Synoptic CB: Porewater SO4/Cl

July 2025 Samples

2025-10-22

Contents

##Add Required Packages

0.1 Run Information

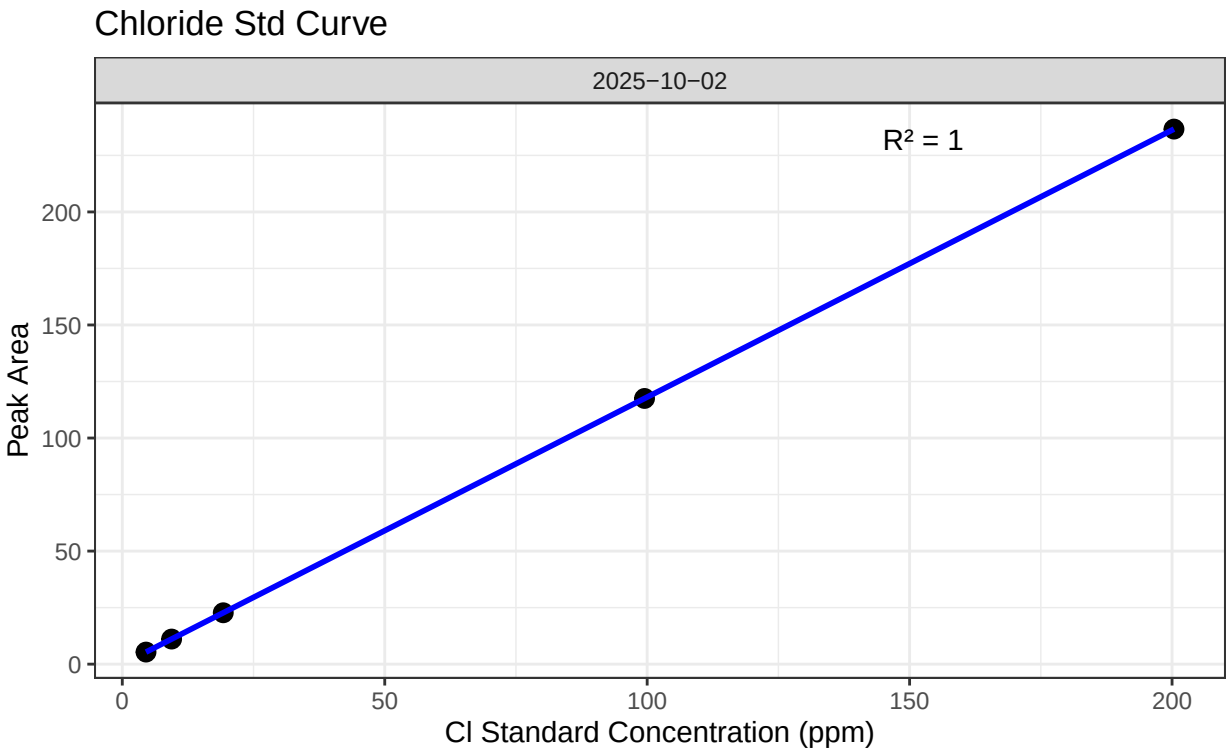
```
###### Run information - PLEASE CHANGE
  Date_Run = "2025-10-02"  #Date that instrument was run
  Run_by = "Zoe Read"  #Instrument user
  Script_run_by = "Zoe Read" #Code user
  run_notes = "Std 1 is lower than the expected concentration.
  Some sample IDs are missing from metadata:
  MSM_202507_UP_LYSB_20CM, MSM_202507_UP_LYSB_45CM, MSM_202507_UP_LYSC_10CM, GCW_202507_TR_LYSA_10CM,
  9, 10, 88, 89 (test samples for Lucie)
