A modeling study of temporal and spatial pCO_2 variability on the biologically active and temperature-dominated Scotian Shelf

Response to Comments by Reviewer 1

(Reviews are included in black font; Responses are in blue font)

This work seeks to identify the role of local event-scale variability – namely upwelling – in determining the regional air-sea carbon dioxide fluxes over the Scotian Shelf through the integration of several different data sets as well as the use of a regional numerical model. The paper features wonderful contextualization of previous flux estimates with observational limitations and integration of multiple kinds of data for this regional problem. The problem itself is quite timely as recent work has identified that the coastal ocean rates of change in carbon dioxide may always reflect the global changes. The manuscript requires additional details in the methods section – most notably about the regressions used to drive the initial and boundary conditions and river values, some issues with time surrounding the observations used and the simulation years, as well as the methods pertaining to evaluation of the model itself. In additional, more attention needs to be paid to the role of the Revelle Factor in driving these interregional differences between the upwelling on this shelf and the CCS. Finally – and most importantly – the authors need to clarify how the upwelling event contributes to the shelf wide estimates more clearly. The paper would be publishable in Biogeosciences if these issues can be addressed by the author team. More specific comments follow.

Response: We appreciate the constructive comments and have paid close attention in our revision to clarify the objectives of our study and to provide or emphasize the methodological details requested by the reviewer. The main objectives of our study are to show (1) that the Scotian Shelf, as a whole, acts as a net source of CO_2 to the atmosphere, (2) that local processes drive seasonal and spatial variability of pCO_2, and (3) to present an assessment of how well our regional model captures these processes. The methodological details are provided as detailed in the responses below. A discussion of the Revelle factor is beyond the intended scope of this study. Likewise, as explained in more detail below, the upwelling event is not a major contributor to the shelf-wide air-sea flux and we did not mean to suggest it is. This is now stated clearly in the manuscript (see response to next comment).

Major Comments:

The main message appears to be that local processes are important for carbon content of the temperate Scotian shelf region. In the context of that message, the authors need to show how the localized upwelling event contributed to the overall regional flux somehow. One way might be to show this flux as a map. While there is quite a bit of information on the in situ observed location's variability, there is very little about how that compares to the region as a whole – is it representative? For instance, where in Figure 1 does this upwelling occur (at the buoy and along the black line/transect?) – and how does the simulated flux at the surface of the entire region compare to this localized event? How fine of a resolution do we need to observe to get the shelf-based flux estimate direction right? Also, how does this flux compare with other regional/broader scale fluxes reported for the North Atlantic?

Response:

First, we would like to emphasize again that the main objectives of our study are to show (1) that the Scotian Shelf, as a whole, acts as a net source of CO_2 to the atmosphere, (2) that local processes drive seasonal and spatial variability of pCO_2, and (3) to present an assessment of how well our regional model captures these processes. We accomplish this by combining two high-resolution data sets, a timeseries (CARIOCA buoy) and regular cross-shelf transects (Atlantic Condor cruises) with a high-resolution regional model.

In response to: "the authors need to show how the localized upwelling event contributed to the overall regional flux somehow.":

One of the main messages of our paper is that the flux across the shelf is relatively uniform and that these localized summer upwelling events do not contribute significantly to shelf-wide fluxes but would be more important locally. We believe this is an interesting contrast to other shelves with summer upwelling (e.g. the California Current System or CCS), where these events have been shown to contribute significantly to air-sea fluxes.

This is now stated more clearly in section 4.3 Regional Flux Estimates (line 287ff in the revised manuscript) where we have added:

"*Bin 1 along the Atlantic Condor transect (Halifax Harbour/upwelling bin, Figure 1) has an annually integrated flux of +2.2* ± 0.2 *mmol C* m^{-2} yr^{-1}*, which is comparable to the annual flux of bin 2 (Deep Panuke/shelfbreak bin, Figure 1) at +2.0* ± 0.2 *mmol C* m^{-2} yr^{-1} *and the simulated flux at the buoy location. These results indicate that cross-shelf variability in the air-sea* CO_2 *flux is small.*"

In section 5 Discussion (line 344ff in the revised manuscript) we have added:

"*Additionally, the simulated annual air-sea* CO_2 *flux in bin 1 (upwelling bin, Figure 1) is +2.2* ± 0.2 *mmol C* m^{-2} yr^{-1} *and similar to bin 2 (shelfbreak bin, Figure 1) where the annual flux is +2.0* ± 0.2 *mmol C* m^{-2} yr^{-1}*. For comparison, the annual flux for the entire shelf flux is +1.7* ± 0.2 *mmol C* m^{-2} yr^{-1} *and the flux at the CARIOCA buoy is +2.3* ± 0.1 *mmol C* m^{-2} yr^{-1}*. Our results indicate that the short-term upwelling events in summer do not significantly affect the shelfwide fluxes on an annual scale.*"

In response to: "where in Figure 1 does this upwelling occur (at the buoy and along the black line/transect?)":

We have added the location of the CARIOCA buoy and condor transect to the upwelling figure (top panel Figure 6).

In response to: "How fine of a resolution do we need to observe to get the shelf-based flux estimate direction right?":

As mentioned above, air-sea flux is rather homogenous across the shelf and the localized upwelling events do not noticeably affect shelf-wide air-sea flux. Although more observations would be better, of course, it appears that the combination of the high-resolution time series and the cross-shelf transects provide adequate resolution to support our conclusions.

In response to: "how does this flux compare with other regional/broader scale fluxes reported for the North Atlantic":

We provide such reported fluxes in Figure 9 where we compare our flux estimates to other regional and global fluxes reported for the region (from Grand Banks to Gulf of Maine).

Secondly, it is critical to clarify time in this work. 2005 was the year when the warming started intensely on the east coast of North America. The model runs happen before that, but the comparisons are to data after that…. How does that impact the results? What about the time variability of carbon dioxide in the atmosphere over these various intervals?
Response: We have updated our manuscript using an extended simulation from 1999-2014. We now focus on model years 2006-2014, which encompasses the observation years from the CARIOCA buoy (2007-2014). When plotting model and observations from different years in the same graph, we perform a simple detrending where we map these observations onto the common year using the long-term atmospheric pCO_2 trend of ~ + 2 µatm/year (see lines 190ff and Supplement Figure S1). Analysis of the warming observed on the east coast of North America is beyond the intended scope of this paper, which aims to address seasonal variability (now emphasized throughout the revised manuscript, for example at lines 11, 67, 68, 310, 371, 396). A model analysis of long-term trends with the same model is forthcoming.

The comparison to the California Current or other traditionally upwelling situations is not entirely accurate as the vertical gradient in DIC (presented in the figure here) is nearly half what it is in the CCS (Feely et al. 2004). The phytoplankton growth at the surface is quite efficient unless the winds blow too strongly and the phytoplankton can no longer grown in place. This aspect of the upwelling system is neglected in the text. The signature of the phytoplankton drawdown can be seen very far offshore as it takes nearly a year for CO2 to equilibrate at the surface. In addition, the two systems likely experience very different temperature, salinity, and alkalinity parameter spaces – all of which are important to consider for the response of the carbon system.
Response:
We fully agree with the Reviewer that the Scotian Shelf and the CCS behave very differently. In fact, we believe this is one of the interesting findings of our study and we have made this clearer in the Discussion section by referring and comparing to Feely et al. (2008).

We have added the following to the discussion section (see lines 328ff in the revised manuscript): "*There are, however, large differences between the Scotian Shelf and the typical upwelling scenario of the CCS. For instance, the size and geometry of these shelves are quite different, which affects the type of water being upwelled to the surface. The California Shelf is an active margin shelf approximately 10 km wide (Fennel et al. 2019) compared to the passive-margin Scotian Shelf with approximately 120-240 km width (Shadwick et al. 2010). As a result, upwelling in the CCS brings DIC rich water (~2200-2250 umol kg^{-1}) from deep in the water column (below (150-200 m) of the open ocean across the shelf break to the surface of the shelf (Feely et al. 2008). On the Scotian Shelf, it is only subsurface shelf water from between ~20-25 m depth that is being upwelled, which is at a similar temperature to the upwelled water in the CCS (7-8^{o}C) but at a much lower DIC concentration (2050 mmol C m^{-3}).*"

The Revelle Factor influence on the differences between what is observed on the Scotian Shelf and in the CCS should be included – for an example described in more detail see here: https://www.sciencedirect.com/science/article/pii/S0278434317303643#f000

Because the Revelle Factor is important to consider within the context of this issue, it would be important to evaluate DIC and TA with in situ observations locally, here within this manuscript. Please add DIC and TA evaluation of the model fields. Do observations of these fields exist for the simulated period?

Response:

We agree with the Reviewer that an evaluation of DIC and TA is useful. We have added this using in-situ observations available from the Department of Fisheries and Oceans (DFO) Atlantic Zone Monitoring Program (AZMP) and have added a brief evaluation of DIC and TA to these observations in the supplement (Section S4; Figures S6 – S8). A discussion of the Revelle factor is beyond the intended scope of this manuscript.

The methods require quite a bit more detail. Specifically, what is the model skillful in (Lines 112) from other studies? Was it evaluated mostly at the surface? Over annual timescales? Or events like in this work? The K1 and K2 constants chosen are not meant for regions that experience a lot of freshwater influence. Can you justify their choice in this region by discussing the salinity ranges that this region observes? What atmospheric carbon dioxide concentration was used?

Response:

Regarding Lines 114ff, we have expanded the text as follows (Lines 114-119 in revised manuscript; additions in bold italics): "*For a detailed description and validation of the biological model, we refer to Laurent et al. (2021),* ***who compared the model output with glider transects of temperature, salinity and chlorophyll, and in situ measurements of chlorophyll and nitrate. The model was evaluated on a seasonal scale for the entire model domain, mainly in the surface (top 100 m). Laurent et al. (2021) showed that the model outperforms global models for the region for all variables and that the timing of the spring bloom is well represented, but the model slightly underestimates the magnitude of the bloom and tends to slightly overestimate nitrate throughout the year.*** "

Regarding our use of our K1 and K2 constants, we have modified the text to (lines 120-123 in the revised manuscript; additions in bold italics): *"…we use dissociation constants (K1 and K2) from Millero et al. (1995) using Mehrbach et al. (1973) data on the seawater scale* ***which are deemed appropriate for the typical salinity ranges from 27 to 36.6 in the model domain (lower salinities are highly localized in the Gulf of St. Lawrence Estuary)****."*

Regarding atmospheric CO_2 concentrations:
As stated on lines 145-146 in the original text (lines 123 in revised manuscript): "*Atmospheric pCO_2 is set to the seasonal cycle and secular trend derived from Sable Island monitoring data contributed by Environment Canada's Greenhouse Gas Measurement Program (Environment and Climate Change Canada, 2017).*"
We have added the trend equation with seasonal cycle to the Supplement with a figure illustrating (see Supplement S2 and Figure S1).

Most importantly in the methods – the boundary condition DIC and TA relationships and river concentrations require additional documentation. In the case of the boundary conditions, they appear to rely solely on data from the winter months from an unspecified location. Can you add these relationships to supplemental? And describe the data that they rely on? Are they from a similar time period that was simulated? Were adjustments made for time in the DIC field if they were observed more than 5 years earlier/later than the simulations? There are existing hydrographic relationships in the region and globally that could be used instead (McGarry et al. 2021; Xu et al. 2020; CANYON; LIAR) – why generate a new one?

Response:
We have added a more detailed description of the DIC and TA data in the Methods section (they are from DFO's AZMP program mentioned above). The relationships are reported there already (lines 132-138) we have modified the text as follows:

Lines 137ff in revised text (updated text in bold italics): "*The model is initialized on January 1, 1999 from Urrego-Blanco and Sheng's (2012) solution for temperature and salinity. Nitrate (NO_3^-) concentrations are initialized from regional climatologies as in Laurent et al. (2020).* ***DIC and TA initial and boundary conditions were created from observationally based relationships with temperature (T) and salinity (S) using bottle data from regional cruises from 1997-2011 encompassing as far south as the Gulf of Maine and as far north as the Labrador Sea (observations from DFO's AZMP program, see: dfo-mpo.gc.ca/science/data-donnees/azmp-pmza/index-eng.html#publications). Initialization relationships used only observations from December, January and February ($TA = 43S + 800$, $r^2 = 0.96$; $DIC = 1153 – 21.6T + 29.1S – 0.41T^2 + 0.63ST$, $r^2= 0.90$). Boundary conditions used observations that encompass the entire year ($TA = 41S + 875$, $r^2 = 0.92$; $DIC = 912.6 – 2.4T + 35.7S – 0.45T^2 + 0.12ST$, $r^2= 0.80$).***"

Why did we not use other relationships? Aside from the obvious reason of timing (we have been working on the model for a few years while McGarry et al. 2021 and Xu et al. 2020 were just recently published), we know it is crucial to use observations from our shelf region. McGarry et al. (2021) focuses on Gulf of Maine and does not include most of our study region. Similarly, Xu et al. 2020 focuses on MAB and SAB, and not our study region. Since the Gulf of Maine, MAB and SAB are all more strongly influenced by Gulf Stream water than the upstream shelves that we focus on, it is important to use hydrographic relationships that are specific to our region of focus. We do not believe the CANYON fields are appropriate as they are derived from open-ocean not shelf data. Furthermore, as CANYON requires the use of oxygen data in addition to temperature and salinity, which we do not have access to for the entire region, and any workarounds would introduce errors. Likewise, we did not use LIAR because it was optimized for the open ocean not the shelf.

