and amplitudes across global ocean basins, particularly in regions with stable conditions, such as subtropical gyres. On the time scale longer than one year, the model demonstrated its ability to capture higher interannual $sp\text{CO}_2$ variability, particularly during El Niño and La Niña events, with high spatial and temporal coherence. The higher performance is likely due to the incorporation of CMIP6 model and advanced ocean biogeochemical model results during the ViT-based model

training process. This approach allows the model to capture more accurate $sp\text{CO}_2$ variability in these data-sparse regions. Additionally, it captures the global ocean carbon sink's long-term strengthening, consistent with rising atmospheric CO_2 . However, uncertainties remain in high-latitude regions due to challenges in resolving complex oceanic processes. Despite this, the model's output aligns with the uncertainty ranges of existing datasets, demonstrating its reliability for global CO_2 exchange assessments.

This study highlights machine learning's potential in $sp\text{CO}_2$ reconstruction, while identifying key challenges, such as input data limitations and model interpretability. Future work should extend this approach to higher spatial and temporal resolutions, integrate more biogeochemical parameters, and couple the model with ocean-atmosphere models for improved long-term projections. Additionally, enhancing model interpretability will be crucial for understanding the drivers of $sp\text{CO}_2$ variability. The approach shows promise for reconstructing other carbonate system parameters, contributing to a more comprehensive global ocean carbon data product. This will support climate change research, carbon neutrality policies, and global carbon management efforts.

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Author contributions. EL conceived the original idea of this work, acquired funding, and provided continuous guidance. XZ conducted the main analysis, developed the code, performed the experiments, and drafted the manuscript. SL supported the setup of the computational environment and assisted with access to HPC resources. WL, ZW, GW, and XMZ supervised the overall progress of the study, reviewed the manuscript, and provided critical feedback and revisions. All authors contributed to the final version of the manuscript.

Competing interests. The contact author has declared that none of the authors has any competing interests.

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References

- Adcroft, A., Anderson, W., Balaji, V., Blanton, C., Bushuk, M., Dufour, C. O., Dunne, J. P., Griffies, S. M., Hallberg, R., Harrison, M. J., Held, I. M., Jansen, M. F., John, J. G., Krasting, J. P., Langenhorst, A. R., Legg, S., Liang, Z., McHugh, C., Radhakrishnan, A., Reichl, B. G., Rosati, T., Samuels, B. L., Shao, A., Stouffer, R., Winton, M., Wittenberg, A. T., Xiang, B., Zadeh, N., and Zhang, R.: The GFDL Global Ocean and Sea Ice Model OM4.0: Model Description and Simulation Features, *J. Adv. Model. Earth Syst.*, 11, 3167–3211, <https://doi.org/10.1029/2019MS001726>, 2019.
- Arcucci, R., Zhu, J., Hu, S., and Guo, Y.-K.: Deep Data Assimilation: Integrating Deep Learning with Data Assimilation, *Appl. Sci.*, 11, 1114, <https://doi.org/10.3390/app11031114>, 2021.
- Arrigo, K. R. and Dijken, G. L. V.: Secular trends in Arctic Ocean net primary production, *J. Geophys. Res.-Oceans*, 116, C09011, <https://doi.org/10.1029/2011JC007151>, 2011.
- Arrigo, K. R., Dijken, G. V., and Pabi, S.: Impact of a shrinking Arctic ice cover on marine primary production, *Geophys. Res. Lett.*, 35, L19603, <https://doi.org/10.1029/2008GL035028>, 2008.
- Bakker, D. C. E., Pfeil, B., Landa, C. S., Metzl, N., O'Brien, K. M., Olsen, A., Smith, K., Cosca, C., Harasawa, S., Jones, S. D., Nakaoka, S.-I., Nojiri, Y., Schuster, U., Steinhoff, T., Sweeney, C., Takahashi, T., Tilbrook, B., Wada, C., Wanninkhof, R., Alin, S. R., Balestrini, C. F., Barbero, L., Bates, N. R., Bianchi, A. A., Bonou, F., Boutin, J., Bozec, Y., Burger, E. F., Cai, W.-J., Castle, R. D., Chen, L., Chierici, M., Currie, K., Evans, W., Featherstone, C., Feely, R. A., Fransson, A., Goyet, C., Greenwood, N., Gregor, L., Hankin, S., Hardman-Mountford, N. J., Harlay, J., Hauck, J., Hoppema, M., Humphreys, M. P., Hunt, C. W., Huss, B., Ibáñez, J. S. P., Johannessen, T., Keeling, R., Kitidis, V., Körtzinger, A., Kozyr, A., Krasakopoulou, E., Kuwata, A., Landschützer, P., Lauvset, S. K., Lefèvre, N., Lo Monaco, C., Manke, A., Mathis, J. T., Merlivat, L., Millero, F. J., Monteiro, P. M. S., Munro, D. R., Murata, A., Newberger, T., Omar, A. M., Ono, T., Paterson, K., Pearce, D., Pierrot, D., Robbins, L. L., Saito, S., Salisbury, J., Schlitzer, R., Schneider, B., Schweitzer, R., Sieger, R., Skjelvan, I., Sullivan, K. F., Sutherland, S. C., Sutton, A. J., Tadokoro, K., Telszewski, M., Tuma, M., Van Heuven, S. M. A. C., Vandemark, D., Ward, B., Watson, A. J., and Xu, S.: A multi-decade record of high-quality $f\text{CO}_2$ data in version 3 of the Surface Ocean CO_2 Atlas (SOCAT), *Earth Syst. Sci. Data*, 8, 383–413, <https://doi.org/10.5194/essd-8-383-2016>, 2016.
