Computed (from pH) surface partial pressure and air-water flux of carbon dioxide in the mainstem Chesapeake Bay from 1998 to 2018

Website: https://www.bco-dmo.org/dataset/887398
Data Type: model results
Version: 1
Version Date: 2023-02-17

Project
» Collaborative Research: Multiple Stressors in the Estuarine Environment: What drives changes in the Carbon Dioxide system? (Estuarine Stressors)

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Abstract
The data products are calculated partial pressure and air-sea flux of carbon dioxide in the main stem of Chesapeake Bay from 1998 to 2018 and include all the inputs to the calculation as well.

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Coverage

Spatial Extent: **N**:40 **E**:-75 **S**:36 **W**:-78
Temporal Extent: 1998 - 2018

Dataset Description

This research was supported with funding from the National Science Foundation's Chemical Oceanography

Program (OCE-1536996 and OCE-1537013). Additional support was provided by NASA through Grants NNX14AM37G and NNX14AF93G.

The data products are calculated partial pressure and air-sea flux of carbon dioxide in the main stem of Chesapeake Bay; the dataset also includes all the inputs to the calculation.

The data were derived from the Chesapeake Bay program's Water Quality Database, United States Geological Survey monitoring data, North American Regional Reanalysis, World Data Centre for Greenhouse Gases, and 2016-2018 carbonate system measurements the Chesapeake (Shadwick et al., 2019). See Related Datasets section.

The data are in the form of seven netCDF files:

1. results-pco2-gasex.nc: calculated monthly pCO_2 and air-sea CO_2 flux in the Chesapeake Bay mainstem, separated into 8 segments and for the total bay (point estimates and Monte Carlo ensembles).
2. atmosph-apres-wspd2_xco2.nc: atmospheric data (squared wind speed, atmospheric pressure, and CO_2 mole fraction) used as inputs to the CO_2 flux calculation; also provided are intermediate calculation results (airpCO_2, CO_2 solubility, and gas transfer velocity).
3. nontidal-susquehanna-alk-dic: alkalinity and DIC at the non-tidal station in the Susquehanna River at Conowingo, Maryland (USGS gauge number 01578310).
4. tidal-33stations-database.nc: measured (Chesapeake Bay Program) and calculated variables at the 33 tidal stations in the Chesapeake Bay mainstem (temperature, salinity, oxygen, pH and alkalinity); at the surface- and at the native time resolution of the Chesapeake Bay Program.
5. shadwick2019a-buoy-pco2.nc: hourly *p*CO2 calculated from the high-frequency measurements of temperature, salinity, and pH at the York River buoy (Shadwick et al. 2019a).
6. shadwick2019b-cruises-alk-dic.nc: surface alkalinity and DIC measurements from 2016-2018 cruises in the Chesapeake Bay mainstem (Shadwick et al. 2019b).
7. cbp-cruises-alk.nc: surface alkalinity measurements from 1986-1991 cruises in the Chesapeake Bay mainstem (Chesapeake Bay Program)

Methods & Sampling

*p*CO2 and the air–water CO2 flux were computed at monthly resolution from 1998 to 2018 from tidal fresh to polyhaline waters.

Detailed description of processing of pH, temperature, salinity, and dissolved oxygen data

