TEMPEST: Porewater SO4/Cl

June (1-71) 2024 Samples

2025-10-02

Contents

##Add Required Packages

0.1 Run Information

```
###### Run information - PLEASE CHANGE
  Sample_Year = "2024"
  Date_Run = "2025-08-14"  #Date that instrument was run
  Run_by = "Zoe Read"  #Instrument user
  Script_run_by = "Zoe Read" #Code user
  run_notes = "Check standard 1 is low for SO4, so <80% of Sulfate Check
  Standards are within range of expected concentration. The peaks look uniform,
  so I'm not sure why the standard is low.
  The 1st duplicate has high CV for both Cl and SO4, the 6th dup has high cv for Cl only - check peaks
  The 1st spk was low and was probably not spiked.
  Some sample IDs are missing from metadata: TMP_C_H6_20240610_15CM, TMP_SW_H3_20240612_15CM_T3
  " #any notes from the run

###### File Names - PLEASE CHANGE
#file path and name for raw summary data file
  raw_file_name_cl = "Raw Data/COMPASS_TEMPEST_202406_1-71_Cl.txt"
  raw_file_name_so4 = "Raw Data/COMPASS_TEMPEST_202406_1-71_SO4.txt"

#file path and name of processed data file
  processed_file_name = "Processed Data/COMPASS_TEMPEST_Processed_Cl_SO4_202406_1-71.csv"

###### Log Files - PLEASE CHECK

#qaqc log file path for this year copied over from COMPASS GitHub
  Log_path = "Raw Data/COMPASS_Synoptic_Cl_SO4_QAQClog_2024.csv"
```
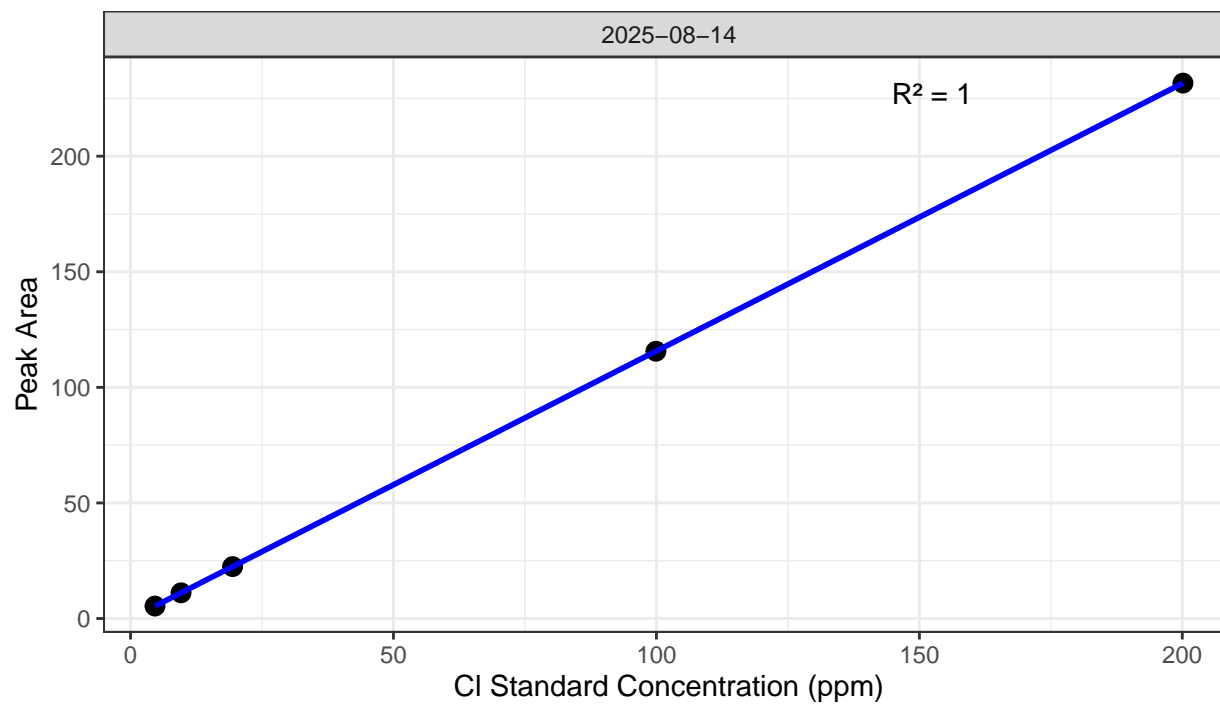
##Set Up Code - constants and QAQC cutoffs

