Response letter to Reviewer#2

Overview

The authors are presenting a new, regional pCO_2-product specifically designed for the North American Atlantic coastal region that provides monthly pCO_2 at a .25-degree spatial resolution from 1993-2021. The product uses integrated random forest and linear regression methods incorporating observational products in order to generate their monthly reconstructed pCO_2-product. This allows for analysis of regional, seasonal, and yearly trends in addition to an uncertainty calculation. The authors find through validation that their product provides high accuracy, improving public access for more precise, higher resolution coastal carbon dynamics in the NAACOM region.

There is great need for products like these to be publicly accessible, and this contributes an important resource to the scientific community. The authors do a nice job of introducing the field, the data gaps, and where this product can contribute to those gaps. I do recommend for publication, following a few edits as outlined below.

General responses: We sincerely appreciate the reviewer's recognition of the value of our work. We have carefully addressed the reviewer's suggestions for strengthening our contribution through more detailed explanations and thorough analyses. The manuscript has been extensively revised to incorporate feedback from both reviewers. Major improvements include:

1. Clarified the usage and distinction between fCO_2 and pCO_2 throughout different sections of the manuscript
2. Enhanced the presentation and explanation of Mean Bias Error (MBE) in Section 3.2 and Fig. 5 to avoid potential confusion
3. Substantially revised Section 3.3 to better explain why product-estimated pCO_2 and SOCAT observations show discrepancies in the northern areas, attributing these differences to limited observational coverage
4. Restructured Section 3.4 and Fig. 7 to clearly differentiate between previously documented regional variations and newly identified phenomena revealed by our product

Additionally, we have made an important revision regarding model evaluation. In our previous version, we reported the model outputs for the training dataset (80% of X1) using results from 10-fold cross-validation. We have now updated our methodology to use direct predictions from the final trained model [y = f(X1)] for these data points. This revision aligns with machine learning best practices, as the final data product should utilize predictions from the complete trained model rather than intermediate cross-validation results. The cross-validation metrics remain valuable for model evaluation during the development phase, while the final product benefits from the full model trained on the entire training dataset. For uncertainty quantification, we maintain the use of validation set RMSE, as it aligns well with 10-fold cross-validation results and provides a more comprehensive assessment of model uncertainty. Noted that this revision did not essentially change the results of this work.

All revisions are highlighted in red in the manuscript and are detailed in this response letter.

R2C1. One edit I have for the paper regards the interchangeable use of fCO_2 and pCO_2. In section 2.1 the authors mention that "both are commonly used in oceanographic studies", which is accurate. However, they are not interchangeably used. At the end of Section 2.2 an equation to convert pCO_2 to fCO_2 is provided, but it's unclear at what point this conversion is made. Figure 2 shows values in fCO_2, but the rest of the figures use pCO_2. I recommend a clear statement about conversion with the introduction of fCO_2, as well as consistency in the figures (I would convert Figure 2 to showing pCO_2 or at least have a clear statement on the conversion and reason for fCO_2 presentation in the figure caption).

Response: We thank the reviewer for highlighting this important distinction between fCO_2 and pCO_2. Throughout the main text, we primarily focused on pCO_2 comparisons, as this parameter was directly provided by other products. We discovered an error, which actually shows pCO_2 values in our Python codes but was incorrectly written as fCO_2 in both the color bar and caption for Figure 2. We have now corrected these labels and added a clarifying sentence to the caption. The modified Figure 2 is attached for reference.

