ACIDIFICATION OF THE GLOBAL SURFACE OCEAN

WHAT WE HAVE LEARNED FROM OBSERVATIONS

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DATA SYNTHESIS METHODS

Within each time interval, all data were adjusted to their respective middle year (i.e., 1975, 1995, 2005, and 2015) using the Empirical Seawater Property Estimation Routines (ESPER) algorithm, an algorithm that uses sea surface temperature (SST), sea surface salinity (SSS), and other variables (Carter et al., 2021). The international Surface Ocean CO_2 Atlas (SOCAT), total alkalinity (TA), silicate, and phosphate contents needed for carbon system calculations were calculated using ESPER from temperature, salinity, longitude, latitude, and depth. For the Global Ocean Data Analysis Project Version 2 (GLODAPv2) and the Common Online Data Analysis Platform in North America (CODAP-NA), only data with at least a pair of dissolved inorganic carbon (DIC) and TA, DIC and pH, or TA and pH, and a water depth of less than 20 m were used. If all three parameters were available, DIC and TA were used. For each of these intervals, data from the three data products were pooled as one observational database before it was interpolated onto a global surface ocean 1° × 1° grid (Jiang et al., 2023). Interpolation and gap-filling were done with a Julia version of the Data-Interpolating Variational Analysis (DIVAnd.jl, https://github.com/gher-ulg/DIVAnd.jl; Barth et al., 2014). The correlation lengths of 21° latitudinally and 42° longitudinally, as well as the signal-to-noise ratio of 0.1, were selected to strike a balance between retaining some local regional variability and smoothing over fine-scale variability that is present in synoptic measurements but not representative of climatological conditions (see also Jiang et al., 2021).

The ocean acidification indicators for this study—fugacity of carbon dioxide ($f CO_2$), carbonate ion content ($[CO_3^{2-}]$), total hydrogen ion content ($[H^+]_T$), pH on total scale (pH_T), aragonite saturation state (Ω_{ar}), and calcite saturation state (Ω_{cal})—were calculated following the six steps as below:

1. For each of the three ocean carbon data products, SOCAT, GLODAPv2, or CODAP- NA, all data points from one of the periods (e.g., 1961 to 1990) were grouped together.

2. DIC and TA, if they were not already available, were calculated using CO2SYS with the available carbon system parameters, depending on the ocean carbon data products. The SOCAT, TA, silicate, and phosphate contents needed for carbon system calculations were calculated using ESPER, an empirical algorithm that uses SST, SSS, and other variables (Carter et al., 2021). For GLODAPv2 and CODAP-NA, only data with at least a pair of DIC and TA, DIC and pH, or TA and pH, and a water depth of less than 20 m were used. If all three parameters were available, DIC and TA were used.

3. Delta DIC (ΔDIC) changes from the sampling year to the respective middle years was calculated out of two sets of ESPER calculations based on the input parameters of temperature, salinity, longitude, latitude, and depth, but different output years: sampling year and middle year. The difference between the two DIC output values was assumed to be the delta DIC change during the period.

4. The adjusted DIC values in the middle year were calculated as the sum of the DIC values of the sampling year from Step 2 and the ΔDIC derived from Step 3.

5. The OA indicators were then calculated based on TA and the adjusted DIC values. This is repeated for all four periods and all three data products.
6. For each of the four time intervals, data from the three data products were pooled as one observational database. Then, each ocean acidification indicator for the period was interpolated onto a global surface ocean 1° × 1° grid.

The CO_2 system calculation was performed using a Julia version of the CO2SYS (CO2System.jl, v2.0.5, https://github.com/mvdh7/CO2System.jl; Humphreys et al., 2022) with the dissociation constants and parameters as recommended by Jiang et al. (2021), that is, dissociation constants for carbonic acid of Lueker et al., 2000), bisulfate (HSO_4^-) of Dickson (1990), hydrofluoric acid (HF) of Perez and Fraga (1987)), and total borate content of Lee et al. (2010). Interpolation and gap-filling was done with a Julia version of DIVAnd.jl (Barth et al., 2014). The correlation lengths of 21° latitudinally and 42° longitudinally and the noise to signal ratio of 0.1 were selected to strike a balance between retaining some local regional variability and smoothing over fine-scale variability that is present in synoptic measurements but not representative of climatological conditions (see also Jiang et al., 2021).

The model output results are from a model-data fusion product that was created by combining 14 latest Earth System Models from the Coupled Model Intercomparison Project Phase 6 (CMIP6) with the three latest observational ocean carbon data products, SOCAT, GLODAPv2, and CODAP-NA (Jiang et al., 2023). The temporal evolution of surface ocean acidification indicators as decadal averages from historical conditions (1850–2010) to two future shared socioeconomic pathways (2020–2100): SSP1-1.9 and SSP5-8.5, were used as a reference for the observational data-based temporal changes.

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