0.2 Pull in active porewater tracking inventory sheet from Google Drive:

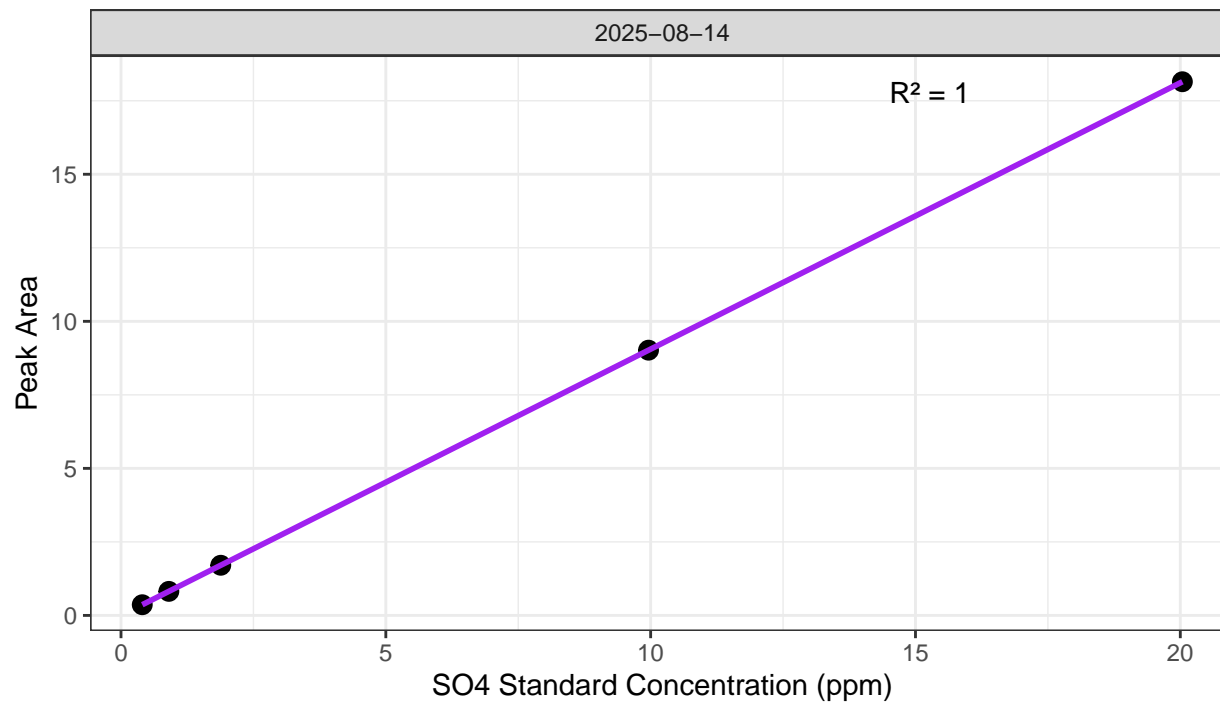##Create similar sample IDs to match with run samples
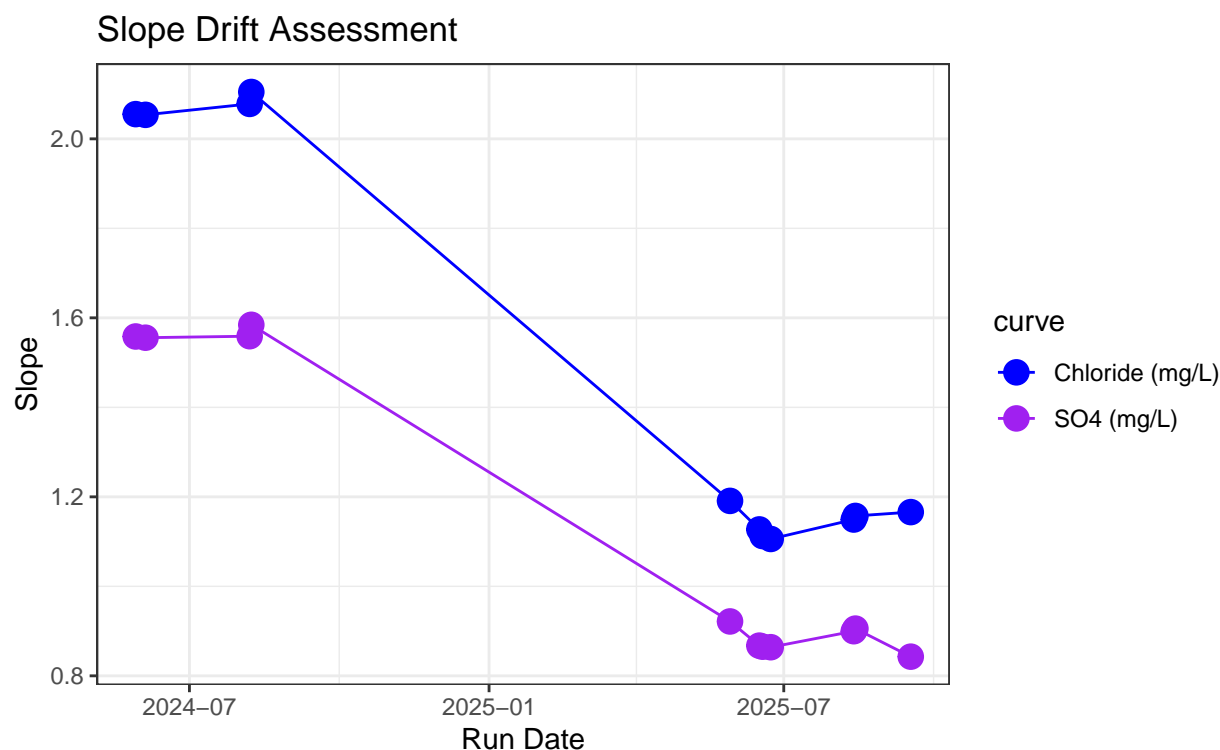
##Import Sample Data

