Synoptic CB: Porewater SO4/Cl

April 2024 Samples

2025-09-08

Contents

##Add Required Packages

0.1 Run Information

```r
###### Run information - PLEASE CHANGE
  Date_Run = "2024-05-29"  #Date that instrument was run
  Run_by = "Zoe Read"  #Instrument user
  Script_run_by = "Zoe Read" #Code user
  run_notes = "Std curve slopes higher than other 2024 runs because this run was put on
      before major changes to the dionex. The output values have been checked against those run
      at later dates and look good / comparable. We are accepting this slope deviation." #any notes fro
  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_202404_Cl.txt"
  raw_file_name_so4 = "Raw Data/COMPASS_Synoptic_CB_MonMon_202404_SO4.txt"

#file path and name of processed data file
  processed_file_name = "Processed Data/COMPASS_SynopticCB_PW_Processed_Cl_SO4_202404.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"
```
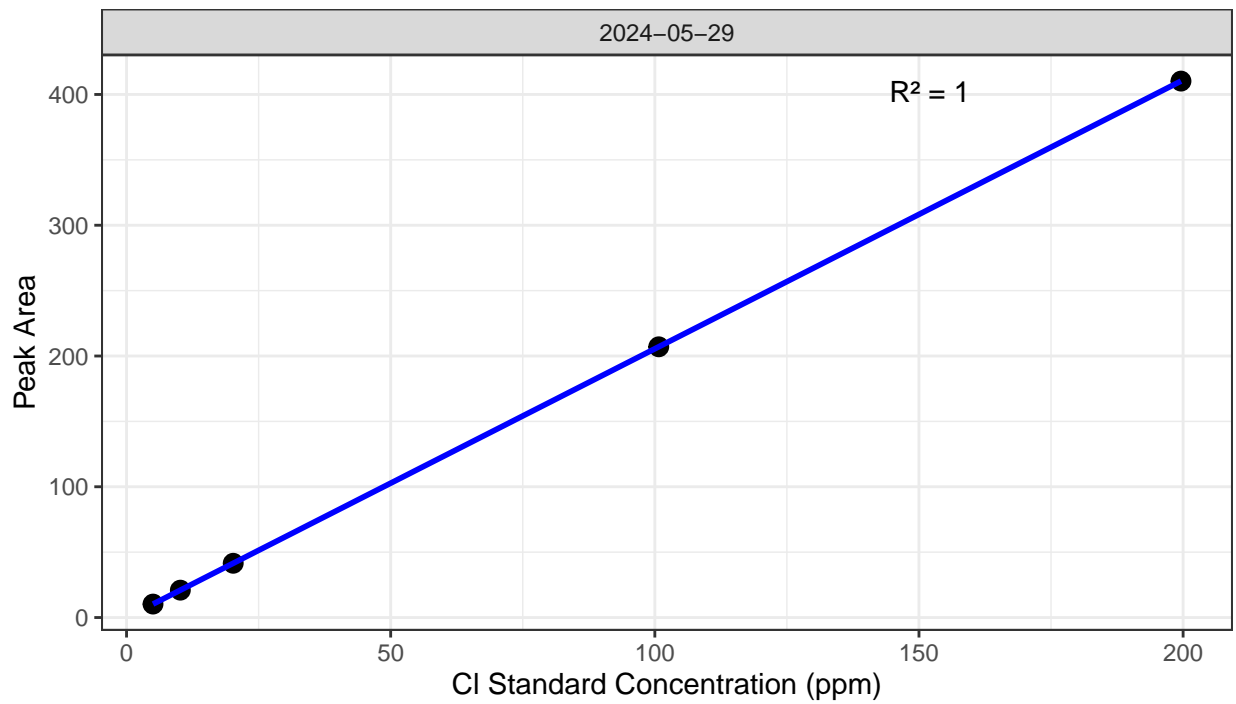
##Set Up Code - constants and QAQC cutoffs