Data from the beginning of the regular monitoring program in 1985 through 2018 were downloaded from the Chesapeake Bay Program's Data Hub (see related datasets), with the original intention of producing a 33-year analysis of the air–water CO2 flux. However, a close examination of the pH data led us to question some measurements in the early part of the record. We found a dramatic difference in long-term trends between stations measured by institutions in the state of Virginia and stations measured by the state of Maryland, particularly from late spring to early fall. The boundary between the station groups runs east–west within the mesohaline portion of the bay in segment 5, where the Potomac River estuary intersects the mainstem bay. The boundary separates strong negative linear trends to the south (Virginia stations) from neutral and weakly positive linear trends to the north (Maryland stations). A closer examination of summer data at two stations straddling the boundary between the states (CB5.3 and CB5.4) revealed a distinct separation of the data before 1998 and convergence thereafter. The Virginia measurement protocols changed around this time (Chesapeake Bay Program, 2012). Specifically, Old Dominion University (ODU) took over sampling from the Virginia Institute of Marine Science (VIMS) in 1996. VIMS measured pH by first collecting a water sample and then inserting a pH probe into that sample whereas ODU and Maryland measured pH with an *in situ* probe. In 1997, ODU switched from using a Hydrolab Surveyor II sonde to a YSI 6000 sonde. It seems likely that the data quality of the Virginia measurements improved greatly after 1997 and we thus chose to limit our analysis to 1998–2018. For this shorter time period, the four parameters were measured exclusively with in situ probes from YSI® and Hydrolab®, and pH was reported on the NBS scale. The specific models used are described in Chesapeake Bay Program (2012) and probe accuracies can be found in the respective user manuals. As an example, the user manual for the YSI 6-series multiparameter water quality sondes provide accuracies of 0.15 ºC for temperature, 1% or 0.1 part per thousand (whichever is greater) for salinity, 0.2 for pH, and 2% or 6.25 mmol m–3 (whichever is greater) for dissolved oxygen measured with a polarographic sensor and half these values for an optical sensor.

Surface time series of pH, temperature, salinity, and dissolved oxygen were subset from the full Chesapeake Bay Program database depth profiles as the shallowest available measurement in the upper 2 m (36% at 0.5 m, 50% at 1 m, and 14% at 2 m). The native temporal resolution of the measurements was preserved in the surface subset. All data flagged with “Problem” by the Chesapeake Bay Program were removed (<0.1% of data for temperature and salinity, 0.6% for pH, and 0.4% for oxygen). The oxygen supersaturation was computed as the oxygen concentration minus the saturation concentration (computed from temperature and salinity, Garcia & Gordon, 1992). Surface values of pH, temperature, salinity, and dissolved oxygen supersaturation were quality controlled by removing gross outliers in three steps. First, pH was converted to hydrogen ion concentration. Second, the interquartile range for each variable for the whole 1998–2018 data set was computed. Third, all data 20 interquartile ranges above or below the 75th and 25thpercentiles, respectively, were removed. pH was the only variable affected by this filtering, resulting in removal of 0.26% of the pH data. pH was subjected to a second round of quality control following the same procedure, but this time on a station-by-station basis using 10 interquartile ranges as the threshold, leading to removal of 0.5 to 3.5% of the pH data from 18 of the 33 stations.

Because pH is a non-linear function of hydrogen ion, any time the pH data were manipulated in the analyses that follow (e.g., calculation of monthly averages), pH was converted to hydrogen ion concentration, the hydrogen ion data were processed, and the results were converted back to pH.

Data Processing Description

The Matlab programming language was used for the subsetting and quality control of input data and for the calculation of *p*CO2 and the air–water CO2 flux. NetCDF files were created from the native Matlab files.

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Data Files

File

atmosph_apres_wspd2_xco2.nc (NetCDF, 87.60 KB)

MD5:2a8616005496a20bcee37e189c571738

```
netcdf atmosph_apres_wspd2_xco2 {

dimensions:

        rows = 252 ;

        column = 8 ;

        nchar8 = 8 ;

        nchar10 = 10 ;

variables:

        double daten(rows) ;

                daten:units = "decimal_days" ;

                daten:long_name = "number of days from January 0, 0000" ;

        char dates(nchar10, rows) ;

                dates:units = "N/A" ;

                dates:long_name = "date string in the form YYYY-MM-DD" ;



// global attributes:

                :date_created = "20-May-2020" ;

                :creator = "Maria Herrmann, mxh367@psu.edu" ;

                :manuscript = "Challenges in quantifying air?water carbon dioxide flux using estuarine water quality data: Case study for
Chesapeake Bay, Journal of Geophysical Research - Oceans" ;

                :dataset_description = "atmospheric data (squared wind speed, atmospheric pressure, and CO2 mole fraction) used as
inputs to the CO2 flux calculation; also provided are intermediate calculation results (pCO2air, CO2 solubility, and gas transfer
velocity)" ;

                :missing_data_code = "NaN" ;

}
```

