Version 2020. Release August 26 , 2020

**Gridded surface water fugacity of CO2 observations, and calculated pH, aragonite saturation state and air–sea CO2 ﬂuxes in the northern Caribbean Sea from 2002 through 2019.**

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**Summary**

Here we provide an update of gridded surface water fugacity of CO2, fCO2w, observations and calculated inorganic carbon parameters in the northern Caribbean Sea (15˚ N to 28˚ N, and 62˚ W to 88˚ W) by adding data from January 2019 through December 2019. The data products are derived from observations made on Royal Caribbean International (RCI) ships. The *Allure of the Seas* (*ALoS*), International Council for the Exploration of the Sea (ICES) ship code BHAF, completed 46 cruises, and the *Equinox* (*Eqnx*), ICES ship code MLCE, did 41 cruises in the northern Caribbean area. For 2019 there were a total of 198,396 observations.

The dataset and derived quantities are binned and averaged on a 1◦ monthly grid and are available at NCEI at http://accession.nodc.noaa.gov/0207749 and fully described in Wanninkhof et al. (2020). The derived quantities include total alkalinity (TA), acidity (pH), aragonite saturation state (Ar) and air–sea CO2 ﬂux and cover the region from 15◦ to 28◦ N and 88˚ to 62◦ W. Methodologies to derive the TA, pH and Ar and to calculate the ﬂuxes from fCO2w, temperature and salinity are described in Wanninkhof et al. (2020), and interpretation of data from 2002 through 2018 is presented in Wanninkhof et al. (2019).

**Data package**

This package contains 5 files covering the time period from January 1, 2002 through December 30, 2019. The data product through 2018 are available at: (<https://doi.org/10.25921/2swk-9w56>).

The current files extend the products by one year and provide uniform areal coverage from 15˚ N to 28˚ N, and 62◦ W to 88˚ W for the whole time period. The previous dataset had slight inconsistencies in coverage and land blanking of the mapped products. As in the previous data products all data are presented on 1˚ grids and monthly times.

**Data files**

A.Multi linear regression (MLR) coefficients. File name: **Summary\_MLR\_coefficients\_2002-2019.xlsx**. The MLR from 2002 – 2018 are unchanged from Table 1 in Wanninkhof et al. 2020. The coefficients and their uncertainty (1-sigma) for 2019 are added to the file. The MLRs are based on regressions of fugacity of CO2 in seawater on a 1˚ by 1˚ by month grid against longitude, latitude, sea surface temperature SST, mixed layer depth (MLD), and sea surface salinity (SSS). Mixed layer depth is from the output of the HYCOM model. The MLR coefficients for 2019 are based on 1056 grid cells and give a correlation coefficient, r2 of 0.92 and a root mean square error in fCO2w of 5 µatm.

Column headers and description1:

|  |  |  |
| --- | --- | --- |
| Coefficient2 | Independent parameter | Description |
|  a | (LON) | Longitude, ˚E. Note: western longitude will be negative. |
| b | (LAT) | Latitude, ˚N. |
|  c | (SST) | Sea surface temperature, ˚C. To create the MLR, in situ SST is used; to apply it, the OISST is used.  |
| d | (MLD) | Mixed layer depth, m from the HYCOM model. |
| e | (SSS) | Sea surface salinity, permil. To create the MLR, in situ SSS is used; to apply it, SSSHYCOM is used |
| f | (Icept) | Intercept |
| Standard error fCO2w,MLR |  | Standard error of the calculated fCO2w in µatm. |
| r2 |  | Correlation coefficient |
| #points |  | Number of grid points used to create the MLR (data average 1˚ by 1˚ by mo).  |

1: These annual regressions were used to create the mapped fCO2wMLR fields using the 1˚ by 1˚ by month gridded data product. The second row of the entires (in italics) for each annual entry is the error of the coefficient.

2: fCO2wMLR = a Longitude + b Latitude + c OISST + d MLDHYCOM + e SSSHYCOM + f

B. All gridded data from 2002-2019. File name: **Gridded\_Observations\_2002-2019.xlsx**

 The 2019 data is appended to the 2002-2018 data set. For 2019, the 198,396 observations of fCO2w, SST, and SSS were binned and averaged in 1˚ by 1˚ by month grid with a total of 1056 grid cells. The quality controlled original data can be found at https://www.aoml.noaa.gov/ocd/ocdweb/occ.html and at NCEI: https://www.nodc.noaa.gov/ocads/oceans/VOS\_Program/explorer.html. It is also ingested in SOCAT v.2020 (<https://www.socat.info/index.php/data-access/>).