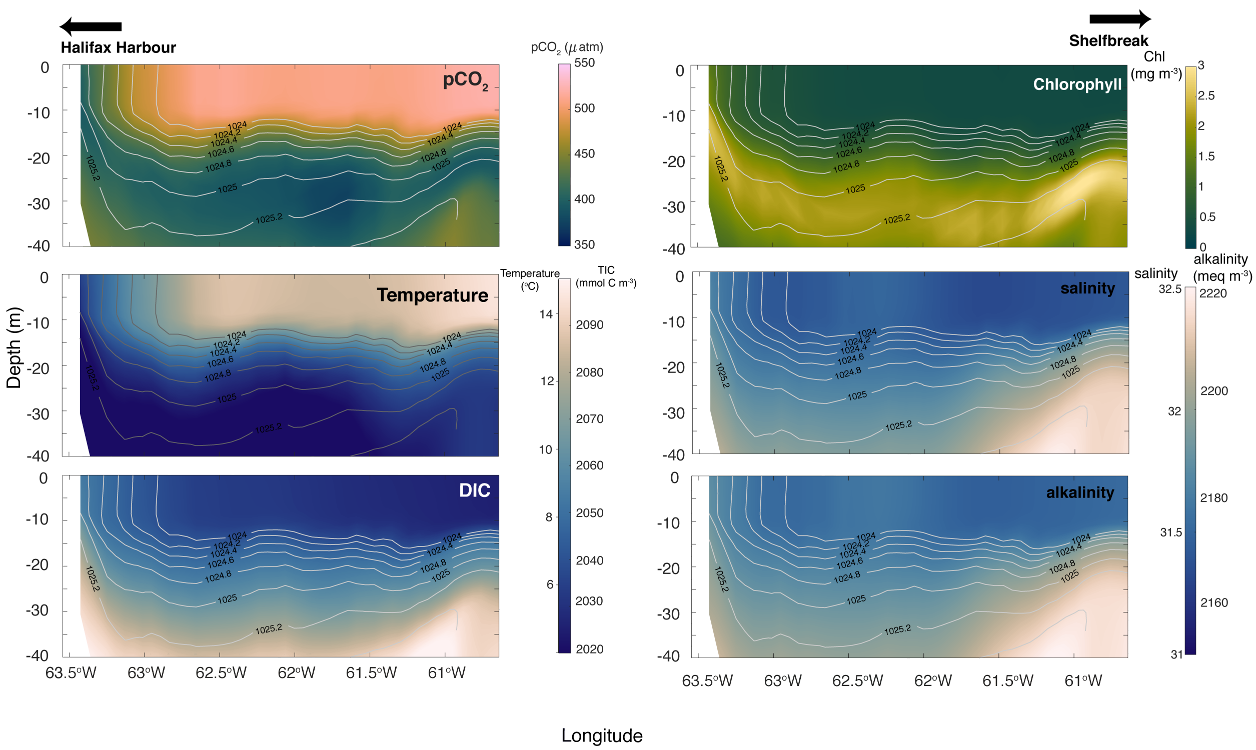
Finally, the point that the upwelling event signal leads to reduced outgassing compared to the rest of the shelf (Line 280-281) is not clearly shown and is related to the main point of the work. The reader is still considering (because none of the other fields were shown) that maybe the phytoplankton growth rate in relationship to the winds -documented in Evans et al. (2015) could also be contributing to this. What does the subsurface pool of pco2 look like prior to these events? Is that getting efficiently drawn down or is the biological response week and so the physical transport is the main control over the surface carbon concentration? See more discussion on the role of event based air-sea carbon fluxes in annual variability for a region here: https://agupubs.onlinelibrary.wiley.com/doi/epdf/10.1029/2010JC006625
Response:

We have reworded lines 280ff to de-emphasize the upwelling events. As stated above, we do not see this as the main focus of our paper as these are short-term events that have no marked influence on annual or shelf-wide fluxes.

In addition to comparing the annually integrated air-sea flux in the upwelling bin to the shelfbreak bin (see previous response), these lines have now been reworded to (see lines 340ff in revised manuscript; changes are in bold italics): "***Our regional model shows*** *that upwelling events* ***could be a large contributor to setting*** *the CO_2 signal in the summer on the inner portion of the Scotian Shelf, act****ing*** *to lower pCO_2* ***here*** *and* ***slightly reducing*** *outgassing compared to the* ***outer*** *shelf.*"

Regarding the comment on phytoplankton growth, we have added the transects below to the supplement (Section S6 and Figure S11) so readers are informed of other variables at the time of the upwelling event. Our interpretation is that during the event, physical transport is the main control on the spatial variability.

In addition, as per the suggestion from the other Reviewer, we have added a Taylor decomposition to better illustrate how these different factors are affecting the pCO_2 signal during the upwelling events (see lines 149ff in the Methods, lines 263ff and Figure 7 in the Results, and lines 322ff in the Discussion).



Minor Comments:
Line 52-52: Please add the Feely et al. 2008 citation here (https://science.sciencemag.org/content/320/5882/1490).
Response: Yes, we have added this reference (see line 52 in revised text).

The model gas transfer function chosen is Ho et al. (2006), which is different than the earlier Fennel model iterations. How does this choice (between all of the existing gas transfer functions available) influence your results?
Response: Since we are not focusing on short-term, high-wind events, most of the gas transfer functions yield similar results without much divergence. A few years ago, we updated from Wanninkhof (1993), which is the gas transfer function originally used in the Fennel model, to Ho et al. (2006) because we were criticized for using on outdated parameterization. Although it is thought that Wanninkhof (1993) potentially overestimates gas transfer, particularly at higher wind speeds (Ho et al. 2006), both gas transfer functions yield similar results for the air-sea CO_2 fluxes in our model.

Lines 213-214: Can you add statistics to support "good agreement" here?
Response: We have moved the figure that this sentence references to the Supplement and removed this sentence from the main text. However, in Figure 3, we do report overall statistics comparing the model to the Atlantic Condor transect, with an RMSE of 28.7 µatm and a bias of 13.9 µatm.

Line 292: If you averaged your two regions together - would your results be more in line with theirs?
Response: No, if we averaged our two regions together our estimate would not be more in line with the estimate from Laruelle et al. (2015).

Line 314: " thermodynamic signal in pCO2 outweighs the influence of biological activity " This is not clearly shown in this work.
Response: Agree, this statement is a reference to Shadwick & Thomas (2014). We have modified the text to (see lines 376ff in revised text): *"In summer, temperature-normalized pCO_2 continues to decrease rather than follow the increasing temperature signal of non-normalized pCO_2. Previous studies have noted that, in summer, the thermodynamic signal in pCO_2 outweighs the influence of biological activity (Shadwick et al. 2011; Shadwick & Thomas 2014), which could explain the differences in seasonality between pCO_2 and temperature-normalized pCO_2 in the present study. We believe this thermodynamic influence is an important factor driving the net outgassing observed on the Scotian Shelf, particularly when combined with the delivery of DIC-rich water from the Labrador Sea."*

Figure 2 - Add statistics (RMSE etc) directly to these plots. Is the smoothing of the model part of the issue? what about the time/spatial mismatch? Is the socat data being interpolated to the location of the mooring? was the model? how was that extracted? These details need to be added to the methods as well – evaluation methods.
Response: We have added the RMSE and bias directly to the plots. The model was not smoothed and model and data are shown in the same location (no spatial mismatch). We now focus on only one year from the extended model simulation, but include the shaded area as the range from multiple years to illustrate the temporal variability. We have redone all figures and are now correcting for the long-term trend by mapping values from different years onto the same reference year. We believe the main issue is that the magnitude of the bloom is not large enough in the model to capture the rapid and large decline in pCO_2, as stated in the text. The model

output was extracted at the buoy location. The SOCAT data was averaged over the Scotian Shelf, as indicated in the figure caption.

Figure 3 – The summer gradient generated by the upwelling (observed) does not appear to be captured by model. Can you address this with respect to the localized mechanism that is the focus of this work? Please add some discussion of this to the text. Is the time period the same between simulated and observed?
Response: Is the Reviewer perhaps referring to Figure 4? Figure 3 is not intended to show evidence of summer upwelling in either observations or the model but shows the annual and shelf-scale changes in pCO_2. Upwelling in the model is also illustrated in Figures 5 and 6.

Figure 4 – the longitudinal gradient in the observations does not appear to be well captured by the model. Is there additional evidence that the model simulates the upwelling in this area well?
Response: The occurrence of summer upwelling is well-documented on the Scotian Shelf (see some examples from satellite and models below). The intensity of an upwelling event and the width of the coastal band of cold water varies from event to event and is directly related to the strength and duration of the upwelling-favourable wind. Hence upwelling bands are wider in some events than in others. We are not directly comparing the same event in the model as in the observations since the model simulation does not extend to 2018/2019 (the time period of the Condor transect observations), therefore we do not expect the extent of the upwelling area to be the same between the model and observations.

Examples of upwelling events and the associated band of upwelled water on the Scotian Shelf: Petrie et al. (1987) used satellite images of the region to show the development of a band of cool water along the southern shore of Nova Scotia over the month of July 1984 caused by upwelling-favourable winds (see Figure below).

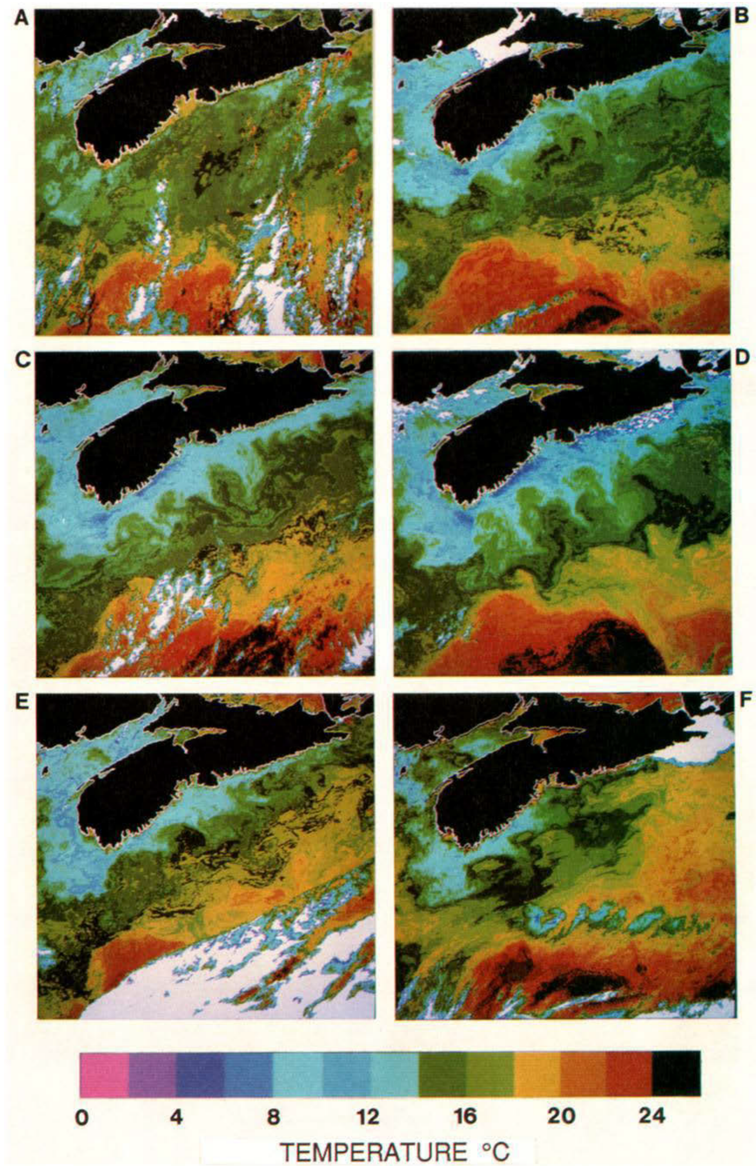


Figure 1: Satellite infrared imagery of sea surface temperatures from (a) July 7, (b) July 14, (c) July 21, (d) July 25, (e) July 31 and (f) August 6, 1984. Image is from Petrie et al. (1987) illustrating narrow band of cool water on the southern shore of Nova Scotia during a period of upwelling-favourable winds.

A more recent example from Shan (2016) showing both satellite images and simulated model snapshots of SST in July 2012 is given below and illustrates again the band of cool upwelled waters on the southern shore of Nova Scotia in the vicinity of the coast. Shan (2016) noted two distinct upwelling events during 2012, one that peaked July 22 and the other September 1, 2012.

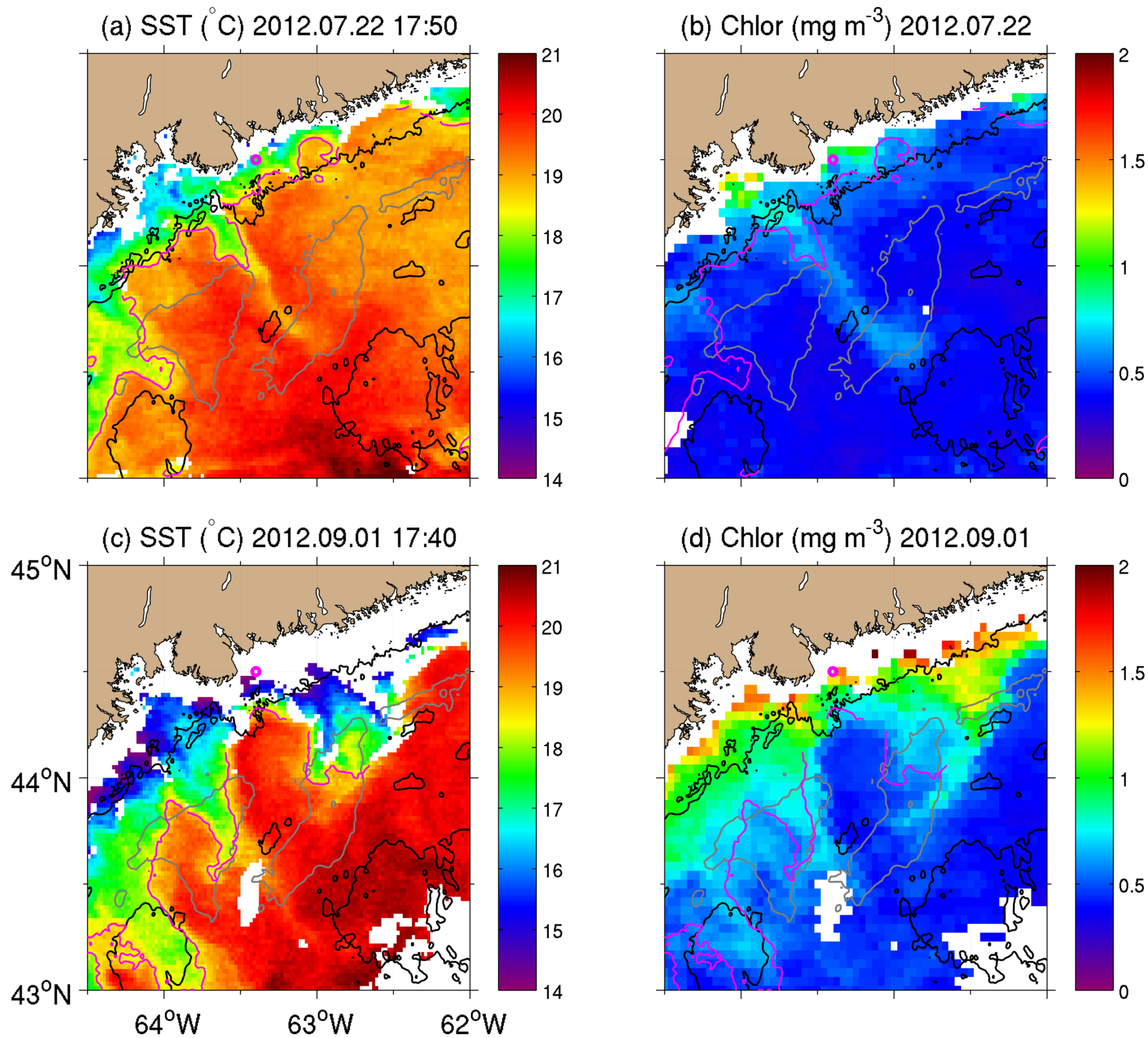


Figure 2: MODIS satellite remote sensing data of SST and Chlorophyll concentrations over the central Scotian Shelf and adjacent waters from July 22 and September 1, 2012 (from Shan 2016). Note that the shelf break is outside the frames. 100 m and 200 m isobaths are shown in black and gray contour lines, respectively.