  " #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_202507_Cl.txt"
  raw_file_name_so4 = "Raw Data/COMPASS_Synoptic_CB_MonMon_202507_SO4.txt"

#file path and name of processed data file
  processed_file_name = "Processed Data/COMPASS_SynopticCB_PW_Processed_Cl_SO4_202507.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_2025.csv"

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

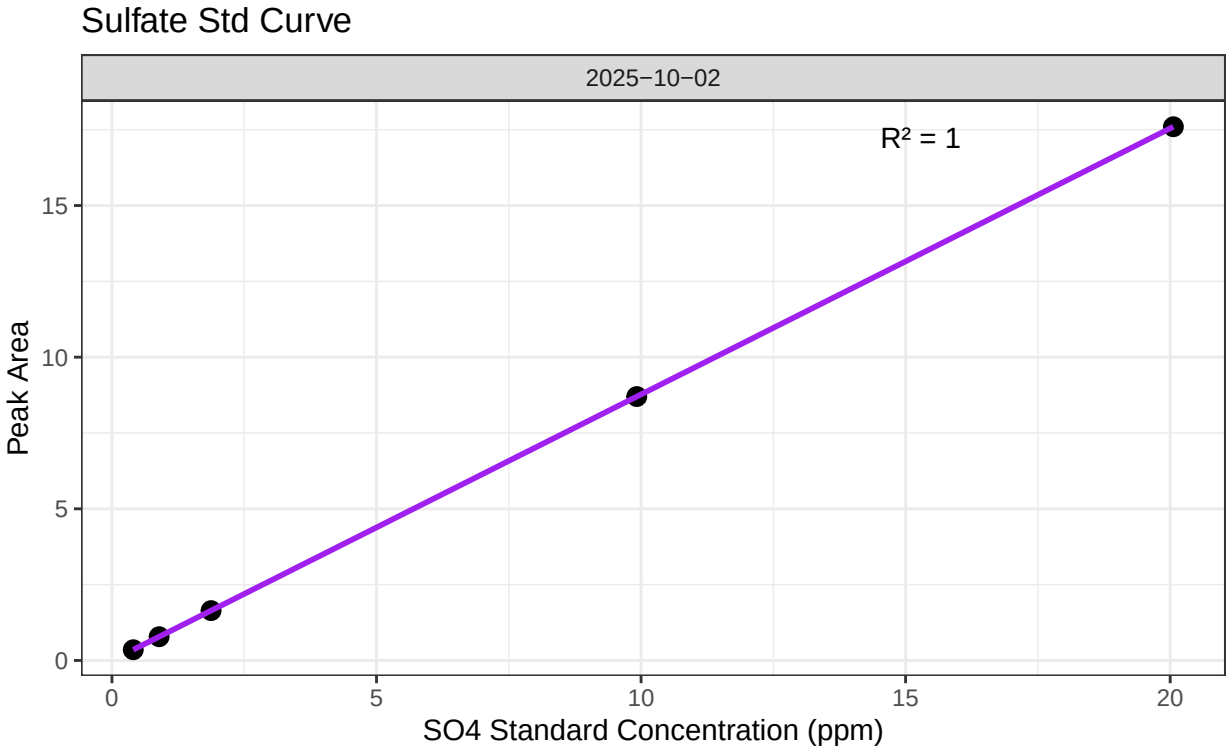
##Set Up Code - constants and QAQC cutoffs

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

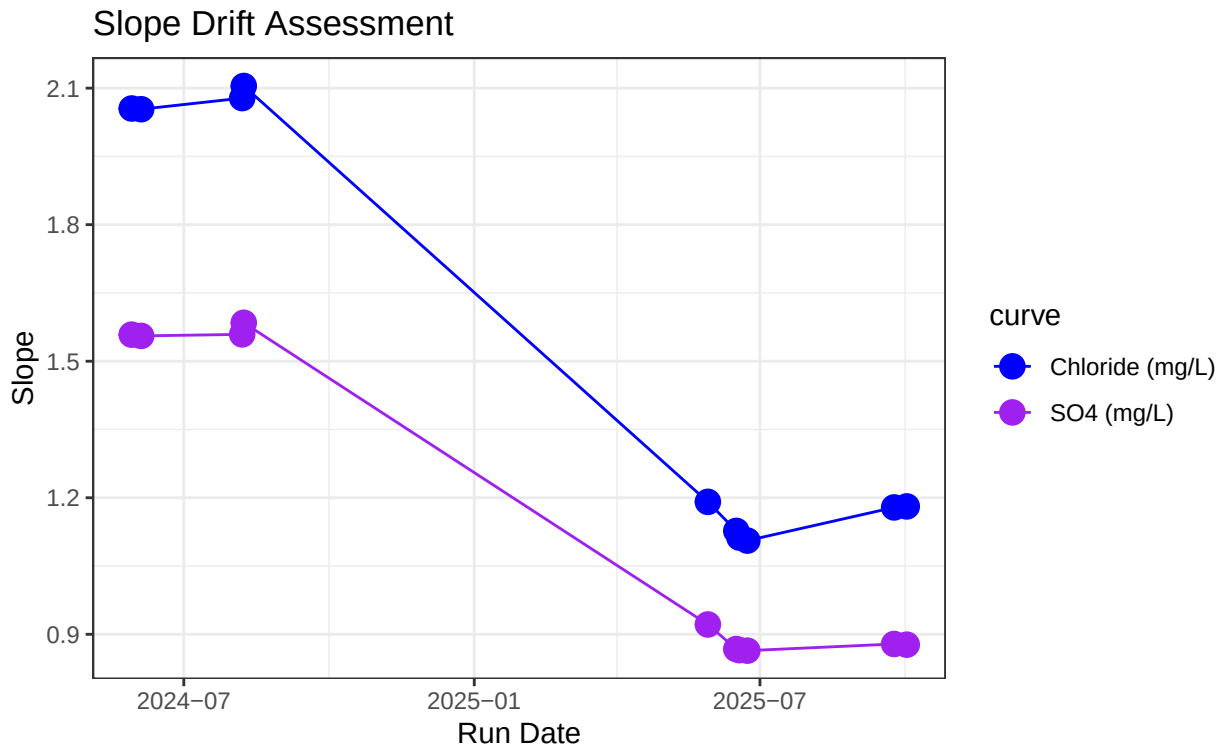
##Import Sample Data

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"
```

