Synoptic CB: Porewater SO4/Cl

June 2024 Samples

2025-09-16

Contents

##Add Required Packages

0.1 Run Information

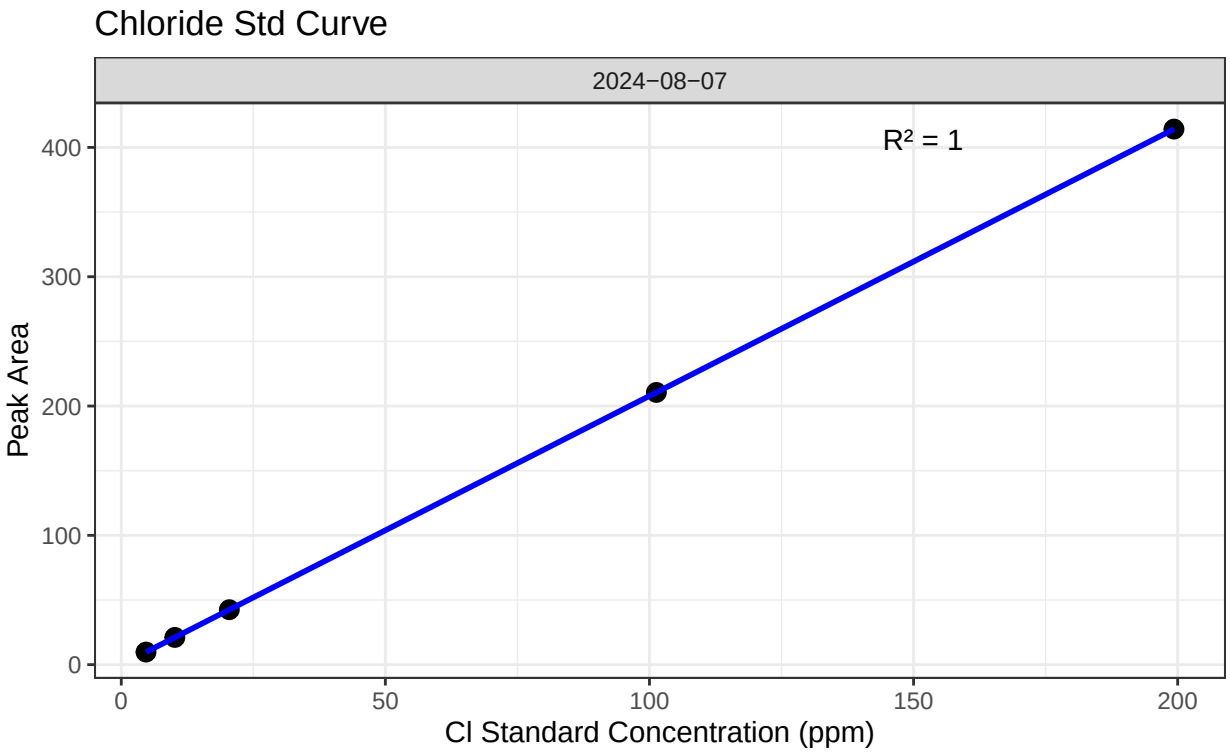
```
###### Run information - PLEASE CHANGE
  Date_Run = "2024-08-07"  #Date that instrument was run
  Run_by = "Zoe Read"  #Instrument user
  Script_run_by = "Zoe Read" #Code user
  run_notes = "<80% of Sulfate Check Standards are within range of expected concentration - REASSESS,
  specifically check standards 1 and 2 were lower than expected;
  <80% (2/4) of Sulfate Duplicates have a CV <10% - REASSESS,
  although one of the dups had a CV of 15 which was not too much higher than the cutoff of 10;
  <80% (3/4) of SO4 spikes have a recovery between the high and low cutoff - REASSESS;
  The two samples from the FTS were adl;
  One blank was high
  Some sample IDs are missing from metadata:
  FTS_1630_20230816
  FTS_1730_20230816
  " #any notes from the run
  samples <- c("GCW", "GWI", "MSM", "SWH") #whatever identifies your samples within the same names
  samples_pattern <- paste(samples, collapse = "|")
    #samples_pattern <- "GCW" #use this instead of the line above if you have only one site code

###### File Names - PLEASE CHANGE
#file path and name for raw summary data file
  raw_file_name_cl = "Raw Data/COMPASS_Synoptic_CB_MonMon_202406_Cl.txt"
  raw_file_name_so4 = "Raw Data/COMPASS_Synoptic_CB_MonMon_202406_SO4.txt"

#file path and name of processed data file
  processed_file_name = "Processed Data/COMPASS_SynopticCB_PW_Processed_Cl_SO4_202406.csv"

###### Log Files - PLEASE CHECK
#downloaded metadata csv - downloaded from Google drive as csv for this year
  Raw_Metadata = "Raw Data/COMPASS_SynopticCB_PW_SampleLog_2024.csv"

#qaqc log file path for this year
  Log_path = "Raw Data/COMPASS_Synoptic_Cl_SO4_QAQClog_2024.csv"
```

