1. Introduction

To create an integrated database of discrete water quality measurements in the San Francisco Estuary, we combined data from 14 boat-based surveys with the R statistical programming language (R Core Team 2020). The data integration code was packaged into the R package discretewq v2.2.0: https://github.com/sbashevkin/discretewq (Bashevkin and Perry 2022).

The surveys included in the integrated database are long-term monitoring surveys managed by federal agencies, state agencies, and the University of California, Davis. Eight surveys are primarily focused on collecting fish abundance data but collect water quality data alongside fish samples. These include the California Department of Fish and Wildlife (CDFW) Fall Midwater Trawl (FMWT), CDFW Summer Townet Survey (STN), CDFW Spring Kodiak Trawl (SKT), CDFW 20-mm Survey (20mm), CDFW San Francisco Bay Study (Bay Study), CDFW Smelt Larva Survey (SLS), California Department of Water Resources (DWR) Yolo Bypass Fish Monitoring Program (YBFMP), United States Fish and Wildlife Service (USFWS) Enhanced Delta Smelt Monitoring (EDSM), USFWS Delta Juvenile Fish Monitoring Program (DJFMP), and University of California, Davis Suisun Marsh Fish Study (Suisun Study). An additional 3 surveys are primarily focused on water quality data: the DWR Environmental Monitoring Program (EMP), DWR Stockton Dissolved Oxygen Survey (SDO), United States Bureau of Reclamation Sacramento Deepwater Shipping Channel Survey (SDSCS), and the United States Geological Survey San Francisco Bay Survey (SFBS) (see Delta\_Integrated\_WQ\_metadata.csv).

The primary aim of this data integration was to combine datasets to facilitate analyses of water quality trends in the upper San Francisco Estuary. The focal water quality variables included water temperature, conductivity (or salinity), Secchi depth, *Microcystis* concentration, and chlorophyll concentration. Key nutrient variables were retained from the SFBS and EMP surveys. These variables were all collected from the surface of the water column. In addition, water temperature from the bottom of the water column was retained when available. Not all surveys measured all focal variables. Some surveys (particularly the water quality surveys) measured more water quality variables than were retained in this integrated dataset.

While we describe some of the methods here, it is highly recommended to inspect the documentation of the component surveys (see provenance and below for citations) for more information on their methods.

2. Survey methods

Methods for measuring water quality variables were generally consistent among the component surveys, but there were slight differences. All surface water samples were collected within the upper 1 m, but the exact depth differed slightly among studies. SFBS collected some surface temperatures at depths of 2 m, but we only retained samples collected at 1 m or shallower for compatibility with the other studies. The only exception to this is for nutrient data collected by the SFBS survey. Nutrient samples were sometimes collected deeper than the surface water quality data. In these cases, we selected the shallowest nutrient data available. The maximum depth of surface nutrient data is 4 m and these depths are available in the dataset. Bottom temperature samples were collected within 1 m of the bottom (see Delta\_Integrated\_WQ\_metadata.csv). More detailed methods and protocols for most component surveys can be found in the data source links in Delta\_Integrated\_WQ\_metadata.csv or the provenance citations.

2.1. Water temperature

While all surveys now measure water temperature with digital sensors, older surveys used less precise handheld thermometers in earlier years. More precise sensors were first used by FMWT in 1995, STN in 1994, and DJFMP in 2014. All other surveys used more precise methods to measure temperature since inception. SKT had notes on some temperature records that they were transcribed from a different monitoring program (CDEC) so these values were all removed.

2.2. Conductivity/Salinity

Most surveys reported specific conductivity except SFBS which reported salinity. DJFMP and EDSM could not verify their conductivity metric for data collected before June 2019 so conductivity values collected before that date are removed from the integrated dataset.

2.3. Secchi depth

Secchi depth was measured on the shady side of the boat (when possible) in all surveys that measured this variable. It is important to note that the Secchi data are right-censored, since in some cases the disk was still visible at the deepest depth to which it could be extended. In these cases, the maximum extension depth was usually recorded, even if the disk was still visible.