 The column headers and brief explanation (if necessary):

|  |  |  |
| --- | --- | --- |
| Parameter | Unit | Description |
| Year |  |  |
| Month |  | 1 (January) through 12 (December) |
| Latitude (Lat) | Degrees | North is positive. Location is the center point of the grid cell. That is, 15.5˚ N is the grid box spanning 15˚ N to 16˚ N |
| Longitude (Lon) | Degrees | East is positive. All values in the Caribbean are negative. Location is center point of the grid cell. That is, -87.5 is the grid box spanning 87˚ W to 88˚ W. |
| Area | Km2 | Area of grid box excluding land where appropriate |
| #\_Obs |  | Number of fCO2w observations in the particular grid box for the particular month. |
| SST\_OBS | ˚C | Sea surface temperature measured at the intake (average of the grid box) |
| SST\_STDEV | ˚C | Standard deviation of SST. |
| SSS\_OBS | permil | Sea surface salinity measured by thermosalinograph (average of the grid box). |
| SSS\_STDEV | permil | Standard deviation of SSS |
| fCO2w\_OBS | µatm | Fugacity of CO2 in seawater (average of the grid box). |
| fCO2w\_STDEV | µatm | Standard deviation of fCO2w observations in the grid box |
| TA | µmol kg-1 | Total alkalinity calculated from a relationship salinity TA = 57.3 SSS\_OBS+ 296.4 (Cai et al., 2010) using the measured SSS |
| pHT |  | pH on the total scale at SST calculated from fCO2w\_OBS and TA using the CO2SYS program of Pierrot et al. (2006) with pH Scale: Total scale (mol/kg-SW) at OISST; CO2 Constants: K1, K2 from Lueker et al. (2000); KSO4- for Dickson (1990); KF from Perez and Fraga (1987) and Total Boron from Uppström (1974). |
| ΩAr |  | Aragonite saturation state calculated using CO2SYS with fCO2w\_OBS and TA as input parameters and the same dissociation constants as used for pHT. |
| OISST | ˚C | Optimal interpolated sea surface temperature (Reynolds et al., 2007) for the particular grid box. |
| SSSHYCOM | permil | Sea surface salinity from the HYCOM model.  |
| fCO2wMLR | µatm | Fugacity of CO2 in seawater determined from annual MLRs (see Table 1) with Lat, Lon, SST, OISST, SSSHYCOM, and MLDHYCOM.  |

C. Mapped products for 15˚ N to 28˚ N, and 62˚ W to 88˚ W from 2002-2019. File name: **Mapped**

 **product\_2002-2019.xlsx**. The column headers and brief explanation (if necessary):

|  |  |  |
| --- | --- | --- |
| Parameter | Unit | Description |
| Year |  |  |
| Month |  | 1 (January) through 12 (December) |
| Latitude (Lat) | Degrees | North is positive. Location is center point of the grid cell. For example, 15.5˚ N is the grid box spanning 15˚ N to 16˚ N. |
| Longitude (Lon) | Degrees | East is positive. All values in Caribbean are negative. Location is center point of the grid cell. For example, -87.5 is the grid box spanning 87˚ W to 88˚ W. |
| Area | Km2 | Area of grid box excluding land where appropriate. |
| OISST | ˚C | Optimal interpolated sea surface temperature (Reynolds et al., 2007). |
| SSSHYCOM | permil | Sea surface salinity Sea surface salinity from the HYCOM model. |
| MLDHYCOM | m | Mixed layer depth from the HYCOM model.  |
| fCO2wMLR | µatm | Fugacity of CO2 in seawater determined from annual MLRs with Lat, Lon, OISST, SSSHYCOM, and MLDHYCOM. |
| fCO2a | µatm | Fugacity of CO2 in air using the average value between atmospheric sampling station KEY and RBP. |
| ∆fCO2 | µatm | Air-water fugacity difference, fCO2w -fCO2a. |
| TA | µmol kg-1 | Total alkalinity calculated from a relationship salinity TA = 57.3SSSHYCOM+ 296.4 (Cai et al., 2010).  |
| pHT |  | pH calculated from fCO2w and TA with the CO2SYS program of Pierrot et al. (2006) with pH Scale: Total scale (mol/kg-SW) at OISST; CO2 Constants: K1, K2 from Lueker et al. (2000); KSO4- for Dickson (1990); KF from Perez and Fraga (1987) and Total Boron from Uppström (1974). |
| ΩAr |  | Aragonite saturation state calculated using CO2SYS with fCO2wMLR, TA, OISST, and SSSHYCOM as input parameters with same dissociation constants as used for pHT. |
| <u2> | m2 s-2 | Second moment of the wind based on ¼˚ 6-h CCMP-2 product (Atlas et al., 2011). |
| CO2\_Flux | mol m-2 yr-1 | Monthly air-sea CO2 flux calculated according to Eqs. 5 and 6, with fCO2wMLR @ OISST. |