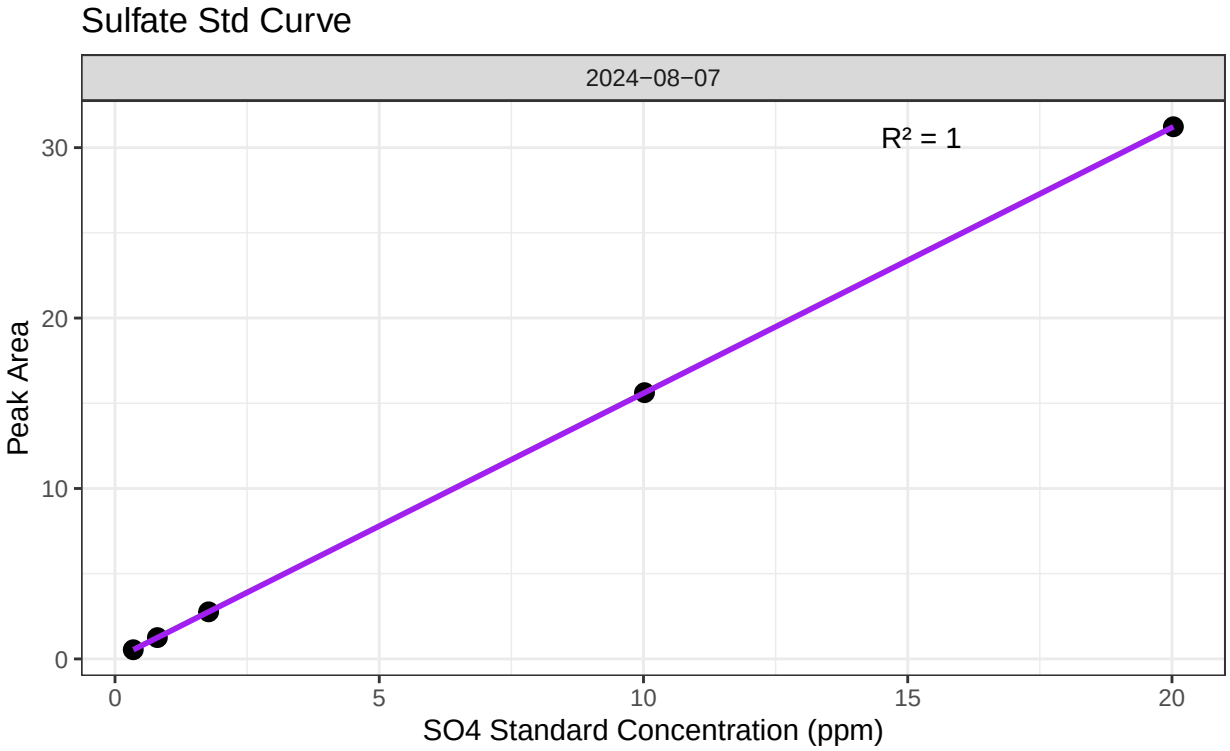
##Set Up Code - constants and QAQC cutoffs

