Raw water temperature data are uploaded to the California Data Exchange Center (CDEC) by state and federal agencies. Some agencies do have their own websites for posting and sharing data, which may include water quality that has undergone quality checks, and additional water quality stations; however, we used CDEC data to ensure we could treat all data consistently. Additionally, existing data packages made it efficient to download all existing CDEC data in a streamlined way (R code available in this package).

We used CDEC’s station locator map (https://cdec.water.ca.gov/cdecstations) to download metadata from stations in our area of interest – the San Francisco Estuary. We filtered stations to include those that had water temperature data that was either collected hourly or every 15-minutes (labeled as event in CDEC). Water temperature sensors are labeled as sensor numbers 25 (temperature in degrees Fahrenheit) and 146 (temperature in degrees Celsius). Data were downloaded and processed in R version 3.6.2.

*Metadata Template*

We contacted agency managers and supervisors to locate station manager names and contact information.

We created a template of relevant metadata regarding water temperature sensors and available data, and requested station managers fill out the template.

We edited responses for consistency, and standardized habitat types (see below).

*Habitat Type Definitions*

Tidal River Channel (brackish) - a natural brackish river (higher salinity than freshwater, resulting from a mixture of estuarine river and seawater) whose flow and level are influenced by tides.

Tidal River Channel (brackish, marsh) - a natural brackish river within the boundaries of a defined marsh whose flow and level are influenced by tides.

Tidal River Channel (freshwater) - a natural river, mainly freshwater, whose flow and level are influenced by tides.

Non-Tidal River Channel (freshwater) - a channel of freshwater that is not affected by the ebb and flow of tides.

Tidal Canal (freshwater) - an artificial waterway of freshwater constructed to allow the passage of boats or ships, or to transport water for agriculture.

Tidal Flooded Island (freshwater) - a man-made flooded island that contains freshwater.

Tidal Embayment (brackish) - a recess in a waterway or coastline forming a bay with brackish water.

Tidal Slough - a backwater to a larger body of water that is tidally influenced, with high water residence time and low water velocity.

Non-Tidal Slough - a backwater to a larger body of water that is non-tidal, with high water residence time and low water velocity.

Concrete-lined Reservoir - a large natural or artificial lake used as a source of water supply that is lined with concrete.

Aqueduct - a wide artificial channel or canal used for transporting water.

Note: Prior to conducting analyses, please read “Comments” column in the Water Temperature Sensor Metadata Table for additional relevant information about sensors. We tried to keep columns in consistent formats, so most of the additional text was added to Comments.

*Raw Integrated Dataset*

1. Data Download: The CDECRetrieve package https://github.com/FlowWest/CDECRetrieve was used to download data. All versions of temperature data for each station were downloaded (Event-Fahrenheit, Event-Celsius, Hourly-Fahrenheit, Hourly-Celsius), then combined.

2. Standardization: Fahrenheit temperatures were converted to Celsius.

3. Conversion to hourly temperature points: Data were grouped and organized by station, date, hour. The first value for each grouping was kept, while the rest of the data for each station was removed. This resulted in one temperature value for each station-date-hour.

4. Saved files: The raw hourly temperature dataset was saved as Temp\_all\_H.csv and Temp\_all\_H.rds (this compressed file is smaller and reads faster into R; this is also the file used for subsequent QC code and app code). The code is in the file DownloadData\_CDEC.Rmd.

*Quality Control Filters*

Quality control (QC) filters were informed by NOAA’s Manual for Real-Time Quality Control In-Situ Temperature and Salinity Data, which can be found at: https://cdn.ioos.noaa.gov/media/2017/12/qartod\_temperature\_salinity\_manual.pdf.

QC filters were applied to the raw temperature data, and each temperature value was either flagged (Y) or not flagged (N) for each filter:

QC1: Temperature Range​: Values outside of 1-40 degreesC were flagged/ filtered.​

QC2: Missing Values​: Days with >4 missing values were flagged/ filtered​. Data were grouped by station and date, and summarized for number of values per grouping. Days with less than 20 temperature values were flagged. Dates were merged back to full temperature dataset to flag all values that had a flagged day.

QC3: Repeating Values​: Values that repeat 18+ times were flagged/ filtered​. Each value was compared with the prior value. A column was created to indicate whether or not they were the same (same = 1 if values are not the same, 0 if values are different). The total number of repeating values was summed. If the number of repeating values was > 18, the repeating values were flagged/filtered.

QC4: Flag anomalies​: Data were separated into seasonal, trend and remainder components, and remainder component outliers were flagged/filtered. This analysis was conducted by the anomalize package in R. Seasonal decomposition method: Loess​. Trend: Set at 6 months​. Outlier detection: Used threshold of 3\*IQR to flag/filter outliers​

QC5: Spike: Values that “spike” compared to the value before and after were flagged/filtered. Data were grouped by station, and arranged by Station and Datetime. Each value was compared with the average of the prior and subsequent values. If the difference was > 5 degreesC, the value was flagged/ filtered.​

QC6: Rate of change: ​Values with a rate of change greater than 5 \* standard deviation of values from the past 50 hours (~ 2 tidal cycles) were flagged/filtered. Data were grouped by station, and arranged by station and datetime. A = The difference between each value and the prior value. B = The standard deviation of the past 50 temperature values (hours). If A>B, the value was flagged/ filtered.

Saved Files: Flagged Dataset: Contains all raw data, with a column for each QC filter above filled in with either a “Y” or “N.” Saved as Temp\_flagged.csv. Filtered Dataset: Removed any data that was flagged for at least one QC filter. Saved as Temp\_filtered.csv. Code: WaterTemp\_QC.Rmd

RShiny: An RShiny app was also created to allow individuals to select their own filtering criteria and download individual station data according to their needs. Code: app.R. Shortly after EDI data publication, this app will be hosted on the Delta Science Program’s Shiny server at: https://deltascience.shinyapps.io/Home/. There may be minor changes made to the Rshiny code after publication of this dataset.

Specific values used for QC filters were initially selected by real-time water quality experts as values deemed reasonable. Once values were selected, filters were applied to the raw temperature data, and were visualized in an R Shiny app, which highlighted data that were flagged under each filter. Some values were then modified as deemed appropriate to prevent over- or under-flagging. For one filter, the QC4 trend (see above), visualization was not deemed enough to make a selection. Thus, a subset of stations was selected for further analysis. For the subset of stations, 3-month, 6-month, and 12-month trends were applied, and downloaded into separate datasets. Each dataset was analyzed for maximum temperatures, days with maximum temperatures > 27 degreesC, and whether outliers flagged by QC4 corresponded with heat waves. The 6-month trend was chosen based on comparisons of the results from the three datasets.

*Additional Notes on Data Review and Quality:*

USGS water temperature time-series data are reviewed, quality-assured, and aged within the National Water Information System (NWIS: https://nwis.waterdata.usgs.gov/nwis) using procedures outlined in Wagner and others (2006). USGS data released on EDI were imported as raw data and filtered as described so may not be identical to approved USGS data published on NWIS.

Our QC methods were meant to efficiently review water temperature data from a large number of stations by using overarching code for the entire dataset. However, we did not review every point at every station in depth, and we recognize there are some points that may have been flagged incorrectly, or not flagged when they should be flagged. We leave it to the data user to further review data for their own analysis needs.