- Bates, N. R. and Mathis, J. T.: The Arctic Ocean marine carbon cycle: evaluation of air–sea CO_2 exchanges, ocean acidification impacts and potential feedbacks, *Biogeosciences*, 6, 2433–2459, <https://doi.org/10.5194/bg-6-2433-2009>, 2009.
- Bauer, J. E., Cai, W.-J., Raymond, P. A., Bianchi, T. S., Hopkinson, C. S., Regnier, P. A. G., Bauer, J. E., Cai, W.-J., Raymond, P. A., Bianchi, T. S., Hopkinson, C. S., and Regnier, P. A. G.: The changing carbon cycle of the coastal ocean, *Nature*, 504, 61–70, <https://doi.org/10.1038/nature12857>, 2013.
- Behrenfeld, M. J., O'Malley, R. T., Siegel, D. A., McClain, C. R., Sarmiento, J. L., Feldman, G. C., Milligan, A. J., Falkowski, P. G., Letelier, R. M., and Boss, E. S.: Climate-driven trends in contemporary ocean productivity, *Nature*, 444, 752–755, <https://doi.org/10.1038/nature05317>, 2006.
- Boyce, D. G., Lewis, M. R., and Worm, B.: Global phytoplankton decline over the past century, *Nature*, 466, 591–596, <https://doi.org/10.1038/nature09268>, 2010.
- Brajard, J., Carrassi, A., Bocquet, M., and Bertino, L.: Combining data assimilation and machine learning to infer unresolved scale parametrization, *Philos. T. Roy. Soc. A*, 379, 1–16, <https://doi.org/10.1098/rsta.2020.0086>, 2021.
- Cai, W.-J., Xu, Y.-Y., Feely, R. A., Wanninkhof, R., Jönsson, B., Alin, S. R., Barbero, L., Cross, J. N., Azetsu-Scott, K., Fassbender, A. J., Carter, B. R., Jiang, L.-Q., Pepin, P., Chen, B., Hussain, N., Reimer, J. J., Xue, L., Salisbury, J. E., Hernández-Ayón, J. M., Langdon, C., Li, Q., Sutton, A. J., Chen, C.-T. A., Gledhill, D. K., Cai, W.-J., Xu, Y.-Y., Feely, R. A., Wanninkhof, R., Jönsson, B., Alin, S. R., Barbero, L., Cross, J. N., Azetsu-Scott, K., Fassbender, A. J., Carter, B. R., Jiang, L.-Q., Pepin, P., Chen, B., Hussain, N., Reimer, J. J., Xue, L., Salisbury, J. E., Hernández-Ayón, J. M., Langdon, C., Li, Q., Sutton, A. J., Chen, C.-T. A., and Gledhill, D. K.: Controls on surface water carbonate chemistry along North American ocean margins, *Nat. Commun.*, 11, 1–13, <https://doi.org/10.1038/s41467-020-16530-z>, 2020.
- Chau, T. T., Gehlen, M., and Chevallier, F.: A seamless ensemble-based reconstruction of surface ocean $p\text{CO}_2$ and air–sea CO_2 fluxes over the global coastal and open oceans, *Biogeosciences*, 19, 1087–1109, <https://doi.org/10.5194/bg-19-1087-2022>, 2022.
- Chen, C., Zhang, H., Shi, W., Zhang, W., and Xue, Y.: A novel paradigm for integrating physics-based numerical and machine learning models: A case study of eco-

- hydrological model, *Environ. Model. Softw.*, 163, 105669, <https://doi.org/10.1016/j.envsoft.2023.105669>, 2023.
- Claustre, H., Johnson, K. S., and Takeshita, Y.: Observing the Global Ocean with Biogeochemical-Argo, *Annu. Rev. Mar. Sci.*, 12, 23–48, <https://doi.org/10.1146/annurev-marine-010419-010956>, 2020.