0.3 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"
```
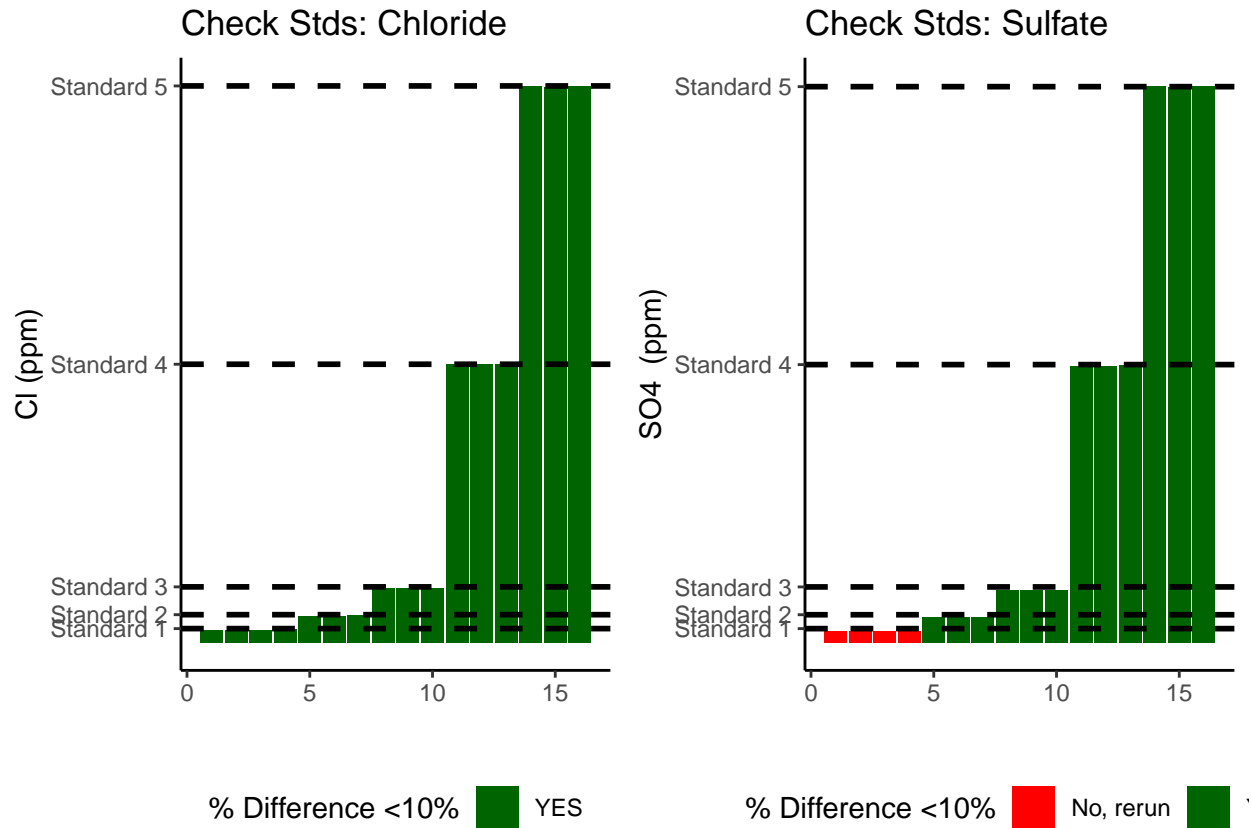
0.4 Assess Check Standards