File

cbp_cruises_alk.nc (NetCDF, 21.21 KB)

MD5:17a9b50fb287e4adfa27007f500a2660

```
netcdf cbp_cruises_alk {
dimensions:
        rows = 514 ;
        nchar6 = 6 ;
        nchar10 = 10 ;
variables:
        char sta(nchar6, rows) ;
                sta:units = "N/A" ;
                sta:long_name = "tidal monitoring station ID" ;
        double daten(rows) ;
                daten:units = "decimal_days" ;
                daten:long_name = "number of days from January 0, 0000" ;
        char dates(nchar10, rows) ;
                dates:units = "N/A" ;
                dates:long_name = "date string in the form YYYY-MM-DD" ;
        double salt(rows) ;
                salt:units = "ppt" ;
                salt:long_name = "salinity" ;
                salt:comment = "measured" ;
        double alk(rows) ;
                alk:units = "mol/m3" ;
                alk:long_name = "total alkalinity" ;
                alk:comment = "measured" ;

// global attributes:
                :date_created = "20-May-2020" ;
                :creator = "Maria Herrmann, mxh367@psu.edu" ;
                :manuscript = "Challenges in quantifying air-water carbon dioxide flux using estuarine water quality data: Case study for Chesapeake Bay, Journal of Geophysical Research - Oceans" ;
                :dataset_description = "surface alkalinity measurements from 1986-1991 cruises in the Chesapeake Bay mainstem (Chesapeake Bay Program)" ;
                :missing_data_code = "NaN" ;
}
```

File

nontidal_susquehanna_alk_dic.nc (NetCDF, 12.02 KB)

MD5:81d42d94d4855f0d1f020aa06ae1f715

```
netcdf nontidal_susquehanna_alk_dic {

dimensions:

        rows = 252 ;

        nchar8 = 8 ;

        nchar10 = 10 ;

variables:

        double daten(rows) ;

                daten:units = "decimal_days" ;

                daten:long_name = "number of days from January 0, 0000" ;

        char dates(nchar10, rows) ;

                dates:units = "N/A" ;

                dates:long_name = "date string in the form YYYY-MM-DD" ;

        double flow(rows) ;

                flow:units = "m3/s" ;

                flow:long_name = "monthly average streamflow" ;

                flow:comment = "calculated as the arithmetic average of daily streamflow" ;

        double ealk(rows) ;

                ealk:units = "mol/m3" ;

                ealk:long_name = "effective monthly mean alkalinity concentration" ;

                ealk:comment = "the daily fluxes were summed for each month to get monthly fluxes and then an effective monthly mean alkalinity concentration was determined by dividing the monthly alkalinity flux by the monthly streamflow" ;

        double edic(rows) ;

                edic:units = "mol/m3" ;

                edic:long_name = "effective monthly mean DIC concentration" ;

                edic:comment = "the daily fluxes were summed for each month to get monthly fluxes and then an effective monthly mean DIC concentration was determined by dividing the monthly DIC flux by the monthly streamflow" ;



// global attributes:

                :date_created = "20-May-2020" ;

                :creator = "Maria Herrmann, mxh367@psu.edu" ;

                :manuscript = "Challenges in quantifying air-water carbon dioxide flux using estuarine water quality data: Case study for Chesapeake Bay, Journal of Geophysical Research - Oceans" ;

                :dataset_description = "monthly timeseries in the Susquehanna River at Conowingo, MD (USGS gauge number 01578310), see Supplement Text S2 and Section 4.3 of the manuscript" ;

                :missing_data_code = "NaN" ;
```

}

File

results_pco2_gasex.nc (NetCDF, 34.65 MB)