- de Boyer Montégut, C., Madec, G., Fischer, A. S., Lazar, A., and Iudicone, D.: Mixed layer depth over the global ocean: An examination of profile data and a profile-based climatology, *J. Geophys. Res.-Oceans*, 109, C12003, <https://doi.org/10.1029/2004JC002378>, 2004.
- Denvil-Sommer, A., Gehlen, M., Vrac, M., and Mejia, C.: LSCE-FFNN-v1: a two-step neural network model for the reconstruction of surface ocean $p\text{CO}_2$ over the global ocean, *Geosci. Model Dev.*, 12, 2091–2105, <https://doi.org/10.5194/gmd-12-2091-2019>, 2019.
- DeVries, T.: Atmospheric CO_2 and Sea Surface Temperature Variability Cannot Explain Recent Decadal Variability of the Ocean CO_2 Sink, *Geophys. Res. Lett.*, 49, e2021GL096018, <https://doi.org/10.1029/2021GL096018>, 2022.
- DeVries, T., Holzer, M., and Primeau, F.: Recent increase in oceanic carbon uptake driven by weaker upper-ocean overturning, *Nature*, 542, 215–218, <https://doi.org/10.1038/nature21068>, 2017.
- Dickson, A. G., Sabine, C. L., and Christian, J. R.: Guide to best practices for ocean CO_2 measurements, PICES Special Publication 3, 3, 191, <https://doi.org/10.1159/000331784>, 2007.
- Dlugokencky, E. J., Thoning, K. W., Lang, P. M., and Tans, P. P.: NOAA Greenhouse Gas Reference from Atmospheric Carbon Dioxide Dry Air Mole Fractions from the NOAA ESRL Carbon Cycle Cooperative, Global Air Sampling Network [data set], <https://www.esrl.noaa.gov/gmd/ccgg/mbl/data.php> (last access: 20 February 2025), 2019.
- Dosovitskiy, A., Beyer, L., Kolesnikov, A., Weissenborn, D., Zhai, X., Unterthiner, T., Dehghani, M., Minderer, M., Heigold, G., Gelly, S., Uszkoreit, J., and Houslsby, N.: An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale, *arXiv [preprint]*, *arXiv:2010.11929*, <https://doi.org/10.48550/arXiv.2010.11929>, 2020.
- Fennel, K., Long, M. C., Algar, C., Carter, B., Keller, D., Laurent, A., Mattern, J. P., Musgrave, R., Oschlies, A., Ostiguy, J., Palter, J. B., and Whitt, D. B.: Modelling considerations for research on ocean alkalinity enhancement (OAE), in: *Guide to Best Practices in Ocean Alkalinity Enhancement Research*, edited by: Oschlies, A., Stevenson, A., Bach, L. T., Fennel, K., Rickaby, R. E. M., Satterfield, T., Webb, R., and Gattuso, J.-P., Copernicus Publications, State Planet, 2-oae2023, 9, <https://doi.org/10.5194/sp-2-oae2023-9-2023>, 2023.
- Friedlingstein, P., O'Sullivan, M., Jones, M. W., Andrew, R. M., Bakker, D. C. E., Hauck, J., Landschützer, P., Le Quéré, C., Luijkx, I. T., Peters, G. P., Peters, W., Pongratz, J., Schwingshackl, C., Sitch, S., Canadell, J. G., Ciais, P., Jackson, R. B., Alin, S. R., Anthoni, P., Barbero, L., Bates, N. R., Becker, M., Bellouin, N., Decharme, B., Bopp, L., Brasika, I. B. M., Cadule, P., Chamberlain, M. A., Chandra, N., Chau, T.-T.-T., Chevallier, F., Chini, L. P., Cronin, M., Dou, X., Enyo, K., Evans, W., Falk, S., Feely, R. A., Feng, L., Ford, D. J., Gasser, T., Ghattas, J., Gkritzalis, T., Grassi, G., Gregor, L., Gruber, N., Gürses, Ö., Harris, I., Hefner, M., Heinke, J., Houghton, R. A., Hurtt, G. C., Iida, Y., Ilyina, T., Jacobson, A. R., Jain, A., Jarníková, T., Jersild, A., Jiang, F., Jin, Z., Joos, F., Kato, E., Keeling, R. F., Kennedy, D., Klein Goldewijk, K., Knauer, J., Korsbakken, J. I., Körtzinger, A., Lan, X., Lefèvre, N., Li, H., Liu, J., Liu, Z., Ma, L., Marland, G., Mayot, N., McGuire, P. C., McKinley, G. A., Meyer, G., Morgan, E. J., Munro, D. R., Nakaoka, S.-I., Niwa, Y., O'Brien, K. M., Olsen, A., Omar, A. M., Ono, T., Paulsen, M., Pierrot, D., Pockock, K., Poulter, B., Powis, C. M., Rehder, G., Resplandy, L., Robertson, E., Rödenbeck, C., Rosan, T. M., Schwinger, J., Séférian, R., Smallman, T. L., Smith, S. M., Sospedra-Alfonso, R., Sun, Q., Sutton, A. J., Sweeney, C., Takao, S., Tans, P. P., Tian, H., Tilbrook, B., Tsujino, H., Tubiello, F., van der Werf, G. R., van Ooijen, E., Wanninkhof, R., Watanabe, M., Wimart-Rousseau, C., Yang, D., Yang, X., Yuan, W., Yue, X., Zaehle, S., Zeng, J., and Zheng, B.: Global Carbon Budget 2023, *Earth Syst. Sci. Data*, 15, 5301–5369, <https://doi.org/10.5194/essd-15-5301-2023>, 2023.
