Supplement of Biogeosciences, 18, 6271–6286, 2021
https://doi.org/10.5194/bg-18-6271-2021-supplement
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Supplement of

A modelling study of temporal and spatial $p$CO$_2$ variability on the biologically active and temperature-dominated Scotian Shelf

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S0. Introduction

The following supplementary information is divided into six parts.

S1 includes a table outlining the location (latitude, longitude) and year/month of sampling of the observational datasets used.

S2 includes details about the long-term trend in atmospheric $pCO_2$ and the regression used in ROMS.

S3 includes figures comparing the seasonal cycle of $pCO_2$ in each year of the model simulation at different locations in the model.

S4 includes model validation of Dissolved Inorganic Carbon (DIC) and Total Alkalinity (TA).

S5 includes further comparison of $pCO_2$ and temperature in the Halifax Harbour bin versus the Deep Panuke/Shelfbreak bin along the Atlantic Condor transect.

S6 includes further figures describing the upwelling event of July 3, 2006 in the model.

S1. Observational Datasets

Table S1 indicates the location (latitude, longitude) and years/months of sampling of $pCO_2$ at the CARIODCA buoy and from the Atlantic Condor Transect.

Table S1: Summary of observational datasets, including latitude, longitude location and month/year of sampling.

<table>
<thead>
<tr>
<th>Observational Dataset</th>
<th>Location</th>
<th>Year &amp; month of sampling</th>
</tr>
</thead>
<tbody>
<tr>
<td>CARIODCA Buoy</td>
<td>44.3°N, 63.3°W</td>
<td>2007: May, Jun, July, Aug, Sept, Oct</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2008: Jan, Feb, Mar, Apr, May, Jul, Aug, Sept, Oct, Dec</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2009: Sept, Oct, Nov, Dec</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2010: Jan, Apr, May, Jun, Jul, Aug, Sept</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2011: Jul, Aug, Sept, Oct, Nov, Dec</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2012: Jan, Feb, Mar, Apr, May</td>
</tr>
<tr>
<td>Atlantic Condor Transect</td>
<td>43.8°N, 60.6°W to 44.6°N, 63.5°W</td>
<td>2018: Feb, Mar, Apr, May, Jun, Jul, Sept, Oct, Nov</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2019: Jun, Jul, Oct, Nov</td>
</tr>
</tbody>
</table>
S2. Atmospheric $pCO_2$

Figure S1 illustrates the secular and seasonal cycle in atmospheric $pCO_2$. The black points are observations taken at Sable Island and the red line is the regression used in ROMS:

\[
pCO_{2,\text{atm}} = 273.9904 + 1.9738 \cdot t + 5.3132 \cdot \cos 2\pi t + 4.0601 \cdot \sin 2\pi t \\
- 0.5814 \cdot \cos 4\pi t - 2.1740 \cdot \sin 4\pi t - 0.5009 \cos 6\pi t \\
+ 0.5904 \cdot \sin 6\pi t
\]

where \( t = \text{year} - 1951 + \text{yearday}/365 \).

The blue dashed line is the long term linear fit of \( \sim +2 \mu\text{atm yr}^{-1} \) used to map model years and observations onto the same year for comparison.

Figure S1: Atmospheric $pCO_2$ observations (black points) taken on the Scotian Shelf and fit to a regression (red line) used in ROMS and a linear long term fit (blue dashed line) for mapping surface ocean $pCO_2$ onto the same year.

S3. Interannual variability of surface water $pCO_2$

Figures S2 – S5 illustrate $pCO_2$ at the CARIOCA buoy, and averaged on the Scotian Shelf, Grand Banks and Gulf of Maine, respectively, throughout the model simulation (excluding the spin-up year). Each panel in these figures compares year 2000 to each subsequent year in the model simulation. Years 2001-2014 are mapped to year 2000 using the linear atmospheric trend \( \sim 2 \mu\text{atm yr}^{-1} \) to eliminate the long term trend in $pCO_2$. 
Figure S2: Surface pCO$_2$ at the CARIOCA buoy (see Figure 1) comparing year 2000 with each subsequent year. Years 2001 to 2014 were mapped onto year 2000 using the longterm linear trend in atmospheric pCO$_2$.

Figure S3: Surface pCO$_2$ averaged over the Scotian Shelf comparing year 2000 with each subsequent year. Years 2001 to 2014 were mapped onto year 2000 using the longterm linear trend in atmospheric pCO$_2$. 
Figure S4: Surface $pCO_2$ averaged over the Grand Banks comparing year 2000 with each subsequent year. Years 2001 to 2014 were mapped onto year 2000 using the longterm linear trend in atmospheric $pCO_2$.