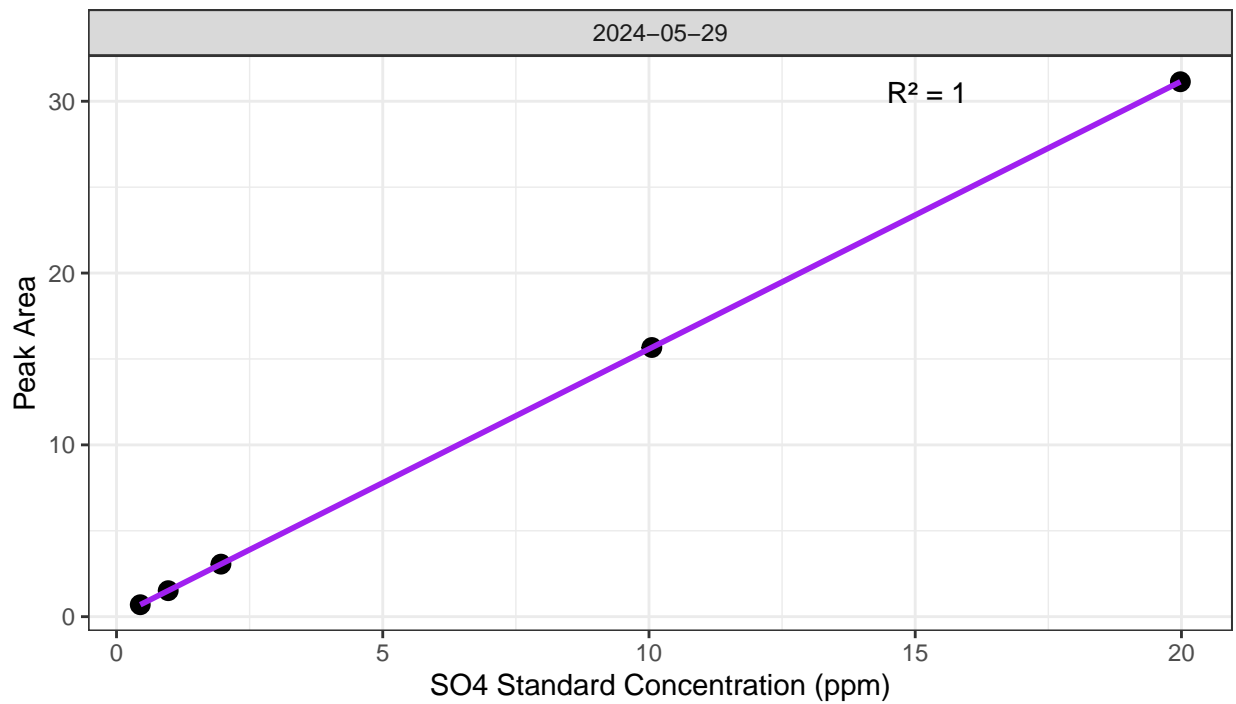##Read in metadata and create similar sample IDs for matching to samples

##Import Sample Data
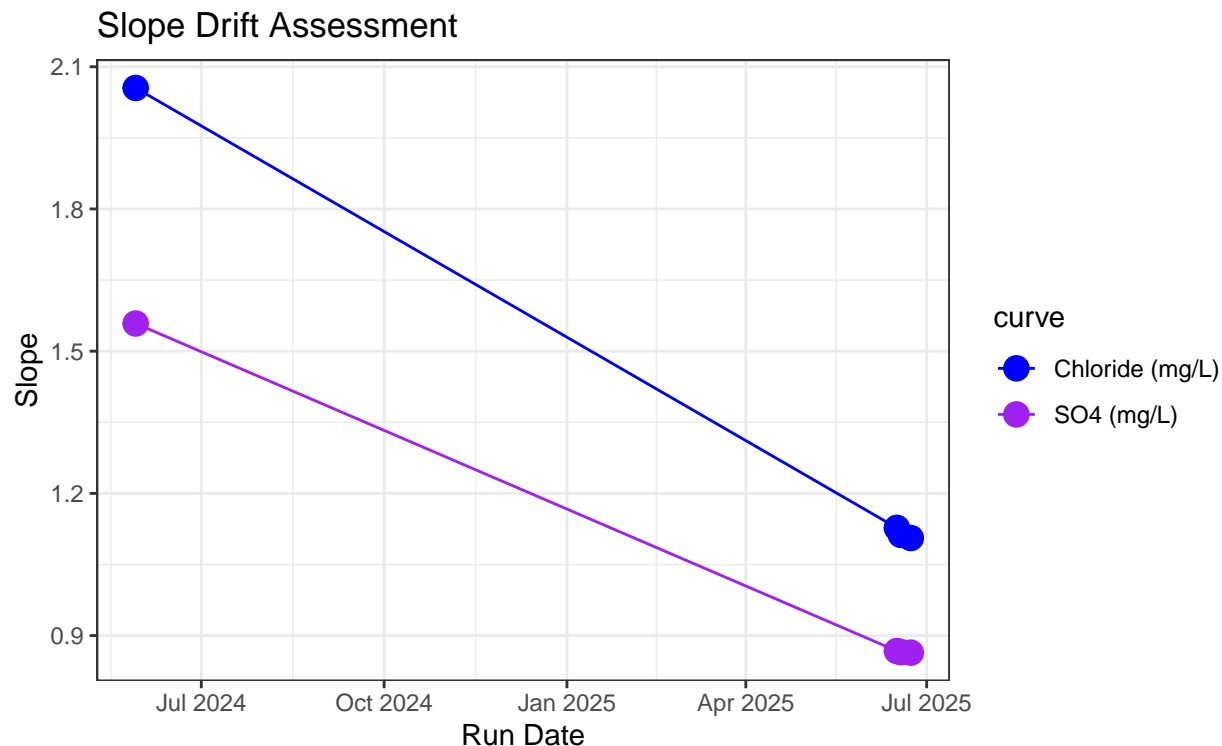
0.2 Assess Standard Curves