##Read in metadata and create similar sample IDs for matching to samples

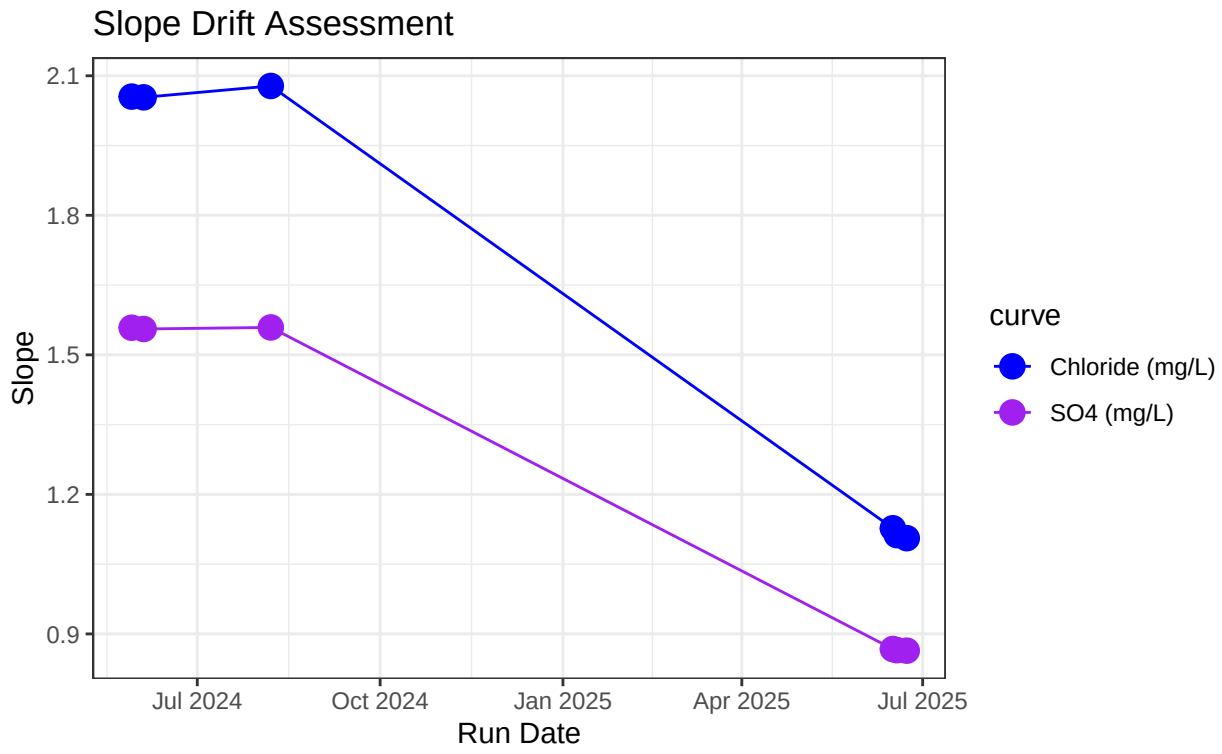
##Import Sample Data

0.2 Assess Standard Curves






```
## [1] "QAQC log file exists and has been read into the code."
```




```
## [1] "Cl Curve r2 GOOD"
```

```
## [1] "SO4 Curve r2 GOOD"
```

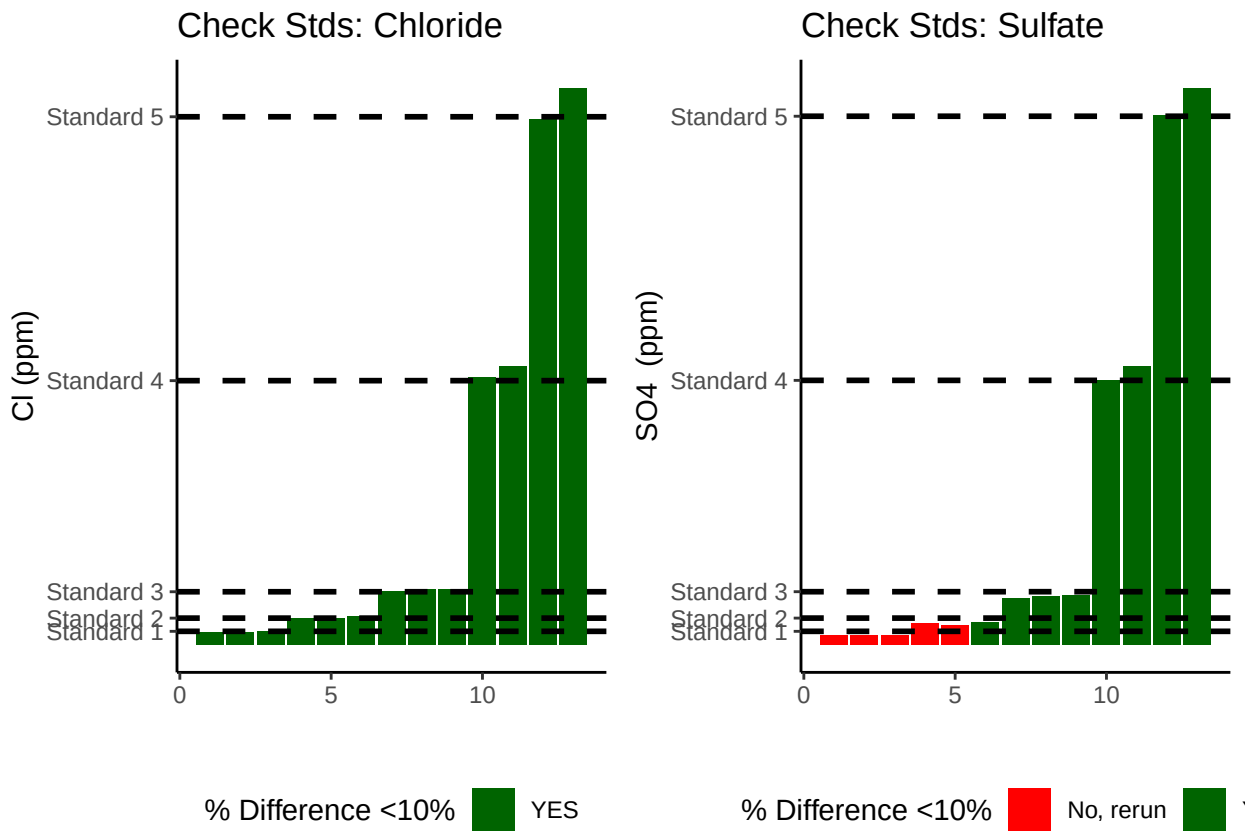
0.3 Assess Check Standards

```
## # A tibble: 5 x 5
##   sample_ID  mean_Cl sd_Cl  cv_Cl flag_Cl
##   <chr>        <dbl> <dbl>  <dbl> <chr>
## 1 Standard 1    4.84 0.164 0.0338 Chloride Check Standard RSD within Range - PR~
## 2 Standard 2   10.2  0.373 0.0364 Chloride Check Standard RSD within Range - PR~
## 3 Standard 3   20.8  0.315 0.0151 Chloride Check Standard RSD within Range - PR~
## 4 Standard 4  103.   2.98  0.0289 Chloride Check Standard RSD within Range - PR~
## 5 Standard 5  205.   8.32  0.0405 Chloride Check Standard RSD within Range - PR~
```

```
## # A tibble: 5 x 5
##   sample_ID  mean_SO4 sd_SO4 cv_SO4 flag_SO4
##   <chr>         <dbl>  <dbl>  <dbl> <chr>
## 1 Standard 1    0.359 0.0128 0.0356 Sulfate Check Standard RSD within Range - P~
## 2 Standard 2    0.802 0.0599 0.0746 Sulfate Check Standard RSD within Range - P~
## 3 Standard 3    1.83  0.0496 0.0271 Sulfate Check Standard RSD within Range - P~
## 4 Standard 4   10.3   0.369  0.0359 Sulfate Check Standard RSD within Range - P~
## 5 Standard 5   20.6   0.748  0.0364 Sulfate Check Standard RSD within Range - P~
```

```
## [1] ">80% of Chloride Check Standards have RSD within range - PROCEED"
```

```
## [1] ">80% of Sulfate Check Standards have RSD within range - PROCEED"
```