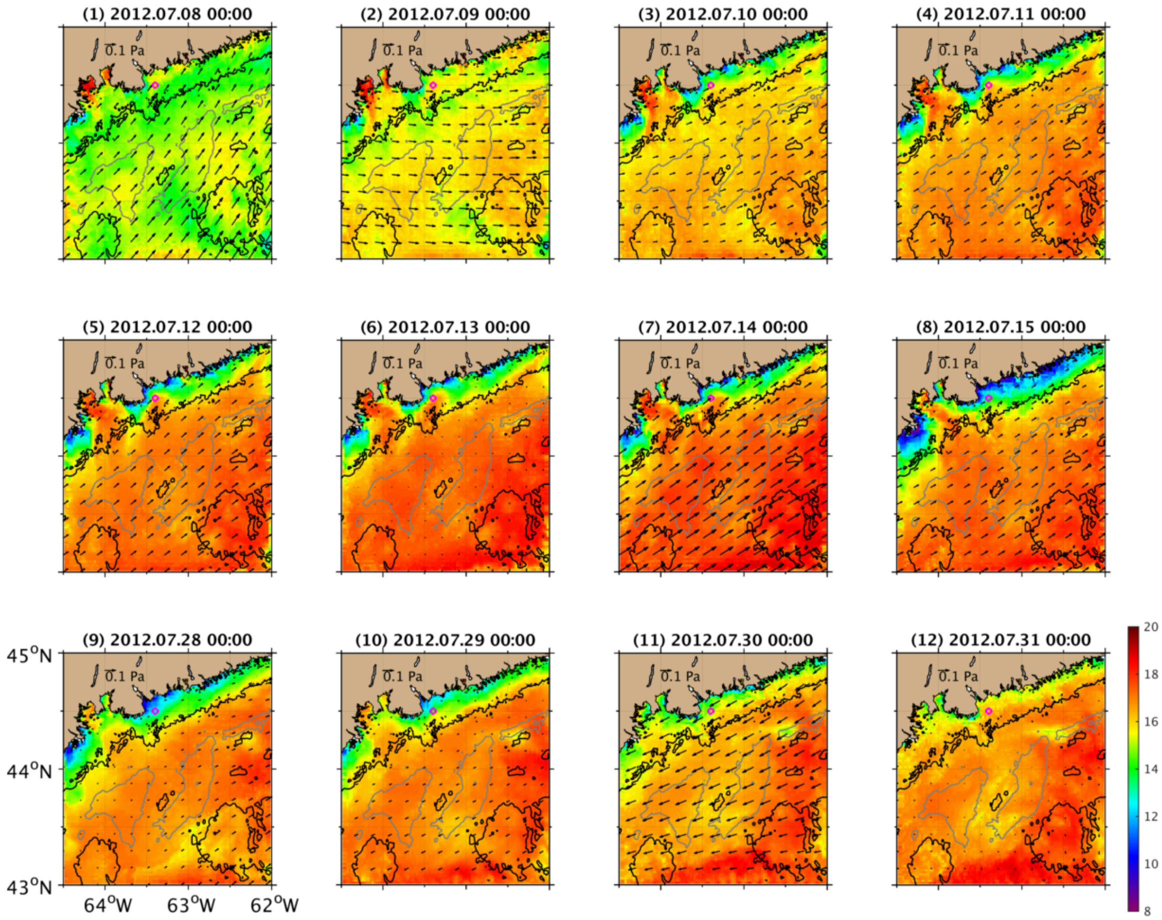


Figure 3: Snapshots of simulated SST over the central Scotian Shelf in July 2012 with instantaneous wind stress vectors plotting as black arrows (DalCoast-CSS model from Shan 2016).

These references further illustrate that some upwelling events create larger bands of upwelled water along the coastline, such as in Figure 1 and panel (c) in Figure 2.

References:

Petrie, B., B. Topliss, and D. Wright, Coastal upwelling and eddy development off Nova Scotia, *Journal of Geophysical Research*, 92, 12979-12991, 1987.

Shan, S. Eulerian and Lagrangian studies of circulation on the Scotian Shelf and adjacent deep waters of the North Atlantic with biological implications, PhD thesis, Dalhousie University, Halifax, NS, 2016.

Figure 6 - Highlight the "nearshore" region you mention in the text on this figure. The DIC gradient is not as severe as in the CCS. Consider putting it in this space: https://www.sciencedirect.com/science/article/pii/S0278434317303643#f0005

Response: Indeed, this upwelling is very different from the upwelling in the CCS (see above comments).

Figure 7 – Please add other parameter time series to this plot including temperature, salinity and most important winds (both modeled and observed).
Response: We have added more parameters to this time series, now Figure 5 in the revised manuscript.

Figure 8- More detail needs to be added to methods about how these comparisons were made.
Response: We added more detail to the figure caption, which now reads (additions in bold italics) "*Monthly and annual air-sea CO_2 flux calculated from the model on the entire Scotian Shelf (pink), **extracted** at the CARIOCA buoy location (black), and from the buoy observations (blue). **Flux is averaged over simulation years 2006-2014 for the model, and years 2007-2014 for the CARIOCA observations. Error bars are +/- 1 standard deviations between years**.*"

Figure 9 – Please add vandemark discussion to the text. What is the far right "section"?
Response: We have added Vandemark to the discussion (see line 354). The rightmost section is a "merged" location as both Laruelle papers define a larger area and not solely the Scotian Shelf or Gulf of Maine. We have relabelled this accordingly.

Finally, the title would be more informative if it were about the science question the paper is trying to address.
Response: We believe the Reviewer may have misunderstood our intended science question and hope this is clarified by the above responses.

McGarry, K., Siedlecki, S. A., Salisbury, J., & Alin, S. R. (2021). Multiple linear regression models for reconstructing and exploring processes controlling the carbonate system of the northeast US from basic hydrographic data. Journal of Geophysical Research: Oceans, 126, e2020JC016480. https://doi.org/10.1029/2020JC016480

Xu, Y.âY., Cai, W.âJ., Wanninkhof, R., Salisbury, J., Reimer, J., & Chen, B. (2020). Long-Term Changes of Carbonate Chemistry Variables Along the North American East Coast. Journal of Geophysical Research: Oceans, 125, e2019JC015982. https://doi.org/10.1029/2019JC015982

A modeling study of temporal and spatial pCO2 variability on the biologically active and temperature-dominated Scotian Shelf

Response to Comments by Reviewer 2

(Reviews are included in black font; Responses are in blue font)

The authors use output from a regional oceanic biogeochemical model and mooring/ship-board observations to study the seasonal cycle of surface pCO2 and sea-air CO2 fluxes. The general findings are that the Scotian Shelf acts as a net annual source of CO2 to the atmosphere and that biological activity and temperature are the main drivers of the pCO2 variability. The authors also try to show that coastal upwelling is responsible for low near-shore surface pCO2 in summer. Overall, I find the manuscript well organized. However, I have several concerns (see below) that need to be addressed.

Response: We appreciate the constructive comments and have addressed them as described below.

Line 14: Might be good to mention here by how much pCO2 changes due to this steep increase in temperature.

Response: Agree, we have modified the text as follows (addition in bold italics; lines 12-15 in the revised manuscript): "*Surface pCO_2 undergoes a strong seasonal cycle **with an amplitude of ~200-250 µatm**. **These changes are** associated with both a strong biological drawdown of Dissolved Inorganic Carbon (DIC) in spring **(corresponding to a decrease in pCO_2 of 100-200 µatm)**, and pronounced effects of temperature, which ranges from 0°C in the winter to near 20°C in the summer**, resulting in an increase in pCO_2 of ~ 200-250 µatm.***"

Lines 33-36: Since you specify the type of measurements that suggest that the Scotian Shelf is a net CO2 source, it would be interesting to know what type of data suggests that it is a net sink.

Response: It is the same type of measurement (surface ocean pCO_2), but different data sets are used in these studies. We have modified the text as follows (addition in bold italics; lines 36-38 in the revised manuscript): "These findings are in contrast to other studies ***using observations from the SOCAT database,*** indicating that the Scotian Shelf follows the global trend and acts as a net sink of CO_2 (Laruelle et al. 2014; Laruelle et al. 2015; Signorini et al. 2013)."

Line 63: I would be careful calling any model "accurate"! If the model has been evaluated properly (if the region has an adequate amount of observations), then I bet these studies identified some deficiencies. I would suggest to briefly summarizing the previous model evaluation here and state unknowns due to lack of data, if applicable.

Response: Agree, we have modified this as follows (added/modified text in bold italics; lines 64-65 in the revised manuscript):

*"In the present study, we employ a high-resolution biogeochemical model of the northwest North Atlantic to examine the magnitude, variability and sign of the air-sea CO_2 flux on the Scotian Shelf. Previous studies **evaluated** our **model's ability to** represent the physical (Brennan et al. 2016, Rutherford & Fennel 2018) and biological (Laurent et al. 2020) dynamics of the region."*

We have also added more detail about these evaluations in the methods, where we describe the physical and biological model set up.

Line 105: What are the possible implications of using a river climatology to force the model? Is anything known about interannual or longterm changes to the riverine input?
Response: The intended purpose of this paper is to focus on the seasonal variability not interannual or long-term changes. River inputs make up a very small fraction of the water on the Scotian Shelf (see Rutherford & Fennel 2018) and variations in riverine chemistry over this short period would be negligible. We have emphasized throughout the revised manuscript that the focus of this study is on a seasonal scale (see for example lines 11, 67, 68, 310, 371, 396 in the revised manuscript).

Line 102: Again, a brief summary of deficiencies and skills of the model would be good.
Response: Agree, we have added the following (addition/modification in bold italics):

Lines 114-119 in the revised manuscript: "*For a detailed description and validation of the biological model, we refer to Laurent et al. (2021),* ***who compared the model output with glider transects of temperature, salinity and chlorophyll, and in situ measurements of chlorophyll and nitrate. The model was evaluated on a seasonal scale for the entire model domain, mainly in the surface (top 100 m). Laurent et al. (2021) showed that the model outperforms global models for the region for all variables and that the timing of the spring bloom is well represented, but the model slightly underestimates the magnitude of the bloom and tends to slightly overestimate nitrate throughout the year.*** "

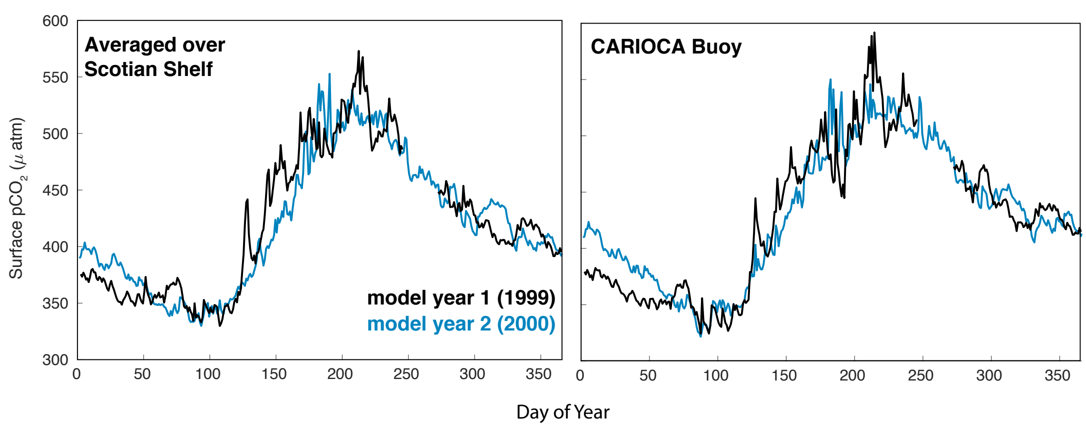
Lines 107-110 in the revised manuscript: *"Full details on the physical model setup and its validation can be found in Brennan et al. (2016) and Rutherford & Fennel (2018).* ***These studies have shown that our model simulates the vertical structure and seasonal cycling of temperature and salinity on the shelf well. The model captures mesoscale features and coastal upwelling events, and simulates the volume transport throughout the region in agreement with observation-based estimates.***"

Line123: Why is it drifting and how does the nudging impact the actual model skill. I was surprised that so much nudging was done for a relatively small model domain. Are the nudged areas not used in the analysis? And if these areas are used, how do you deal with them? Would be helpful to show the nudged areas in Figure 1.
Response: The nudging zones along the boundary are not used in the analysis, which we have stated explicitly in the revised manuscript. It is common to apply boundary nudging in regional domains as a method to impose low-frequency variability from outside the domain. The nudging timescale is long (60 days at the boundary, linearly decreasing to zero at the inner edge of the nudging zone). This means that nudging is weak. Since the internal dynamics of the Labrador Sea, which set the seasonal cycle of physical and biogeochemical conditions at the northeastern boundary, are not represented in our regional shelf-focussed domain, boundary nudging is applied essentially to impose information from outside the domain in a band along the model's open boundary. This benefits model skill by eliminating unrealistic drifts.
We have updated the manuscript as follows: (Lines 130-134 in the revised manuscript, added text is in bold italics): "*DIC is nudged in an 80-grid-cell wide buffer zone along the eastern boundary, with nudging linearly decaying away from* ***a nudging timescale of 60 days at*** *the boundary to a value of 0 in the 81st grid cell. At all other boundaries, a 10-grid buffer zone is*

used, as with temperature and salinity. ***Use of a wider boundary nudging zone along the eastern boundary was found to be beneficial in imposing low-frequency variability from the Labrador Sea at the northeastern boundary. The nudging zones are not used in the analysis.***

Line 131: Model spin-up of a biogeochemical model usually takes 6-10 years. Can you show that 1 year is enough and the model won't drift anymore? For example run the model for 10 years perpetually, using the 2000 conditions. Does DIC remain relatively stable, without drifting?
Response: We have now run a longer simulation (1999-2014), which has been analyzed and replaced the previous 6-year simulation (1999-2004) from the original manuscript. We now focus on the years 2006-2014 of the longer simulation, which encompass the observation years. In addition, we have included figures in the supplement (see supplement section S2 and Figures S2-S5) with a timeseries of surface pCO_2 on each of our shelves for the years 2000-2014 to illustrate the interannual variability in the model and show that there is no noticeable model drift in these years.