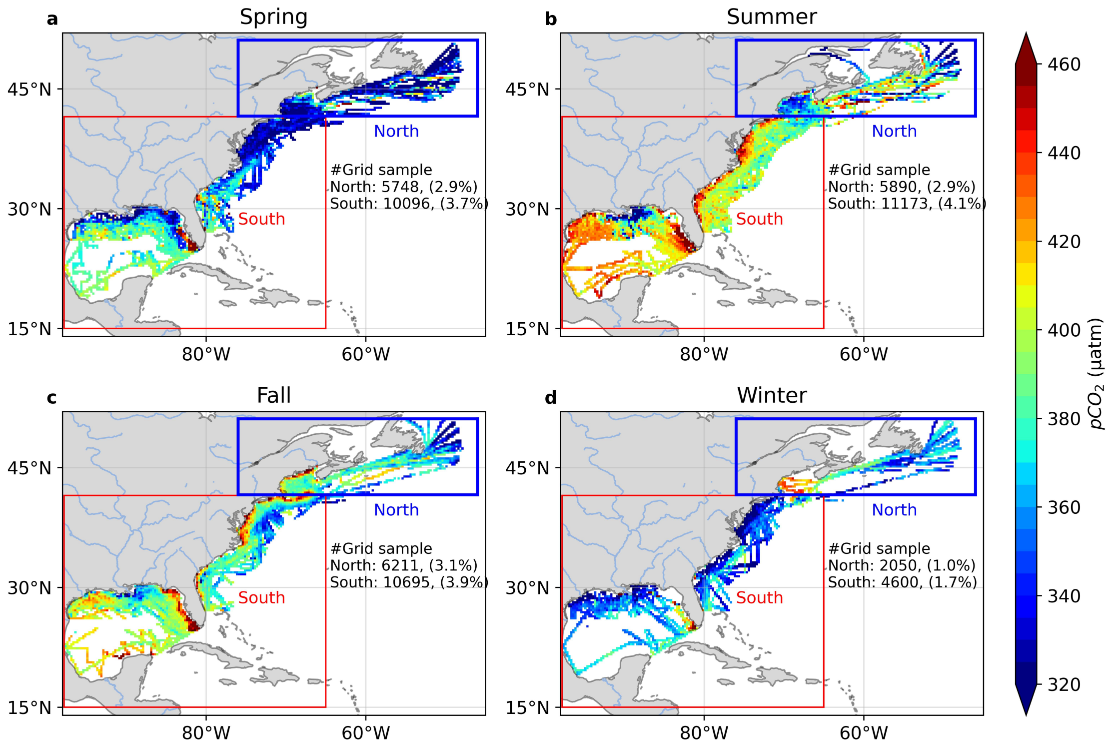

Figure 2. Spatial distribution of sea surface pCO_2 observations from SOCAT database (version 2023) in the NAACOM across four seasons from 1993 to 2021. Grid samples with data were counted by season: **(a)** Spring (March to May), **(b)** Summer (June to August), **(c)** Fall (September to November), and **(d)** Winter (December to February). The study region is divided into northern (blue box) and southern (red box) areas at approximately 41.5°N (Cape Cod). The number and percentage of grid samples are indicated for each region per season. Color scale represents pCO_2 values in µatm. Higher

sampling density is evident in the southern area. Winter shows the lowest overall sampling coverage. Note that the SOCAT database provides quality-controlled fCO_2 measurements as the default parameter, which are subsequently converted to pCO_2 using Eq. (2).

Regarding the usage of fCO_2 in our study, because SOCAT reports fCO_2 directly rather than pCO_2, we specifically use it as the label during model training. Based on our previous work on carbonate dynamic in the Gulf of Mexico (Wu et al., 2024), we decided to provide both reconstructed fCO_2 and pCO_2 in our final product. The model trains and outputs fCO_2 directly, and the predicted fCO_2 values are subsequently converted to pCO_2 using OISST data. This process was briefly mentioned in the last paragraph of Section 2.2:

"Finally, the trained model is applied to all satellite and reanalysis data to generate the final gap-free reconstructed fCO_2 data. As most products reported seawater CO_2 concentration as pCO_2, our final product reports both fCO_2 and pCO_2, with the fCO_2 values being converted to pCO_2 using the following equation (Takahashi et al., 2019)."

To further clarify this, we have made the following modifications:

1) We updated Figure 3 to show that the model first outputs 3D fCO_2, which is then converted to pCO_2
2) A clarifying sentence was added at the beginning of Section 2.2 (Model design, line 148): "During the model development phase, fCO_2 measurements served as training labels for the machine learning algorithm."
3) We modified the last paragraph of Section 2.2 to emphasize that fCO_2 was used in the model development phases before conversion to pCO_2

The revised Figure 3 is attached for reference."