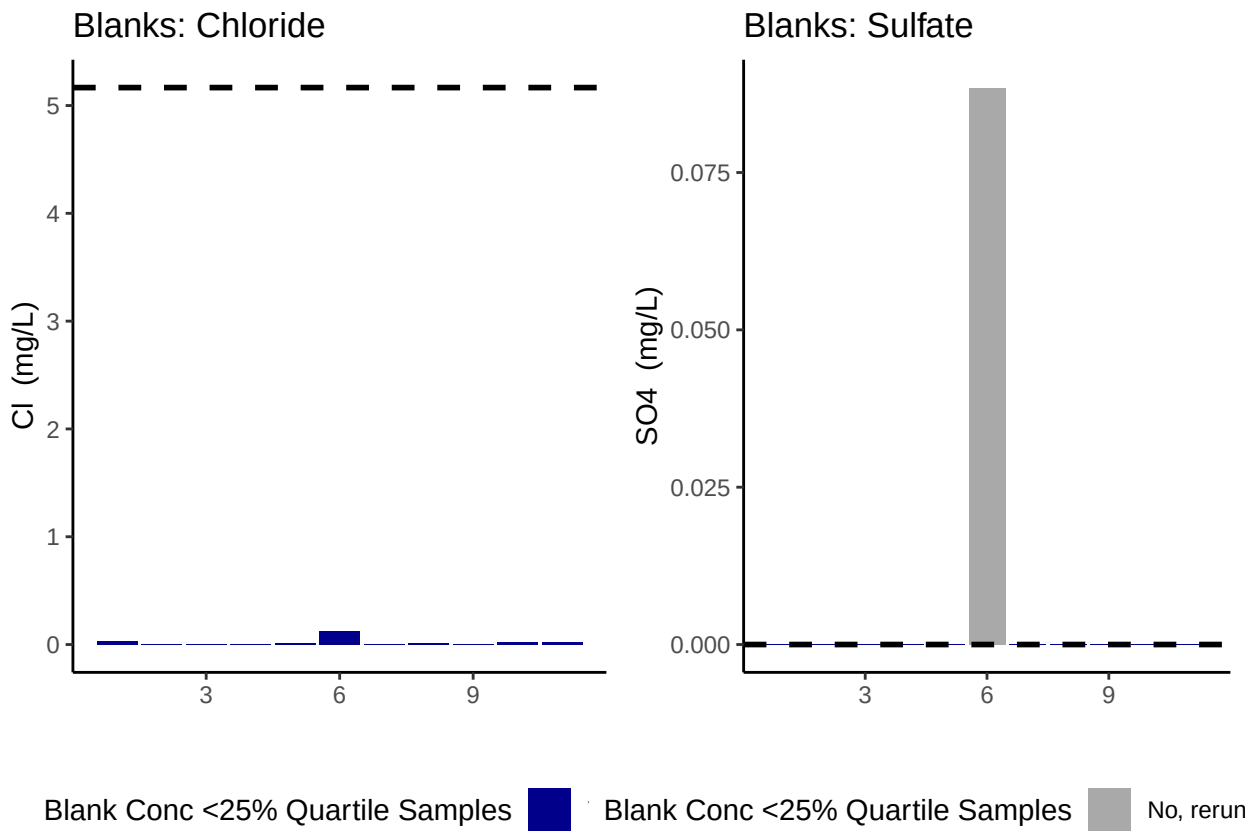

```
## [1] ">80% of Chloride Check Standards are within range of expected concentration - PROCEED"
```

```
## [1] "<80% of Sulfate Check Standards are within range of expected concentration - REASSESS"
```

