LTRM Water Data Cleaning

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TLDR

Here's what we did. ("Samples" refers to rows of the data.)

1. Filter for surface level samples.
2. Filter for non-fixed site samples (and select 11 important continuous variables and 7 identifier variables).
3. Change variable values with bad QF code values to `NA`.
4. Collapse duplicate `SHEETBAR`s by taking the average.
5. Replace negative values in 11 continuous variables with `NA`.

Concerns

- Only 82k rows left in the data (look at the sidenote: fixed sites account for almost half of the original dataset!)
- When should we keep negative values (look at the graphs at the bottom)

Summary

One important goal before we interpolate missing values is to clean the data. Cleaning includes filtering for relevant rows and selecting the relevant variables. This will decide on the scope of our analysis. We will also see that removing duplicate rows will reduce the missing values (that aren't actually missing), thus making the interpolation step significantly easier.

In cleaning the LTRM Water Quality dataset, we encounter the following questions:

1) Which variables (columns) are the most important for us to keep (out of the 133 total variables)?
2) Why do duplicate rows happen, and how do we deal with them?
3) Which samples (rows) are high enough quality for us to keep? (This involves the QF codes.) We want to set low quality data to `NA` for interpolation later.

The LTRM Water Quality dataset has duplicate rows for the same `SHEETBAR`, which is problematic because `SHEETBAR` is a unique identifier for a water data sheet (sample at a date, time, and location).

Load libraries

```r
library(tidyverse)
library(ggplot2)
library(lubridate)
library(corrplot)
library(RColorBrewer)
library(kableExtra)
```

Read data

```r
# set working directory to source file location
# setwd("~/Documents/GitHub/UMR-TDA-2021")

water20 <- read.csv(file = "../LTRM data/ltrm_water_data_lat_long.csv")
```

1. These are the important variables

```r
water_var <- c('TN','TP','TEMP','DO','TURB',
               'COND','VEL','SS','WDP','CHLcal','SECCHI')

waterQF_var <- paste(water_var, "QF", sep = "")

identifier_var <- c('SHEETBAR', 'DATE', 'LATITUDE', 'LONGITUDE', 'FLDNUM', 'STRATUM', 'LOCATCD')
```

```r
waterQF_var <- waterQF_var[waterQF_var != "WDPQF" &
                             waterQF_var != "CHLcalQF"]

waterQF_var <- c(waterQF_var, "ZMAXQF")
```

We decided that the 11 continuous variables of importance were: total nitrogen, total phosphorous, temperature, dissolved oxygen, turbidity, water condition, velocity, suspended solids, water depth, chlorophyll-a, and Secchi distance.

In addition, we will want to include the QA/QC codes, along with identifier variables like `SHEETBAR` and date.

Lastly, we manually edit these variable strings because:

- The water depth variable is `WDP`, but the corresponding quality factor is `ZMAXQF` rather than `WDPQF`.
- `CHLcal`, calibrated fluorometric chlorophyll a, does not have a corresponding quality factor code. According to the metadata: "`CHLcal` is generated by calibration of fluorometric chlorophyll readings (`CHLF`) to season and year specific measurements of spectrophotometric chlorophyll (`CHLS`). Data from sites where CHLS and CHLF are both collected are used to build river-specific calibration curves for these data. Values are corrected for pheophytin. Units are micrograms per liter.“

2. Investigating duplicate SHEETBARs in the data

At the same sheetbar, multiple samples can be taken at different water depths.

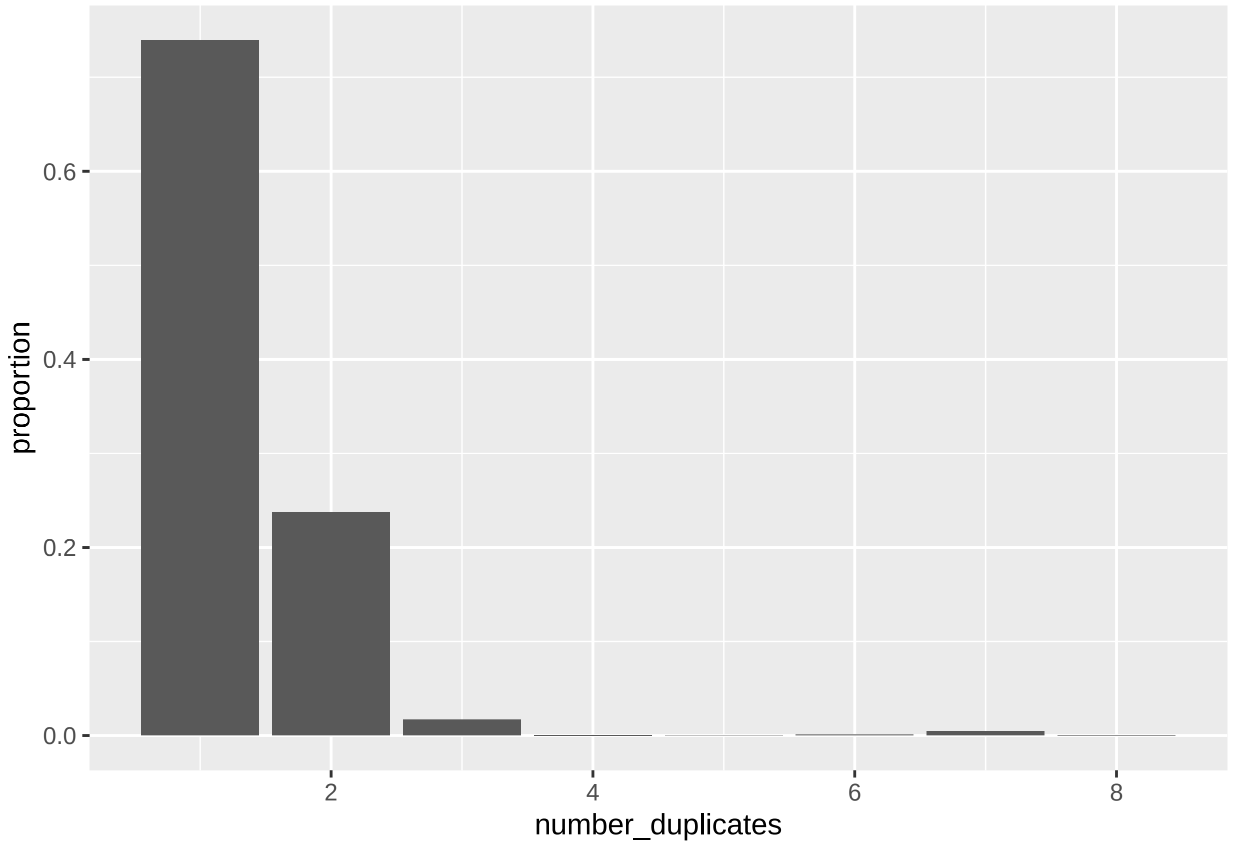
There are 204305 total rows in the LTRM water quality dataset. Of these rows, there are 156474 distinct `SHEETBAR` codes.