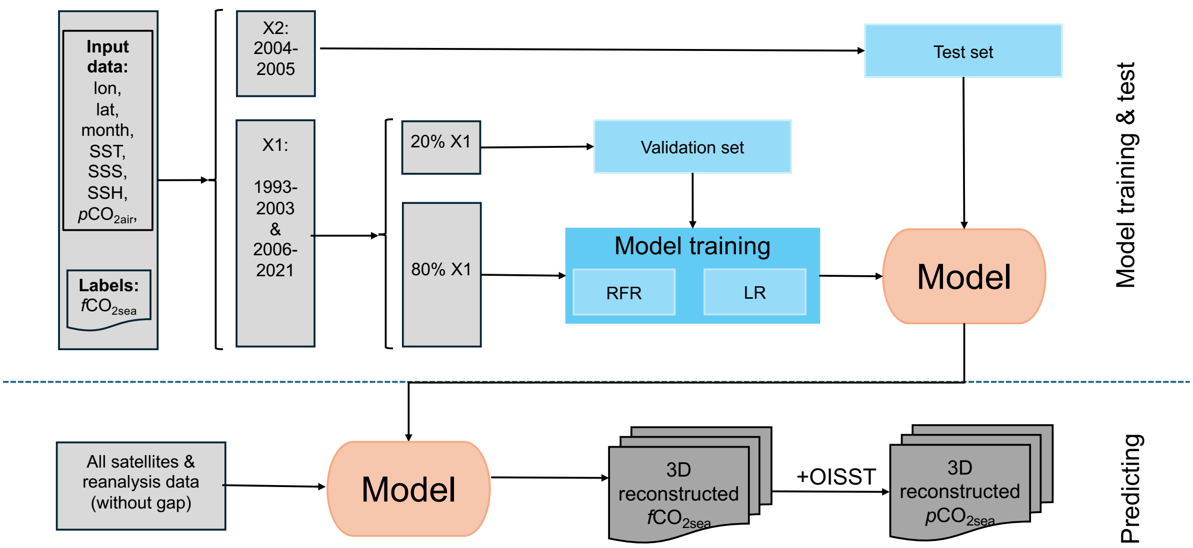

Figure 3. A flowchart of the two-step machine learning regression model for generating the reconstructed pCO_2 product. Grey boxes represent the input and output datasets, blue boxes illustrate the model training, validation testing, and independent test processes, and orange boxes represent the final trained model for predicting the reconstructed product. The two models in the orange boxes are

identical. The training data, consisting of paired input variables (lon, lat, month, sea surface temperature (SST), sea surface salinity (SSS), sea surface height (SSH), and atmospheric pCO_2 (pCO_{2air}) and corresponding sea surface fCO_2 (fCO_{2sea}) labels), is divided into two sets: X1 (1993-2003 and 2006-2021) and X2 (2004-2005). X1 is further randomly divided into subsets for model training set (80%) and validation set (20%). The predictive model combines a random forest regression (RFR) and a linear regression (LR) algorithm. The trained and validated regression model is then applied to all satellite and reanalysis data (without gaps) to generate the 3D reconstructed fCO_{2sea} product, which was then converted to pCO_{2sea} with satellite SST data.

R2C2. My second edit has to do with the calculation of uncertainty. There is a calculation representing the inputs (u_{inputs}), but some of the products are in the original resolution and others are linearly interpolated to that resolution. Does the interpolation introduce more error, and is this taken into account?

Response: We appreciate the reviewer's inquiry regarding our input variables. Our model uses sea surface height (SSH), sea surface temperature (SST), sea surface salinity (SSS), and atmospheric pCO_2 as input variables. To clarify, 1) both SSH and SST are at 0.25° resolution and monthly timescale, averaged from daily data. 2) Atmospheric pCO_2 has a very small spatial gradient when compare with the sea surface pCO_2. Thus, interpretation won't introduce additional uncertainty. In our previous studies, we found that even Mauna Loa pCO_2 data would closely approximate the pCO_2 observed at U.S. East Coast stations, as pCO_2 typically varies little globally (Wu et al., 2024).

SSS is the variable most likely to introduce uncertainty due to interpolation. It's crucial as it reflects the interaction between terrestrial and open ocean waters. While SODA is a widely used and respected salinity product, its uncertainty in our study region is not well-defined. Therefore, we adopted a conservative approach: **we doubled the uncertainty reported in the SODA paper for our calculations.** To clarify this in our methods, we've added a sentence in the Method section (lines 210-211):

"Noted that such interpolation could potentially introduce additional errors. We doubled the SSS uncertainty in the region, assuming this would encompass its true uncertainty (see **Appendix B**)."