- Gal, Y. and Ghahramani, Z.: Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning, *arXiv [preprint]*, *arXiv:1506.02142*, <https://doi.org/10.48550/arXiv.1506.02142>, 2016.
- Geurts, P., Ernst, D., Wehenkel, L., Geurts, P., Ernst, D., and Wehenkel, L.: Extremely randomized trees, *Mach. Learn.*, 63, 3–42, <https://doi.org/10.1007/s10994-006-6226-1>, 2006.
- Gloege, L., McKinley, G. A., Landschützer, P., Fay, A. R., Frölicher, T. L., Fyfe, J. C., Ilyina, T., Jones, S., Lovenduski, N. S., Rodgers, K. B., Schlunegger, S., and Takano, Y.: Quantifying Errors in Observationally Based Estimates of Ocean Carbon Sink Variability, *Global Biogeochem. Cy.*, 35, e2020GB006788, <https://doi.org/10.1029/2020GB006788>, 2021.
- Good, S. A., Martin, M. J., and Rayner, N. A.: EN4: Quality controlled ocean temperature and salinity profiles and monthly objective analyses with uncertainty estimates, *J. Geophys. Res.-Oceans*, 118, 6704–6716, <https://doi.org/10.1002/2013JC009067>, 2013.
- Graven, H. D., Gruber, N., Key, R., Khatriwala, S., and Giraud, X.: Changing controls on oceanic radiocarbon: New insights on shallow-to-deep ocean exchange and anthropogenic CO_2 uptake, *J. Geophys. Res.-Oceans*, 117, C10005, <https://doi.org/10.1029/2012JC008074>, 2012.
- Gregor, L. and Gruber, N.: OceanSODA-ETHZ: a global gridded data set of the surface ocean carbonate system for seasonal to decadal studies of ocean acidification, *Earth Syst. Sci. Data*, 13, 777–808, <https://doi.org/10.5194/essd-13-777-2021>, 2021.
- Gregor, L., Kok, S., and Monteiro, P. M. S.: Interannual drivers of the seasonal cycle of CO_2 in the Southern Ocean, *Biogeosciences*, 15, 2361–2378, <https://doi.org/10.5194/bg-15-2361-2018>, 2018.
- Gregor, L., Lebehot, A. D., Kok, S., and Scheel Monteiro, P. M.: A comparative assessment of the uncertainties of global surface ocean CO_2 estimates using a machine-learning ensemble (CSIR-ML6 version 2019a) – have we hit the wall?, *Geosci. Model Dev.*, 12, 5113–5136, <https://doi.org/10.5194/gmd-12-5113-2019>, 2019.
- Gruber, N., Bakker, D. C. E., DeVries, T., Gregor, L., Hauck, J., Landschützer, P., McKinley, G. A., and Müller, J. D.: Trends and variability in the ocean carbon sink, *Nat. Rev. Earth Environ.*, 4, 119–134, <https://doi.org/10.1038/s43017-022-00381-x>, 2023.
- Hauck, J., Nissen, C., Landschützer, P., Rödenbeck, C., Bushinsky, S., and Olsen, A.: Sparse observations induce large biases

- in estimates of the global ocean CO_2 sink: an ocean model subsampling experiment, *Philos. T. Roy. Soc. A*, 381, 1–24, <https://doi.org/10.1098/rsta.2022.0063>, 2023.
- Hersbach, H., Bell, B., Berrisford, P., Biavati, G., Horányi, A., Muñoz Sabater, J., Nicolas, J., Peubey, C., Radu, R., Rozum, I., Schepers, D., Simmons, A., Soci, C., Dee, D., Thépaut, J.-N.: ERA5 monthly averaged data on single levels from 1940 to present, Copernicus Climate Change Service (C3S) Climate Data Store (CDS), <https://doi.org/10.24381/cds.f17050d7>, 2023.
- Huang, B., Liu, C., Banzon, V., Freeman, E., Graham, G., Hankins, B., Smith, T., Zhang, H.-M., Huang, B., Liu, C., Banzon, V., Freeman, E., Graham, G., Hankins, B., Smith, T., and Zhang, H.-M.: Improvements of the Daily Optimum Interpolation Sea Surface Temperature (DOISST) Version 2.1, *J. Climate*, 34, 2923–2939, <https://doi.org/10.1175/JCLI-D-20-0166.1>, 2021.