Chloride Std Curve

Sulfate Std Curve


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

Slope Drift Assessment


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

```
## [1] "SO4 Curve r2 GOOD"
```
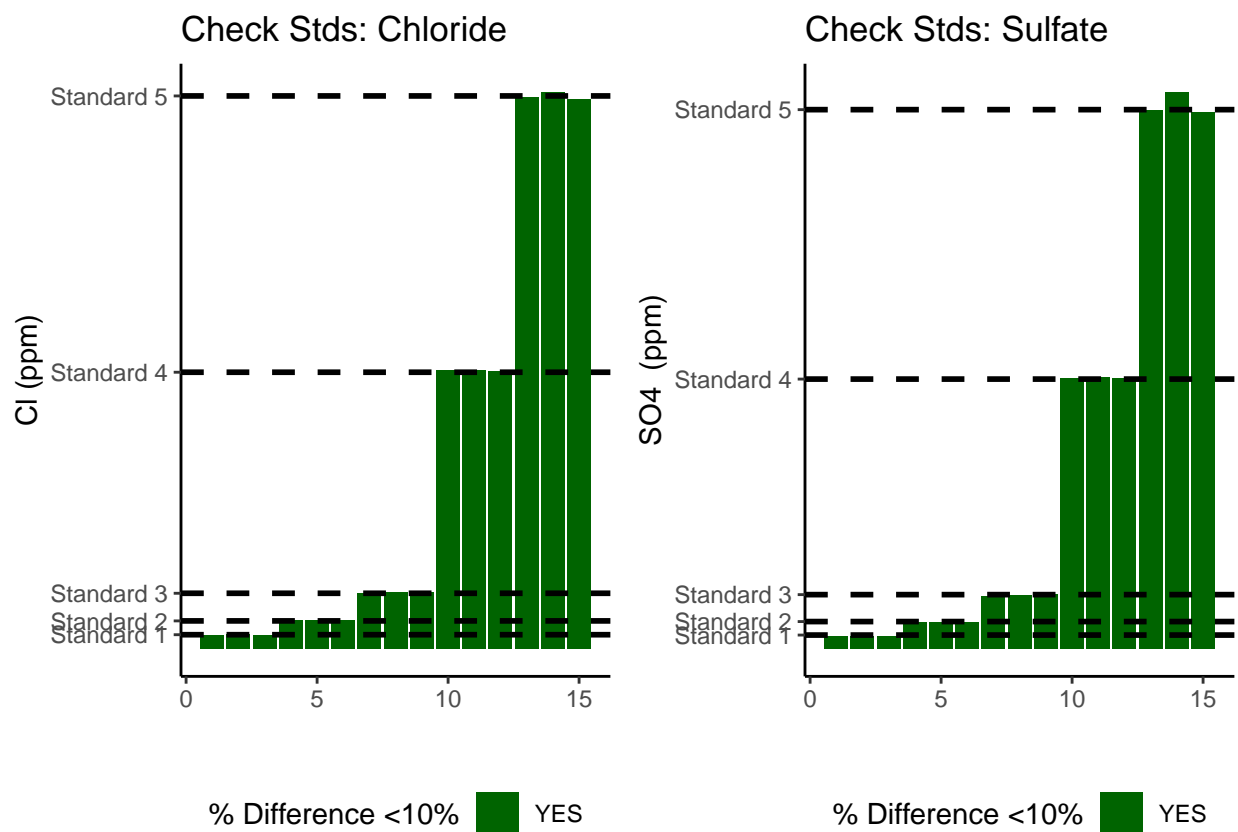
0.3 Assess Check Standards

```
## # A tibble: 5 x 5
##   sample_ID  mean_Cl  sd_Cl    cv_Cl flag_Cl
##   <chr>        <dbl>  <dbl>    <dbl> <chr>
## 1 Standard 1    5.05 0.0338 0.00669 Chloride Check Standard RSD within Range - ~
## 2 Standard 2   10.3  0.0690 0.00673 Chloride Check Standard RSD within Range - ~
## 3 Standard 3   20.3  0.0836 0.00412 Chloride Check Standard RSD within Range - ~
## 4 Standard 4  101.   0.223  0.00222 Chloride Check Standard RSD within Range - ~
## 5 Standard 5  200.   1.42   0.00710 Chloride Check Standard RSD within Range - ~
```