We visualize duplicates as follows. To identify the duplicate rows, we count the number of occurences of each unique `SHEETBAR` value in the dataset. Then, we can calculate and plot the distribution of `SHEETBAR` duplicates.

```
duplicates <- water20 %>%
  select(SHEETBAR) %>%
  group_by(SHEETBAR) %>%
  summarize(count = n())

duplicates %>% head()
```

```
## # A tibble: 6 x 2
##   SHEETBAR count
##      <int> <int>
## 1 -4604348     1
## 2 -4604347     2
## 3 -4604346     2
## 4 -4604345     2
## 5 -4604344     1
## 6 -4604343     2
```

```
count_n_duplicates <- function(n, df) {
  return((df %>% filter(count == n) %>% dim())[1]/156474) #156k distinct sheetbars
}

count_duplicates <- data.frame(proportion = sapply(1:8, count_n_duplicates,
                                                   duplicates),
                               number_duplicates = 1:8)

ggplot(count_duplicates, aes(x = number_duplicates, y = proportion)) +
  geom_bar(stat = "identity")
```



SHEETBAR	Z	CALCZCD	DO	TP	TN
-4604347	0.2	SF	7.4	0.265	7.49
-4604347	4.8	BT	7.5	NA	NA

SHEETBAR	Z	CALCZCD	DO	TP	TN
41015929	0.2	SF	14.4	0.075	2.557
41015929	1.0	OT	14.8	NA	NA
41015929	2.0	OT	14.9	NA	NA
41015929	3.0	OT	15.0	NA	NA
41015929	4.0	OT	15.2	NA	NA
41015929	4.6	BT	15.2	NA	NA

```
count_duplicates %>% kbl(booktabs = T)
```

proportion	number_duplicates
0.7393497	1
0.2377072	2
0.0166481	3
0.0006199	4
0.0002365	5
0.0007605	6
0.0046781	7
0.0000000	8

The proportion of SHEETBARs with at least one duplicated row is0.2606503 (representing about 47,000 rows). When do duplicated rows occur?

We look at two SHEETBARs with duplicated rows.

```
water20 %>%
  filter(SHEETBAR == -4604347) %>%
  select(SHEETBAR, Z, CALCZCD, DO, TP, TN) %>%
  kbl(booktabs = T) %>%
  kable_styling(latex_options = "striped")
```

```
water20 %>%
  filter(SHEETBAR == 41015929    ) %>%
  select(SHEETBAR, Z, CALCZCD, DO, TP, TN) %>%
  kbl(booktabs = T) %>%
  kable_styling(latex_options = "striped")
```

Here, we see that TP and TN, total phosphorous and total nitrogen, are measured only at the surface level (when CALCZCD == "SF"). The variable CALCZCD is a categorical variable with levels surface, middle, bottom, and other. It is calculated with the sample depth and the total water depth (of the river site).

In contrast, dissolved oxygen DO is measured at various depths (denoted by Z) because different parts of the water column have different levels of DO. It would be inappropriate to average the dissolved oxygen levels because they were taken at different sample depths.

Thus, this missing values of TP and TN are occuring at different sample depths at the same sampling site. These missing values aren't *really* missing values; they would be redundant to interpolate.

We can reasonably keep only the samples taken at the surface level

We decided to filter for rows that were labelled as surface level,`CALCZCD == "SF"`. Implicitly, this filtering step removes samples for which the sample depth is missing.

```
table(water20$CALCZCD)
```

```
##
##             BT     MD     OT     SF
##   8436  34991   2971  10736 147171
```

More than 70% of the samples were taken on the surface level. Of these measurements taken at the surface level, the eleven important continuous variables (in `water_var`) were recorded with a recording rate of at least 50%. This is a good sanity check because `TN` and `TP` are never recorded in the middle and bottom water depths. we checked to see the recording rate of the eleven important variables and found recording rates greater than 50%.

```
sapply(water20 %>%
         filter(CALCZCD == "SF") %>%
         select(all_of(water_var)),
       function(x) sum(is.na(x)/length(x)))
```

```
##         TN         TP       TEMP         DO       TURB       COND        VEL
## 0.49246115 0.50078480 0.01157837 0.01390220 0.01440501 0.01510488 0.39597475
##         SS        WDP     CHLcal     SECCHI
## 0.17570717 0.07648925 0.26196058 0.09751921
```

What if CALCZCD is missing?

There are are about 8000 samples with missing `CALCZCD`. However, we will see this is okay because when `CALCZCD` is missing, nearly all of our 11 continuous variables are missing too. These samples are not particularly useful.

```
(water20 %>%
  filter(CALCZCD == "") %>%
  dim())[1]
```

```
## [1] 8436
```

```
sapply((water20 %>%
  filter(CALCZCD == "") %>%
  select(all_of(water_var))), function(x) sum(is.na(x)/length(x)))
```

```
##        TN        TP      TEMP        DO      TURB      COND       VEL        SS
## 0.9998815 0.9998815 0.9992888 0.9992888 0.9996444 0.9992888 0.9997629 0.9996444
##       WDP    CHLcal    SECCHI
## 0.8488620 0.9996444 0.9665718
```

When `CALCZCD` isn't recorded, the rest of the variables aren't recorded. Since these samples represent 0.041 percent of the original data, we decide that it is okay to exclude these observations.