- Iida, Y., Takatani, Y., Kojima, A., and Ishii, M.: Global trends of ocean CO_2 sink and ocean acidification: an observation-based reconstruction of surface ocean inorganic carbon variables, *J. Oceanogr.*, 77, 323–358, <https://doi.org/10.1007/s10872-020-00571-5>, 2020.
- Jackson, T., Sathyendranath, S., and Mélin, F.: An improved optical classification scheme for the Ocean Colour Essential Climate Variable and its applications, *Remote Sens. Environ.*, 203, 152–161, <https://doi.org/10.1016/j.rse.2017.03.036>, 2017.
- Jaegle, A., Gimeno, F., Brock, A., Zisserman, A., Vinyals, O., and Carreira, J.: Perceiver: General Perception with Iterative Attention, *arXiv [preprint]*, *arXiv:2103.03206*, <https://doi.org/10.48550/arXiv.2103.03206>, 2021.
- Ji, J., He, J., Lei, M., Wang, M., and Tang, W.: Spatio-Temporal Transformer Network for Weather Forecasting, *IEEE T. Big Data*, 11, 372–387, <https://doi.org/10.1109/TBDATA.2024.3378061>, 2025.
- Kepler, L., Landschützer, P., Gruber, N., Lauvset, S. K., and Stemmler, I.: Seasonal Carbon Dynamics in the Near-Global Ocean, *Global Biogeochem. Cy.*, 34, e2020GB006571, <https://doi.org/10.1029/2020GB006571>, 2020.
- Kern, S., McGuinn, M. E., Smith, K. M., Pinardi, N., Niemeyer, K. E., Lovenduski, N. S., and Hamlington, P. E.: Computationally efficient parameter estimation for high-dimensional ocean biogeochemical models, *Geosci. Model Dev.*, 17, 621–649, <https://doi.org/10.5194/gmd-17-621-2024>, 2024.
- Lakshminarayanan, B., Pritzel, A., and Blundell, C.: Simple and Scalable Predictive Uncertainty Estimation using Deep Ensembles, *arXiv [preprint]*, *arXiv:1612.01474*, <https://doi.org/10.48550/arXiv.1612.01474>, 2016.
- Landschützer, P., Gruber, N., Bakker, D. C. E., Schuster, U., Nakaoka, S., Payne, M. R., Sasse, T. P., and Zeng, J.: A neural network-based estimate of the seasonal to inter-annual variability of the Atlantic Ocean carbon sink, *Biogeosciences*, 10, 7793–7815, <https://doi.org/10.5194/bg-10-7793-2013>, 2013.
- Landschützer, P., Gruber, N., Bakker, D. C. E., and Schuster, U.: Recent variability of the global ocean carbon sink, *Global Biogeochem. Cy.*, 28, 927–949, <https://doi.org/10.1002/2014GB004853>, 2014.
- Landschützer, P., Gruber, N., and Bakker, D. C. E.: Decadal variations and trends of the global ocean carbon sink, *Global Biogeochem. Cy.*, 30, 1396–1417, <https://doi.org/10.1002/2015GB005359>, 2016.
- Landschützer, P., Gruber, N., Bakker, D. C. E., Stemmler, I., Six, K. D., Landschützer, P., Gruber, N., Bakker, D. C. E., Stemmler, I., and Six, K. D.: Strengthening seasonal marine CO_2 variations due to increasing atmospheric CO_2 , *Nat. Clim. Change*, 8, 146–150, <https://doi.org/10.1038/s41558-017-0057-x>, 2018.
- Landschützer, P., Laruelle, G. G., Roobaert, A., and Regnier, P.: A uniform $p\text{CO}_2$ climatology combining open and coastal oceans, *Earth Syst. Sci. Data*, 12, 2537–2553, <https://doi.org/10.5194/essd-12-2537-2020>, 2020.
- Leal, A. M. M., Kyas, S., Kulik, D. A., and Saar, M. O.: Accelerating Reactive Transport Modeling: On-Demand Machine Learning Algorithm for Chemical Equilibrium Calculations, *Transp. Porous Media*, 133, 161–204, <https://doi.org/10.1007/s11242-020-01412-1>, 2020.
- Liao, E., Resplandy, L., Liu, J., and Bowman, K. W.: Amplification of the Ocean Carbon Sink During El Niños: Role of Poleward Ekman Transport and Influence on Atmospheric CO_2 , *Global Biogeochem. Cy.*, 34, e2020GB006574, <https://doi.org/10.1029/2020GB006574>, 2020.