MD5:178cc6808849edff9a092bd2e5f7a967

```
netcdf results_pco2_gasex {

dimensions:

        rows = 252 ;

        column = 9 ;

        pages = 1000 ;

        nchar5 = 5 ;

        nchar10 = 10 ;

variables:

        char segm(nchar5, column) ;

                segm:units = "none" ;



// global attributes:

                :date_created = "20-May-2020" ;

                :creator = "Maria Herrmann, mxh367@psu.edu" ;

                :manuscript = "Challenges in quantifying air?water carbon dioxide flux using estuarine water quality data: Case study for Chesapeake Bay, Journal of Geophysical Research - Oceans" ;

                :dataset_description = "calculated monthly pCO2 and CO2 flux in the Chesapeake Bay mainstem, separated into 8 segments and for the total bay (point estimates and Monte Carlo ensembles)" ;

                :missing_data_code = "NaN" ;

}
```

shadwick2019a_buoy_pco2.nc (NetCDF, 371.40 KB)

MD5:ee2a970159e37f2e15ff6915fffd5f2e

```
netcdf shadwick2019a_buoy_pco2 {

dimensions:

        rows = 6528 ;

        nchar10 = 10 ;

variables:

        double daten(rows) ;

                daten:units = "decimal_days" ;

                daten:long_name = "number of days from January 0, 0000" ;

        char dates(nchar10, rows) ;

                dates:units = "N/A" ;
```

File	dates:long_name = "date string in the form YYYY-MM-DD" ;

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        double temp(rows) ;
                temp:units = "degC" ;
                temp:long_name = "water temperature" ;
                temp:comment = "high-frequency measurements at York River Buoy, see Section 2.6.2" ;
        double salt(rows) ;
                salt:units = "ppt" ;
                salt:long_name = "salinity" ;
                salt:comment = "high-frequency measurements at York River Buoy, see Section 2.6.2" ;
        double ph(rows) ;
                ph:units = "NBS scale" ;
                ph:long_name = "pH" ;
                ph:comment = "high-frequency measurements at York River Buoy, see Section 2.6.2" ;
        double alk(rows) ;
                alk:units = "mol/m3" ;
                alk:long_name = "total alkalinity" ;
                alk:comment = "calculated; see Section 2.6.2" ;
        double pco2(rows) ;
                pco2:units = "atm" ;
                pco2:long_name = "partial pressure of CO2 in the water" ;
                pco2:comment = "calculated, see Section 2.6.2" ;


// global attributes:
                :date_created = "20-May-2020" ;
                :creator = "Maria Herrmann, mxh367@psu.edu" ;
                :manuscript = "Challenges in quantifying air-water carbon dioxide flux using estuarine water quality data: Case study for Chesapeake Bay, Journal of Geophysical Research - Oceans" ;
                :dataset_description = "hourly pCO2 calculated from the high-frequency measurements of temperature, salinity, and pH at the York River buoy (Shadwick et al. 2019a)" ;
                :missing_data_code = "NaN" ;
}
```

shadwick2019b_cruises_alk_dic.nc (NetCDF, 10.60 KB)
MD5:656dab2a755276dc8fa2764fa464c119

```
netcdf shadwick2019b_cruises_alk_dic {
dimensions:
        rows = 168 ;
```

File

```
        nchar6 = 6 ;
        nchar10 = 10 ;
variables:
        char sta(nchar6, rows) ;
                sta:units = "N/A" ;
                sta:long_name = "tidal monitoring station ID" ;
        double daten(rows) ;
                daten:units = "decimal_days" ;
                daten:long_name = "number of days from January 0, 0000" ;
        char dates(nchar10, rows) ;
                dates:units = "N/A" ;
                dates:long_name = "date string in the form YYYY-MM-DD" ;
        double temp(rows) ;
                temp:units = "degC" ;
                temp:long_name = "water temperature" ;
                temp:comment = "measured" ;
        double salt(rows) ;
                salt:units = "ppt" ;
                salt:long_name = "salinity" ;
                salt:comment = "measured" ;
        double alk(rows) ;
                alk:units = "mol/m3" ;
                alk:long_name = "total alkalinity" ;
                alk:comment = "measured" ;
        double dic(rows) ;
                dic:units = "atm" ;
                dic:long_name = "dissolved inorganic carbon (DIC)" ;
                dic:comment = "measured" ;