(Sidenote) Water column variables and SITETYPE

What is the difference between WDP, ZMAX, CALCZCD, SAMPZCD? (Could be answered later because not all these variables will be used in our analysis)

- received suggestion to filter `Z >= 0.2`

- SITETYPE should be for random samples, not fixed sites. SITETYPE == 2 means fixed sites.

```
table(water20$SITETYPE)
```

```
##
##      0      1      2
## 104759   4702  94844
```

Filter for surface level observations at fixed sites

This eliminates most of the duplicates. We will return to the duplicates discussion later. We also will not be using any of the fixed sites for interpolation or TDA. We will remove these rows with the SITETYPE value '2' because... TODO.

```
water20 <- water20 %>%
  filter(CALCZCD == "SF") %>%
  filter(SITETYPE != 2) %>%
  select(all_of(c(identifier_var, water_var, waterQF_var)))
```

3. QA/QC filtering

We have 11 continuous water quality variables. They have corresponding QA/QC codes which describe the quality of the data collected. *For the collected data are too compromised, we set their value to NA to interpolate later.* The low quality data values will not be used in our subsequent analysis.

The QA/QC codes that we do not want are as follows:

- 7 of them, TURBQF, TEMPQF, DOQF, VELQF, ZMAXQF, SECCHIQF, and CONDQF, will be filtered out if they are "A" or "0" (in Python, pandas reads each column as characters and integers, so 0 must also be filtered for if using pandas. In R, the entire column is converted to character type).
- 3 of them, TNQF, TPQF, and SSQF, will be filtered out if they are 8 or 64.
- 1 of them, CHLcal, doesn't have a corresponding QF code. TODO

The code works as follows:

1. Define two character vectors, one for which QF codes of "A" and "0" are problematic; one for which QF codes of 8 and 64 are problematic.
2. Create a temporary index tmp_idx for each row in the dataset because, as we know, SHEETBARs are not unique identifiers!
3. For the entire water dataset, do the following:

a. Define two functions that appropriately set the water variable values to NA. There are two functions because there are two QF code rules ("A" and "0"; 8 and 64). Each function will iterate through pairs of columns (of the variable and corresponding QF code variable) to set the variable column to NA.
b. Join the pairs of columns (by tmp_idx). This join happens twice, once for each function.
c. Join the two dataframes (by tmp_idx).
d. Join with the entire water dataset to get the identifier_var.

```
qf_A0 <- c("TURBQF", "TEMPQF", "DOQF", "VELQF", "ZMAXQF",
                 "SECCHIQF", "CONDQF")

qf_864 <- c("TNQF", "TPQF", "SSQF")
```

```r
water20$tmp_idx <- 1:nrow(water20)
```

```r
qfcodes_setNA <- function(qf_AO, qf_864, water_df,
                          identifier_var, water_var, waterQF_var){
  # qf_AO is a character vector of the variable qf names for which
  # A, O qf codes are bad

  # qf_864 is a character vector of the variable qf names for which
  # 8, 64 qf codes are bad

  # water_df is the entire water_df

  # last 3 variables are just for naming

  replace_na_qf <- function(qf_str, df, two_badqfval){

    # remove QF at the end of qf_str
    var_str <- substr(qf_str, 1, nchar(qf_str)-2)

    if (var_str == "ZMAX") { var_str <- "WDP"}

    df <- df %>%
      # !!sym is for non standard evaluation
      mutate(!!sym(var_str) := case_when(!!sym(qf_str) == two_badqfval[1] ~ NA_real_,
                                         # specify the type of NA correctly
                                         !!sym(qf_str) == two_badqfval[2] ~ NA_real_,
                                         TRUE ~ !!sym(var_str))) %>%
                                         # other QF code values are fine, keep data
      select(all_of(c("tmp_idx", var_str, qf_str))) # keep sheetbar for joins

    return(df)

    }
  # remove_864 <- function(qf_str, df){
  #
  #   # remove the QF at the end
  #   var_str <- substr(qf_str, 1, nchar(qf_str)-2)
  #
  #   df <- df %>%
  #     mutate(!!sym(var_str) := case_when(!!sym(qf_str) == 8 ~ NA_real_,
  #                                        # use correct NA type and !!sym for NSE
  #                                        !!sym(qf_str) == 64 ~ NA_real_,
  #                                        TRUE ~ !!sym(var_str))) %>%
  #                                        # remaining QF code values are fine
  #     select(all_of(c("tmp_idx", var_str, qf_str))) # sheetbars for joining
  #
  # }

  remove_AO_df <- bind_cols(lapply(qf_AO, replace_na_qf, water_df, c("A", "O"))) %>%
    rename(tmp_idx = `tmp_idx...1`) %>%
    select(!contains("..."))

  remove_864_df <- bind_cols(lapply(qf_864, replace_na_qf, water_df, c(8, 64))) %>%
    rename(tmp_idx = `tmp_idx...1`) %>%
    select(!contains("..."))

  fixedqf_df <- inner_join(remove_864_df, remove_AO_df, by = "tmp_idx") %>%
    inner_join(water_df, by = c("tmp_idx", waterQF_var)) %>%
    # this causes duplicate columns for water_var, which we do want
    # because water_df has the old (wrong) values for water_var
    select(!contains(".y")) %>% # remove the old (wrong) values from water_df
    rename_with(~ gsub(".x", "", .), contains(".x")) %>% # rename
    select(all_of(c(identifier_var, water_var, waterQF_var))) # reorder columns

  return(fixedqf_df)

}

qfwater20 <- qfcodes_setNA(qf_AO, qf_864, water20,
                           identifier_var, water_var, waterQF_var)
```

check that `qfwater20` is working as we want.