- Liao, E., Lu, W., Xue, L., and Du, Y.: weakening Indian ocean carbon uptake in 2015: the role of amplified basin-wide warming and reduced Indonesian throughflow, *Limnol. Oceanogr. Lett.*, 4, 442–451, <https://doi.org/10.1002/lol2.10397>, 2024.
- Liu, Y., Lu, W., Wang, D., Lai, Z., Ying, C., Li, X., Han, Y., Wang, Z., and Dong, C.: Spatiotemporal wave forecast with transformer-based network: A case study for the northwestern Pacific Ocean, *Ocean Model.*, 188, 102323, <https://doi.org/10.1016/j.ocemod.2024.102323>, 2024.
- Mackay, N. and Watson, A.: Winter Air-Sea CO_2 Fluxes Constructed From Summer Observations of the Polar Southern Ocean Suggest Weak Outgassing, *J. Geophys. Res.-Oceans*, 126, e2020JC016600, <https://doi.org/10.1029/2020JC016600>, 2021.
- McKinley, G. A., Fay, A. R., Eddebar, Y. A., Gloege, L., and Lovenduski, N. S.: External Forcing Explains Recent Decadal Variability of the Ocean Carbon Sink, *AGU Adv.*, 1, e2019AV000149, <https://doi.org/10.1029/2019AV000149>, 2020.
- Mongwe, N. P., Vichi, M., and Monteiro, P. M. S.: The seasonal cycle of $p\text{CO}_2$ and CO_2 fluxes in the Southern Ocean: diagnosing anomalies in CMIP5 Earth system models, *Biogeosciences*, 15, 2851–2872, <https://doi.org/10.5194/bg-15-2851-2018>, 2018.
- Müller, S. A., Joos, F., Plattner, G.-K., Edwards, N. R., and Stocker, T. F.: Modeled natural and excess radiocarbon: Sensitivities to the gas exchange formulation and ocean transport strength, *Global Biogeochem. Cy.*, 22, GB3011, <https://doi.org/10.1029/2007GB003065>, 2008.
- Nguyen, T., Brandstetter, J., Kapoor, A., Gupta, J. K., and Grover, A.: ClimaX: A foundation model for weather and climate, *arXiv [preprint]*, *arXiv:2301.10343*, <https://doi.org/10.48550/arXiv.2301.10343>, 2023.
- Rayner, N. A., Parker, D. E., Horton, E. B., Folland, C. K., Alexander, L. V., Rowell, D. P., Kent, E. C., and Kaplan, A.: Global analyses of sea surface temperature, sea ice, and night marine air temperature since the late nineteenth century, *J. Geophys. Res.-Atmos.*, 108, 4407, <https://doi.org/10.1029/2002JD002670>, 2003.
- Reichstein, M., Camps-Valls, G., Stevens, B., Jung, M., Denzler, J., Carvalhais, N., and Prabhat, M.: Deep learning and process understanding for data-driven Earth system science, *Nature*, 566, 195–204, <https://doi.org/10.1038/s41586-019-0912-1>, 2019.

- Resplandy, L., Hogikyan, A., Müller, J. D., Najjar, R. G., Bange, H. W., Bianchi, D., Weber, T., Cai, W.-J., Doney, S. C., Fennel, K., Gehlen, M., Hauck, J., Lacroix, F., Landschützer, P., Quéré, C. L., Roobaert, A., Schwinger, J., Berthet, S., Bopp, L., Chau, T. T. T., Dai, M., Gruber, N., Ilyina, T., Kock, A., Manizza, M., Lachkar, Z., Laruelle, G. G., Liao, E., Lima, I. D., Nissen, C., Rödenbeck, C., Séférian, R., Toyama, K., Tsujino, H., and Regnier, P.: A Synthesis of Global Coastal Ocean Greenhouse Gas Fluxes, *Global Biogeochem. Cy.*, 38, e2023GB007803, <https://doi.org/10.1029/2023GB007803>, 2024.
- Reynolds, R. W., Smith, T. M., Liu, C., Chelton, D. B., Casey, K. S., and Schlax, M. G.: Daily High-Resolution-Blended Analyses for Sea Surface Temperature, *J. Climate*, 20, 5473–5496, <https://doi.org/10.1175/2007JCLI1824.1>, 2007.
- Rödenbeck, C., Bakker, D. C. E., Metzl, N., Olsen, A., Sabine, C., Cassar, N., Reum, F., Keeling, R. F., and Heimann, M.: Interannual sea–air CO_2 flux variability from an observation-driven ocean mixed-layer scheme, *Biogeosciences*, 11, 4599–4613, <https://doi.org/10.5194/bg-11-4599-2014>, 2014.