```
## # A tibble: 5 x 5
##   sample_ID  mean_SO4 sd_SO4  cv_SO4 flag_SO4
##   <chr>         <dbl>  <dbl>   <dbl> <chr>
## 1 Standard 1    0.466 0.0182  0.0391 Sulfate Check Standard RSD within Range - ~
## 2 Standard 2    0.985 0.0124  0.0126 Sulfate Check Standard RSD within Range - ~
## 3 Standard 3    1.99  0.0243  0.0122 Sulfate Check Standard RSD within Range - ~
## 4 Standard 4   10.1   0.0281 0.00280 Sulfate Check Standard RSD within Range - ~
## 5 Standard 5   20.2   0.417   0.0207 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"
```
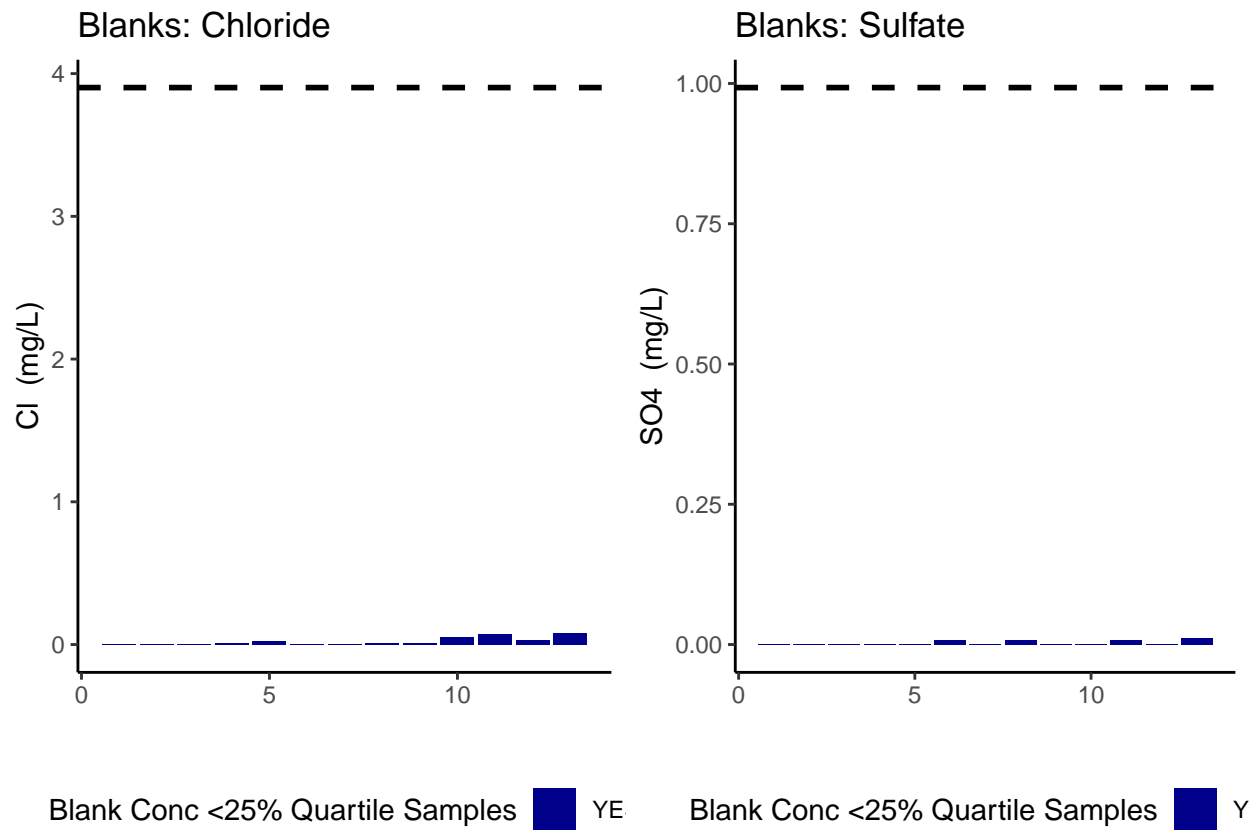
Check Stds: Chloride — Check Stds: Sulfate