Below is a figure of surface pCO_2 averaged on the Scotian Shelf and locally at the CARIOCA buoy comparing year 1999 to year 2000 (i.e. years 1 and 2 of the simulation) to illustrate the model spin-up. Model spin-up is seen mainly within the first 75 days (or first 3 months) where pCO_2 is lower and relatively constant in 1999 compared with 2000 (and all other subsequent years, see Figure S2 and S3). This spin-up period aligns with the residence time on the Scotian Shelf of ~ 3 months (see Rutherford and Fennel 2018).



Line 147: Need to label the location of the Halifax and Deep Panuke gas platform.
Response: Agree, we have added this to Figure 1 and updated the text as follows (additions in bold italics, see lines 176-177 in revised manuscript): "*The ship transits weekly to biweekly between the Halifax* ***Harbour (Bin 1)*** *and the Deep Panuke gas platform off Sable Island* ***(Bin 2)*** *on the Scotian Shelf (Figure 1).*"

Line 163: "from top to bottom…" belongs into caption and not into main text. Also, describe method you used to temperature normalize pCO2 in caption.
Response: Agree, we have modified this accordingly.

Line 164: To me it is confusing to talk about days and months. I would just stick to months, since days are less obvious – The reader would have to first convert to the month before understanding what time of the year you are referring to. I don't see how pCo2 is relatively constant between day 0

to 75. Are you referring to the temp normalized pCO2? But even temp normalized pCO2 is increasing during this time. Might be better to give a range here?
Response: We prefer using the day of year for this section because it is more specific than referring to months and believe it is clear.

Line178: add "buoy" to "… at the low end of the **buoy** observations
Response: Agree, this change was made.

Line 182: I don't think the word "consistent" is appropriate here? The model seems to underestimate the DIC drawdown due to primary production compared to both types of observations (temp norm. pCO2).
Response: Agree. We have modified this line to (now 216-217; modification in bold italics): *"The bloom-related minimum in pCO_2 in the model is approximately 50-75 µatm higher than the buoy observations* ***and approximately 25-50 µatm higher than*** *the Atlantic Condor observations."*

Line 189: verb is missing.
Response: This has been corrected, and now reads as follows (see 224-225 in revised manuscript, changes in bold italics): "*The model tends* ***towards*** *slightly higher pCO_2 across the shelf* ***compared to*** *the ship data,* ***but the bias along the ship track is about half the magnitude as that at the buoy."***

Line 209: Figure 4 shows how the model struggles to simulate the spatial variability, which should be pointed out.
Response: We have added a sentence at the end of the first paragraph stating that the model does not show the small-scale variations in pCO_2 that are seen in the Condor transect. However, we would like to add that this is not surprising. It is common that models produce much less variations than underway pCO_2 observations. We would also point out that underway measurements are prone to many errors and that the variations may at least partly be due to measurement artefacts. See lines 240ff in the revised manuscript for this addition: "***Small-scale spatial variability in the observations is not captured by the model, but may, at least in part, be due to measurement artefacts of the underway system."***

Line 212: add east or west to longitude description
Response: Yes, we have added this throughout the paper.

Line 216: I don't think these events are all that obvious in the observations. There were only a total 3 inner shelf observations during this time period, two of which are actually higher than an outer shelf observation point (also the only one during this period). I agree, that this is obvious in the model, but would be more careful with this statement for the observations. I just don't think that the observations can be interpreted that way… Im also not conviced by the proposed mechanism that leads to low pCO2, despite high DIC. What does the salinity profile look like? I think this section needs something like a Taylor decomposition to show that what is responsible for the low pCO2 (see details in
Rheuban, J. E., Doney, S. C., McCorkle, D. C., and Jakuba, R. W.: Quantifying the effects of nutrient enrichment and freshwater mixing on coastal ocean acidification, J. Geophys. Res.-Oceans, 124, 9085–9100, https://doi.org/10.1029/2019JC015556, 2019.
Or

Hauri, C., Schultz, C., Hedstrom, K., Danielson, S., Irving, B., Doney, S.C., Dussin, R., Curchitser, E.N., Hill, D.F, and Stock, C.A.: A regional hindcast model simulating ecosystem dynamics, inorganic carbon chemistry, and ocean acidification in the Gulf of Alaska, Biogeosciences, 17, 3837–3857, https://doi.org/10.5194/bg-17-3837-2020, 2020.

Response: The observations with higher pCO_2 nearshore have been removed from the analysis, due to measurement system error. There is 1 instance in the observations where this low pCO_2 signal is very clear, which is associated with cold temperatures (refer to Figure 5 in the original manuscript; now Figure S9 in the supplement). We agree that with only 1 instance in the observations of low pCO_2 nearshore, it is difficult to draw unequivocal conclusions about the mechanisms driving this. We have therefore rephrased this section as using the model to hypothesize what could be driving this low pCO_2 nearshore. See the following changes in the revised manuscript:

Add at lines 245ff: "***With more obvious examples in the model than in the observations, we use the model to investigate into a possible explanation for this decreased pCO_2 nearshore."***

And lines 312ff (additions in bold italics): ***"Notable occurrences of spatial variability of pCO_2 on the Scotian Shelf occur throughout the summer months in both the model and observations. With only 1-2 clear examples of lower pCO_2 within ~ 25 km of shore in the observations, we used our model to hypothesize about a possible mechanism driving this variability. In the model, we found that*** *coastal upwelling events are driving* ***the summertime*** *spatial variability in pCO2 on the Scotian Shelf* ***and could explain the variability in the observations as well."***

We additionally have added more variables along the transect to the supplementary info (see section S6 and figure S11). We also have added a Taylor Decomposition (in the revised manuscript, see lines 149ff in the Methods, lines 263ff and Figure 7 in the Results, and lines 322ff in the Discussion).

Line 264: "Accurate" means: "correct in all details; exact"- as menti0oned earlier, I yet have to see a model that can be described as "accurate". I would tone it down… especially because you start the sentence with "This limitation aside…"

Response: Agree, we have changed the word "accurately" to "well captured" (see line 310 in revised manuscript).

Line 270: would be nice to calculate how much the temperature change affects pCO2 and how much DIC increases affect pCO2….

Response: Agree, we have used the Taylor Decomposition to accomplish this. At line 323ff in the modified text, we have added: "***In the example explored in the present study, the upwelled water comes from ~ 20-25 m depth that has a pCO_2 approximately 100 uatm lower than the rest of the shelf. Temperature in the upwelled water is acting to lower pCO_2 by ~ 150 uatm whereas DIC is acting to increase pCO_2 by ~ 50 uatm compared to the rest of the shelf. If deeper water was being upwelled to the surface, DIC would likely start to be the dominant factor in setting pCO_2 during these events (Figure 7)."***

Figures – I really like the color choices of the figures!

Response: Thank you!

Figure 1: It would be nice to give the reader a better understanding of where the Scotian Shelf is located. Maybe a zoomed-out map as an insert? Label all location names you are mentioning in the paper e.g. Halifax Harbor. What are bin 1 and bin 2? Please describe in caption. Also, LAt and Lon labels are missing, including whether it is north or south, and east or west. This should be adjusted for all figures throughout.
Response: We have made these changes as suggested.

Figure 2: Correct "Glider obser**v**ations"
Identify grey band in legend for consistency.
What are the two different x-axis?
Response: We have made these changes. We included a DOY and month x-axis to help the reader (since we refer to DOY in the text).

Figure 4: What are these inserts? Zoom in? Does not seem to show what you see in the smaller box below. This figure is kind of confusing. What are we actually looking at? Are there 365/5 lines total per figure?
Response: We have made the caption for this figure clearer and more descriptive.

Figure 5: On the left, there is no top and lower panel... please adjust accordingly. Also, maybe identify "thick black line" as "vertical black line"
Response: Agree, these have been modified. This figure has also been moved to the supplement since we have expanded Figure 7 (now Figure 5) to replace it.

Figure 6:Please identify the variable that goes with each unit next to the colorbar. Always good to specify units of all variables in the caption too. Also, define abbreviations in all figures e.g. dissolved inorganic carbon (DIC). Figures and captions should be readable without reading the manuscript. Since you refer from figure 5 to this figure, you should mention here that July 11, 2000 is indicated in figure 5. Please show the transect line again in the map and label it with lat and lon. Why not also show a profile of pCO2 here to make the point that pCO2 decreases during upwelling event.
Response: Agree. We have made these changes.

Figure 7: Add "the" to …the values from **the** nearshore bin…
Response: Done.

Figure 8: What do the error bars mean? What are they based on? What are the numbers behind +/-? 1 STD? Needs to be defined in caption.
Response: Error bars are standard deviation between years. We have added this to the figure caption.

Figure 9: Why are some bars faded? Are all ingassing bars faded? Needs to be defined.
Response: Yes, all ingassing bars are faded. We have added this to the figure caption.

A modeling study of temporal and spatial pCO_2 variability on the biologically active and temperature-dominated Scotian Shelf

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Abstract. Continental shelves are thought to be affected disproportionately by climate change and are a large contributor to global air-sea carbon dioxide (CO_2) fluxes. It is often reported that low-latitude shelves tend to act as net sources of CO_2 whereas mid- and high-latitude shelves act as net sinks. Here, we combine a high-resolution regional model with surface water time-series and repeat transect observations from the Scotian Shelf, a mid-latitude region in the northwest North Atlantic, to determine what processes are driving the temporal and spatial variability of partial pressure of CO_2 (pCO_2) on a seasonal scale. In contrast to the global trend, the Scotian Shelf acts as a net source. Surface pCO_2 undergoes a strong seasonal cycle with an amplitude of ~ 200-250 µatm. These changes are associated with both a strong biological drawdown of Dissolved Inorganic Carbon (DIC) in spring (corresponding to a decrease in pCO_2 of 100-200 µatm), and pronounced effects of temperature, which ranges from 0ºC in the winter to near 20ºC in the summer, resulting in an increase in pCO_2 of ~ 200 µatm). Throughout the summer, events with low surface-water pCO_2 occur nearshore associated with coastal upwelling. This effect of upwelling on pCO_2 is also in contrast to the general assumption that upwelling increases surface pCO_2 by delivering DIC-enriched water to the surface. Aside from these localized events, pCO_2 is relatively uniform across the shelf. Our model agrees with regional observations, reproduces seasonal patterns of pCO_2, and simulates annual outgassing of CO_2 from the ocean of +1.7 ± 0.2 mol C m^{-2} yr^{-1} for the Scotian Shelf, net uptake of CO_2 by the ocean of -0.5 ± 0.2 mol C m^{-2} yr^{-1} for the Gulf of Maine and uptake by the ocean of -1.3 ± 0.3 mol C m^{-2} yr^{-1} for the Grand Banks.

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1 Introduction

The global ocean acts as a major sink of CO_2 from the atmosphere (e.g., Le Quéré et al 2018; Gruber et al. 2019; Landschützer et al. 2014; Rodenbeck et al. 2015), but it has been suggested that flux density (or flux per unit area) on continental shelves is larger than in the open ocean (Chen et al. 2013; Laruelle et al. 2014). Therefore, compared to their size, continental shelves are thought to disproportionately contribute to global air-sea CO_2 fluxes (Laruelle et al. 2010). Additionally, they are susceptible to climate change on much shorter timescales than the open ocean (Cai et al. 2010) and are experiencing increasing impacts of human activity (Cai 2011; Doney 2010; Gruber 2015). Given their high susceptibility to negative impacts from climate change, and their potentially significant contribution to global air-sea CO_2 fluxes, it is important to understand the drivers underlying inorganic carbon dynamics on continental shelves.

It is generally thought that continental shelves at mid to high latitudes act as net sinks of atmospheric CO_2 while those at low latitudes act as net sources (e.g. Chen & Borges 2009; Cai et al. 2006; Laruelle et al. 2014; Roobaert et al. 2019). There are, however, notable deviations from this global-scale pattern. The Scotian Shelf, a mid-latitude shelf off the coast of eastern Canada, is one example with large discrepancies between independent estimates of air-sea CO_2 flux (Fennel et al. 2019). Direct measurements made using a moored CARIOCA buoy on the Scotian Shelf indicate that the shelf acts as a net source of CO_2 to the atmosphere (Shadwick et al. 2010; Shadwick et al. 2011; Shadwick & Thomas 2014). These findings are in contrast to other studies using observations from the SOCAT database, indicating that the Scotian Shelf follows the global trend and acts as a net sink of CO_2 (Laruelle et al. 2014; Laruelle et al. 2015; Signorini et al. 2013). These contrasting results for the Scotian Shelf emphasize the large uncertainty inherent in shelf-wide CO_2 flux estimates.

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Continental shelves are highly complex and dynamic regions where many biological and physical processes modulate CO_2 flux (Laruelle et al. 2014; Laruelle et al. 2017; Roobaert et al. 2019). The partial pressure of CO_2 (pCO_2) in the ocean is one of the key factors which determines the air-sea CO_2 flux. Recent global studies found that thermal controls dominate the seasonality of pCO_2 but that these alone cannot describe observed pCO_2 variations, particularly in temperate and high latitudes (Roobaert et al. 2019). High rates of primary production on continental shelves (Chen & Borges 2009) are another important driver of seasonal changes in pCO_2.