And in Appendix B, line 535:

"Their analysis (their Fig. 8) indicates an RMSE exceeding 0.3 psu in the vicinity of our area of interest. In addition, interpolating the 0.5° SSS data to 0.25° resolution could potentially introduce more errors. To maintain a conservative approach in our uncertainty quantification, we doubled the uncertainty and adopted a value of 0.6 psu as the SSS uncertainty for our calculations."

We acknowledge that SODA SSS may not be optimal in our outer study region. Our Monte Carlo simulations indicate that the SSS-induced uncertainty (around 4 µatm) is small compared to the final uncertainty around 20 µatm, but we agree that a more accurate SSS product would be preferable. To the best of our knowledge, currently, no such reliable coastal SSS data are publicly available for this region. We are developing an improved SSS product for this area, which requires further evaluation. Once we are confident in its reliability, we plan to make it publicly available and incorporate it into ReCAD version 2.

R2C3. Additionally, I will note that I greatly appreciate the inclusion of an uncertainty calculation and the strength it lends to the product. I would have liked to see it highlighted a bit more in the rest of the paper results—some of the data could also be discussed with uncertainty included, rather than purely keeping the uncertainty in one section at the end of the paper. I think the addition of the uncertainty calculation makes this product stronger, and should be displayed as such.

Response: We appreciate the reviewer raising this important point. While writing the manuscript, we deliberated but ultimately decided not to include error analysis for the monthly mean and regional average, to avoid confusion and maintain focus and conciseness. Please see **R2C10** for detailed explanation.

R2C4. Finally, Figure 5 and figure 7, and the associated discussions in 3.2 and 3.4, present some extremely interesting data. We compare some of the regional differences and the products effectiveness of capturing broader $p\mathrm{CO_2}$ patterns across the North Atlantic coast. I would have loved to had this extrapolated on a little further, and perhaps seen more numbers broken down by region. We can visually look at the figures, but it's a little hard to assess and I think the paper would be strengthened by expanding this section a little more with increased quantitative results.

Response: We thank the reviewer for this constructive suggestion. We have enhanced the quantitative presentation of our results in several ways. Figure 5 illustrates the spatial distribution of mean bias error (MBE), these values complement the subregional MBE statistics already provided in the last column of Table 2. To make this more clear, we have now incorporated the average MBE values for all six subregions directly within the figure. We have also expanded the discussion section with additional quantitative analysis of regional patterns. **Please see our response to R2C8 for further details of these modifications.**

Regarding Figure 7 in Section 3.4, our previous work (Wu et al., 2024) indicated that existing $p\mathrm{CO_2}$ products did not adequately meet our requirements for regional analysis. Therefore, one of our primary objectives of this work was to develop a product to capture these regional variations. The $p\mathrm{CO_2}$ distribution shows a clear south-to-north decreasing gradient, with distinct regional patterns superimposed on this large-scale distribution. We selected specific regions where $p\mathrm{CO_2}$ variations have been well-documented in previous studies, including elevated $p\mathrm{CO_2}$ in the West Florida Shelf (WFS), and low $p\mathrm{CO_2}$ in the Mississippi River estuary.

Our product also reveals several interesting features, such as relatively higher $p\mathrm{CO_2}$

values in the Gulf of Maine (GoMe, compared to surrounding waters) that potentially associated with local high-pCO_2 river estuary waters, and notable regional variations in northern areas. The northern regions are particularly interesting as previous studies have reported conflicting results, with some identifying these areas as CO_2 sinks and others as CO_2 sources. However, those spatial variations haven't been confidently confirmed by observations yet.

Following the reviewer's suggestion, we have expanded Section 3.4 to provide a more comprehensive analysis. The revised section now presents two distinct components: (1) validation of previously confirmed regional variations, and (2) discussion of novel patterns revealed by our product that warrant future investigation. The expanded Section 3.4 is provided below:

"The ReCAD-NAACOM-pCO_2 product demonstrates superior alignment with SOCAT observations in capturing these regional features that have been reported in previous observation-based studies (**Fig. 7b**) ….