// global attributes:
                :date_created = "20-May-2020" ;
                :creator = "Maria Herrmann, mxh367@psu.edu" ;
                :manuscript = "Challenges in quantifying air-water carbon dioxide flux using estuarine water quality data: Case study for Chesapeake Bay, Journal of Geophysical Research - Oceans" ;
                :dataset_description = "surface alkalinity and DIC measurements from 2016-2018 cruises in the Chesapeake Bay mainstem (Shadwick et al. 2019b)" ;
```

File	:missing_data_code = "NaN" ;
}	

tidal_33stations_database.nc (NetCDF, 607.79 KB)
MD5:e53d12d15de0d7f2f2544151650bd41e

```
netcdf tidal_33stations_database {

dimensions:

        rows = 9694 ;

        nchar6 = 6 ;

        nchar10 = 10 ;

variables:

        char sta(nchar6, rows) ;



// global attributes:

                :date_created = "20-May-2020" ;

                :creator = "Maria Herrmann, mxh367@psu.edu" ;

                :manuscript = "Challenges in quantifying air-water carbon dioxide flux using estuarine water quality data: Case study for Chesapeake Bay, Journal of Geophysical Research - Oceans" ;

                :dataset_description = "measured (Chesapeake Bay Program) and calculated variables at the 33 tidal stations in the Chesapeake Bay mainstem (temp, salt, oxysu, ph, alk); at surface; at native time resolution of the Chesapeake Bay Program" ;

                :missing_data_code = "NaN" ;