Continental margins are also subject to intense horizontal transport processes, which act as additional drivers of CO_2 fluxes. For example, the Continental Shelf Pump, a term first coined by Tsunogai et al. (1999) in relation to the East China Sea, describes the movement of shelf water high in dissolved inorganic carbon (DIC) across the shelfbreak to the subsurface open ocean leading to an influx of atmospheric CO_2. This mechanism is thought to mainly occur at mid- to high-latitude shelves since it relies on winter cooling to create dense shelf water that is transported to the open ocean's subsurface layers. Upwelling is another well-studied transport mechanism driving shelf-wide CO_2 dynamics. The California Current system is a typical example of an upwelling system (Chavez et al. 2017; Hickey 1998; Fennel et al. 2019; Feely et al. 2008). Here, winds drive coastal upwelling, which brings DIC-rich water to the surface along the continental shelf and creates favourable conditions for CO_2 outgassing to the atmosphere.

Altogether, these complex shelf dynamics lead to large spatial and temporal variability of pCO_2 (Previdi et al. 2009). Such large variability combined with limited data availability for many continental shelves make it difficult to accurately constrain CO_2 fluxes. Limited data availability in space and time, often with seasonal biases, is a prime source of uncertainty in flux estimates that can only be overcome with more uniformly distributed sampling. To fully capture how ocean margins are reacting to perturbations caused by the steady input of anthropogenic CO_2 to the atmosphere, it is important to understand the processes underlying both spatial and temporal evolution of shelf-wide pCO_2.

Numerical models can be useful when investigating such complex interactions and constraining CO_2 flux since they can interpret sparse measurements through the mechanistic representations of relevant processes. In the present study, we employ a high-resolution biogeochemical model of the northwest North Atlantic to examine the magnitude, variability and sign of the air-sea CO_2 flux on the Scotian Shelf. Previous studies have evaluated our model's ability to represent the physical (Brennan et al. 2016, Rutherford & Fennel 2018) and biological (Laurent et al. 2020) dynamics of the region. Here, we focus solely on the model representation of inorganic carbon dynamics, especially the spatial and temporal variability of $p$$CO_2$ on a seasonal scale on the Scotian Shelf in light of new, high-resolution, shelf-wide observations.

Our overall goal is to show how both biological and transport processes work together seasonally on the Scotian Shelf to set shelf-wide surface $p$$CO_2$. We additionally discuss event-based variability of the air-sea CO_2 flux, and, especially, how short-term, upwelling-favourable wind events throughout the summer create spatial variability of CO_2 on the Scotian Shelf. To accomplish these goals, our paper: (1) discusses the seasonal cycle of $p$$CO_2$ across the shelf; (2) investigates the spatial variability of $p$$CO_2$, particularly during the summer months and (3) reports shelf-wide air-sea CO_2 flux estimates in comparison to previously reported estimates. We discuss the importance of our findings in terms of global patterns of air-sea CO_2 flux and carbon cycling.

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2 Study Region

The Scotian Shelf (Figure 1) is uniquely located at the junction of the subpolar and subtropical gyres (Loder et al. 1997; Hannah et al. 2001). Regional circulation is dominated by southward transport of the Labrador Current (Loder et al. 1998; Fratantoni & Pickart 2007). As a result, cool Arctic-derived water accumulates along the northwestern North Atlantic continental shelf separating fresh shelf waters from warmer and salty slope waters (Beardsley & Boicourt 1981; Loder et al. 1998; Fratantoni & Pickart 2007).

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The Scotian Shelf in particular is controlled by inshore and shelf-break branches of the southwestward moving current. The shelf-break branch inhibits the movement of water across the shelf break of the Scotian Shelf (Rutherford & Fennel 2018). As a result, water moves predominantly along-shelf so that residence times in the region are relatively long, with water being retained on the Scotian Shelf for an average of 3 months before moving further southwest on the shelf (Rutherford & Fennel 2018). In terms of vertical structure, the Scotian Shelf shifts between a two-layer system in the winter, when a cold, fresh layer sits over a warm, salty deep layer, and a three-layer system in the spring and summer, when a warm surface layer forms in the top 20 m above the cold intermediate layer between 20 – 100 m, and the warm and salty deep layer (Dever et al. 2016).

The Scotian Shelf is additionally characterized by a large, shelf-wide spring bloom initiated in late-March (Ross et al. 2017; Fournier et al. 1977; Mills & Fournier 1979), when the mixed layer is still relatively deep and temperature is at its coldest (Craig et al. 2015). The initiation of the spring bloom in late-March has rapid and large impacts on the observed $p$$CO_2$ seasonality (Shadwick et al. 2010; Shadwick et al. 2011).

3 Methods

3.1 Model setup & initialization

3.1.1 Physical Model Setup

We employ a biogeochemical model, based on Fennel et al. (2006), Fennel & Wilkin (2009) and Laurent et al. (2020) that is part of the Regional Ocean Modelling System (ROMS, v.3.5; Haidvogel et al. 2008). The physical model implementation, described in more detail in Brennan et al. (2016), has 30 vertical levels and approximately 10-km horizontal resolution (240x120 horizontal grid cells), uses the GLS vertical mixing scheme (Umlauf & Burchard 2003; Warner et al. 2005), atmospheric surface forcing from the European Centre for Medium-Range Weather Forecasts (ECMWF) global atmospheric reanalysis (Dee et al. 2011) and the "*h*igh-order *s*patial *i*nterpolation at the *m*iddle *t*emporal level" (HSIMT) advection scheme for tracers (Wu & Zhu 2010). Physical initial and boundary conditions are defined using the regional physical ocean model of the northwest North Atlantic of Urrego-Blanco & Sheng (2012). Temperature and salinity are nudged toward the climatology of Geshelin et al. (1999) in a 10-grid-cell wide buffer zone along open boundaries. Nudging strength decays linearly away from the boundaries to a value of zero in the 11th grid cell from the boundary. Tides are imposed from Egbert & Erofeeva (2002). Climatological river discharge is imposed for 12 major rivers and uses observed long-term monthly means from Water Survey Canada. Full details on the physical model setup and its validation can be found in Brennan et al. (2016) and Rutherford & Fennel (2018). These studies have shown that our model simulates the vertical structure and seasonal cycling of temperature and salinity on the shelf well. The model captures mesoscale features and the coastal upwelling events, and simulates the volume transport of throughout the region in agreement with observation-based estimates.

3.1.2 Biogeochemical Module

The biogeochemical model is based on the nitrogen-cycle model with inorganic carbon component of Fennel et al. (2006) and Fennel & Wilkin (2009) but was recently expanded to include 2 phytoplankton and 2 zooplankton functional groups (Laurent et al. 2021). For a detailed description and validation of the biological model, we refer to Laurent et al. (2021), who compared the model output with glider transects of temperature, salinity and chlorophyll and in situ measurements of chlorophyll and nitrate. The model was evaluated on a seasonal scale for the entire model domain, mainly in the surface (top 100 m). Laurent et al. (2021) showed that the model outperforms global models for the region for all variables and that the timing of the spring bloom is well represented, but the model slightly underestimates the magnitude of the bloom and tends to overestimate nitrate throughout the year.

For calculating air-sea CO_2 flux, according to the carbonate chemistry model of Zeebe & Wolf-Gladrow (2001), we use dissociation constants (K1 and K2) from Millero et al. (1995) using Mehrbach et al. (1973) data on the seawater scale which are deemed appropriate for the typical salinity ranges from 27 to 36.6 in the model domain (lower salinities are highly localized in the Gulf of St. Lawrence Estuary). Atmospheric pCO_2 is set to the seasonal cycle and secular trend derived from Sable Island monitoring data contributed by Environment Canada's Greenhouse Gas Measurement Program (Environment and

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Climate Change Canada, 2017). The long term linear trend in the atmospheric pCO_2 is ~ +2 µatm year^{-1} (see Supplement for the full trend equation and figure). CO_2 solubility is calculated with the Weiss (1974) formulation. The gas transfer coefficient of Ho et al. (2006) is used and depends on wind speed at 10 m above the sea surface and the Schmidt number. Further details of the biogeochemical model, including the carbonate chemistry equations, can be found in Laurent et al. (2017, Supporting Information). Carbon initialization, boundary conditions and climatological nudging are calculated from relationships with temperature and salinity determined from bottle data for the region. DIC is nudged in an 80-grid-cell wide buffer zone along the eastern boundary, with nudging linearly decaying away from a nudging timescale of 60 days at the boundary to a value of 0 in the 81st grid cell. At all other boundaries, a 10-grid buffer zone is used, as with temperature and salinity. Use of a wider boundary nudging zone along the eastern boundary was found to be beneficial in imposing low-frequency variability from the Labrador Sea at the northeastern boundary. The nudging zones are not used in the analysis.

Nitrate concentrations in rivers are prescribed from Global NEWS model output Seitzinger et al. (2005). DIC and total alkalinity (TA) in rivers were calculated by fitting a linear relationship with salinity from Gulf of St. Lawrence bottle data and extrapolating to river water salinity. The model is initialized on January 1, 1999 from Urrego-Blano and Sheng's (2012) solution for temperature and salinity. Nitrate (NO_3^-) concentrations are initialized from the regional climatologies as in Laurent et al. 2020. DIC and TA initial and boundary conditions were created from observationally based relationships with temperature (T) and salinity (S) using bottle data from regional cruises from 1997-2011 encompassing as far south as the Gulf of Maine and as far north as the Labrador Sea (observations from DFO's AZMP program, see: dfo-mpo.gc.ca/science/data-donnees/azmp-pmza/index-eng.html#publications). Initialization relationships used only observations from December, January and February (TA = 43S + 800, r^2 = 0.96; DIC = 1153 – 21.6T + 29.1S – 0.41T^2 + 0.63ST, r^2= 0.90). Boundary conditions used observations that encompassed the entire year (TA = 41S + 875, r2 = 0.92 ; DIC =912.6 – 2.5T + 35.7S – 0.45T^2 + 0.12ST, r2 = 0.80). The model is run for 16 years (1999-2014) with daily output. The present study analyses the model output from 2006-2014, with focus on year 2006. See the Supplement for a comparison of surface pCO_2 throughout the simulation and a brief validation of TA and DIC.

3.1.3 Taylor Decomposition of Upwelling Events

To better understand the effects of coastal upwelling on surface pCO_2, we perform a Taylor Decomposition on the model output during one of the upwelling events focused on in this study, following a similar methodology to Rheuban et al. (2019) and Hauri et al. (2020). Here, we investigate into the influence of T, S, DIC and TA on pCO_2 following the equation:

$$pCO_2 = f(T, S, DIC, TA)$$

where f indicates the CO2SYS set of equations. We calculated anomalies, ΔpCO_2, from a reference value, $pCO_{2,0}$:

$$\Delta pCO_2 = pCO_2 - pCO_{2,0}$$

The reference values for each variable were calculated as the average of that variable along the Condor transect (see Fig 1) in the upper 40 m (i.e., the part of the water column affected by the upwelling event). We decomposed ΔpCO_2 relatively simply into perturbations related to T, S, DIC, and TA calculated as follows:

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$$\Delta pCO_{2,T} = f(T, S_0, DIC_0, TA_0) - pCO_{2,0}$$

$$\Delta pCO_{2,S} = f(T_0, S, DIC_0, TA_0) - pCO_{2,0}$$

$$\Delta pCO_{2,DIC} = f(T_0, S_0, DIC, TA_0) - pCO_{2,0}$$

$$\Delta pCO_{2,TA} = f(T_0, S_0, DIC_0, TA) - pCO_{2,0}$$

We refer the reader to Rheuban et al. (2019) for a more detailed description of the Taylor Decomposition methodology.

3.2 Observational Datasets

The moored CARIOCA buoy was located at Station 2 on the Halifax Line. Station 2 (HL2; 44.3ºN, 63.3ºW) is located about 30 km offshore from Halifax, Nova Scotia, and occupied monthly by Bedford Institute of Oceanography. The buoy measured surface water (at approximately 1 m depth) temperature, conductivity, pCO_2, salinity and Chl-a fluorescence every hour and was deployed from 2007 to 2014 with several gaps in data due to calibration and maintenance (see Table S1 in Supplement). pCO_2 was estimated using an automated spectrophotometric technique (Lemay et al. 2018). The raw pCO_2 data contained high-amplitude spikes, with increases from 400 µatm to over 1000 µatm within a few hours, which were measuring artifacts and did not represent $pCO2$ of surrounding water. These spikes were removed by binning all years of the pCO_2 observations into a 365-day of year (DOY) seasonal cycle. Any points that were outside 1.5 standard deviations of the 1-month moving average pCO_2 where discarded. This method removed only the extreme values and maintained much of the observed variability (see Figure 2).

The sensor-based underway system, Dal-SOOP (Arruda et al., 2020), was installed on the multipurpose platform supply vessel Atlantic Condor (operated by Atlantic Towing Ltd.) and has been measuring a suite of biogeochemical parameters, including pCO_2, in the surface water since May 2017. The ship transits weekly to biweekly between the Halifax Harbour (Bin 1) and the Deep Panuke gas platform off Sable Island (Bin 2) on the Scotian Shelf (Figure 1). The Atlantic Condor pCO_2 data underwent standard QA/QC procedures, which included pre-, post-deployment and regular zero-calibration of the pCO_2 sensor (Pro-Oceanus Inc, Canada) and associated data corrections. The QC'd data has been deposited into the Surface Ocean CO_2 Atlas (SOCAT v.2020), where it was attributed an accuracy of ±10 µatm. Performance of the novel Dal-SOOP system was assessed during a 2-month transatlantic cruise in comparison with a conventional pCO_2 equilibrator and showed good agreement with the latter (i.e. −5.7 ± 4.0 µatm; Arruda et al., 2020).

During the QC/QA procedure, some data collected in close proximity to Halifax, and corresponding to the outbound transects, were removed. Some of these data were biased high and attributed to prolonged ship layover in port allowing for a build-up of high pCO_2 within the Dal-SOOP system due to respiration. The active pumping that delivers fresh seawater to the measurement system is triggered by a GPS signal when the ship leaves the harbour; as a result, there can be a delayed response from the pCO_2 sensor to the much lower pCO_2 signals observed immediately outside the harbour. To account for the bias, values that were 2 standard deviations from the mean pCO_2 value for the latitudinal bin closest to the Halifax Harbour were removed for some transects. Only three transects were removed.

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The CARIOCA and Atlantic Condor transect observations were mapped onto year 2006 for comparison directly with this year in the model using the linear trend in atmospheric pCO_2 (+ 2 µatm year^{-1}). Where numbers are reported comparing the model mean to observations, the observations were mapped to year 2010 (the median year of our model simulation). For comparison of the modelled flux to the flux estimates from the CARIOCA buoy, years 2006-2014 in the model were used and no mapping of the observations was performed.