0.4 Assess Blanks

```
## [1] ">80% of Chloride Blank concentrations are lower 25% quartile of samples"
```

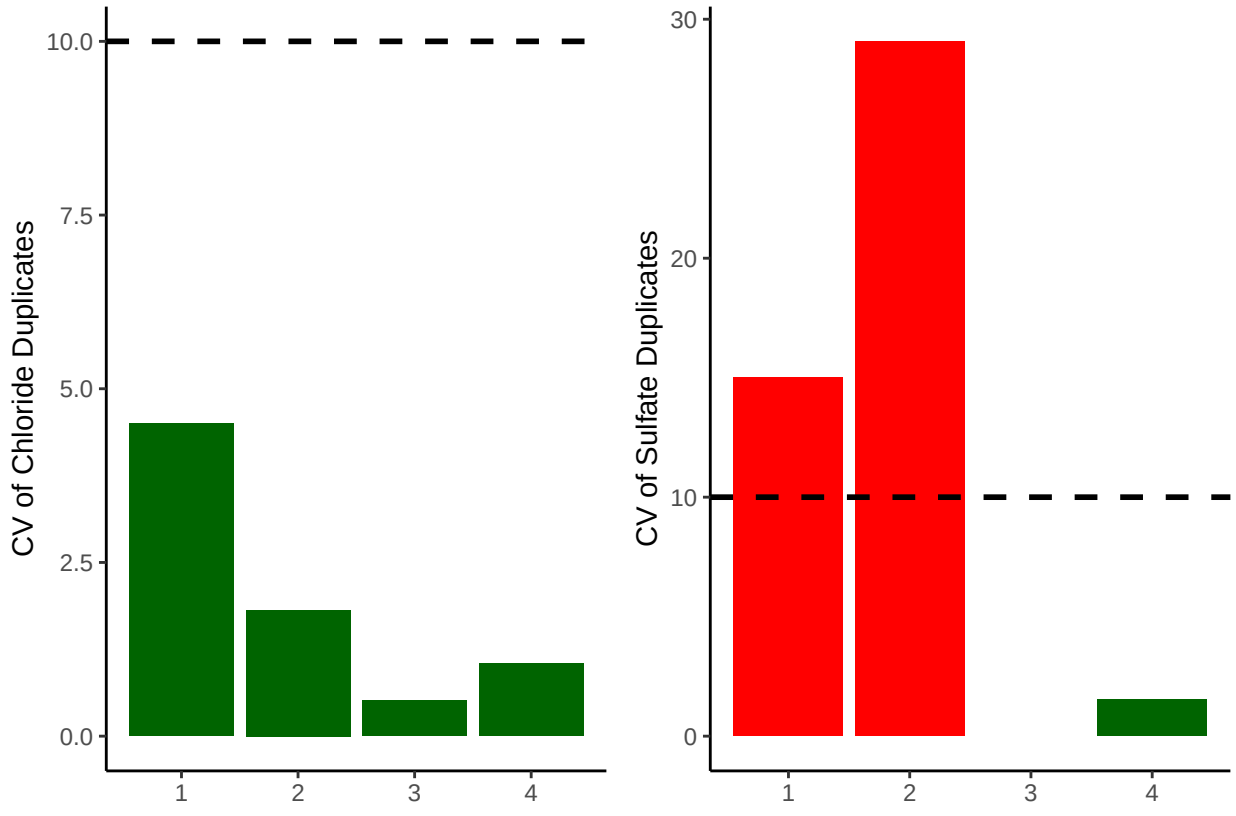
```
## [1] ">80% of Sulfate Blank concentrations are lower 25% quartile of samples"
```




```
## Chloride blanks mean ppm:

## [1] 0.02226364

## Sulfate blanks mean ppm:

## [1] 0.008045455
```

0.5 Assess Duplicates

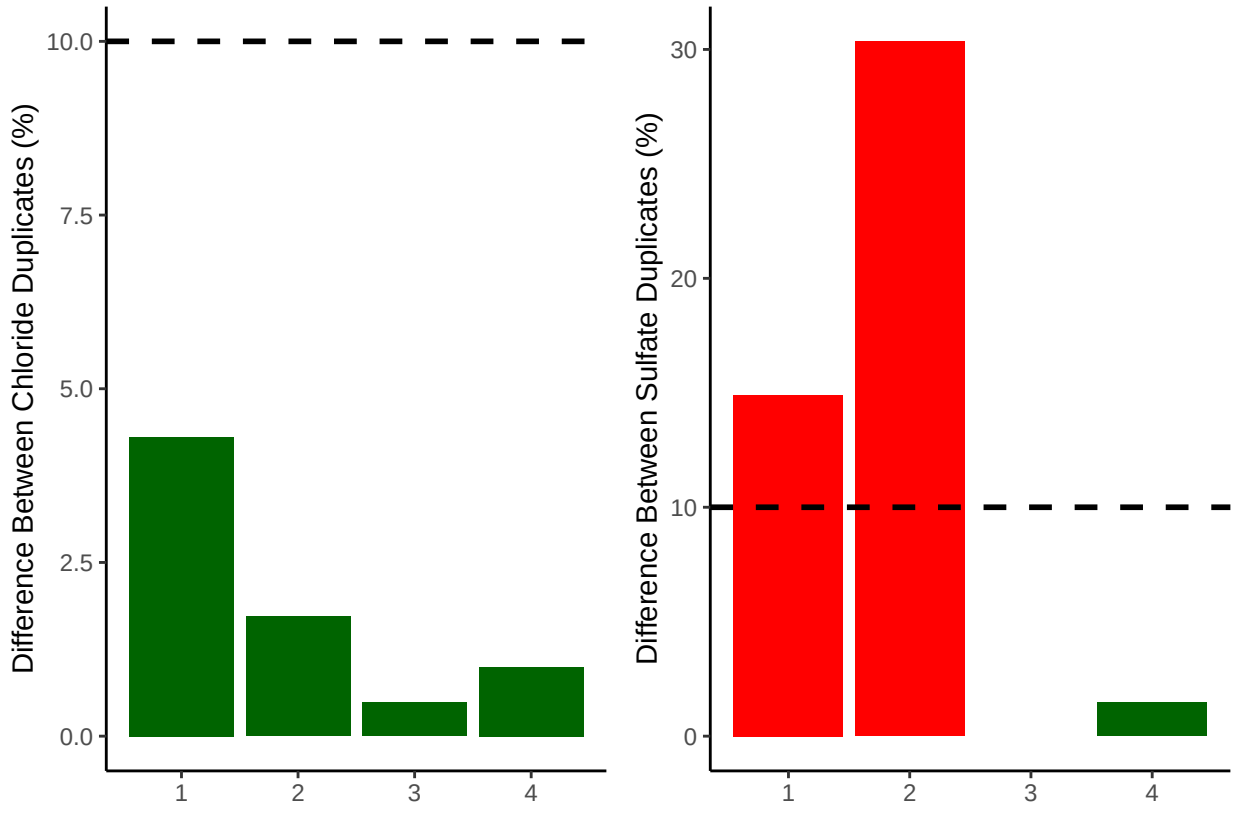
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## (`geom_bar()`).
```