% Difference <10% YES

[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 - PROCEED"

0.4 Assess Blanks

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

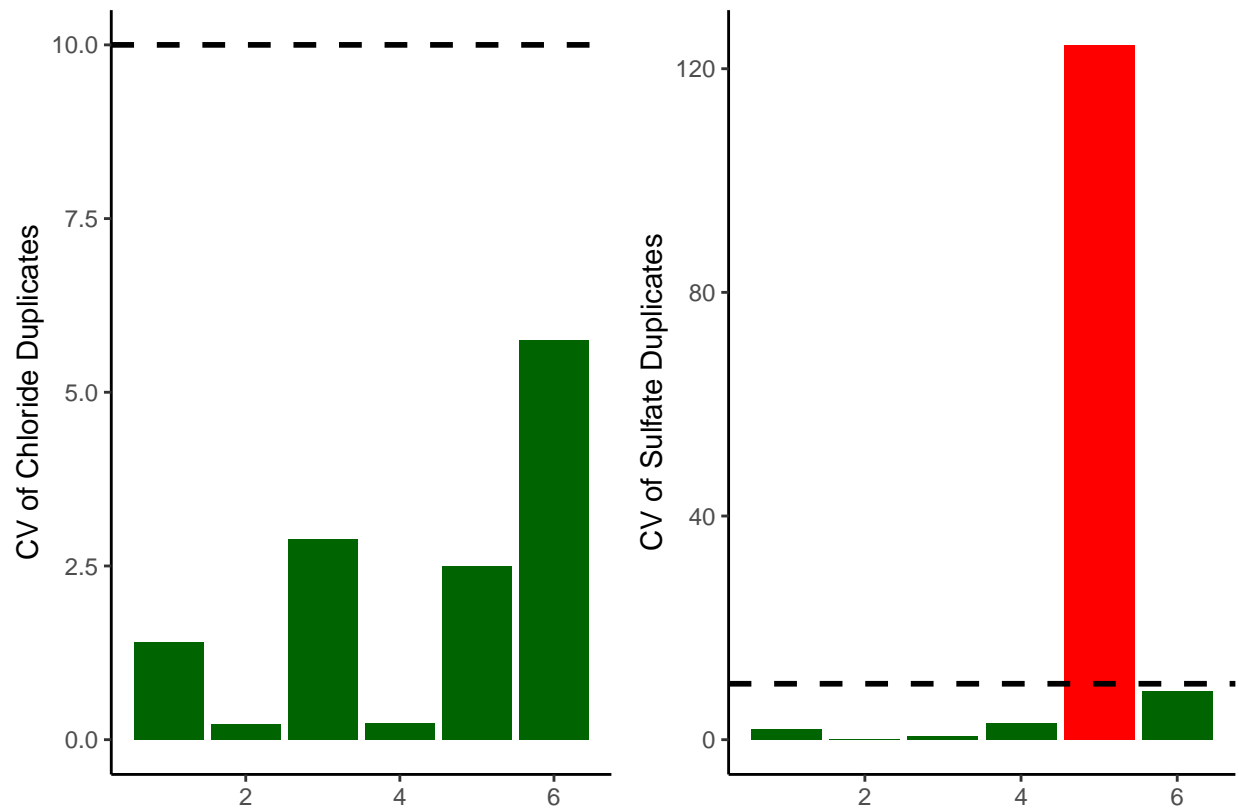## [1] ">80% of Sulfate Blank concentrations are lower 25% quartile of samples"

Blanks: Chloride

Blanks: Sulfate

Cl (mg/L)

SO4 (mg/L)

Blank Conc <25% Quartile Samples   YE

Blank Conc <25% Quartile Samples   Y

Chloride blanks mean ppm:

[1] 0.02266923

Sulfate blanks mean ppm:
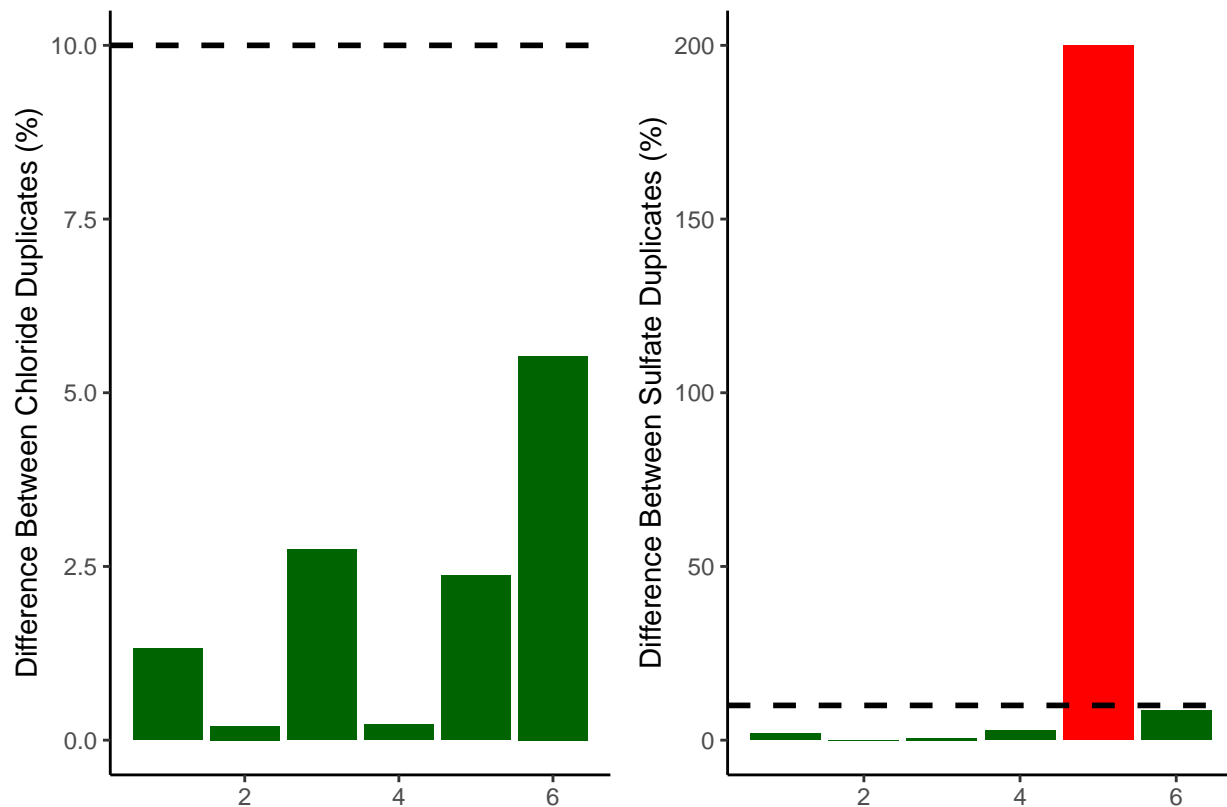
[1] 0.002707692