This test function iterates through each variable (and its corresponding QF code):

1. `badqf_length` is the number of rows with bad qf codes
2. `badqf_sum` is the sum of NA values among the bad qf codes
3. We want `badqf_length == badqf_sum`.

```r
qfcodes_check <- function(qf_str, df, two_badqfval){

  var_str <- substr(qf_str, 1, nchar(qf_str)-2)
  if (var_str == "ZMAX") {var_str = "WDP"}

  badqf_length <- df %>%
    filter(!!sym(qf_str) == two_badqfval[1] | !!sym(qf_str) == two_badqfval[2]) %>%
    pull(!!sym(var_str)) %>%
    length()

  badqf_sum <- df %>%
    filter(!!sym(qf_str) == two_badqfval[1] | !!sym(qf_str) == two_badqfval[2]) %>%
    pull(!!sym(var_str)) %>%
    is.na(.) %>%
    sum()

  if (badqf_length != badqf_sum) {return(qf_str)}
  return(badqf_length == badqf_sum)

}

c(unlist(lapply(qf_AO, qfcodes_check, qfwater20, c("A", "O"))),
  unlist(lapply(qf_864, qfcodes_check, qfwater20, c(8, 64))))
```

```
##  [1] TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
```

4. Removing duplicates (continued): combine the rows that have the same SHEETBAR code

The purpose of this next component is to clean the current data set and remove the remaining rows with non-unique barcodes (SHEETBAR). This will be done by combining or "collapsing" the rows with he same barcode. While filtering for the samples taken at the surface of the river (CALCZCD == "SF") accounted for a majority of the rows with identical barcodes, there are still several rows that need to be removed.

It is important that our data sets consists only of unique barcodes because it removes issues when using interpolating the data and predicting our missing continuous variable values. Some of the TN and TP values that appear to be missing for a sample sites are in fact not missing and can be found in a different row of the data with the same sample site. In other words, if a missing value is actually just misplaced, there is no need to interpolate it.

In each instance of multiple rows with the same SHEETBAR, there will be some combinations of sample and NA values for each continuous variable. Since our goal is combine it to combine the rows with the same SHEETBAR, we will find the average for each column, excluding the DATE, STRATUM, LOCATCD, LATITUDE and LONGITUDE columns.

The data set at this point should have already been filtered for the surface samples and bad QF codes.

```r
# Collapse the rows with the same SHEETBAR code
row_collapse <- function(data, water_var, identifier_var) {

  # Count how many rows each sheetbar has
  sheetbar_counts <- data %>%
    group_by(SHEETBAR) %>%
    dplyr::summarize(count = n()) %>%
    arrange(-count) # 147130

  # Filter for the sheetbars that have multiple rows
  sheetbar_dups <- sheetbar_counts %>% filter(count > 1) # 33
  data_dups <- data[data$SHEETBAR %in% sheetbar_dups$SHEETBAR, ] # 74

  # Set aside the rows with sheetbars that only occur once
  water_cleaned <- data[!(data$SHEETBAR %in% sheetbar_dups$SHEETBAR), ]


  # Average the continuous vars and re-merge the identifiers to the collapsed rows
  data_dups_ids <- data_dups[identifier_var]

  # Find the mean of the continuous variables
  data_dups <- aggregate(data_dups[water_var],
                         by = list(data_dups$SHEETBAR),
                         FUN = mean,
                         na.rm = TRUE,
                         na.action = na.pass)
  colnames(data_dups)[colnames(data_dups) == 'Group.1'] <- 'SHEETBAR'

  # Rounds the data frame
  is.num <-sapply(data_dups, is.numeric)
  data_dups[is.num] <- lapply(data_dups[is.num], round, 2)

  # Replace NaN with Na to be consistent with the rest of the data
  data_dups[is.na(data_dups)] <- NA
  # Merge the ids back to the water_vars
  data_dups <- unique(merge(data_dups, data_dups_ids, by = 'SHEETBAR'))

  # Add the collapsed rows to the cleaned data
  water_cleaned <- rbind(water_cleaned, data_dups)

  return(water_cleaned)

}
```

```
# Just continuous vars and identifiers (remove QF columns)
qfwater20 <- qfwater20[c(water_var, identifier_var)]

qfwater20 <- row_collapse(qfwater20, water_var, identifier_var)
```