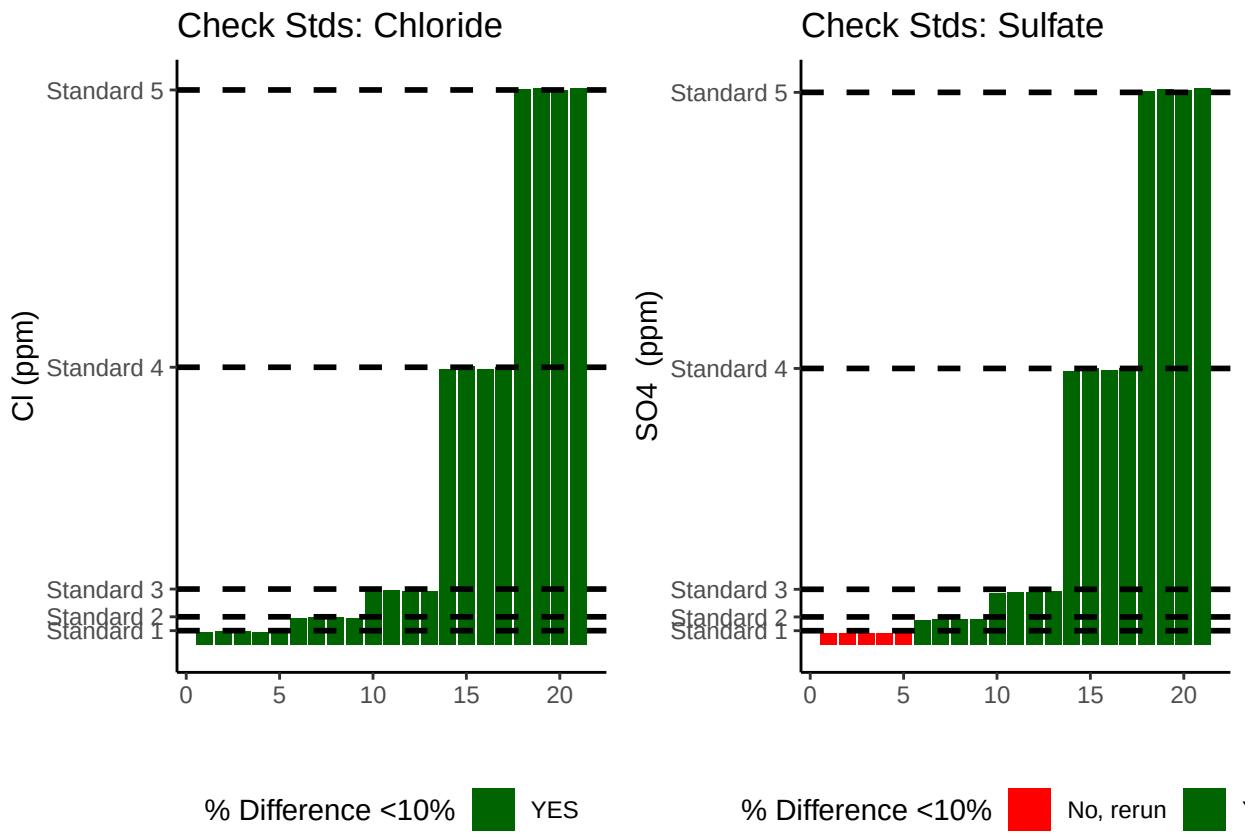
0.3 Assess Check Standards

```
## # A tibble: 5 x 5
##   sample_ID  mean_Cl sd_Cl   cv_Cl flag_Cl
##   <chr>        <dbl> <dbl>   <dbl> <chr>
## 1 Standard 1    4.66 0.133 0.0284  Chloride Check Standard RSD within Range - P~
## 2 Standard 2    9.63 0.218 0.0226  Chloride Check Standard RSD within Range - P~
## 3 Standard 3   19.3  0.206 0.0107  Chloride Check Standard RSD within Range - P~
## 4 Standard 4   99.8  0.526 0.00527 Chloride Check Standard RSD within Range - P~
## 5 Standard 5  201.   0.353 0.00176 Chloride Check Standard RSD within Range - P~
```

```
## # A tibble: 5 x 5
##   sample_ID  mean_SO4 sd_SO4  cv_SO4 flag_SO4
##   <chr>         <dbl>  <dbl>   <dbl> <chr>
## 1 Standard 1    0.419 0.0113 0.0269  Sulfate Check Standard RSD within Range - ~
## 2 Standard 2    0.914 0.0166 0.0182  Sulfate Check Standard RSD within Range - ~
## 3 Standard 3    1.91  0.0238 0.0125  Sulfate Check Standard RSD within Range - ~
## 4 Standard 4    9.98  0.0516 0.00517 Sulfate Check Standard RSD within Range - ~
## 5 Standard 5   20.1   0.0485 0.00241 Sulfate Check Standard RSD within Range - ~
```