```
## [1] ">80% of Chloride Duplicates have a CV <10% - PROCEED"
```

```
## [1] "<80% of Sulfate Duplicates have a CV <10% - REASSESS"
```

```
## Warning: Removed 1 row containing missing values or values outside the scale range
## (`geom_bar()`).
```




```
## [1] ">80% of Chloride Duplicates have a percent difference <10% - PROCEED"
```

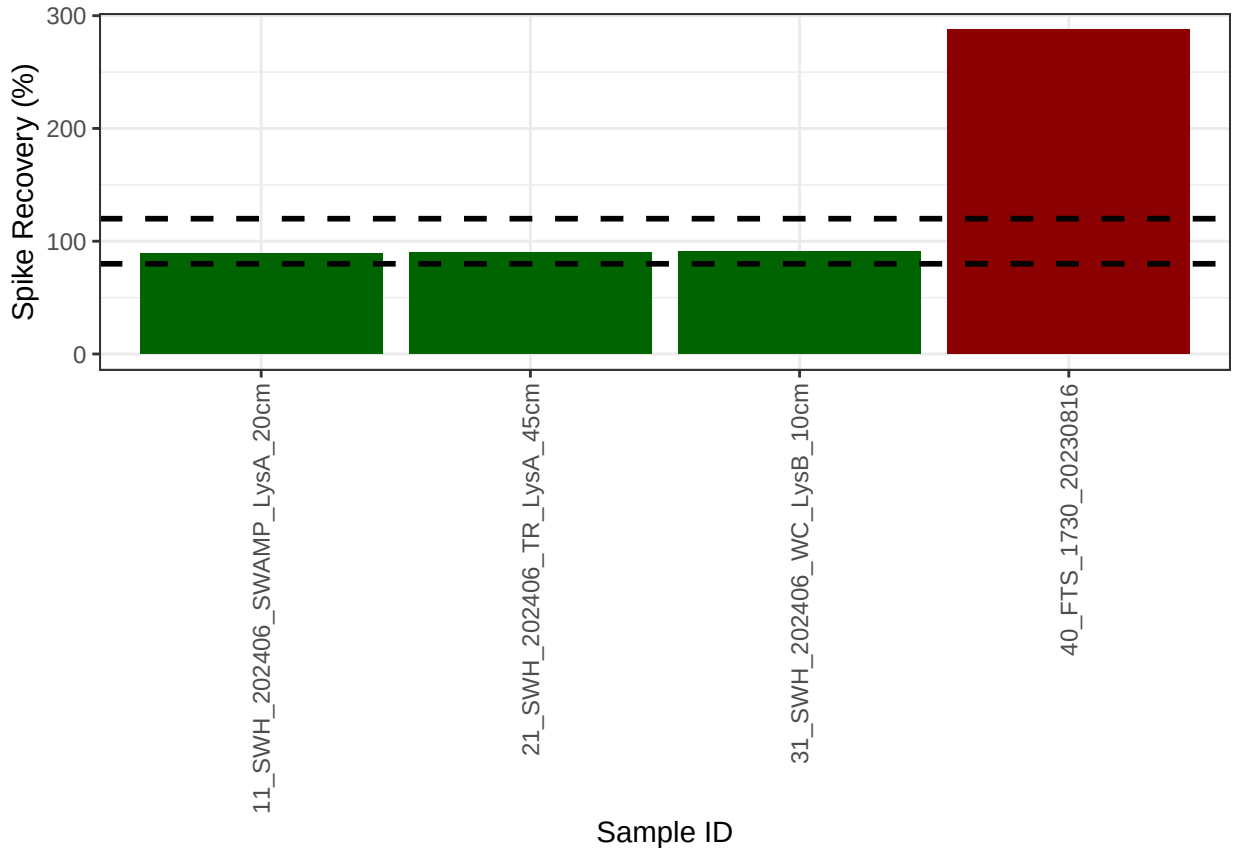
```
## [1] "<80% of Sulfate Duplicates have a CV <10% - REASSESS"
```

0.6 Calculate mmol/L concentrations & salinity, add dilutions