}
```

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Related Publications

Chesapeake Bay Program (2012). Guide to using Chesapeake Bay Program water quality monitoring data. Annapolis, MD: Chesapeake Bay Program.
https://d18lev1ok5leia.cloudfront.net/chesapeakebay/documents/wq_data_userguide_10feb12_mod.pdf
Methods

Mesinger, F., DiMego, G., Kalnay, E., Mitchell, K., Shafran, P. C., Ebisuzaki, W., Jović, D., Woollen, J., Rogers, E., Berbery, E. H., Ek, M. B., Fan, Y., Grumbine, R., Higgins, W., Li, H., Lin, Y., Manikin, G., Parrish, D., & Shi, W. (2006). North American Regional Reanalysis. Bulletin of the American Meteorological Society, 87(3), 343–360. https://doi.org/10.1175/bams-87-3-343 https://doi.org/10.1175/BAMS-87-3-343
Methods

Najjar, R. G., Herrmann, M., Cintrón Del Valle, S. M., Friedman, J. R., Friedrichs, M. A. M., Harris, L. A., Shadwick, E. H., Stets, E. G., & Woodland, R. J. (2020). Alkalinity in Tidal Tributaries of the Chesapeake Bay. Journal of Geophysical Research: Oceans, 125(1). Portico. https://doi.org/10.1029/2019jc015597
https://doi.org/10.1029/2019JC015597
Results

Shadwick, E. H., Friedrichs, M. A. M., Najjar, R. G., De Meo, O. A., Friedman, J. R., Da, F., & Reay, W. G. (2019). High-Frequency CO 2 System Variability Over the Winter-to-Spring Transition in a Coastal Plain Estuary. Journal of Geophysical Research: Oceans, 124(11), 7626–7642. Portico. https://doi.org/10.1029/2019jc015246
https://doi.org/10.1029/2019JC015246
Methods

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Related Datasets

IsDerivedFrom

Chesapeake Bay Data Hub, Water Quality and calculated physical and nutrient parameters accessed [], at URL https://data.chesapeakebay.net/WaterQuality] https://www.chesapeakebay.net/what/downloads/cbp-water-quality-database-1984-present

NCEP North American Regional Reanalysis (NARR) https://psl.noaa.gov/data/gridded/data.narr.html

Shadwick, E. A., De Meo, O. A., & Friedman, J. R. (2019). *Discrete CO2-System Measurements in the Chesapeake Bay Mainstem between 2016 and 2018* [Data set]. Virginia Institute of Marine Science, William & Mary. https://doi.org/10.25773/RNTN-EZ18 https://doi.org/10.25773/rntn-ez18

U.S. Geological Survey, 2001, National Water Information System data available on the World Wide Web (Water Data for the Nation), accessed [], at URL [http://waterdata.usgs.gov/nwis/]. https://nwis.waterdata.usgs.gov/nwis

World Data Centre for Greenhouse Gases (WDCGG) https://gaw.kishou.go.jp/

IsRelatedTo

M. Herrmann, R.G. Najjar, F. Da, S. Goldberger, J. Friedman, M.A.M. Friedrichs, A. Menendez, E.H. Shadwick, E.G. Stets, & P. St-Laurent. (2020). *Dataset for "Challenges in quantifying air–water carbon dioxide flux using estuarine water quality data: Case study for Chesapeake Bay"* [Data set]. scholarsphere. https://doi.org/10.26207/BM5N-N185 https://doi.org/10.26207/bm5n-n185

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Parameters

Parameters for this dataset have not yet been identified

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Project Information

Collaborative Research: Multiple Stressors in the Estuarine Environment: What drives changes in the Carbon Dioxide system? (Estuarine Stressors)

NSF Award Abstract:

Understanding the vulnerability of estuarine ecosystems to anthropogenic impacts requires a quantitative assessment of the dynamic drivers of change to the estuarine carbonate system. Estuaries are currently experiencing multiple environmental stressors that have significant impacts on their carbonate chemistry, making this assessment a major challenge. Although the effects of changes in nutrient run-off (i.e. eutrophication and hypoxia) have been long-studied in many estuaries, much less attention has been given to the impacts of global change on these systems. In this study, a team of field scientists and modelers will attempt to distinguish natural interannual variability in a major US estuary from the impacts of local anthropogenic changes (e.g., nutrient inputs, changing freshwater end member characteristics) and global change (increases in atmospheric temperature, atmospheric carbon dioxide, and sea level), by using numerical models calibrated with CO2-system observations at appropriate spatial and temporal scales. If successful, this will be the first study to quantitatively distinguish between local and global anthropogenic impacts on the CO2 system in an estuary. The results are expected to have important implications for management of Chesapeake Bay because the impact of local anthropogenic stressors on the system, once isolated, may be mitigated by appropriate environmental policy implemented at the regional scale. Two of the PIs have a strong history of proven relationships with Chesapeake Bay managers and policy makers, which will insure direct infusion of these scientific results into ongoing management decisions.

In this project researchers will study the diurnal, seasonal, and interannual variability of the CO2 system in the

Chesapeake Bay, a non-pristine estuary, using a combination of conventional shipboard sampling (of dissolved inorganic carbon, and alkalinity) and new high-frequency autonomous instrumentation (for observations of pH and CO2 partial pressure) to assess the impact of extreme events, like tropical storms and nor?easters on carbonate chemistry. These high-quality observations will afford a rigorous assessment of the uncertainty associated with a 30-year water-quality monitoring time series of pH and alkalinity. The team will use an estuarine-carbon-biogeochemical model evaluated and calibrated with the new and long-term observations. Sensitivity experiments will be applied to disentangle multiple impacts on the CO2 system in the estuary over the last 30 years, including increased atmospheric temperature and CO2, sea-level rise, eutrophication due to increases in nutrient run-off, and changing carbonate characteristics of riverine end-members.

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Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-1537013
NSF Division of Ocean Sciences (NSF OCE)	OCE-1536996
National Aeronautics & Space Administration (NASA)	NNX14AM37G
National Aeronautics & Space Administration (NASA)	NNX14AF93G

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