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4 Results

4.1 CO_2 Timeseries and Transect

Both the model and observations at the CARIOCA buoy location (see Figure 1) are shown as a seasonal cycle in Figure 2 (chlorophyll, pCO_2, temperature and temperature normalized pCO_2). The buoy observations show a distinct and recurring seasonal cycle in pCO_2. Specifically, pCO_2 slightly decreases (from ~450 to 425 µatm) from day 0 to 75. In late March, at approximately day 75, there is a large (100-200 µatm) and rapid (over ~ 25 days) drop of pCO_2 associated with DIC drawdown due to the spring bloom (the dashed line indicates the peak in chlorophyll and its alignment with the lowest pCO_2 value). This drawdown of DIC occurs while the surface temperature is relatively constant and at its annual minimum.

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Following the drop in pCO_2 associated with the spring bloom, around day 100, surface water starts to warm, and this warming dominates the pCO_2 seasonal cycle with a maximum value of approximately 450–500 µatm reached around day 200-250 (mid to late summer). Around day 250, temperatures and pCO_2 start to decrease. Also shown is the temperature-normalized pCO_2 using the Takahashi et al. (2002) method for removing the thermal component of pCO_2 variations. The biological drawdown of DIC is visible in the temperature-normalized pCO_2 during the spring bloom starting around day 75 and a further decline throughout summer from day 150 to 250. This indicates that the overall increase in the non-normalized pCO_2 in summer is driven by increasing temperatures, and that biological process tend to draw down DIC during this period.

Most of the Atlantic Condor observations at this location fall within the envelope of the buoy observations' pCO_2 seasonal cycle. The monthly mean SOCAT v2020 pCO_2 for the entire Scotian Shelf also fall within the spread of buoy observations for most months. Exceptions include February and August when the SOCAT observations are lower than the buoy observations, and September and October when the SOCAT observations are at the low end of the buoy observations.

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In terms of quantitative metrics, the model (year 2006) at the buoy location has an overall bias of 32.2 µatm and RMSE of 64.0 µatm compared to the buoy data. The model underestimates pCO_2 throughout January and February (day 0 - 80) partly because its spring bloom starts earlier than in the observations. The bloom-related minimum in pCO_2 in the model is approximately 50-75 µatm higher than the buoy observations and approximately 25 – 50 µatm higher than the Atlantic Condor observations. Temperature then dominates the pCO_2 seasonality in the model over a similar period as in the observations. During the summer (day 150-300), the model overestimates pCO_2 but follows a similar cycle as the observations throughout the remainder of the year. The temperature-normalized pCO_2 has similar biases (underestimation from day 0-80; overestimation from day 150-300), an RMSE of 66.5 µatm and an overall bias of 23.0 µatm for year 2006.

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A comparison of simulated pCO_2 with the Atlantic Condor Transect observations along the average ship track (Figure 1) is shown in Figure 3. Compared to the Atlantic Condor observations, the model (year 2006) has a bias of 13.9 µatm and an RMSE of 28.7 µatm. The model tends towards slightly higher pCO_2 across the shelf compared to the ship data, but the bias along the ship track is about half the magnitude as that at the buoy. The seasonal cycle along the ship track (Figure 3) is similar to that at the buoy (Figure 2). The top panel of Figure 3 shows qualitatively good agreement between the model and observations across the whole transect, which is reflected in the averaged pCO_2 in the bottom panel. The model does a very good job at representing pCO_2 throughout the winter (November through March) but does not reproduce the full spring bloom drop in pCO_2 across the whole shelf throughout April as observed. The model also overestimates pCO_2 throughout most of June and July. The seasonal cycle across the transect is relatively uniform throughout most of the year; however, there are some exceptions, for example, throughout July pCO_2 is relatively low nearshore in both the model and observations.

4.2 Effects of Upwelling Events

To better understand the effect of physical events on shelf-wide pCO_2, this section focuses on the cross-shelf variations in year 2006. Figure 4 shows the evolution of pCO_2 along the Atlantic Condor transect throughout the year in both model (Figure 4a) and observations (Figure 4b). As in Figure 2 and Figure 3, the seasonal cycle of pCO_2 extends across the entire shelf. Starting in January (light beige), pCO_2 is around 400 µatm. In March (~ day 50; golden orange colour), pCO_2 starts to decrease, reaching a minimum of approximately 325 µatm in the model and around 275-300 µatm in the observations (day 100; dark brown colour). pCO_2 subsequently increases again due to warming in the late-spring/early-summer and reaches a maximum of about 550 µatm in the model and 525 µatm in the observations (day 200; purple values). Following this peak in pCO_2, both the model and observations start to decline, associated with cooling (days 225 to 325; purple to light blue). Small-scale spatial variability in the observations is not captured by the model, but may, at least in part, be due to measurement artifacts of the underway system.

The insets in Figure 4 highlight events in summer (purple), in the northwestern half of the transect closest to Halifax, when pCO_2 decreases by 50 – 100 µatm within ~40 km off the coast in the model and approximately 25 km off the coast in the observations. With more obvious examples in the model than in the observations, we use the model to investigate into a possible explanation for this decreased pCO_2 nearshore. Figure 5 highlights the differences in pCO_2, air-sea CO_2 flux, temperature and DIC between two longitudinal bins along the Atlantic Condor transect throughout summer 2006 in the model. The bin locations are shown in Figure 1 and contrast data closest to the coastline (Halifax Harbour bin, 63.5°W to 63 °W; blue) with data closest to the shelf break (Deep Panuke Bin, 61°W to 60.5 °W; pink). In the model throughout June to August 2006, there are low pCO_2 events nearshore corresponding to low temperature which occurs during upwelling favourable winds. During some of these events, temperature nearshore is about 7°C lower than near the shelf break. These upwelling events and the subsequent low pCO_2 signal result in a short-term lowering of air-sea CO_2 fluxes nearshore (blue) compared to farther offshore (pink) throughout the summer (at approximately half the flux value nearshore versus offshore throughout July).

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The top panel in Figure 6 shows a snapshot of surface pCO_2 from the model during one of the upwelling events (July 3, 2006; vertical dashed line in Figure 5). pCO_2 is relatively uniform across most of the shelf. However, in a narrow band along the coastline, pCO_2 values are nearly 100 µatm lower than the rest of the shelf. The bottom panels in Figure 6 show transects of pCO_2, temperature and DIC with density contours along the Atlantic Condor transect for the same time slice (July 3, 2006). In these panels, the density gradients move upwards towards the coastline, consistent with upwelling events. This upwelling brings cooler temperatures and higher DIC concentrations to the surface along the coastline of Nova Scotia. The low pCO_2 bin ranges from 63.5 ºW to – 63 ºW longitude in the model (approximately 63.5ºW to – 63.3 ºW longitude in the observations; Figure 4), and aligns with the surface area affected by the upwelling events (Figure 6) in the model. See the Supplement for more variables along the Condor transect during the July 3, 2006 upwelling event.

Figure 7 illustrates the results of the Taylor decomposition during the July 3, 2006 upwelling event with lower pCO_2 nearshore compared to a snapshot without upwelling (June 9, 2006) where surface pCO_2 is relatively uniform. The pCO_2 anomalies (ΔpCO_2), show the deviations in each time slice from the mean pCO_2 in the upper 40 m. In both time slices, the surface pCO_2 is ~ 50 µatm higher than the mean pCO_2 value in the upper 40 m. However, in the upwelling case, the upwelled water is 40-50 µatm lower than the mean pCO_2. In both time slices, across most of the transect, temperature is acting to increase pCO_2 ($\Delta pCO_{2,T}$; by ~50-60 µatm on June 9, 2006 and by ~ 75-100 µatm on July 3, 2006) in the top 10-15 m from the mean value whereas DIC is acting to decrease pCO_2 ($\Delta pCO_{2,DIC}$; by ~ 10-20 µatm on June 9, 2006 and by ~40-50 on July 3, 2006). However, in the upwelling region on July 3, temperature has the opposite effect and is acting to decrease pCO_2 by ~ 50-60 µatm and DIC is acting to increase pCO_2 by only ~ 5-10 µatm from the mean pCO_2 in the top 40 m. The effects of alkalinity ($\Delta pCO_{2,TA}$) and salinity ($\Delta pCO_{2,S}$) are much smaller across the shelf and in both time slices (see Supplement Figure S11). Comparisons of $\Delta pCO_{2,T}$ and $\Delta pCO_{2,DIC}$ illustrate that in the upwelled region, anomalies in pCO_2 from temperature are larger than those from DIC. However, if water from below 30m was upwelled, DIC would likely start to outweigh the effect of temperature on pCO_2.

4.3 Regional Flux Estimates

The model-simulated air-sea CO_2 fluxes, integrated by month and year, and averaged over the simulation from 2006-2014, for the Scotian Shelf and at the buoy location are shown in Figure 8 in comparison to the flux calculated from the CARIOCA buoy observations. The uncertainty in the model estimates is calculated as the standard deviation between years. Annually, the averaged flux between the model and observations is comparable, and the flux estimates at the buoy location are significantly larger than the shelf-wide flux estimates. The model-estimated, annually integrated flux for the Scotian Shelf shows outgassing of CO_2 at +1.7 ± 0.2 mmol C m^{-2} yr^{-1}. At the buoy location, just outside the upwelling region, the model estimates net outgassing of +2.3 ± 0.1 mmol C m^{-2} yr^{-1}. From the buoy observations, the annually integrated CO_2 flux is estimated as net outgassing at +1.5 ± 1.4 mmol C m^{-2} yr^{-1}. Although our model-derived estimate is within the upper error-bound of the observation-based estimate, it is higher which may be due to the model's overestimation of pCO_2, particularly throughout the summer months. There are also some differences on the seasonal scale. In the model, the Scotian Shelf flux is lower in magnitude than the flux

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at the buoy location during most of the year, and particularly from June to January. Bin 1 along the Atlantic Condor transect (Halifax Harbour/upwelling bin, Figure 1) has an annually integrated flux of +2.2 ± 0.2 mmol C m^{-2} yr^{-1}, which is comparable to the annual flux of bin 2 (Deep Panuke/shelfbreak bin, Figure 1) at +2.0 ± 0.2 mmol C m^{-2} yr^{-1} and the simulated flux at the buoy location. These results indicate that cross-shelf variability in air-sea CO_2 fluxes is small.

Figure 9 compares the model-derived, annual flux estimates from the present study for the Scotian Shelf (+1.7 ± 0.2 mmol C m^{-2} yr^{-1}), Grand Banks (-1.3 ± 0.3 mol C m^{-2} yr^{-1}) and Gulf of Maine (-0.5 ± 0.2 mol C m^{-2} yr^{-1}) to previously reported estimates. The model estimate for the Scotian Shelf agrees well with the estimates from Shadwick et al. (2011) but disagrees with those from Signorini et al. (2013), Laruelle et al. (2014) and Laruelle et al. (2015). Laruelle et al. (2014) define the shelf region as a larger area that encompasses both the Scotian Shelf and Gulf of Maine. Laruelle et al. (2015) calculate one flux estimate for both the Scotian Shelf and Gulf of Maine. Signorini et al. (2013) calculates separate estimates for Gulf of Maine and Scotian Shelf. The model estimate for the Gulf of Maine agrees best with the estimates from Laruelle et al. (2014) and Laruelle et al. (2015), and disagrees with the estimates from Signorini et al. (2013) and Vandemark et al. (2011).

5 Discussion

We have compared the inorganic carbon dynamics in our medium complexity biogeochemical model of the northwest North Atlantic against two different observational datasets of pCO_2, one of them highly resolved in time from a CARIOCA buoy and the other with high spatial resolution along a cross-shelf transect that is occupied approximately bi-weekly. The largest limitation of the model is that it is unable to capture the speed and magnitude of the DIC drawdown associated with the spring bloom throughout March and April (Figure 2 and Figure 3). The simulated pCO_2 starts to decline earlier and over a longer period than in both the buoy and transect observations, and the transect shows that this timing is consistent across the whole shelf. Additionally, the model does not reach the observed pCO_2 minimum during the bloom across the whole shelf. This discrepancy appears to be a result of the bloom initiation occurring slightly too early and the bloom spanning a longer period of time in the model, and also because chlorophyll levels in the model do not reach the peak values that are observed (Figure 2a). This limitation aside, the overall seasonal cycle and switch between biological- and temperature-dominated signals in pCO_2 are well captured and the model simulates both the seasonal spatial and temporal variability of pCO_2 across the Scotian Shelf reasonably well.

Notable occurrences of spatial variability of pCO_2 on the Scotian Shelf occur throughout the summer months in both the model and observations. With only 1-2 clear examples of lower pCO_2 within ~ 25 km of shore in the observations, we used our model to hypothesize about a possible mechanism driving this variability. In the model, we found that coastal upwelling events are driving the summertime spatial variability of pCO_2 on the Scotian Shelf and could explain the variability in the observations as well. The physical dynamics of coastal upwelling is well-documented on the Scotian Shelf (Petrie et al. 1987; Shan et al. 2016). This upwelling only affects the nearshore region (within ~20-40 km of shore in the model, depending on the event) where water from the cold intermediate layer is transported to the surface. In the model, this creates a coastal band of

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cold water at the surface that is high in DIC and low in pCO_2 (Figure 6). The difference between inshore and offshore temperatures (7ºC and 15ºC, respectively) during these events has a larger influence on the pCO_2 spatial variability than the DIC variations (2050 mmol C m^{-3} inshore and 2020 mmol C m^{-3} offshore; Figure 6) because the thermodynamic influence of temperature outweighs the effect of a slight increase in DIC, thus lowering pCO_2 (see the Taylor decomposition in Figure 7). In the example explored in the present study, the upwelled water comes from ~ 20-25 m depth that has a pCO_2 approximately 100 µatm lower than the rest of the shelf. Temperature in the upwelled water is acting to lower pCO_2 by ~150 µatm whereas DIC is acting to increase pCO_2 by ~ 50 µatm compared to the rest of the shelf. If deeper water was being upwelled to the surface, DIC would likely start to be the dominant factor in setting pCO_2 during these events (Figure 7). For the given range of DIC values (2060 to 2020 mmol C m^{-3}) and a mean temperature of 11ºC, the thermodynamic effect outweighs the effect of DIC differences for temperature changes larger than 4ºC. Typically, it is thought that upwelling of subsurface waters rich in DIC leads to increased surface pCO_2 as is the case for the California Current System (CCS), encompassing the continental shelves off of Washington, Oregon and California, where nearshore outgassing of CO_2 during upwelling events is well documented (Fennel et al. 2019, Chavez et al. 2017, Evans et al. 2015, Fiechter et al. 2014, Turi et al. 2014). There are, however, large differences between the Scotian Shelf and the typical upwelling scenario of the CCS. For instance, the size and geometry of these shelves are quite different, which affects the type of water being upwelled to the surface. The California Shelf is an active margin approximately 10 km wide (Fennel et al. 2019) compared to the passive-margin Scotian Shelf with approximately 120-240 km width (Shadwick et al. 2010). As a result, the upwelling in the CCS brings DIC rich water (~2200-2250 µmol kg^{-1}) from deep in the water column (below 150-200m) of the open ocean across the shelf break to the surface of the shelf (Feely et al. 2008). On the Scotian Shelf, it is only subsurface shelf water from between ~20-25 m depth that is being upwelled, which is at a similar temperature to the upwelled water in the CCS (7-8ºC) but at a much lower DIC concentration (2050 mmol C m^{-3}).