D. Monthly averages for the whole region for 15˚ N to 28˚ N, and 62˚ W to 88˚ W from 2002-2019. File name: **Monthly\_ave\_weighted\_whole\_region\_2002-2019.xlsx.** The results are area weighted to take into account the different size of the 1˚ by 1˚ pixels due to curvature of earth and land coverage. The column headers and brief explanation (if necessary) :

|  |  |  |
| --- | --- | --- |
| Parameter | Unit | Description |
| Year |  |  |
| Month |  | 1 (January) through 12 (December) |
| Area | km2 | Total area of Caribbean region excluding land (15˚ N to 28˚ N and 62˚ W to 88˚ W). |
| OISST | ˚C | Optimal interpolated sea surface temperature (Reynolds et al., 2007) |
| SSSHYCOM  | permil | Sea surface salinity from the HYCOM model.  |
| MLDHYCOM | m | Mixed layer depth from the HYCOM model . |
| fCO2wMLR | µatm | Fugacity of CO2 in seawater determined from annual MLRs with Lat, Lon, SST, SSS, and MLD (see Table 1). |
| fCO2a | µatm | Fugacity of CO2 in air using the average value between atmospheric sampling station KEY and RBP . |
| ∆fCO2 | µatm | Air-water fugacity difference, fCO2w -fCO2a |
| TA | µmol kg-1 | Total alkalinity calculated from a relationship salinity TA = 57.3SSSHYCOM+ 296.4 (Cai et al., 2010). |
| pHT |  | pH calculated from fCO2w and TA with the CO2SYS program of Pierrot et al. (2006) with pH Scale: Total scale at OISST; CO2 Constants: K1, K2 from Lueker et al. (2000); KSO4- for Dickson (1990); KF from Perez and Fraga (1987) and Total Boron from Uppström (1974). |
| ΩAr |  | Aragonite saturation state calculated using CO2SYS with fCO2wMLR, TA, OISST, and SSSHYCOM as input parameters with same dissociation constants as used for pHT. |
| <u2> | m2 s-2 | Second moment of the wind based on ¼˚ 6-h CCMP-2 product (Atlas et al., 2011). |
| CO2\_Flux | mol m-2 mo-1 | Monthly air-sea CO2 flux calculated according to Eqs. 5 and 6. |
| CO2\_FluxTotal | Tg C mo-1 | Total monthly air-sea CO2 flux calculated according to Eqs. 5 and 6 in Teragram of carbon.  |

E. Annual averages 15˚ N to 28˚ N, and 62˚ W to 88˚ W from 2002-2020. The results are based on the monthly averages. File name: **Annual\_ave\_weighted\_whole\_region\_2002-2019.xlsx**. The Column headers for the annual averaged mapped product are:

|  |  |  |
| --- | --- | --- |
| Year |  |  |
| Area | km2 | Total area of Caribbean region, excluding land, from 15˚ N to 28˚ N and 62˚ W to 88˚ W. |
| OISST | ˚C | Optimal interpolated sea surface temperature (Reynolds et al., 2007). |
| SSSHYCOM  | permil | Sea surface salinity from the HYCOM model.  |
| MLDHYCOM | m | Mixed layer depth from the HYCOM model. |
| Area | Km2 | Area of grid box excluding the surface area of land where appropriate. |
| fCO2wMLR | µatm | Fugacity of CO2 in seawater determined from annual MLRs with Lat, Lon, SST, SSS, and MLD (see Table 1). |
| fCO2a | µatm | Fugacity of CO2 in air using the average value between atmospheric sampling station KEY and RBP. |
| ∆fCO2 | µatm | Air water fugacity difference, fCO2w -fCO2a |
| TA | µmol kg-1 | Total alkalinity calculated from a relationship salinity TA = 57.3SSSHYCOM+ 296.4 (Cai et al., 2010). |
| pHT |  | pH calculated from fCO2w and TA with the CO2SYS program of Pierrot et al. (2006) with pH Scale: Total scale at OISST; CO2 Constants: K1, K2 from Lueker et al. (2000); KSO4- for Dickson (1990); KF from Perez and Fraga (1987) and Total Boron from Uppström (1974).  |
| ΩAr |  | Aragonite saturation state calculated using CO2SYS with fCO2wMLR, TA, OISST, and SSSHYCOM as input parameters with same dissociation constants as used for pHT. |
| <u2> | m2 s-2 | Second moment of the wind based on ¼˚ 6-h CCMP-2 product (Atlas et al., 2011). |
| CO2\_Flux | mol m-2 yr-1 | Annual air-sea CO2 flux calculated according to Eqs. 5 and 6. |
| CO2\_FluxTotal | Tg C y-1 | Total annual air-sea CO2 flux calculated according to Eqs. 5 and 6 in Teragram of carbon. |

**References**

Wanninkhof, R., Pierrot, D., Sullivan, K., Barbero, L., & Triñanes, J. (2020). A 17-year dataset of surface water fugacity of CO2 along with calculated pH, aragonite saturation state and air–sea CO2 fluxes in the northern Caribbean Sea. *Earth Syst. Sci. Data, 12*(3), 1489-1509. <https://essd.copernicus.org/articles/12/1489/2020/>

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