```
## # A tibble: 5 x 5
##   sample_ID  mean_Cl  sd_Cl    cv_Cl flag_Cl
##   <chr>        <dbl>  <dbl>    <dbl> <chr>
## 1 Standard 1    4.67 0.0935 0.0200   Chloride Check Standard RSD within Range - ~
## 2 Standard 2    9.62 0.167  0.0173   Chloride Check Standard RSD within Range - ~
## 3 Standard 3   19.6  0.141  0.00719  Chloride Check Standard RSD within Range - ~
## 4 Standard 4  100.   0.107  0.00107  Chloride Check Standard RSD within Range - ~
## 5 Standard 5  200.   0.215  0.00107  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    0.407 0.00382 0.00939  Sulfate Check Standard RSD within Range -~
## 2 Standard 2    0.905 0.00289 0.00320  Sulfate Check Standard RSD within Range -~
## 3 Standard 3    1.89  0.00689 0.00364  Sulfate Check Standard RSD within Range -~
## 4 Standard 4    9.96  0.0134  0.00134  Sulfate Check Standard RSD within Range -~
## 5 Standard 5   20.0   0.0217  0.00108  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% [green] YES

% Difference <10% [red] No, rerun [green] Y

[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"

0.5 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
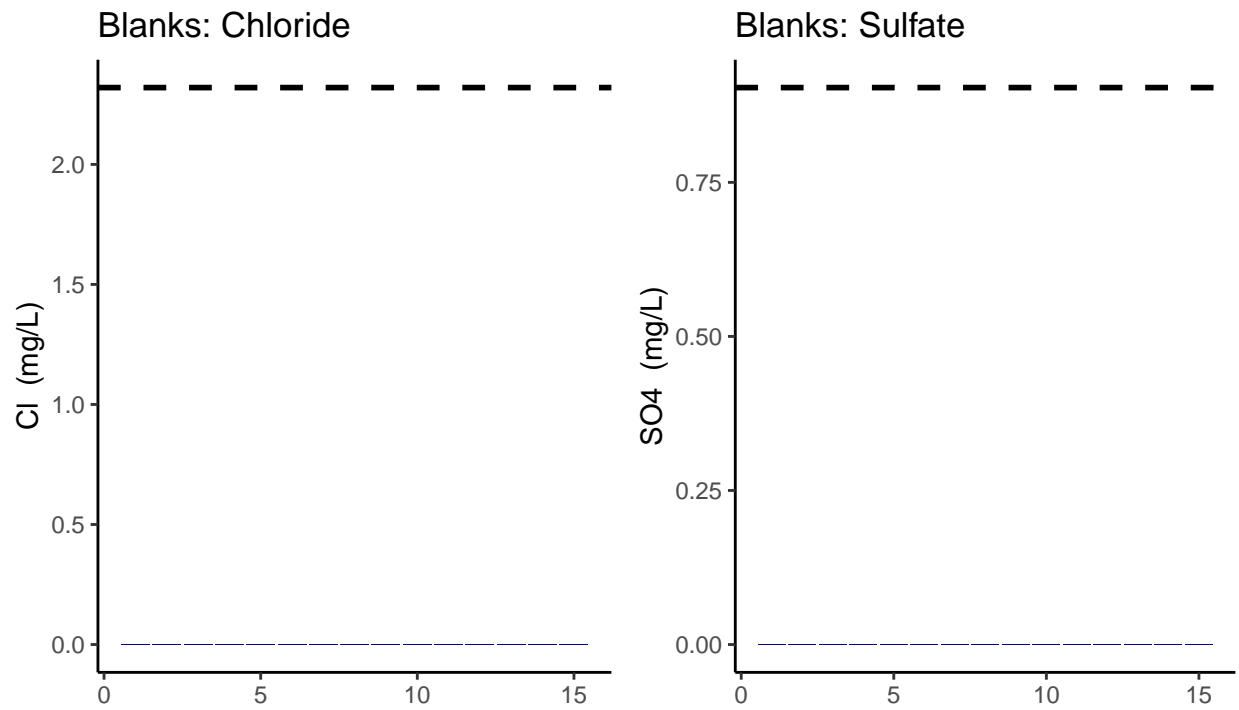
Blanks: Sulfate