2.4. *Microcystis*

Concentration of the toxic microalga *Microcystis* was measured on the same 5-point qualitative scale (absent, low, medium, high, very high) by the 3 surveys that measured this variable. For a short period of time (2012-15), FMWT added a 6th level to the *Microcystis* scale to represent *Microcystis* presence in zooplankton net cod-ends. Outside this short time period, this was measured as a “low” on the 5-point scaled, so all records of this 6th level were converted to “low” for consistency with other surveys and time periods.

2.5. Chlorophyll

Chlorophyll-a methods differed slightly among surveys. EMP filtered water samples through a 1 µm glass fiber filter and measured Chlorophyll concentrations in the lab. SDSCS and SFBS used sonde probes to measure chlorophyll in the field but USGS calibrated these field measurements with filtered water samples collected and analyzed similar to EMP.

2.6. Nutrients

EMP collected and preserved nutrients samples in accordance with standard protocols (Interagency Ecological Program et al. 2021a), after which they were processed in a lab. Nutrients were filtered in the field when applicable. USGS collected, preserved, and processed dissolved inorganic nutrients in a similar manner to EMP. Both surveys collected water using a fixed flow-through pump.

3. Data integration methods

From each dataset, we selected columns corresponding to the water quality variables of interest as well as important accessory information (date, time, station, latitude, longitude, depth, tide, and any notes). We then renamed variables for consistency and converted all variables to consistent units. Salinity was calculated from specific conductivity using the ec2pss function from the wql R package (Jassby et al. 2017). This function uses the Practical Salinity Scale 1978 for salinities between 2 and 42 (Fofonoff and Millard Jr 1983) and the extension of the Practical Salinity Scale (Hill et al. 1986) for salinities below 2. Conductivity data were also retained in the integrated dataset. In most cases, latitude and longitude coordinates of the fixed sampling stations were retained. When these coordinates were not available (e.g. for non-fixed stations), we retained any coordinates that were recorded during the field sampling. To remove duplicate values from the dataset, only one set of values was retained for each recorded date, time, and location. All data integration code can be found in the discretewq R package v2.2.0 (https://github.com/sbashevkin/discretewq; Bashevkin and Perry 2022).

4. Literature cited

Bashevkin, S. M., and S. E. Perry. 2022. discretewq: An Integrated Dataset of Discrete Water Quality in the San Francisco Estuary v2.2.0. Zenodo. doi:10.5281/zenodo.5834909

Fofonoff, N. P., and R. C. Millard Jr. 1983. Algorithms for the computation of fundamental properties of seawater. UNESCO Technical Papers in Marine Science 44.

Hill, K., T. Dauphinee, and D. Woods. 1986. The extension of the Practical Salinity Scale 1978 to low salinities. IEEE Journal of Oceanic Engineering 11: 109–112.

Jassby, A. D., J. E. Cloern, and J. Stachelek. 2017. wql: Exploring Water Quality Monitoring Data.

R Core Team. 2020. R: A Language and Environment for Statistical Computing, R Foundation for Statistical Computing.

5. Data sources

CDFW. 2021a. Fall Midwater Trawl data. https://filelib.wildlife.ca.gov/Public/TownetFallMidwaterTrawl/FMWT%20Data/.

CDFW. 2021b. Summer Townet data. https://filelib.wildlife.ca.gov/Public/TownetFallMidwaterTrawl/TNS%20MS%20Access%20Data/TNS%20data/.

CDFW. 2021c. Bay Study data. https://filelib.wildlife.ca.gov/Public/BayStudy/.