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

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



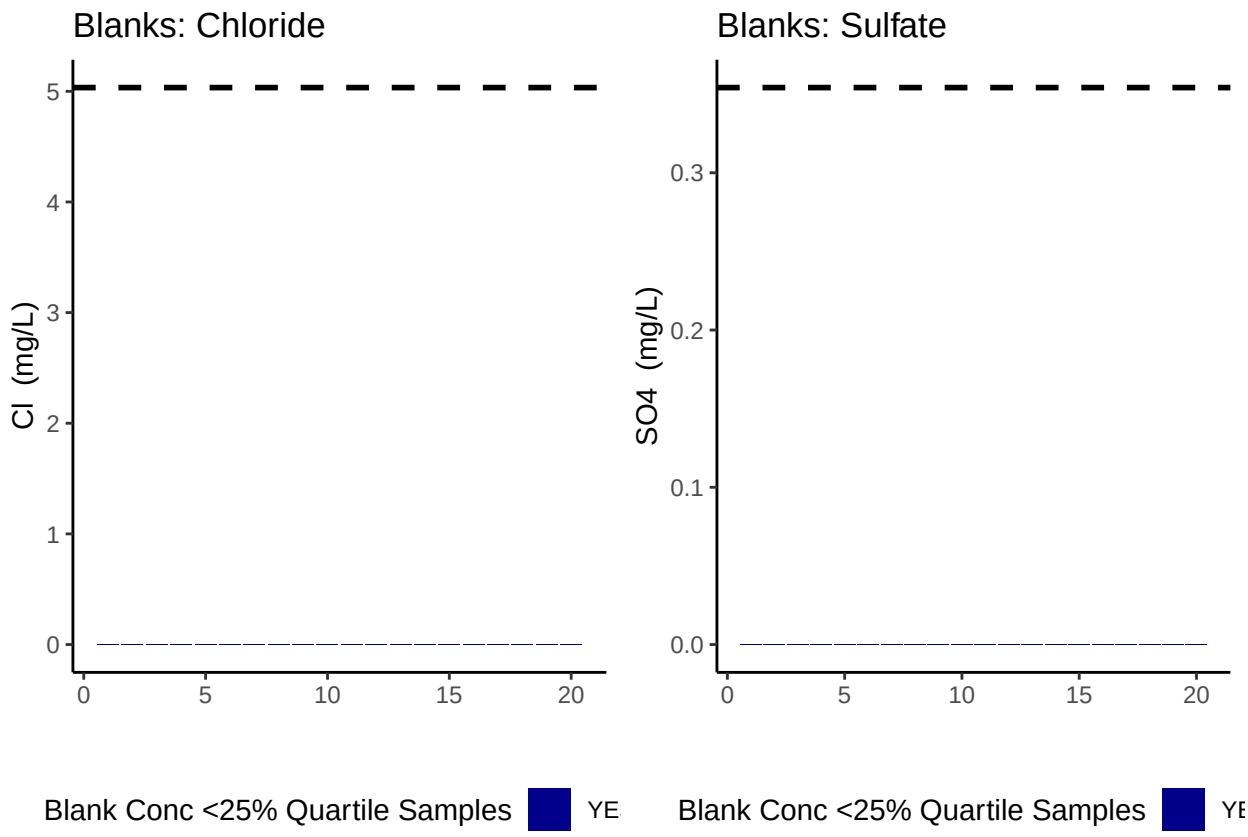

```
## [1] ">80% of Chloride Check Standards are within range of expected concentration - PROCEED"
```