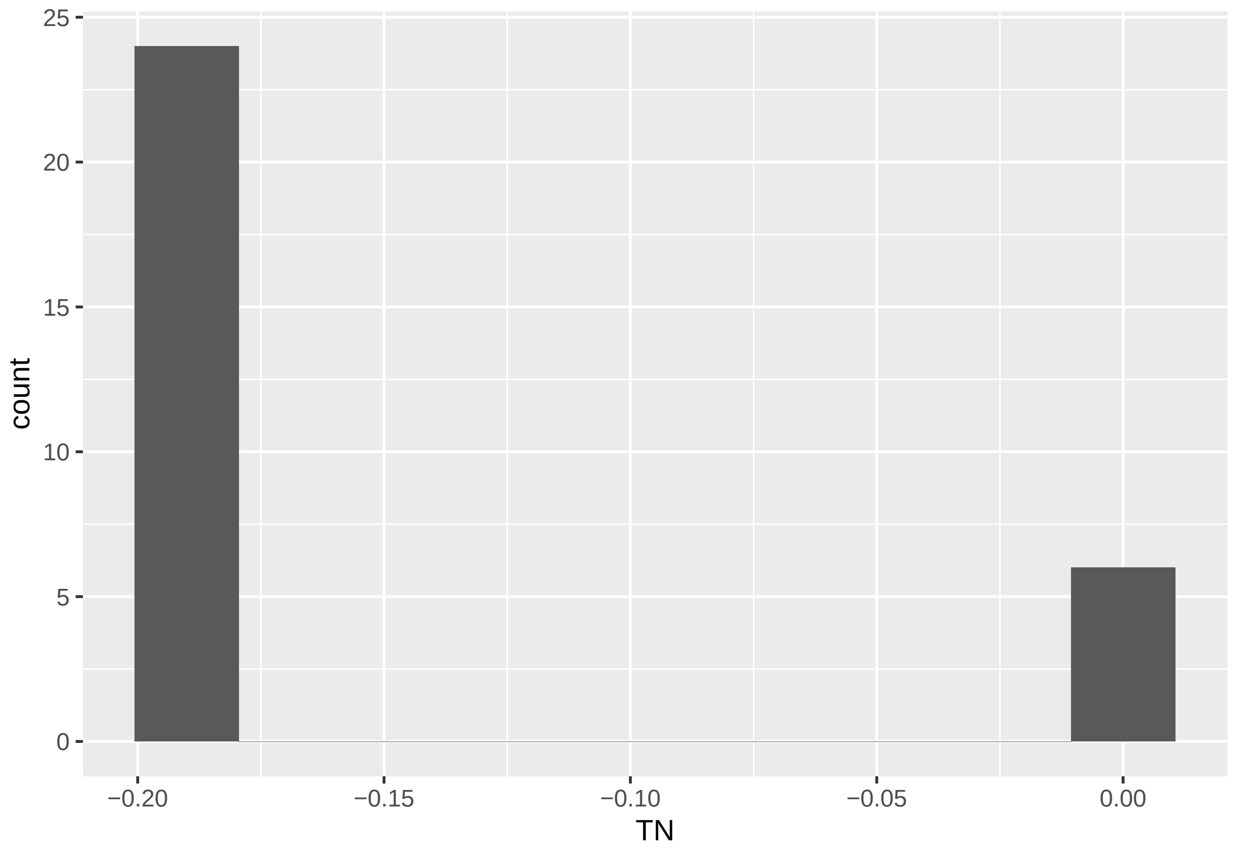
5. Replace negative values with NA

Due to bad readings when sampling, there are negative values for some of the continuous variables. Since we do not want to throw away data that is mostly usable, we will replace the negative value and instead interpolate the value.

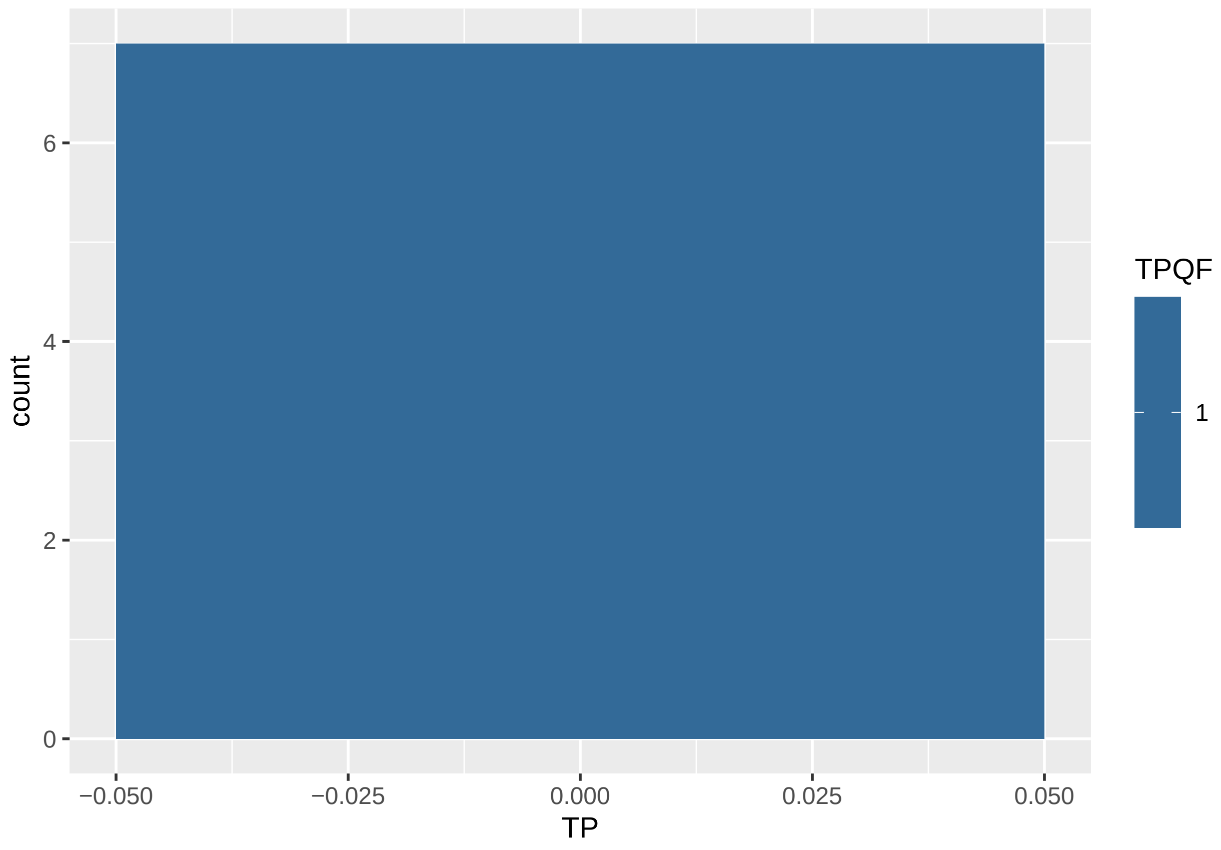
However, notice that there are actually quite a few negative values in the fixed-site, surface-level samples.

```
tmp <- replace(qfwater20[water_var[water_var != "TEMP"]],
               qfwater20[water_var[water_var != "TEMP"]] < 0, NA)


lapply(water_var[!(water_var %in% c("WDP", "CHLcal"))], function(var, df)
  df %>%
    select(all_of(c(var, paste(var, "QF", sep = "")))) %>%
    filter(!!sym(var) < 0) %>%
    mutate(var = paste(var)) %>%
    ggplot(aes(x = !!sym(var))) +
             geom_histogram(aes(fill = !!sym(paste(var, "QF", sep = ""))),
                            bins = 10), water20)
```