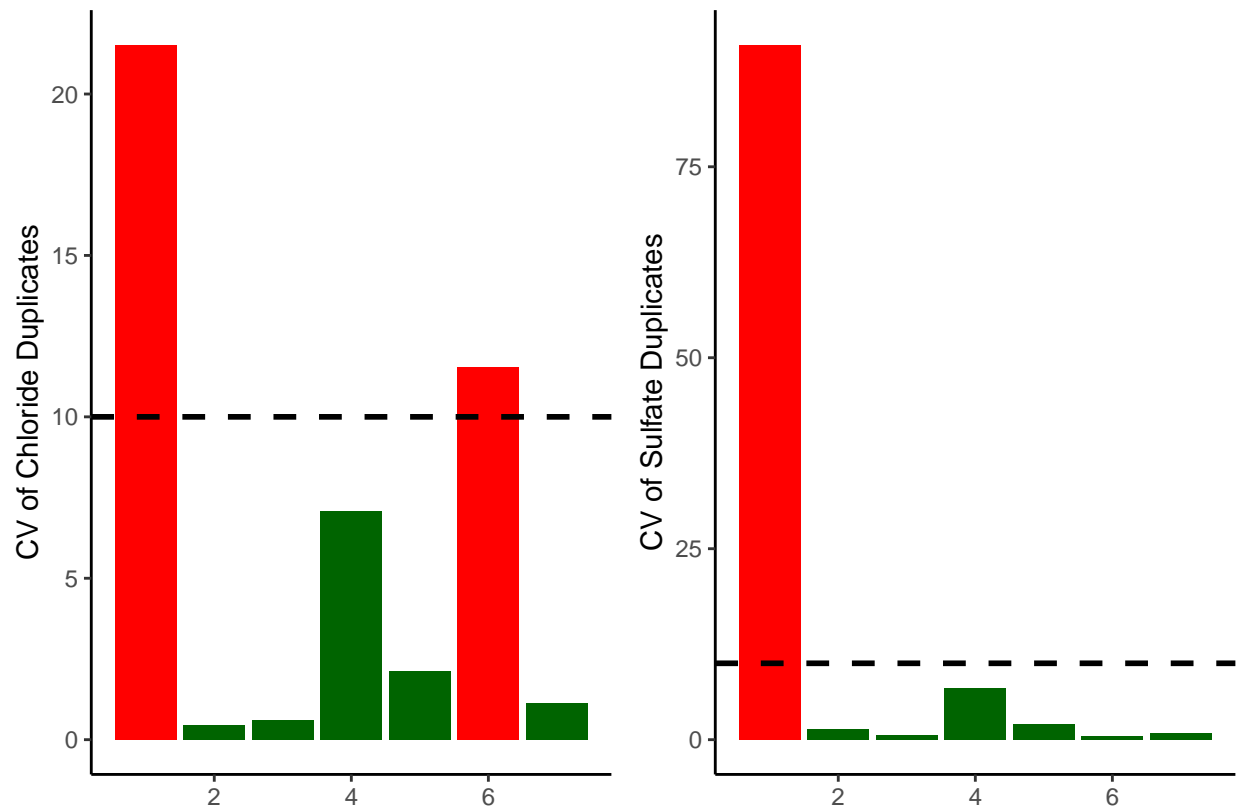Blank Conc <25% Quartile Samples ▉ YE

Blank Conc <25% Quartile Samples ▉ Y

```
## Chloride blanks mean ppm:

## [1] 0

## Sulfate blanks mean ppm:

## [1] 0
```