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

0.4 Assess Blanks

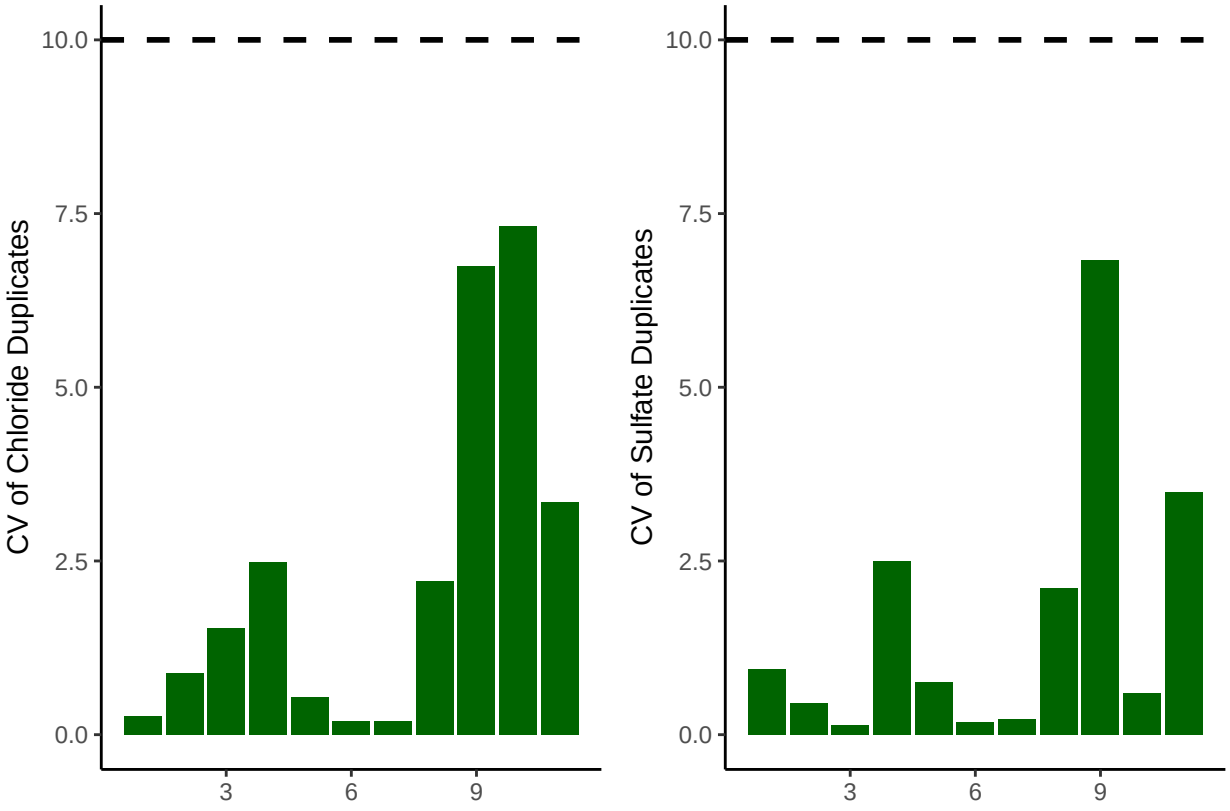
```
## [1] ">80% of Chloride Blank concentrations are lower 25% quartile of samples"
```