Figure S5: Surface $pCO_2$ averaged over the Gulf of Maine comparing year 2000 with each subsequent year. Years 2001 to 2014 were mapped onto year 2000 using the longterm linear trend in atmospheric $pCO_2$.

S4. Model Validation

Figure S7 compares the model (year 2006) to DFO’s AZMP cruise data (see Methods) at the CARIOCA buoy (location indicated in Figure 1, Table S1 and Figure S6). In Dissolved Inorganic Carbon (DIC), there is a similar model-observation comparison as in
$pCO_2$. Mainly, during the bloom (April), surface DIC is overestimated in the model, indicating that the model does not quite capture the magnitude of the bloom and therefore does not capture the magnitude of the associated DIC drawdown. There is subsequently overestimation throughout the year in the model in the surface waters, similar to $pCO_2$ and likely as a result of the low bloom-related drawdown. In total alkalinity (TA), there is relatively good agreement with some overestimation later in the year, mainly in the surface waters. Figure S8 shows further comparison of the model to AZMP cruise data along the Halifax Line (see Figure S6 for location) for different months. There is relatively good qualitative agreement between the model and observations.

Figure 6: Map of the Scotian Shelf with 100 m and 200 m isobaths. The Halifax Line (HAL; from AZMP cruises) is indicated by the black line and the CARIOCA buoy (Station 2 along the Halifax Line) is indicated by the red diamond.

Figure S7: Dissolved Inorganic Carbon (DIC; top panel) and Alkalinity (bottom panel) at the CARIOCA Buoy (Station 2 in the Halifax Line, for location see Figure 1 and Figure S6). Background colour is year 2006 of model simulation. Points are averaged DIC and TA at each depth for each available month from the AZMP cruises.
Figure S8: Dissolved Inorganic Carbon (DIC) and Total Alkalinity (TA) at the CARIOCA Buoy along the Halifax Line (HAL; for location see Figure S6) for (A) April, (B) May, (C) June, and (D) September. Background colour is monthly average DIC or TA for year 2006 of model simulation. Points are averaged DIC and TA at each depth for each available month from the AZMP cruises.

S5. Condor Transect pCO$_2$

Figure S9 shows the full seasonal cycle of $p$CO$_2$ in two bins along the Atlantic Condor transect, both in the model and in the observations (panel a). Panels b through d illustrate the differences in $p$CO$_2$ and panels e through g illustrate temperature in the two bins during three time slices (A-C).
Figure S9: Panel (a) indicates the full seasonal cycle of surface $pCO_2$ in two bins along the Atlantic Condor transect: Halifax Harbour bin (blue) and Deep Panuke/Shelfbreak bin (pink). See figure 1 for the bin locations. Panels (b-d) indicate $pCO_2$ in these bins at three different time slices (A, B and C) which are indicated in panel (a). Panels (e-g) indicate temperature in these bins at the same time slices. The lines indicate the model year 2006 and the points indicate the Atlantic Condor observations.

S6. Upwelling transects
Figure S10 shows additional variables along the Condor transect during the July 3, 2006 upwelling event in addition to the variables in Figure 6 in the main text.

Figure S10: Additional variables along the Atlantic Condor transect during the July 3, 2006 upwelling event. Left panels include (top to bottom): $pCO_2$, temperature and dissolved inorganic carbon (DIC). Right panels include (top to bottom): chlorophyll, salinity, alkalinity. Contours on each panel indicate density. See Figure 1 for the location of the Atlantic Condor transect.

Figure S11 illustrates the complete Taylor decomposition from Figure 7, including the effects of alkalinity ($\Delta pCO_{2,T,A}$) and salinity ($\Delta pCO_{2,S}$).
Figure S11: The full Taylor decomposition of June 9, 2006 (left) versus July 3, 2006 (right). From top to bottom: (a) $p\text{CO}_2$, (b) overall anomaly in $p\text{CO}_2$ ($\Delta p\text{CO}_2$) from the mean $p\text{CO}_2$ in the upper 40 m, (c) anomaly in $p\text{CO}_2$ due to temperature changes ($\Delta p\text{CO}_2,T$), (d) anomaly in $p\text{CO}_2$ due to DIC changes ($\Delta p\text{CO}_2,\text{DIC}$), (e) anomaly in $p\text{CO}_2$ due to alkalinity changes ($\Delta p\text{CO}_2,\text{TA}$), and (f) anomaly in $p\text{CO}_2$ due to salinity changes ($\Delta p\text{CO}_2,S$).