In addition to these previously documented regional variations, our product reveals several notable features not previously captured by observations or other existing products. For instance, the GoMe displays intermediate pCO_2 levels around 380 µatm, distinctly higher than surrounding waters at comparable latitudes, a feature previously documented by a multiple linear regression reconstructed pCO_2 product (Signorini et al., 2013) and five-year (2004-2009) mooring and cruise data (Vandemark et al., 2011) but contradict to another two studies based on numerical models (Cahill et al., 2016; Rutherford et al., 2021). In the southern GStL (S.GStL, box 4 in **Fig. 7**), pCO_2 values are slightly higher compared to adjacent waters at similar latitudes, aligning with high nutrient concentrations typically observed in these river-influenced waters (Lavoie et al., 2021). These regional patterns could not be completely captured by the global products (**Fig. 7c and 7d**). Ability of the ReCAD-NAACOM-pCO_2 product in resolving such regional features demonstrates its potential value for investigating coastal carbon dynamics and their responses to local and regional forcing factors in the NAACOM."

We plan to use this data product to discuss further the spatial and season variability of all sub-regions in NAACOM and the decadal trends in the data-rich MAB and SAB sub-regions in our subsequent publications.

Specific Comments:

R2C5. Figure 1: I felt that the colors of this figure made it difficult to interpret. The way the lines were drawn made the topography difficult to see. For consistency with the other figures in the paper, I would suggest shifting the coastal contour line to being black. Then perhaps make the Gulf stream and Labrador current lines dotted or dashed lines (also, change Gulf Stream's color if you shift contour to black), so they don't block as much topography. I would match the labels of the regions to the lines denoting the regions, and finally increase the deviation in the color scale. Right now, it's not very easy to tell a difference between 800-1000m, and similarly between 0-300m is all about the same tone.

Response: We thank the reviewer for these suggestions to improve the figure's clarity. We agree with the reviewer regarding the visualization challenges of marine terrain data. The bathymetry in our study area presents a particular challenge due to the flat topography on the shelf (0-200 m), but rapid changes on the slope from 200m-2000m depth. For the colors, while we initially attempted to maintain consistent colors for the 200m isobath across all figures, this proved challenging due to the different colormaps required for various figures. To address these concerns, we have made the following modifications to Figure 1:

1) Implemented a light blue background to represent areas within 400 km of the coast
2) Added dashed contour lines for shelf depths (-50 m, -100 m, -200 m) and slope depths (-1000 m, -2000 m, -3000 m, -4000 m)
3) Updated the 200 m isobath to a thick black line in all figures for consistency
4) Modified the Gulf Stream and Labrador Current indicators to dashed arrows, following the reviewer's suggestion. The Gulf Stream is colored red to represent warm current and the Labrador Current is colored blue to represent cold current. Both are semi-transparent to avoid obscuring the contour lines
5) Added a legend to help readers interpret the lines in the figure

We have also revised the figure caption accordingly. The modified Figure 1 is attached for reference:

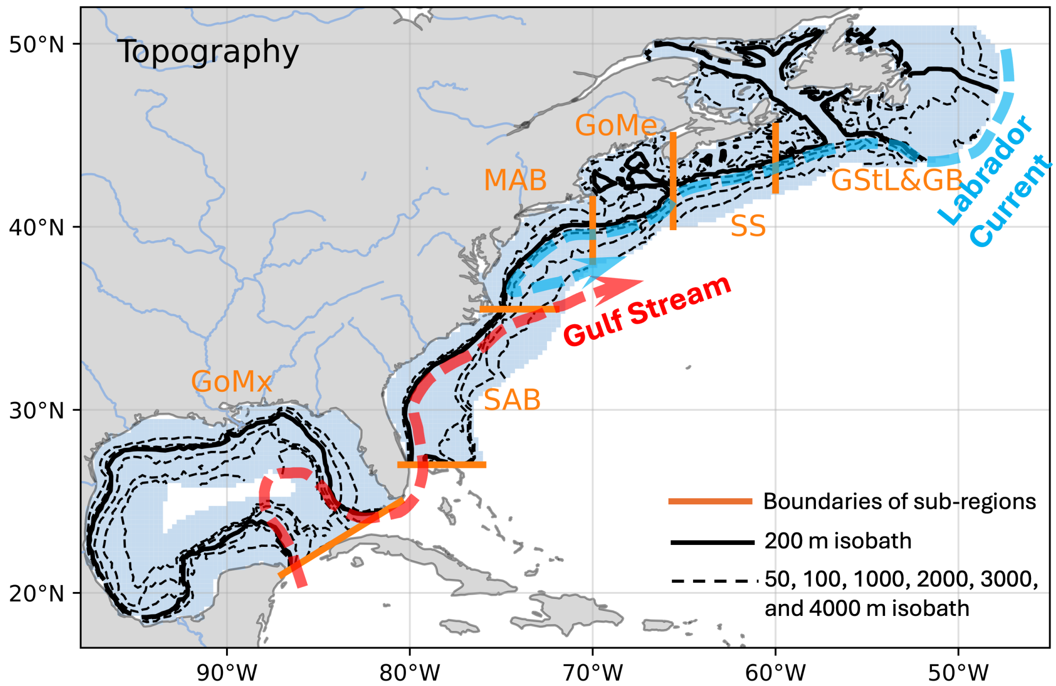

Figure 1. Topography (in meters) and large-scale circulation along the North American Atlantic Coastal Ocean Margin (NAACOM). The study region, defined as coastal areas extending 400 km offshore, is indicated by blue shading. The thick black line is the 200 m isobath, which roughly marks the shelf break and typically defines the continental shelf boundary. The Gulf Stream (thick red dashed

line with an arrow) flows northward along the east coast of the United States before veering eastward into the open Atlantic Ocean around Cape Hatteras. The Labrador Current (thick light blue dashed line with an arrow) flows southward along the east coast of Canada before meeting the Gulf Stream. Following Fennel et al. (2019), the study region is divided into six sub-regions by straight orange lines: the Gulf of Mexico (GoMx), South Atlantic Bight (SAB), Mid-Atlantic Bight (MAB), Gulf of Maine (GoMe), Scotian Shelf (SS), and Gulf of St. Lawrence and Grand Banks (GStL&GB). Dashed contour lines indicate bathymetric depths of 50 m and 100 m on the shelf (from coastline to 200 m isobath), and 1000 m, 2000 m, 3000 m, and 4000 m from the shelf break to the open ocean.

R2C6. Equations: center the equations in the document

Response: We appreciate the reviewer's attention to detail regarding equation formatting. Upon re-examination of the ESSD templates, we have confirmed that left-aligned equations are indeed the default format specified in both the ESSD Microsoft Word and LaTeX templates. We have decided to maintain this alignment to adhere to the journal's standard formatting guidelines, unless otherwise instructed by the editorial team. We thank the reviewer again for their careful revision.

R2C7. Lines 183-184: The nature of this sentence is implying an interchangeable use of fCO_2 and pCO_2, which I don't think is accurate

Response: We appreciate the reviewer's suggestion and agree that clarification was needed. We have modified the sentence as follows (lines 197-198):

"pCO_{2air} represents the atmospheric forcing on the air-sea CO_2 exchange. Including pCO_{2air} is essential for accurately assessing the decadal pCO_2 trend. "

R2C8. Line 284+: Authors show an area-mean bias of +0.17, but with the regional breakdown and discussion, I'd be very curious how that bias varies by region. Can we see numbers for the other regions as well?

Response:

The values shown in this figure represent the Mean Bias Error (MBE). We have updated our methodology to use direct predictions from the final trained model [y = *f*(80% of X1)] for the training dataset (80% of X1), replacing our previous approach that used 10-fold cross-validation outputs. Consequently, the overall MBE for the entire region has been updated to +0.13 ±12.70 µatm. The regional mean bias values are reported in the last column of Table 2. For clarity, we have now incorporated these bias errors with their standard deviations directly into Figure 5:

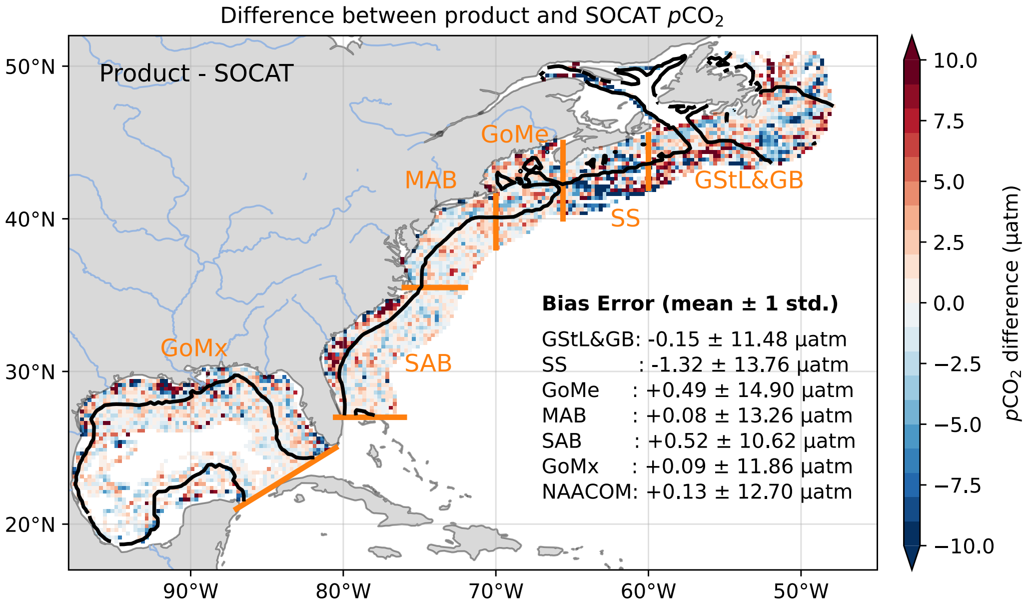

Figure 5. Spatial distribution of mean bias error (MBE) between ReCAD-NAACOM-pCO$_2$ product and SOCAT observations across the NAACOM. The MBE is calculated for each grid cell as the average difference between product estimates and SOCAT observations. Positive values (red) indicate product overestimation, while negative values (blue) indicate underestimation relative to SOCAT. Regional MBE values with one standard deviation are shown for each sub-region, corresponding to the values in the last column of Table 2. The overall bias error for the NAACOM is +0.13 ± 12.97 µatm. Following Fennel et al. (2019), the study region is divided into six sub-regions by straight orange lines: the Gulf of Mexico (GoMx), South Atlantic Bight (SAB), Mid-Atlantic Bight (MAB), Gulf of Maine (GoMe), Scotian Shelf (SS), and Gulf of St. Lawrence and Grand Banks (GStL&GB). The thick black line is the 200 m isobath, which roughly marks the shelf break and typically defines the continental shelf boundary.

We also added two sentences to describe the distribution of MBE more quantitatively in lines 326-329:

"… Regional MBE for different machine learning development phases (training, validation, and test sets) are detailed in Table 2. Despite these regional differences, MBE of both the validation set (-1.0 ~ 1.0 µatm) and independent test set (-4.5 ~ 7.5 µatm) demonstrate minimal values across sub-regions (Table 2), underscoring the product's effectiveness in capturing the broader pCO$_2$ patterns across the NAACOM."

R2C9. Figure 5: Similar edit suggestions to figure 1; update contour line to be black and match the colors of regional names to the lines denoting the regions

Response: We thank the reviewer for these suggestions regarding visual consistency. Following the reviewer's recommendations, we have modified Figure 5 to maintain consistency with Figure 1 by:

1) Updating the 200 m isobath to a thick black line
2) Matching the colors of regional boundary lines and their corresponding region

names
3) Revising the figure caption accordingly

The modified Figure 5 is attached in the previous comment.

R2C10. Figure 6: the error bar denotes one standard deviation of the monthly mean climatology, but didn't the authors also actually calculate a *p*CO_2 error? Why is that not included in any of the figures?

Response: We appreciate the reviewer raising this important point. While writing the manuscript, we deliberated but ultimately decided not to include error analysis for the monthly mean and regional average, to avoid confusion and maintain focus and conciseness. The error metrics shown in our figures serve different purposes:

1) The error bars in Fig. 6 and the values after "±" sign in Fig. 7 represent standard deviations (σ), which characterize the natural variability of pCO2 - temporal variability across the 29-year period (1993-2021) in Fig. 6, and spatial variability in Fig. 7.
2) The uncertainties reported elsewhere in the manuscript and provided in the NetCDF file reflect the propagated errors of individual *p*CO_2 estimates in each grid cell.
3) While these grid-cell uncertainties can be used to calculate uncertainties for area and monthly averages (following methods detailed in Roobaert et al., 2024 and Landschützer et al., 2014), we have deliberately focused this manuscript on establishing the fundamental reliability of our product and decided not to include this part in this manuscript to avoid potential confusion.