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



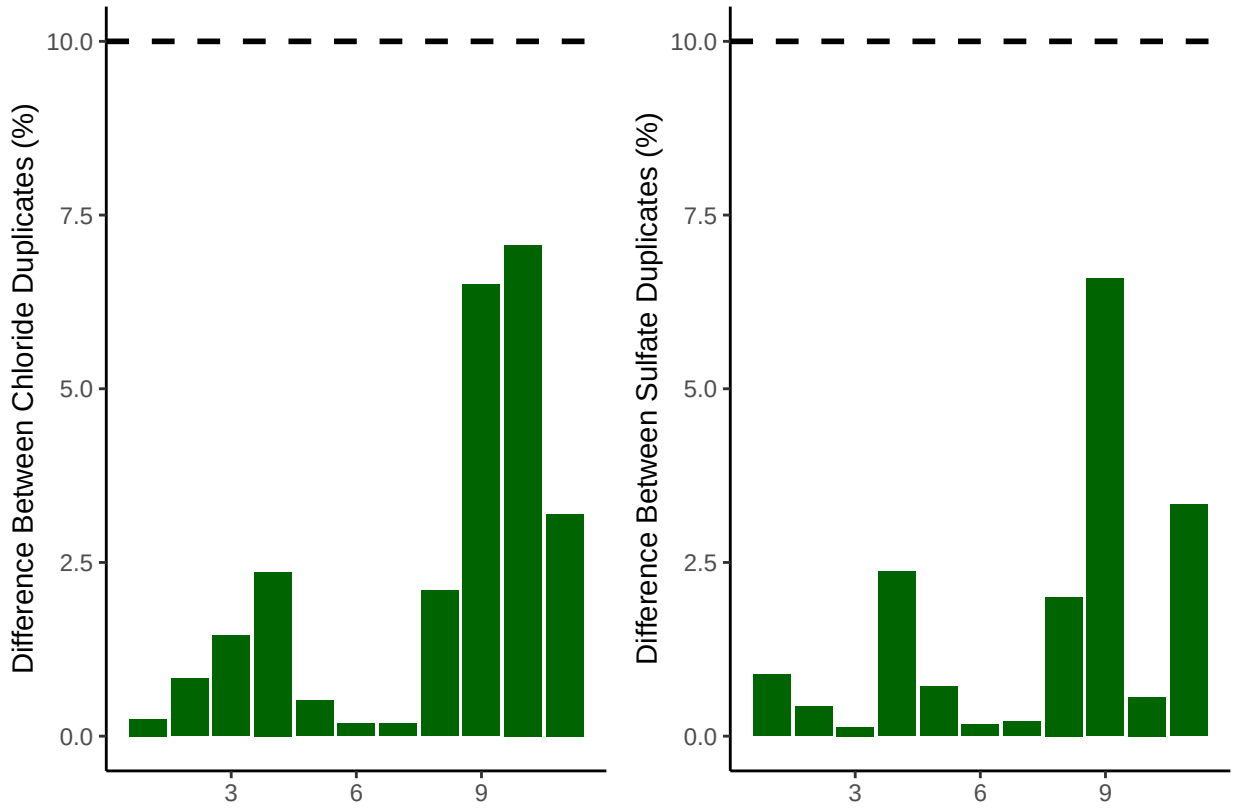

```
## Chloride blanks mean ppm:

## [1] 0

## Sulfate blanks mean ppm:

## [1] 0
```

0.5 Assess Duplicates




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

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




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

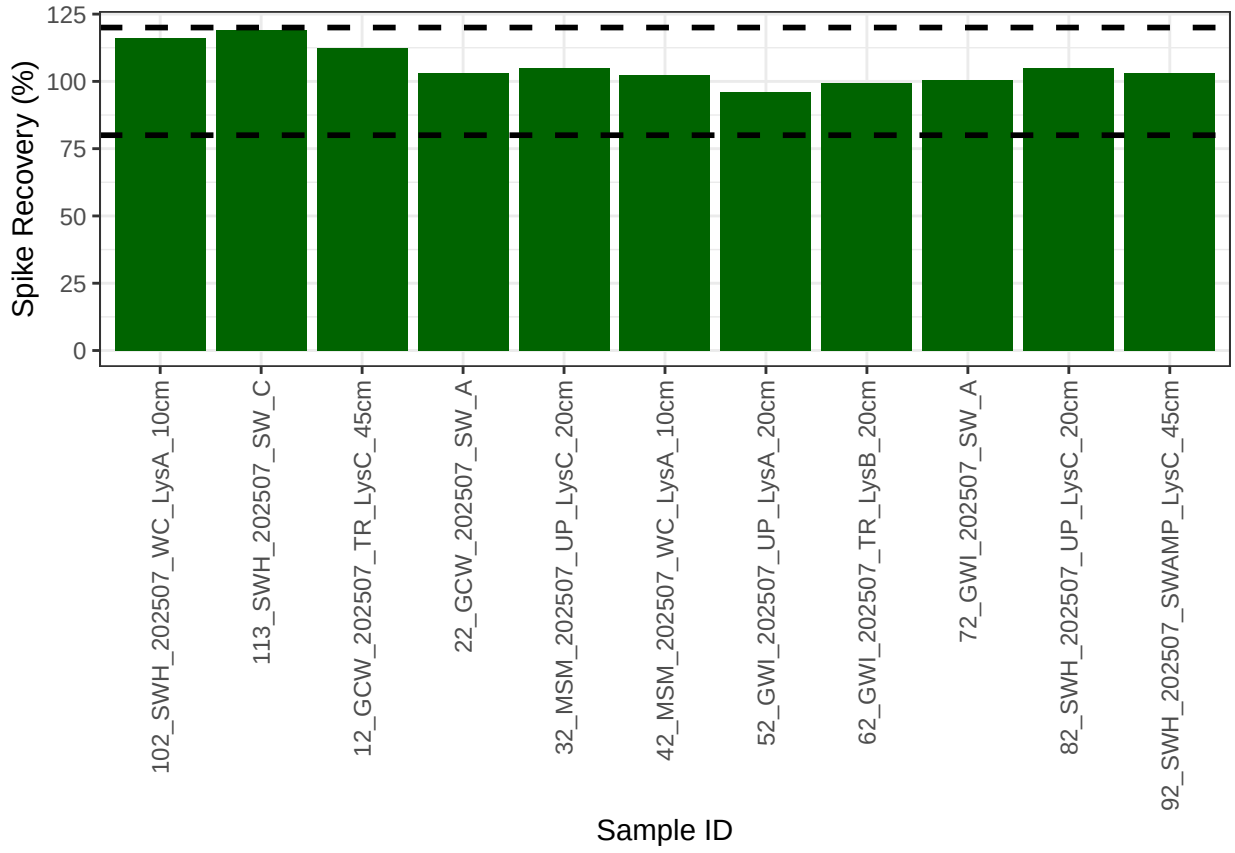
```
## [1] ">80% of Sulfate Duplicates have a percent difference <10% - PROCEED"
```