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

```r
# 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)
```
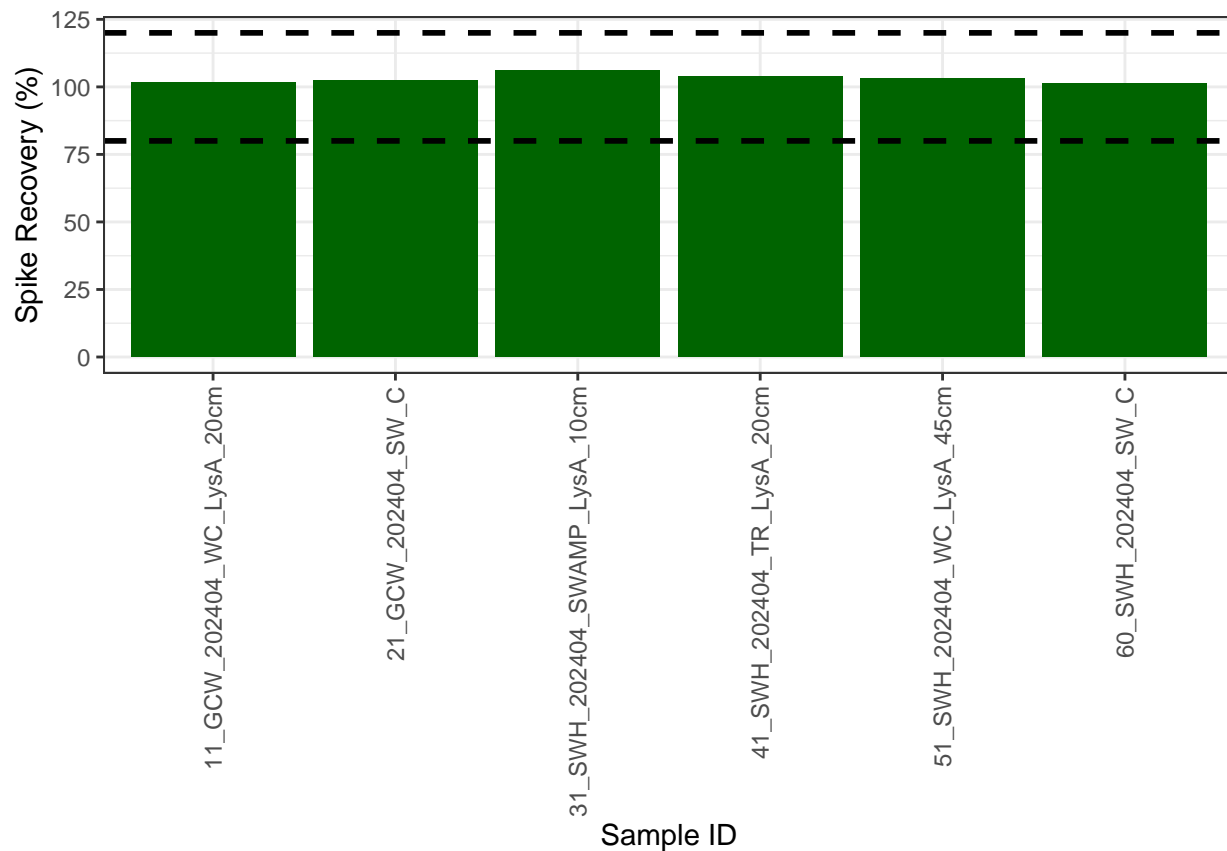
0.7 Assess Analytical Spikes


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

0.8 Check if samples within the range of the standard curve
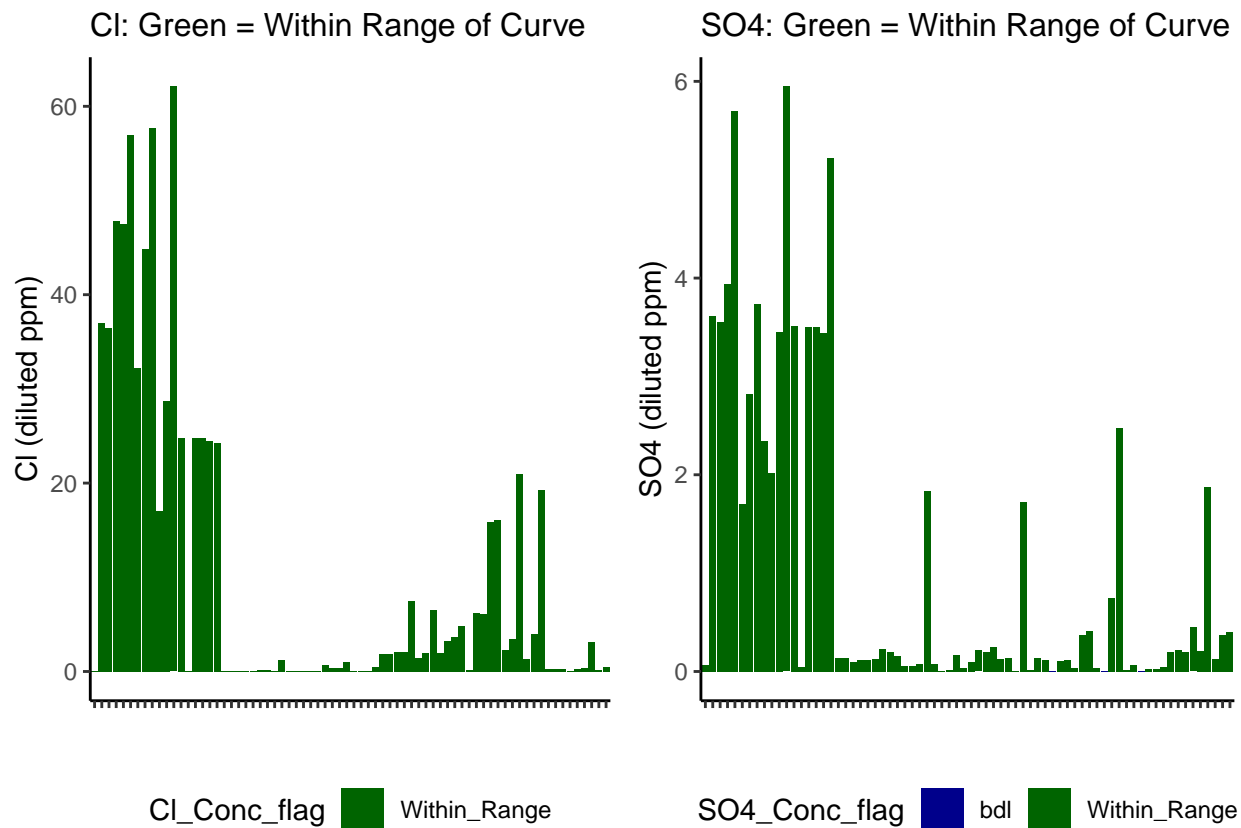
```
## Sample Flagging
```