A comprehensive analysis of uncertainties in regional averages and their implications for CO_2 flux calculations will be presented in our forthcoming manuscript examining *p*CO_2 seasonal cycles, regional variability, and mean seawater CO_2 uptake in the NAACOM. To ensure proper use of our dataset, we have added guidance in lines 459-461:

"… In addition, the uncertainties reported in this section and provided in the NetCDF file represent the propagated errors for individual *p*CO_2 values in each grid cell. Methods to calculate uncertainties in regional averages of *p*CO_2 or air-sea CO_2 fluxes over specific spatial and temporal domains are detailed in Roobaert et al. (2024) and Landschützer et al. (2014)."

Detailed methods for calculating the uncertainty of monthly or area means (which did not appear in the text):

The uncertainty of monthly or regional means (θ_{mean}) can be expressed as:

$$\theta_{mean} = \sqrt{\theta_{stderr}^2 + \theta_{pCO2}^2}$$

where θ_{stderr} is the **standard error** of monthly or regional means, which is a function of the standard deviation (σ_{pCO2}) for each month and the number of samples (N_1 = 29 for monthly means, or N_1 = total grid cells in a specific region for regional average):

$$\theta_{stderr} = \frac{\sigma_{pCO2}}{\sqrt{N_1}}$$

θ_{pCO2} is the uncertainty of product-estimated area-average pCO_2 accumulated from each grid cell, which could be calculated following Landschützer et al. (2014) and Roobaert et al. (2024):

$$\theta_{pCO2} = \sqrt{\frac{u_{obs}^2}{N_2} + \frac{u_{grid}^2}{N_2} + \frac{u_{map}^2}{N_{eff}}}$$

where u_{obs}, u_{grid}, and u_{map} represent observational uncertainties, gridded uncertainty, and mapping uncertainty, respectively, as defined in our manuscript. N_2 denotes the number of grid cells in each region. For u_{map}, the value of N is corrected to effective sample size N_{eff} as individual errors from each grid cell are not spatially independent, which could also be calculated with a Monte Carlo simulation (Landschützer et al., 2018).

We will report the **uncertainty of monthly or regional means** together with our scientific question--what controls regional and seasonal variability--in a separate publication.

R2C11. Line 415: The statement "This uncertainty is deemed reasonable" confused me. Deemed reasonable by who? What metrics are being used? "reasonable" is a very vague term.

Response: We appreciate the reviewer's observation and agree that our original expression lacked precision. We have revised our approach explanation and comparison as follows in lines 453-456:

"Our uncertainty estimation employs a conservative estimation, using maximum values at calculation step. This approach likely overestimates the true uncertainty. Despite this conservative method, our calculated uncertainty for the Atlantic margins is comparable to the 43.4 µatm reported by Sharp et al. (2022) for areas within 100 km of the North American Pacific margins. suggesting a good product performance of our product"

R2C12. Acknowledgments: Make sure to include the SOCAT statement from the website that they ask you to include when you use their product ("The Surface Ocean CO_2 Atlas (SOCAT) is an international effort, endorsed by the International Ocean Carbon Coordination Project (IOCCP), the Surface Ocean Lower Atmosphere Study (SOLAS) and the Integrated Marine Biosphere Research (IMBeR) program, to deliver a uniformly quality-controlled surface ocean CO_2 database. The many researchers and funding agencies responsible for the collection of data and quality control are thanked for their contributions to SOCAT.")

Response: We appreciate the reviewer's suggestion and totally agree on the importance of acknowledging the scientific community's contributions to the data publicly, especially for the SOCAT effort. We have revised our acknowledgments section accordingly and have also carefully reviewed the websites of other datasets used in this work to ensure comprehensive recognition. The updated acknowledgments now read as follows:

"The authors acknowledge the National Oceanic and Atmospheric Administration (NOAA) for providing the OISST data, the University of Maryland Ocean Climate Laboratory for the SODA dataset, and the European Union Copernicus Marine Service Information (CMEMS) for the SSH data. We also express our gratitude to the scientific community for sharing their observational carbonate data in the SOCAT effort. The SOCAT is an international effort, endorsed by the International Ocean Carbon Coordination Project (IOCCP), the Surface Ocean Lower Atmosphere Study (SOLAS) and the Integrated Marine Biosphere Research (IMBeR) program, to deliver a uniformly quality-controlled surface ocean CO_2 database. The many researchers and funding agencies responsible for the collection of data and quality control are thanked for their contributions to SOCAT.

This work is part of Zelun Wu's Ph.D. Dissertation under the University of Delaware-Xiamen University Dual Degree Program in Oceanography."

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