- Rödenbeck, C., Bakker, D. C. E., Gruber, N., Iida, Y., Jacobson, A. R., Jones, S., Landschützer, P., Metzl, N., Nakaoka, S., Olsen, A., Park, G.-H., Peylin, P., Rodgers, K. B., Sasse, T. P., Schuster, U., Shutler, J. D., Valsala, V., Wanninkhof, R., and Zeng, J.: Data-based estimates of the ocean carbon sink variability – first results of the Surface Ocean $p\text{CO}_2$ Mapping intercomparison (SOCOM), *Biogeosciences*, 12, 7251–7278, <https://doi.org/10.5194/bg-12-7251-2015>, 2015.
- Roobaert, A., Resplandy, L., Laruelle, G. G., Liao, E., and Regnier, P.: A framework to evaluate and elucidate the driving mechanisms of coastal sea surface $p\text{CO}_2$ seasonality using an ocean general circulation model (MOM6-COBALT), *Ocean Sci.*, 18, 67–88, <https://doi.org/10.5194/os-18-67-2022>, 2022.
- Roobaert, A., Regnier, P., Landschützer, P., and Laruelle, G. G.: A novel sea surface $p\text{CO}_2$ -product for the global coastal ocean resolving trends over 1982–2020, *Earth Syst. Sci. Data*, 16, 421–441, <https://doi.org/10.5194/essd-16-421-2024>, 2024a.
- Roobaert, A., Resplandy, L., Laruelle, G. G., Liao, E., and Regnier, P.: Unraveling the Physical and Biological Controls of the Global Coastal CO_2 Sink, *Global Biogeochem. Cy.*, 38, e2023GB007799, <https://doi.org/10.1029/2023GB007799>, 2024b.
- Sarmiento, J. L., Gruber, N., Brzezinski, M. A., and Dunne, J. P.: High-latitude controls of thermocline nutrients and low latitude biological productivity, *Nature*, 427, 56–60, <https://doi.org/10.1038/nature02127>, 2004.
- Stock, C. A., Dunne, J. P., Fan, S., Ginoux, P., John, J., Krasting, J. P., Laufkötter, C., Paulot, F., and Zadeh, N.: Ocean Biogeochemistry in GFDL's Earth System Model 4.1 and Its Response to Increasing Atmospheric CO_2 , *J. Adv. Model. Earth Syst.*, 12, e2019MS002043, <https://doi.org/10.1029/2019MS002043>, 2020.
- Sun, C., Liao, E., and Zhu, X.: Asymmetrical ocean carbon responses in the tropical pacific ocean to La Niña and El Niño, *Geophys. Res. Lett.*, 4, e2024GL112039, <https://doi.org/10.1029/2024GL112039>, 2025.
- Sweeney, C., Gloor, E., Jacobson, A. R., Key, R. M., McKinley, G., Sarmiento, J. L., and Wanninkhof, R.: Constraining global air–sea gas exchange for CO_2 with recent bomb ^{14}C measurements, *Global Biogeochem. Cy.*, 21, GB2015, <https://doi.org/10.1029/2006GB002784>, 2007.
- Takahashi, T., Olafsson, J., Goddard, J. G., Chipman, D. W., and Sutherland, S. C.: Seasonal variation of CO_2 and nutrients in the high-latitude surface oceans: A comparative study, *Global Biogeochem. Cy.*, 7, 843–878, <https://doi.org/10.1029/93GB02263>, 1993.
- Takahashi, T., Sutherland, S. C., Sweeney, C., Poisson, A., Metzl, N., Tilbrook, B., Bates, N., Wanninkhof, R., Feely, R. A., Sabine, C., Olafsson, J., and Nojiri, Y.: Global sea–air CO_2 flux based on climatological surface ocean $p\text{CO}_2$, and seasonal biological and temperature effects, *Deep-Sea Res. Pt. II*, 49, 1601–1622, [https://doi.org/10.1016/S0967-0645\(02\)00003-6](https://doi.org/10.1016/S0967-0645(02)00003-6), 2002.
- Takahashi, T., Sutherland, S. C., Wanninkhof, R., Sweeney, C., Feely, R. A., Chipman, D. W., Hales, B., Friederich, G., Chavez, F., Sabine, C., Watson, A., Bakker, D. C. E., Schuster, U., Metzl, N., Yoshikawa-Inoue, H., Ishii, M., Midorikawa, T., Nojiri, Y., Körtzinger, A., Steinhoff, T., and Baar, H. J. W. d.: Climatological mean and decadal change in surface ocean $p\text{CO}_2$, and net sea–air CO_2 flux over the global oceans, *Deep-Sea Res. Pt. II*, 56, 554–577, <https://doi.org/10.1016/j.dsr2.2008.12.009>, 2009.
- Valsala, V., Sreeush, M. G., and Chakraborty, K.: The IOD Impacts on the Indian Ocean Carbon Cycle, *J. Geophys. Res.-Oceans*, 125, e2020JC016485, <https://doi.org/10.1029/2020JC016485>, 2020.