Table 1: SO4 samples

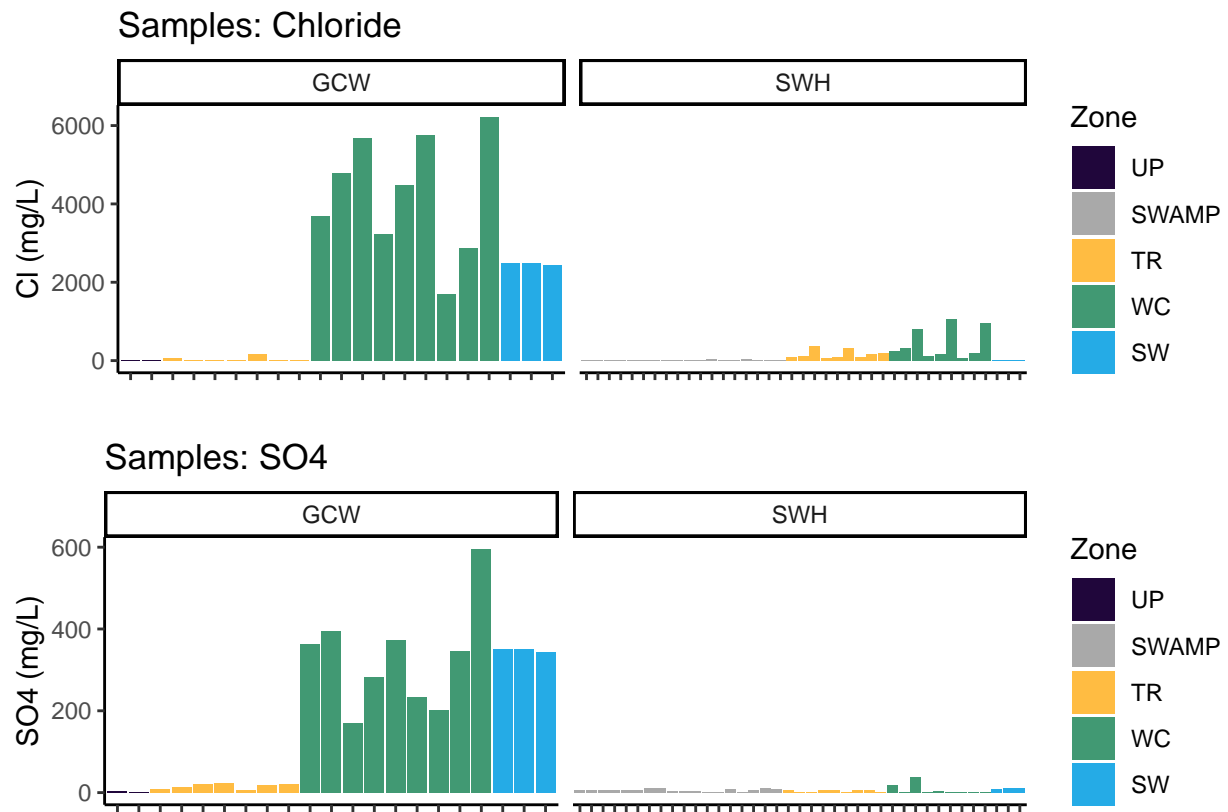| SO4_Conc_flag	Percent_samples
Within_Range	95.833333
bdl	4.166667

Table 2: Cl samples

Cl_Conc_flag	Percent_samples
Within_Range	100

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

```
## All sample IDs are present in metadata.
```

0.10   Visualize Data by Plot

Samples: Chloride

Samples: SO4

0.11   Export Processed Data

#end