Our regional model shows that upwelling events could be a large contributor to setting the CO_2 signal in the summer on the inner portion of the Scotian Shelf, acting to lower pCO_2 here and slightly reducing outgassing compared to the outer shelf. Throughout the remainder of the year, the pCO_2 distribution across the Scotian Shelf is relatively uniform (Figure 3). Comparison of the inner and outer shelf pCO_2 (Figure 4) shows the similar seasonality that is seen across the shelf, both in the model results and Atlantic Condor observations. Additionally, the simulated annual air-sea CO_2 flux in bin 1 (upwelling bin, Figure 1) is +2.2 ± 0.2 mmol C m^{-2} yr^{-1} and similar to bin 2 (shelfbreak bin, Figure 1) where the annual flux is +2.0 ± 0.2 mmol C m^{-2} yr^{-1}. For comparison, the annual flux for the entire shelf flux is +1.7 ± 0.2 mmol C m^{-2} yr^{-1} and the flux at the CARIOCA buoy is 2.3 ± 0.1 mmol C m^{-2} yr^{-1}. Our results indicate that the short-term upwelling events in the summer do not significantly affect the shelfwide fluxes on an annual scale. Overall, the location of the CARIOCA buoy slightly overestimates shelfwide fluxes but is fairly representative of the shelf-wide pCO_2 dynamics overall.

According to the model, the Scotian Shelf acts as a net source of CO_2 to the atmosphere (+1.7 ± 0.2 mol C m^{-2} yr^{-1}), the Gulf of Maine is a net sink of CO_2 (-0.5 ± 0.2 mol C m^{-2} yr^{-1}) and the Grand Banks act as a net sink of CO_2 (-1.3 ± 0.3 mol C m^{-2} yr^{-1}). These results are in agreement with Shadwick et al. (2014) for the Scotian Shelf, and Laruelle et al. (2014, 2015)

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for the Gulf of Maine. Our results disagree, however, with results from other global (Laruelle et al. 2014) and regional studies (Laruelle et al. 2015; Signorini et al. 2013; Vandemark et al. 2011). The discrepancy in reported air-sea CO_2 flux between these studies is partly a result of how each study defines the area of the Scotian Shelf and Gulf of Maine. For example, Laruelle et al. (2015) calculates one estimate for both the Scotian Shelf and Gulf of Maine. The shelves of eastern North America are diverse, particularly in width and circulation features, and defining them as a single region is not representative. Additionally, the Scotian Shelf waters are strongly influenced by cold, carbon-rich Labrador Sea water, which is not the dominant endmember south of the Gulf of Maine (Loder et al. 1998, Rutherford & Fennel 2018; Fennel et al. 2019). Calculating a single flux estimate for the entirety of this dynamically diverse region is problematic and will yield a different estimate than when considering smaller and more specific regions. However, this only partially explains the difference in flux estimates.

Another reason is that the global SOCAT database was missing important regional data until recently. Signorini et al. (2013) used data from version 1.5 and Laruelle et al. (2014, 2015) used data from version 2.0 of the SOCAT database. Neither of the observational datasets used in the present study were included in SOCAT versions 1.5 and 2.0. Figure 10 illustrates the difference between different SOCAT versions for seasonal pCO_2 on the Scotian Shelf. SOCAT v2020 has consistently higher average pCO_2 values than v1.5 and v2, with at least double the number of years and a much larger number of observations going into each monthly average (on the order of 1000 to 10000 measurements in v2020 versus 100 to 1000 in v1.5 and v2). We believe that flux estimates using the updated SOCAT v2020 will agree better with our estimates and those of Shadwick et al. (2014).

In the present study, we have synthesized and compared our model simulations with high-resolution observations to highlight the dependence of Scotian Shelf pCO_2 seasonality on: (1) biological drawdown of DIC during the spring bloom, (2) temperature effects throughout the summer months, and (3) wind-driven coastal upwelling events. In Figure 2d, the temperature-normalized pCO_2 shows the non-thermal pCO_2 signal, which distinguishes the influence of biological and transport processes on pCO_2 (Takahashi et al. 2002). There is a clear decrease of pCO_2 associated with the spring bloom. The simulated decrease in pCO_2 is smaller than in the observations, likely due to the bloom occurring too early and over a more extended period in the model than the observations. In summer, temperature-normalized pCO_2 continues to decrease rather than follow the increasing temperature signal of non-normalized pCO_2. Previous studies have noted that, in summer, the thermodynamic signal in pCO_2 outweighs the influence of biological activity (Shadwick et al. 2011; Shadwick & Thomas 2014), which could explain the differences in seasonality between pCO_2 and temperature-normalized pCO_2 in the present study. We believe this thermodynamic influence is an important factor driving the net outgassing observed on the Scotian Shelf, particularly when combined with the delivery of DIC-rich water from the Labrador Sea.

Understanding what processes presently control CO_2 dynamics is important for projecting how the region will be affected by changes in climate. Previous studies have suggested that the frequency and intensity of coastal upwelling could increase (e.g., Xiu et al. 2018). In the case of the Scotian Shelf, increased upwelling would lead to less outgassing or even net ingassing during summer along the coast of Nova Scotia. Climate change could therefore disproportionately affect the nearshore region here and lead to an intensification of spatial gradients. Such an upwelling signal would be in addition to the

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Formatted: Indent: First line: 1.27 cm effect of increasing atmospheric CO_2, which may be driving the entire Scotian Shelf towards a more neutral system with less outgassing. The effect of the thermal control on Scotian Shelf pCO_2 is also an important aspect to consider. As temperatures continue to rise, summer pCO_2 values will also likely increase, potentially offsetting some of the effect of increased atmospheric CO_2 but also affecting production and respiration rates. Of course, none of these factors act independently and will instead combine to alter both the seasonal and spatial patterns of pCO_2 in the region, making the overall outcome of climate-related perturbations on the Scotian Shelf difficult to predict. However, the implementation of a regional model that resolves current conditions well, as in the present study, is an important step towards projecting future climate-related changes in the region.

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6 Conclusions

In this study, we have validated surface pCO_2 fields on a seasonal scale from a medium-complexity regional biogeochemical model for the northwest North Atlantic shelf region against pCO_2 observations from a CARIOCA buoy and repeated cross-shelf transects from a ship of opportunity that crosses the Scotian Shelf. Except for the strength and speed of the pCO_2 drawdown associated with the spring bloom, the model simulations represent the observed spatial and temporal variability of pCO_2 on the Scotian Shelf well. Contrary to most coastal upwelling systems, upwelling events in summer are acting to lower pCO_2 within ~25 km of the coastline, as cold, carbon-enriched intermediate layer water is brought to the surface. The lowering of surface pCO_2 during these events occurs because the temperature effect leading to a lowering of pCO_2 overwhelms the increase in pCO_2 associated with DIC enrichment. We found pCO_2 to be relatively uniform across the shelf, with the exception of a narrow band near shore impacted by summer upwelling events. Overall, the Scotian Shelf acts as a net source of CO_2 (+1.7 ± 0.2 mol C m^{-2} yr^{-1}), the Gulf of Maine is a net sink of CO_2 (-0.5 ± 0.2 mol C m^{-2} yr^{-1}) and Grand Banks acts as a net sink of CO_2 (-1.3 ± 0.3 mol C m^{-2} yr^{-1}) in our simulation. Combination of the model simulation and the highly resolved observational data sets emphasizes that the seasonal cycle of pCO_2 is driven by strong biological drawdown of DIC in early spring and a dominant thermal control throughout the summer months. Except for the short spring bloom period, surface pCO_2 is oversaturated with respect to atmospheric values, which results in net outgassing. Ongoing changes in climate and carbon cycling will likely alter both the seasonal and spatial patterns of pCO_2 on the Scotian Shelf.

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Acknowledgements

We acknowledge funding by the Marine Environmental Observation, Prediction and Response Network (MEOPAR). This work was additionally funded in part by the Canada Excellence Research Chair (CERC) in Ocean Science and Technology at Dalhousie University and Canada Foundation for Innovation (CFI) project number 29011. We would like to thank the captain and crew of Atlantic Condor for their continuing support in operating the Dal-SOOP underway system. Mike Vining, Jeremy Lai, Dan Kehoe, Kitty Kam and Jordan Sawler contributed to the design, installation and maintenance of the underway system.

We also are grateful for the use of observational datasets to initialize our model from Kumiko Azetsu-Scott (Department of Fisheries and Oceans Canada) and Alfonso Mucci (McGill University). We would also like to acknowledge the use of the scientific colourmaps lapaz, vikO, and batlow (Crameri 2018) used in this study.

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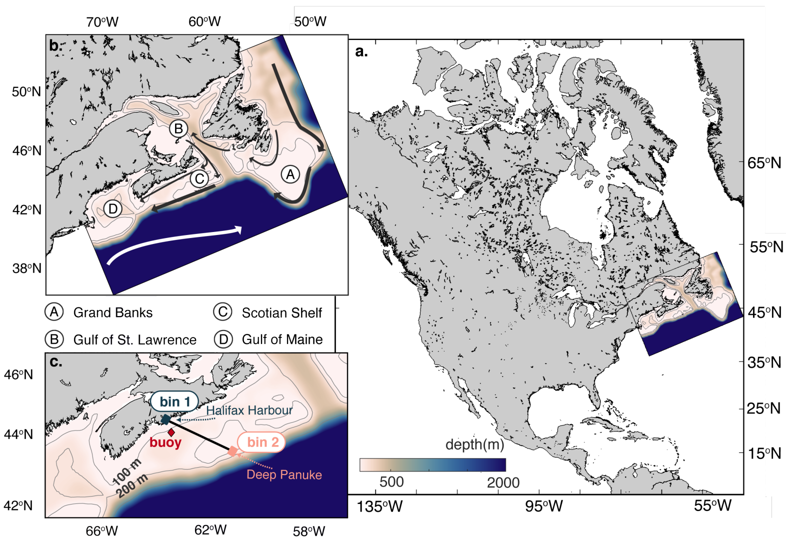

Figure 1: Bathymetric maps of the model domain. (a) Map of North America, including the location of the model domain. (b) A zoomed in map of the model domain with mean current locations. (c) Zoomed in map of the Scotian Shelf, and indicates the location of the CARIOCA buoy (red diamond) and the Atlantic Condor Transect (black line). Bin 1 (Halifax Harbour) and bin 2 (Deep Panuke) are used for analyses of spatial variability. All maps show the 100 m and 200 m isobaths.

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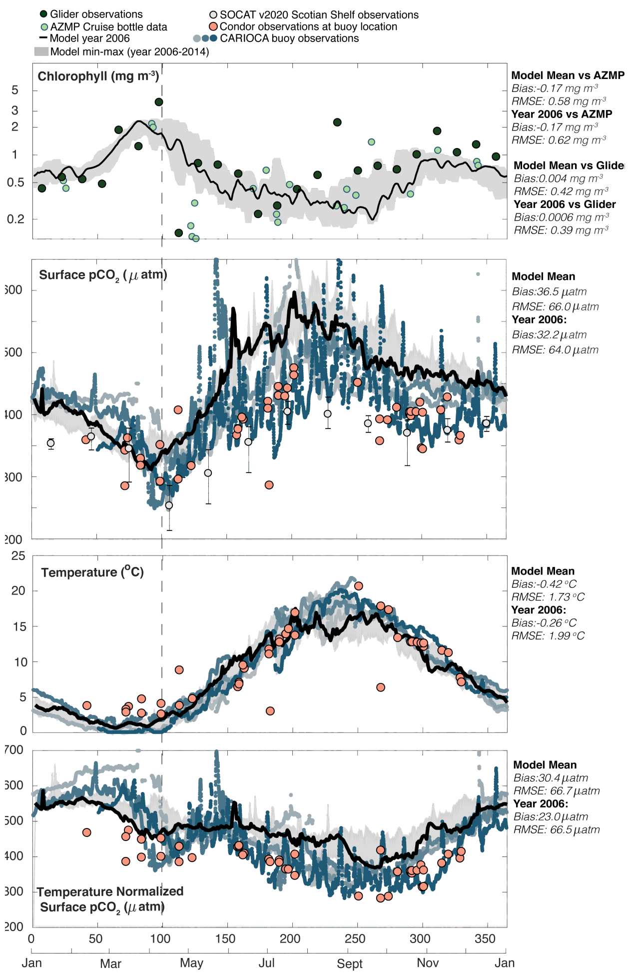

Figure 2: Seasonal (from top to bottom, with RMSE and bias in references to year 2006) (a) chlorophyll (Glider: RMSE: 0.39 mg m^{-3}, bias: 0.0006 mg m^{-3}; AZMP: RMSE: 0.62 mg m^{-3}, bias: -0.17 mg m^{-3}); (b) pCO$_2$ (RMSE: 64.0 µatm, bias: 32.2 µatm); (c) temperature (RMSE: 1.99 °C, bias: -0.26 °C); (d) temperature normalized pCO$_2$ following Takahashi et al. (2002) (RMSE: 66.5 µatm, bias: 23.0 µatm) at STN 2 on the Scotian Shelf. The model year 2006 is shown with the thick black line and min-max in the model from years 2006-2014 with the grey shaded area in all panels. In (a) the dark green points are AZMP bottle data and light

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green points are glider data. In (b-d) observations from the moored CARIOCA buoy are shown as small blue points, with lighter shades of blue indicating earlier observations and darker shades indicating more recent observations, and observations from the Atlantic Condor transects at approximately the same location as the buoy are shown in large pink points. Both the Condor and CARIOCA buoy observations are mapped to year 2006 using the atmospheric trend in *p*CO_2. Light grey points are monthly mean SOCAT observations for the entire Scotian Shelf and the error bars are the 10th and 90th percentiles.