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)

all_dat$Dilution <-  ifelse(str_detect(all_dat$sample_ID, "Lucie"), 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 - PROCEED"
```

0.8 Check if samples within the range of the standard curve

```
## Sample Flagging
```

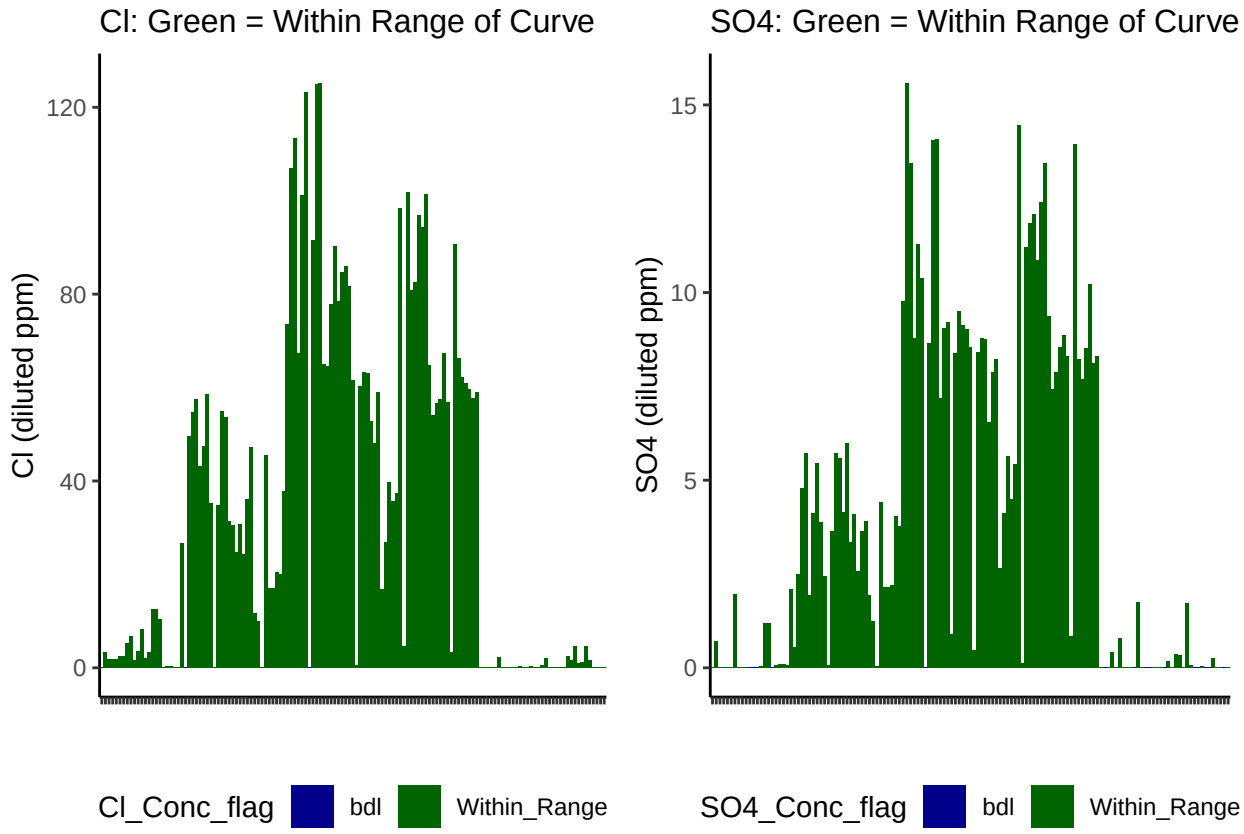


Table 1: SO4 samples

SO4_Conc_flag	Percent_samples
Within_Range	89.20863
bdl	10.79137

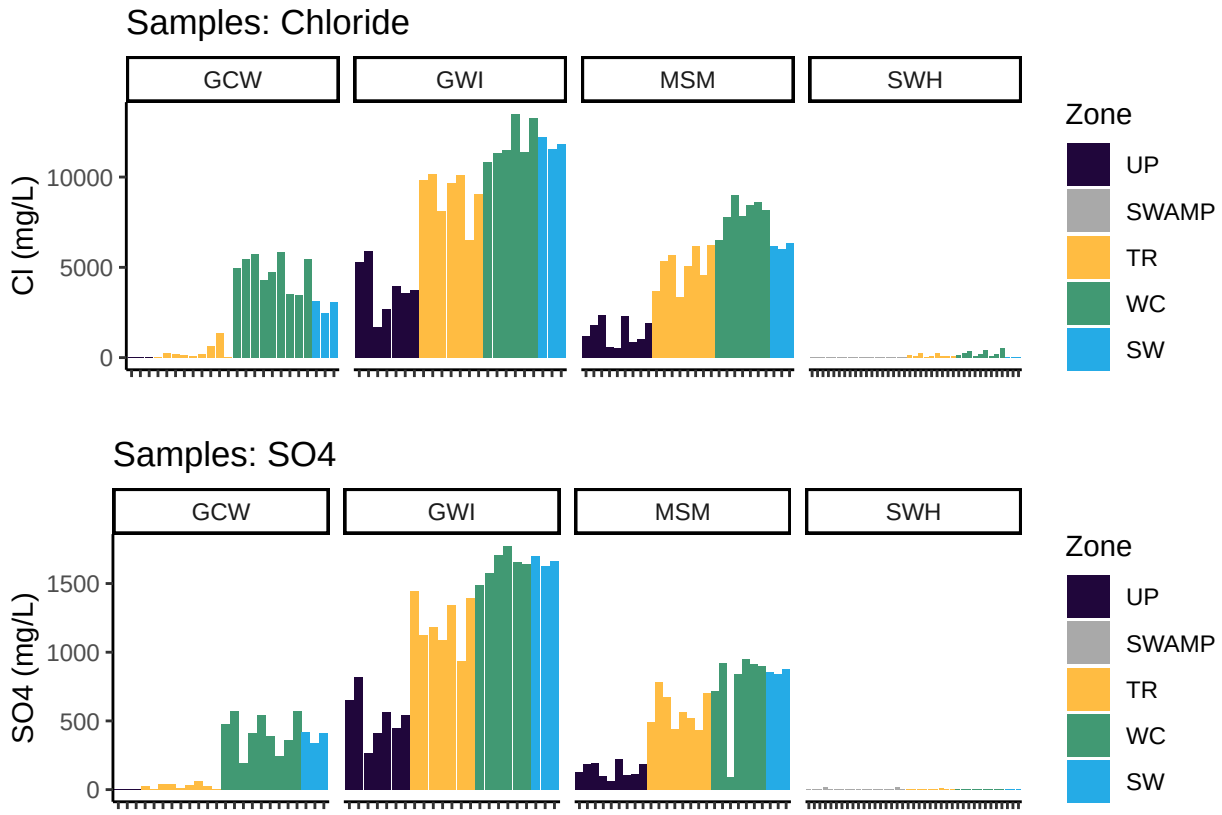
Table 2: Cl samples

Cl_Conc_flag	Percent_samples
Within_Range	98.561151
bdl	1.438849

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

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

## [1] "MSM_202507_UP_LYSB_20CM" "MSM_202507_UP_LYSB_45CM"
## [3] "MSM_202507_UP_LYSC_10CM" "GCW_202507_TR_LYSA_10CM"
## [5] "9"                       "10"
## [7] "88"                      "89"
```

0.10 Visualize Data by Plot



0.11 Export Processed Data

#end