0.6   Assess Duplicates


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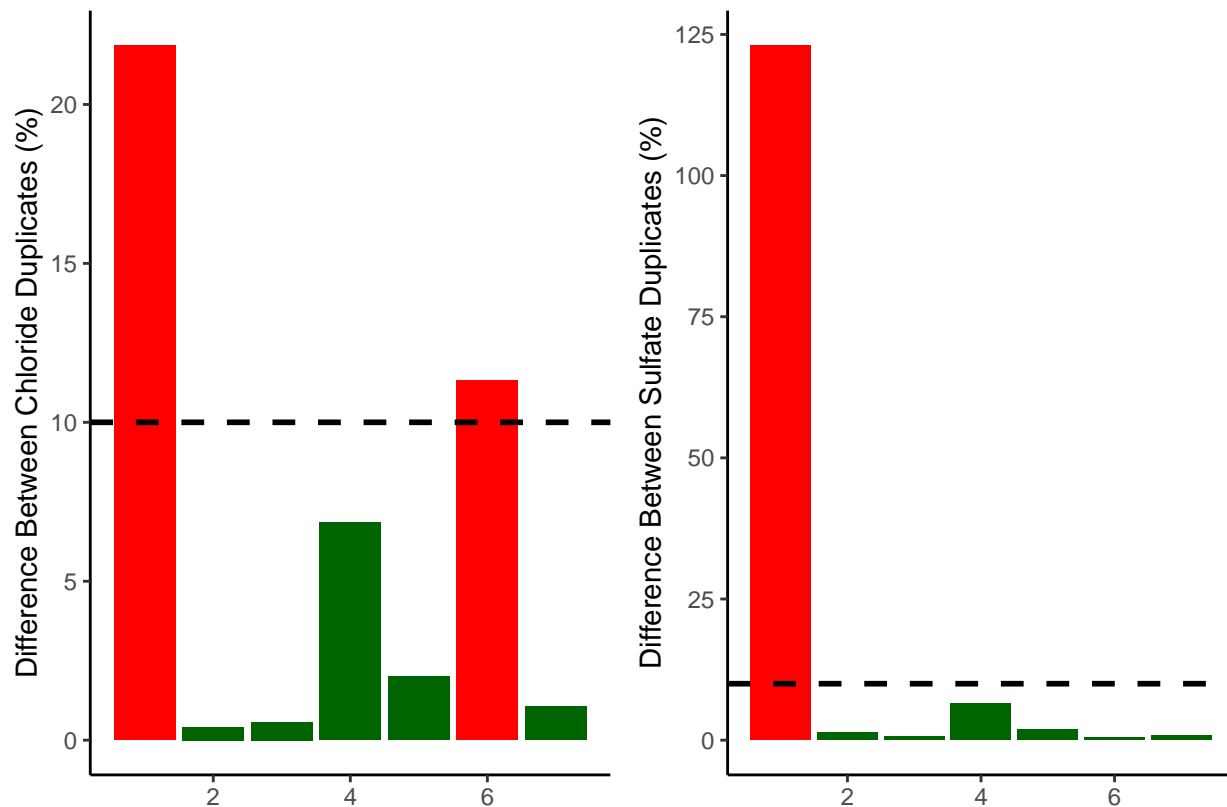
```
## [1] ">80% of Sulfate Duplicates have a CV <10% - PROCEED"
```