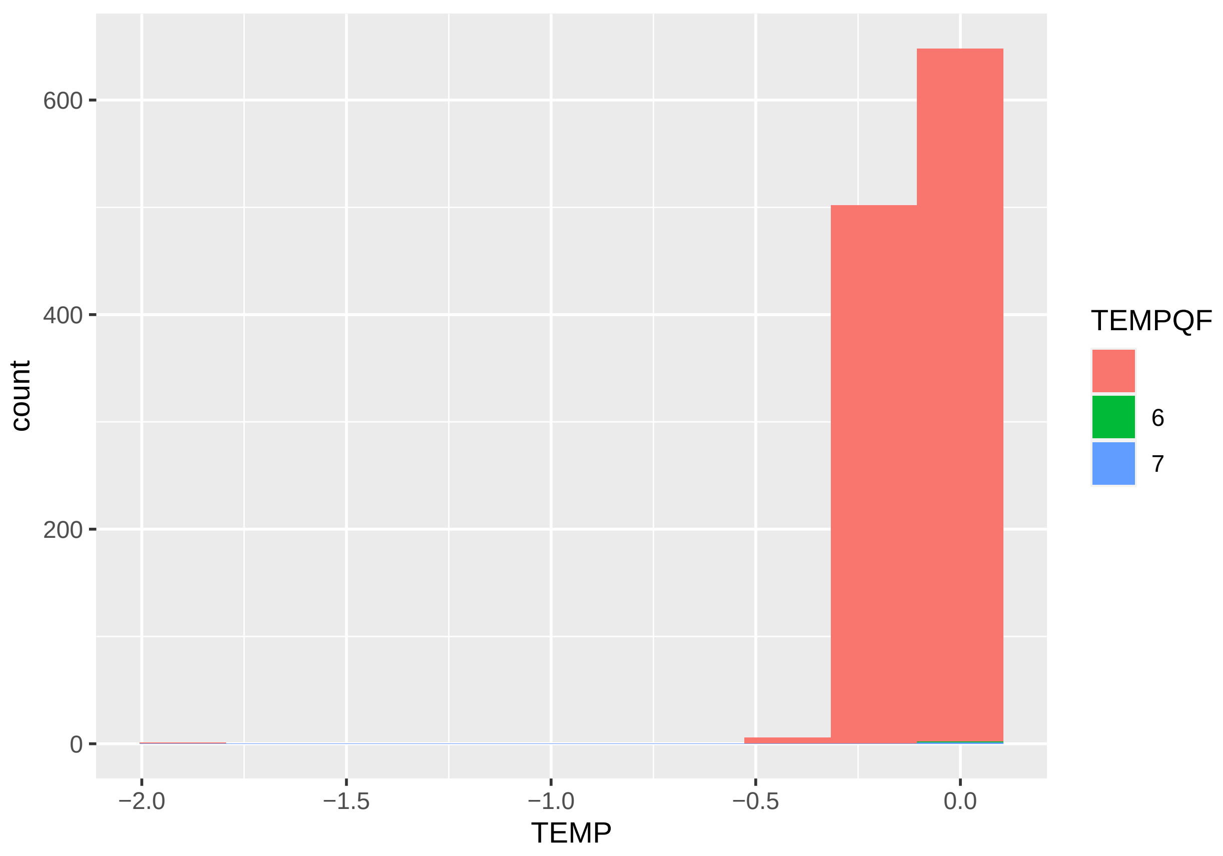
```
## [[1]]
```



```
##
## [[2]]
```

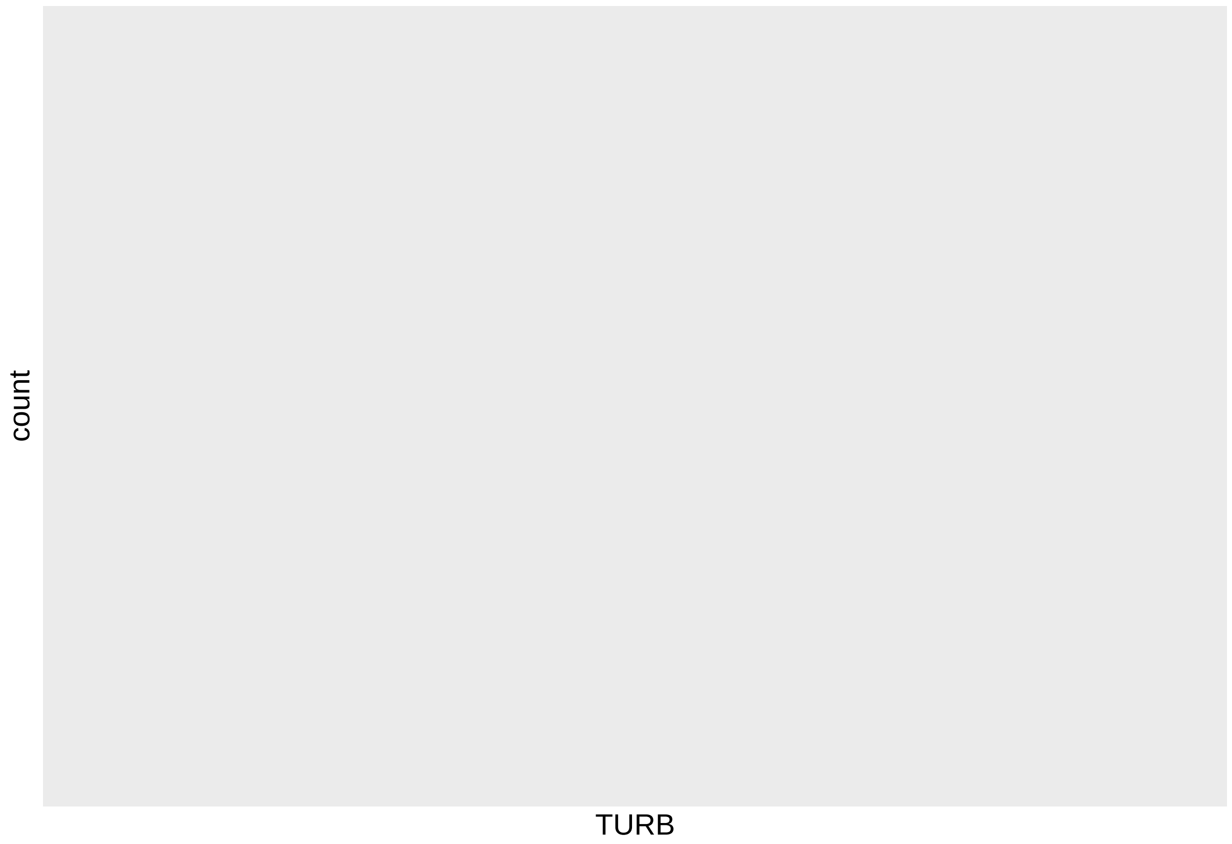