```
# Convert ppm to mmol/L
all_dat$SO4_Conc_mM <- (all_dat$SO4_ppm / s_mw)
all_dat$Cl_Conc_mM <- (all_dat$Cl_ppm / cl_mw)

# Calculate Salinity
# calculated using the Knudsen equation
# Salinity = 0.03 + 1.8050 * Chlorinity
# Ref: A Practical Handbook of Seawater Analysis by Strickland & Parsons (P. 11)
# =((1.807*Cl_ppm)+0.026)/1000
all_dat$salinity <- ((1.8070 * all_dat$Cl_ppm) + 0.026) / 1000

#Need to determine dilution factors for your samples
#for Steph / COMPASS this depends on the site so...
all_dat$Dilution <- 1
all_dat$Dilution <-  ifelse(str_detect(all_dat$sample_ID, "MSM") & str_detect(all_dat$sample_ID, "UP"),
all_dat$Dilution <-  ifelse(str_detect(all_dat$sample_ID, "MSM") & str_detect(all_dat$sample_ID, "TR"),
all_dat$Dilution <-  ifelse(str_detect(all_dat$sample_ID, "MSM") & str_detect(all_dat$sample_ID, "WC"),
```

```r
all_dat$Dilution <-  ifelse(str_detect(all_dat$sample_ID, "MSM") & str_detect(all_dat$sample_ID, "SW"),

all_dat$Dilution <-  ifelse(str_detect(all_dat$sample_ID, "GCW") & str_detect(all_dat$sample_ID, "UP"),
all_dat$Dilution <-  ifelse(str_detect(all_dat$sample_ID, "GCW") & str_detect(all_dat$sample_ID, "TR"),
all_dat$Dilution <-  ifelse(str_detect(all_dat$sample_ID, "GCW") & str_detect(all_dat$sample_ID, "WC"),
all_dat$Dilution <-  ifelse(str_detect(all_dat$sample_ID, "GCW") & str_detect(all_dat$sample_ID, "SW"),

all_dat$Dilution <-  ifelse(str_detect(all_dat$sample_ID, "GWI") & str_detect(all_dat$sample_ID, "UP"),
all_dat$Dilution <-  ifelse(str_detect(all_dat$sample_ID, "GWI") & str_detect(all_dat$sample_ID, "TR"),
all_dat$Dilution <-  ifelse(str_detect(all_dat$sample_ID, "GWI") & str_detect(all_dat$sample_ID, "WC"),
all_dat$Dilution <-  ifelse(str_detect(all_dat$sample_ID, "GWI") & str_detect(all_dat$sample_ID, "SW"),

all_dat$Dilution <-  ifelse(str_detect(all_dat$sample_ID, "SWH"), 50, all_dat$Dilution)

# head(all_dat)
```

0.7 Assess Analytical Spikes




```
## [1] "<80% of SO4 spikes have a recovery between the high and low cutoff - REASSESS"
```

0.8 Check if samples within the range of the standard curve