Cloern, J. E., and T. S. Schraga. 2016. USGS Measurements of Water Quality in San Francisco Bay (CA), 1969-2015 (ver. 3.0 June 2017). U. S. Geological Survey data release. doi:https://doi.org/10.5066/F7TQ5ZPR

Interagency Ecological Program, L. Damon, and A. Chorazyczewski. 2021a. Interagency Ecological Program San Francisco Estuary 20mm Survey 1995 - 2021. ver 4. Environmental Data Initiative. doi:10.6073/pasta/32de8b7ffbe674bc6e79dbcd29ac1cc2

Interagency Ecological Program, L. Damon, and A. Chorazyczewski. 2021b. Interagency Ecological Program San Francisco Estuary Spring Kodiak Trawl Survey 2002 - 2021. ver4. Environmental Data Initiative. doi:10.6073/pasta/f0e2916f4a026f3f812a0855cee74a8d

Interagency Ecological Program, L. Damon, T. Tempel, and A. Chorazyczewski. 2021c. Interagency Ecological Program San Francisco Estuary Smelt Larva Survey 2009 – 2021. ver 4. Environmental Data Initiative. doi:10.6073/pasta/8e1ceb1c02fbc8b0ba7a6b58229109f2

Interagency Ecological Program, S. Lesmeister, and J. Rinde. 2020a. Interagency Ecological Program: Discrete dissolved oxygen monitoring in the Stockton Deep Water Ship Channel, collected by the Environmental Monitoring Program, 1997-2018. ver 2. Environmental Data Initiative. doi:10.6073/PASTA/3268530C683726CD430C81894FFAD768

Interagency Ecological Program, M. Martinez, and S. Perry. 2021d. Interagency Ecological Program: Discrete water quality monitoring in the Sacramento-San Joaquin Bay-Delta, collected by the Environmental Monitoring Program, 1975-2020. ver 4. Environmental Data Initiative. doi:10.6073/pasta/31f724011cae3d51b2c31c6d144b60b0

Interagency Ecological Program, R. McKenzie, J. Speegle, A. Nanninga, and J. Hagen. 2021e. Interagency Ecological Program: Over four decades of juvenile fish monitoring data from the San Francisco Estuary, collected by the Delta Juvenile Fish Monitoring Program, 1976-2021. ver 8. Environmental Data Initiative. doi:10.6073/pasta/8dfe5eac4ecf157b7b91ced772aa214a

Interagency Ecological Program, C. L. Pien, J. B. Adams, and N. Kwan. 2020b. Interagency Ecological Program: Zooplankton catch and water quality data from the Sacramento River floodplain and tidal slough, collected by the Yolo Bypass Fish Monitoring Program, 1998-2018. ver 2. Environmental Data Initiative. doi:10.6073/pasta/baad532af96cba1d58d43b89c08ca081

Interagency Ecological Program, B. Schreier, B. Davis, and N. Ikemiyagi. 2019. Interagency Ecological Program: Fish catch and water quality data from the Sacramento River floodplain and tidal slough, collected by the Yolo Bypass Fish Monitoring Program, 1998-2018. ver 2. Environmental Data Initiative. doi:10.6073/PASTA/B0B15AEF7F3B52D2C5ADC10004C05A6F

O’Rear, T., J. Durand, and P. Moyle. 2021. Suisun Marsh Fish Study. https://watershed.ucdavis.edu/project/suisun-marsh-fish-study.

Schraga, T. S., E. S. Nejad, C. A. Martin, and J. E. Cloern. 2018. USGS measurements of water quality in San Francisco Bay (CA), beginning in 2016 (ver. 3.0, March 2020). U. S. Geological Survey data release. doi:https://doi.org/10.5066/F7D21WGF

United States Fish And Wildlife Service, T. Senegal, R. Mckenzie, and others. 2021. Interagency Ecological Program and US Fish and Wildlife Service: San Francisco Estuary Enhanced Delta Smelt Monitoring Program data, 2016-2021. ver 7. Environmental Data Initiative. doi:10.6073/pasta/65f9297a7077320f4ba31c2acd685f93

USBR, R. Dahlgren, L. Loken, and E. Van Nieuwenhuyse. 2020. Monthly vertical profiles of water quality in the Sacramento Deep Water Ship Channel 2012-2019.