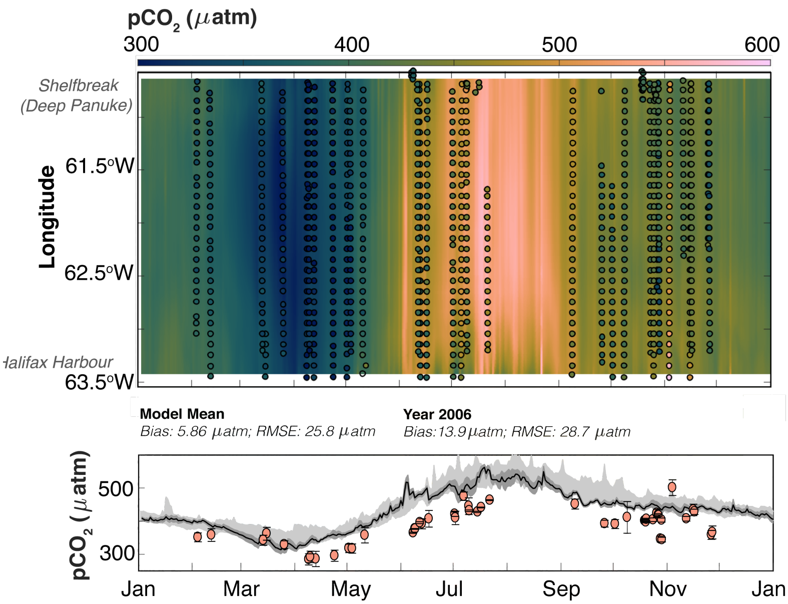

Figure 3: Model-data comparison along the Atlantic Condor transect. The top panel shows *p*CO_2 (in colour) evolving over time (x-axis) along the transect (longitude on the y-axis; Halifax Harbour to Shelfbreak). The background is the model average *p*CO_2 along the transect and the points are the Atlantic Condor data binned into 0.1° longitudinal bins. The bottom panel shows the average *p*CO_2 along the transect (y-axis) as it evolves over the seasonal cycle (x-axis). The line is year 2006 from the model averaged across the transect, the dark grey shaded area is the standard deviation, and the light grey shaded area is the min-max *p*CO_2 along the transect from 2006-2014. The points are the average and the error bars are standard deviation of observational *p*CO_2 across each transect. The Condor observations are mapped to year 2006 in both panels using the atmospheric trend in *p*CO_2. *RMSE: 28.7 µatm; Bias: 13.9 µatm*

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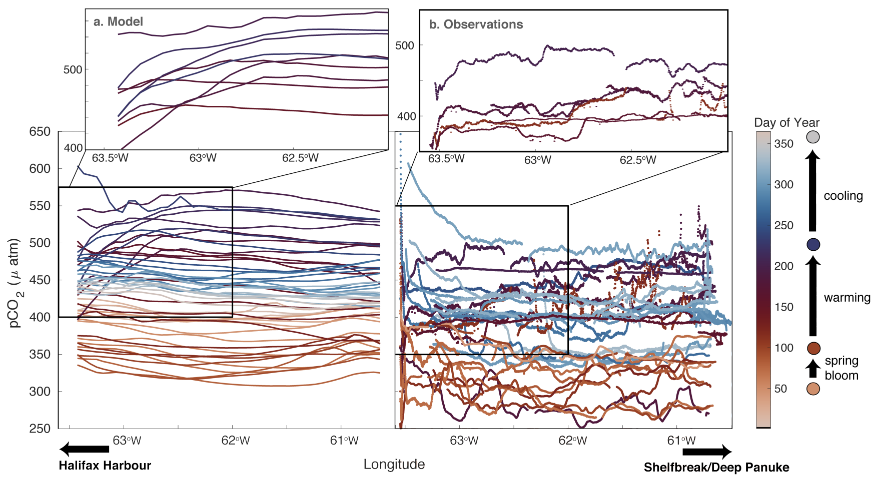

Figure 4: Temporal evolution of pCO_2 across the Atlantic Condor transect. X-axis is longitude, with the Halifax Harbour indicated on the left-hand side and the Shelfbreak indicated on the right-hand side of each panel; Y-axis is pCO_2; and the colour indicates the day of the year. The left panel is year 2006 of the model along the transect every 7 days. The right panel are all of the observations along the transect. The upper insets zoom in on the indicated boxes showing only the events with lower pCO_2 nearshore in the summer months (dark red/purple cololoured lines).

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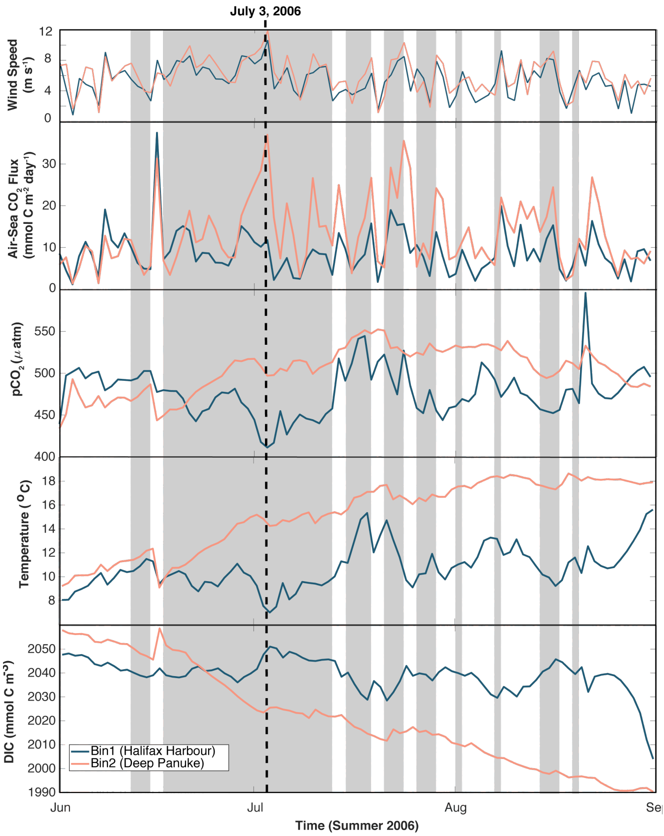

Figure 5: Timeseries of variables in two bins along the Condor Transect (see Figure 1) during summer 2006. From top to bottom: (a) wind speed, (b) air-sea CO_2 flux, (c) *p*CO_2, (d) temperature and (e) dissolved inorganic carbon (DIC). Shaded area indicates when there was upwelling-favourable winds nearshore (Bin 1). The blue lines indicate the values from the nearshore bin closest to the Halifax Harbour and the pink lines indicate values from the offshore bin near the Deep Panuke oil platform.

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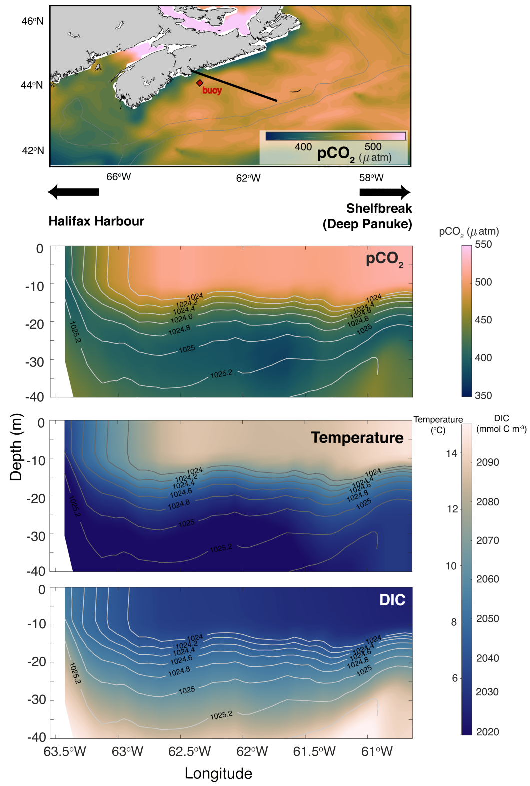

Figure 6: Surface map of pCO$_2$ (top panel), and transects along the average Atlantic Condor ship track of (top to bottom) pCO$_2$, temperature, and dissolved inorganic carbon (DIC) from the model taken during an upwelling event (Jul 3, 2006; see Figure 5). Contours in the transects are density. The top panel indicates the Condor transect with the black line and the location of the CARIOCA buoy with the red diamond.

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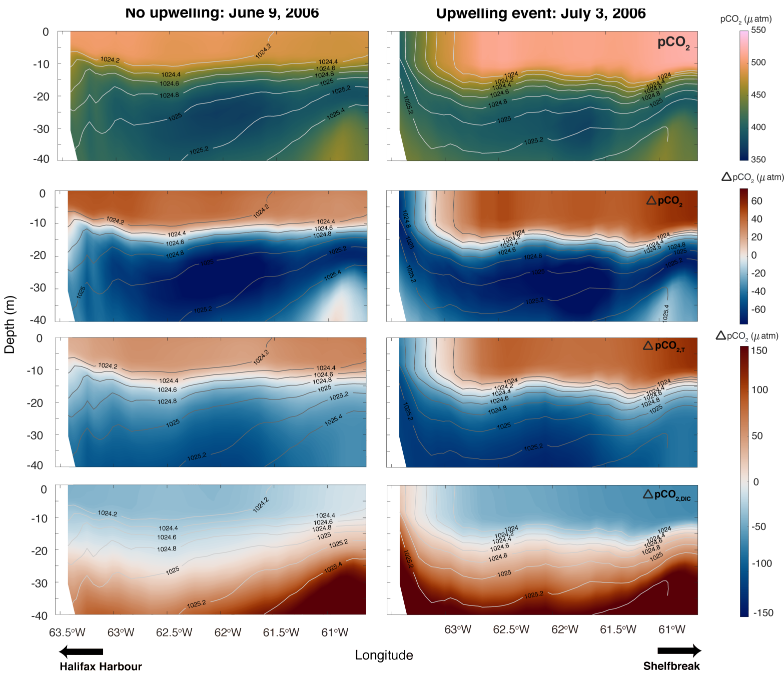

Figure 7: Taylor Decomposition of the upwelling event (right side; July 3, 2006) in Figure 6 compared to a non-upwelling event (left side; June 9, 2006). From top to bottom: (a) pCO_2, (b) overall anomaly in pCO_2 (ΔpCO_2) from the mean pCO_2 in the upper 40 m, (c) anomaly in pCO_2 due to temperature changes ($\Delta pCO_{2,T}$), (d) anomaly in pCO_2 due to DIC changes ($\Delta pCO_{2,DIC}$).

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Figure 7: Taylor Decomposition of upwelling event.¶

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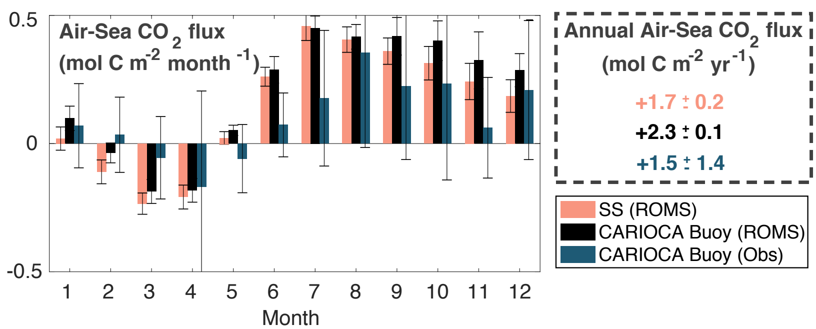

Figure 8: Monthly and annual air-sea CO_2 flux calculated from the model on the entire Scotian Shelf (pink), extracted at the CARIOCA buoy location (black), and from the buoy observations (blue). Flux is averaged over simulation years 2006-2014 for the model, and years 2007-2014 for the CARIOCA observations. Error bars are +/- 1 standard deviations between years.

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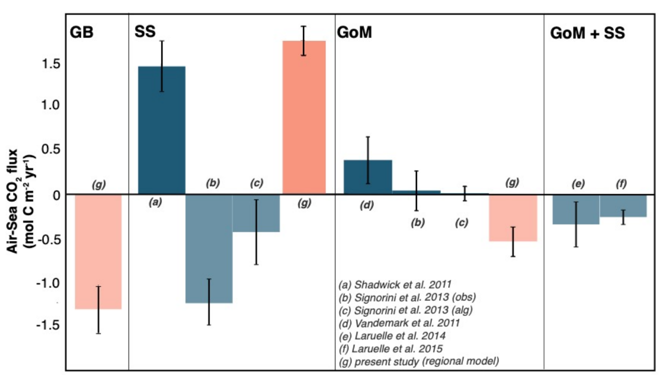

Figure 9: Annually integrated air-sea CO_2 flux for the Grand Banks (GB), Scotian Shelf (SS) and Gulf of Maine (GoM) in the model (pink) compared to literature values (blue). Positive values are net outgassing, indicated by solid bars, and negative values are net ingassing, indicated by faded bars.

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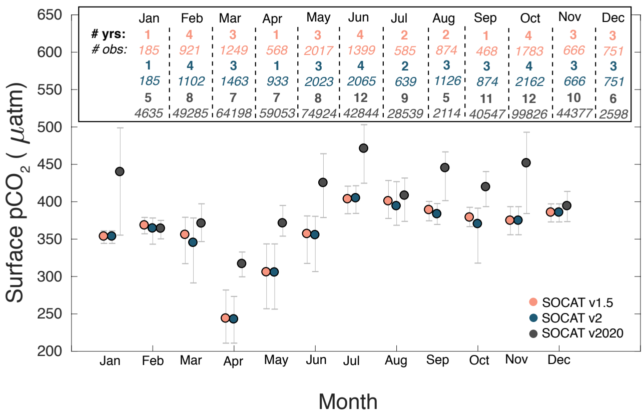

Figure 10: Comparison of the seasonal cycle of pCO_2 for the different versions of SOCAT for the Scotian Shelf, mapped to year 2006. The points indicate the mean for each month and the bars indicate the 5th and 95th percentile. Inset shows the number of years and number of observations used in each month for each version.

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