```
##
## [[3]]
```



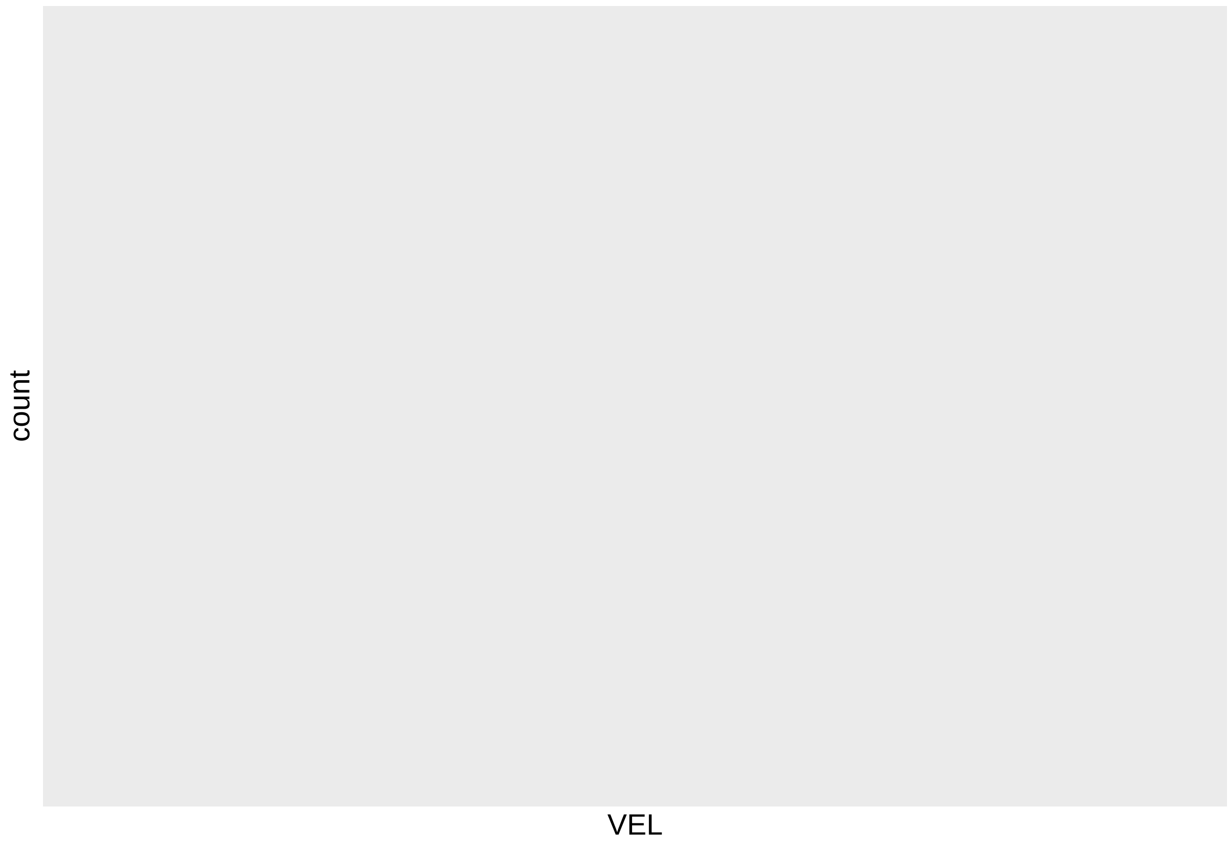
```
##
## [[4]]
```

```
##
## [[5]]
```