- Valsala, V., Sreeush, M. G., Anju, M., Sreenivas, P., Tiwari, Y. K., Chakraborty, K., and Sijikumar, S.: An observing system simulation experiment for Indian Ocean surface $p\text{CO}_2$ measurements, *Prog. Oceanogr.*, 194, 102570, <https://doi.org/10.1016/j.pocean.2021.102570>, 2021.
- Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A. N., Kaiser, L., and Polosukhin, I.: Attention Is All You Need, *arXiv [preprint]*, arXiv:1706.03762, <https://doi.org/10.48550/arXiv.1706.03762>, 2017.
- Wang, H., Hosseini, S. A., Tartakovsky, A. M., Leng, J., and Fan, M.: A deep learning-based workflow for fast prediction of 3D state variables in geological carbon storage: A dimension reduction approach, *J. Hydrol.*, 636, 131219, <https://doi.org/10.1016/j.jhydrol.2024.131219>, 2024.
- Wang, Y.-H. and Gupta, H. V.: A Mass-Conserving-Perceptron for Machine-Learning-Based Modeling of Geoscientific Systems, *Water Resour. Res.*, 60, e2023WR036461, <https://doi.org/10.1029/2023WR036461>, 2024.
- Wanninkhof, R.: Relationship between wind speed and gas exchange over the ocean revisited, *Limnol. Oceanogr. Meth.*, 12, 351–362, <https://doi.org/10.4319/lom.2014.12.351>, 2014.
- Watson, A. J., Schuster, U., Shutler, J. D., Holding, T., Ashton, I. G. C., Landschützer, P., Woolf, D. K., and Goddijn-Murphy, L.: Revised estimates of ocean-atmosphere CO_2 flux are consistent with ocean carbon inventory, *Nat. Commun.*, 11, 1–6, <https://doi.org/10.1038/s41467-020-18203-3>, 2020.
- Weiss, R. F.: Carbon dioxide in water and seawater: the solubility of a non-ideal gas, *Mar. Chem.*, 2, 203–215, [https://doi.org/10.1016/0304-4203\(74\)90015-2](https://doi.org/10.1016/0304-4203(74)90015-2), 1974.
- Willard, J., Jia, X., Xu, S., Steinbach, M., and Kumar, V.: Integrating Scientific Knowledge with Machine Learning for Engineering and Environmental Systems, *arXiv [preprint]*, arXiv:2003.04919, <https://doi.org/10.48550/arXiv.2003.04919>, 2020.

- Willard, J. D., Harrington, P., Subramanian, S., Mahesh, A., O'Brien, T. A., and Collins, W. D.: Analyzing and Exploring Training Recipes for Large-Scale Transformer-Based Weather Prediction, arXiv [preprint], arXiv:2404.19630, <https://doi.org/10.48550/arXiv.2404.19630>, 2024.
- Williams, N. L., Juranek, L. W., Feely, R. A., Johnson, K. S., Sarmiento, J. L., Talley, L. D., Dickson, A. G., Gray, A. R., Wanninkhof, R., Russell, J. L., Riser, S. C., and Takeshita, Y.: Calculating surface ocean $p\text{CO}_2$ from biogeochemical Argo floats equipped with pH: An uncertainty analysis, *Global Biogeochem. Cy.*, 31, 591–604, <https://doi.org/10.1002/2016GB005541>, 2017.
- Wu, H., Xiao, B., Codella, N., Liu, M., Dai, X., Yuan, L., and Zhang, L.: CvT: Introducing Convolutions to Vision Transformers, arXiv [preprint], arXiv:2103.15808, <https://doi.org/10.48550/arXiv.2103.15808>, 2021.
- Wu, Z., Lu, W., Roobaert, A., Song, L., Yan, X.-H., and Cai, W.-J.: A machine-learning reconstruction of sea surface $p\text{CO}_2$ in the North American Atlantic Coastal Ocean Margin from 1993 to 2021, *Earth Syst. Sci. Data*, 17, 43–63, <https://doi.org/10.5194/essd-17-43-2025>, 2025.
- Zeng, J., Nojiri, Y., Landschützer, P., Telszewski, M., and Nakaoka, S.: A Global Surface Ocean fCO_2 Climatology Based on a Feed-Forward Neural Network, *J. Atmos. Ocean. Tech.*, 31, 1838–1849, <https://doi.org/10.1175/JTECH-D-13-00137.1>, 2014.
- Zhang, X., Liao, E., Lu, W., Wu, Z., Wang, G., and Liang, S.: A surface ocean $p\text{CO}_2$ product with improved representation of interannual variability using a vision transformer-based model, Zenodo [data set], <https://doi.org/10.5281/zenodo.15331978>, 2025.
- Zhou, L. and Zhang, R.-H.: A self-attention-based neural network for three-dimensional multivariate modeling and its skillful ENSO predictions, *Sci. Adv.*, 9, eadf282, <https://doi.org/10.1126/sciadv.adf2827>, 2023.