```
## Sample Flagging
```

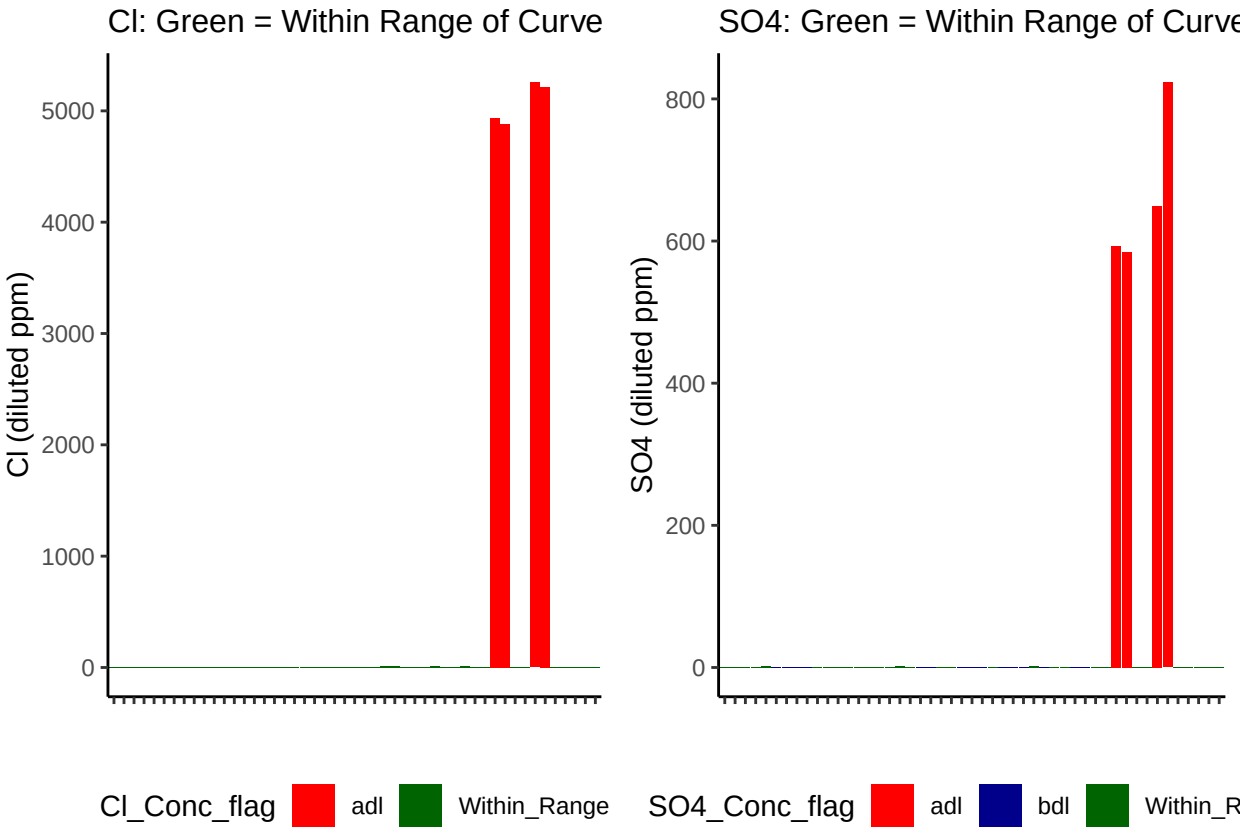


Table 1: SO4 samples

SO4_Conc_flag	Percent_samples
Within_Range	61.224490
adl	8.163265
bdl	30.612245

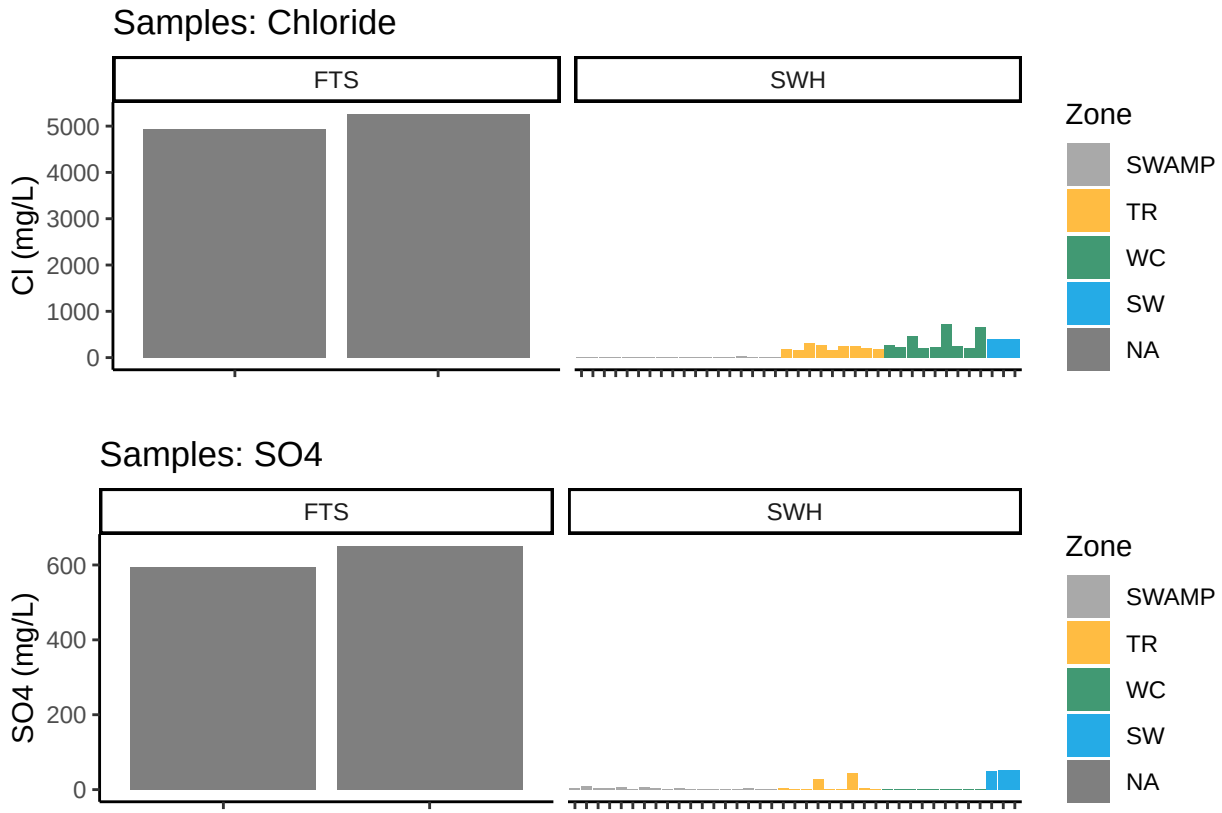
Table 2: Cl samples

Cl_Conc_flag	Percent_samples
Within_Range	91.836735
adl	8.163265

0.9 Check to see if samples run match metadata & merge info

```
## Some sample IDs are missing from metadata.

## [1] "FTS_1630_20230816" "FTS_1730_20230816"
```

0.10 Visualize Data by Plot



0.11 Export Processed Data

#end