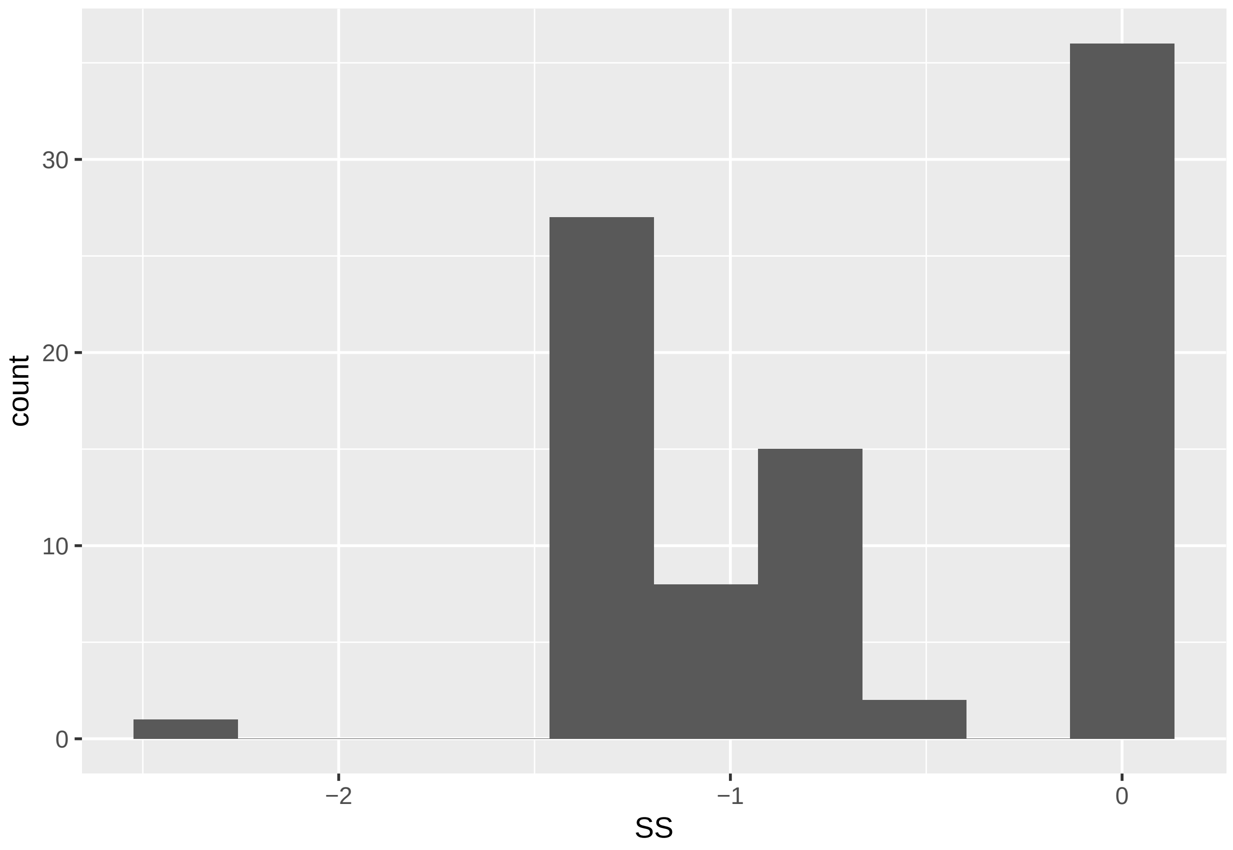


```
##
## [[6]]
```

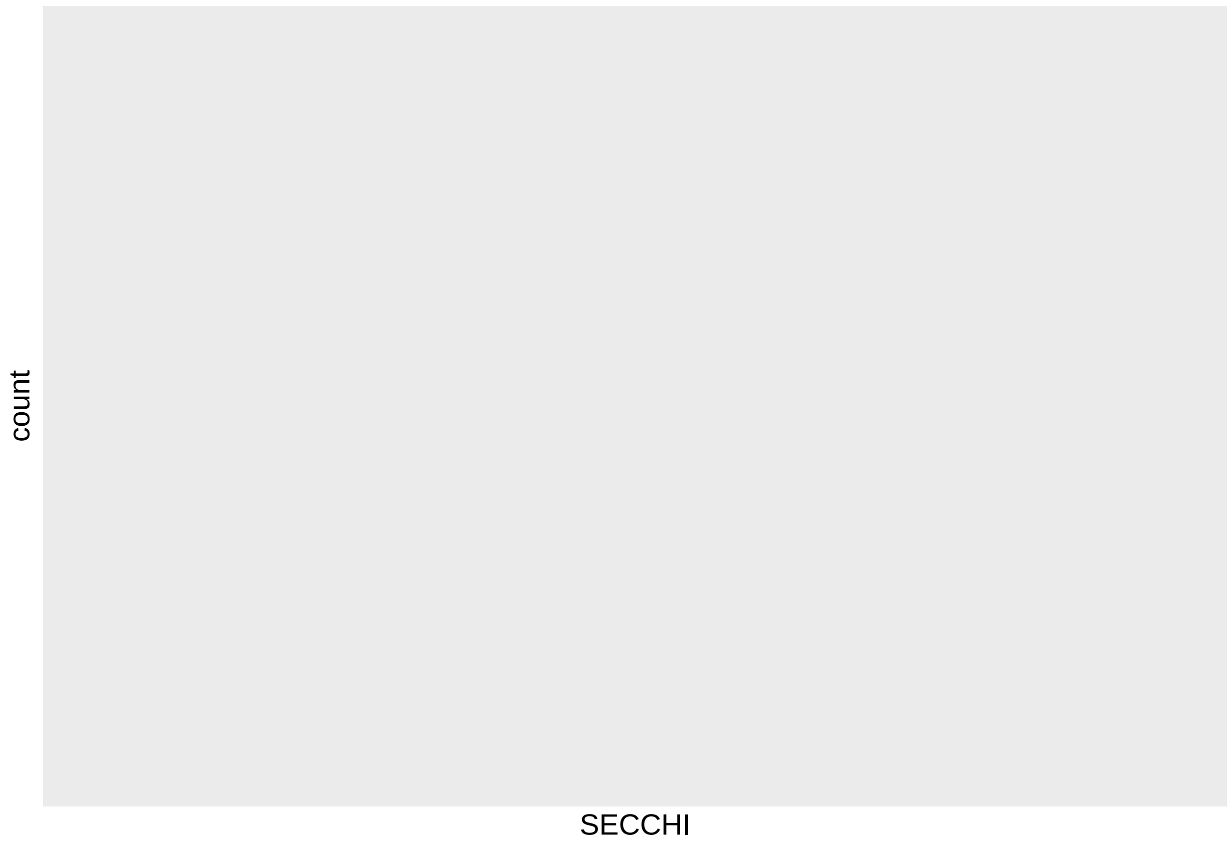
```
##
## [[7]]
```



```
##
## [[8]]
```



```
##
## [[9]]
```



```
# lapply(water_var, function(var, df)
#   df %>%
#     select(var) %>%
#     filter(!!sym(var) < 0) %>%
#     mutate(var = paste(var)), qfwater20)
#
#
# lapply(water_var, function(var, df)
#   df %>%
#     select(var) %>%
#     filter(!!sym(var) < 0) %>%
#     mutate(var = paste(var)), tmp) # this checks that we successfully set negative values to 0
```

```
write.csv(tmp, "../LTRM data/water_data_qfneg.csv", row.names = FALSE)
```