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

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

0.7 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 TEMPEST this depends on the sample so...
all_dat$Dilution <- 1
all_dat$Dilution <-  ifelse(str_detect(all_dat$sample_ID, "TMP"), 50, all_dat$Dilution)
all_dat$Dilution <-  ifelse(str_detect(all_dat$sample_ID, "EST_SourceWater"), 100, all_dat$Dilution)
all_dat$Dilution <-  ifelse(str_detect(all_dat$sample_ID, "SW_SourceWater"), 100, all_dat$Dilution)
```
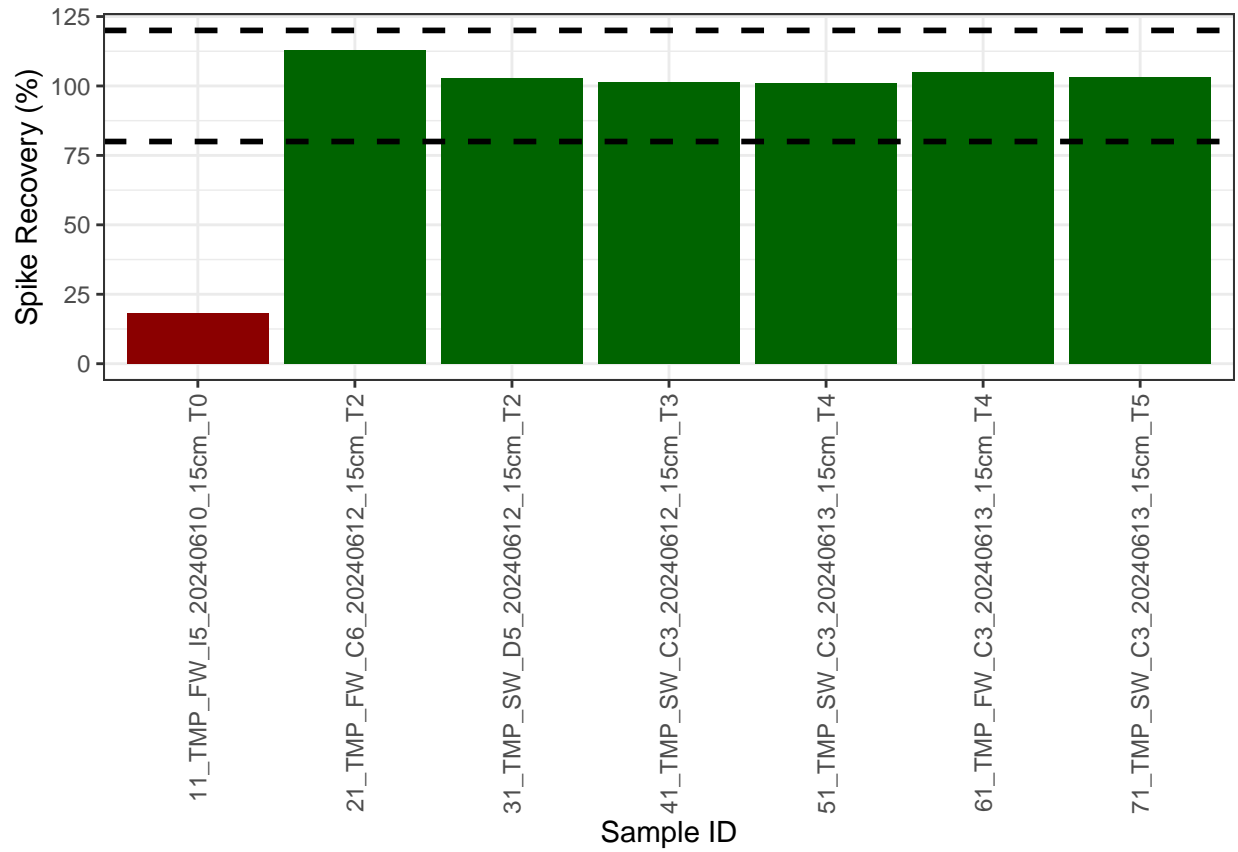
0.8 Assess Analytical Spikes

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

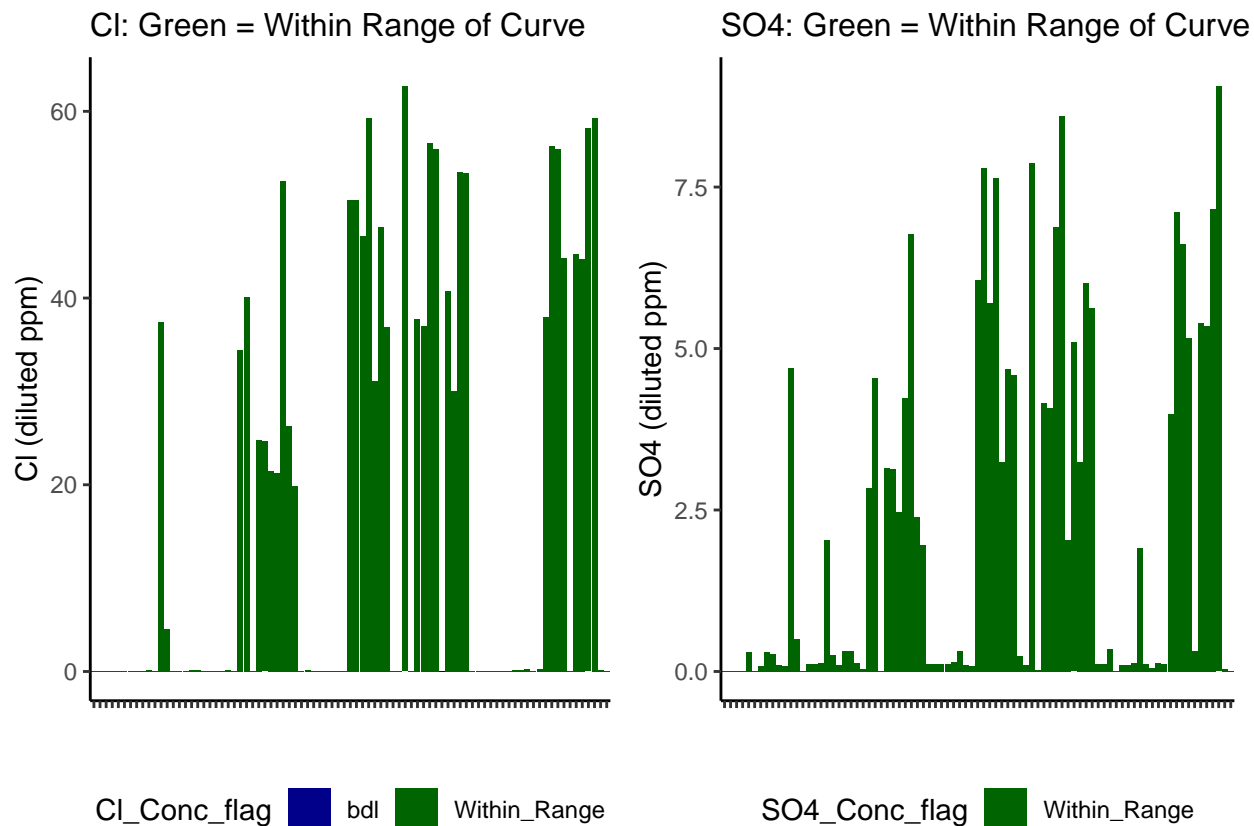## 0.9 Check if samples within the range of the standard curve

Sample Flagging

Table 1: SO4 samples

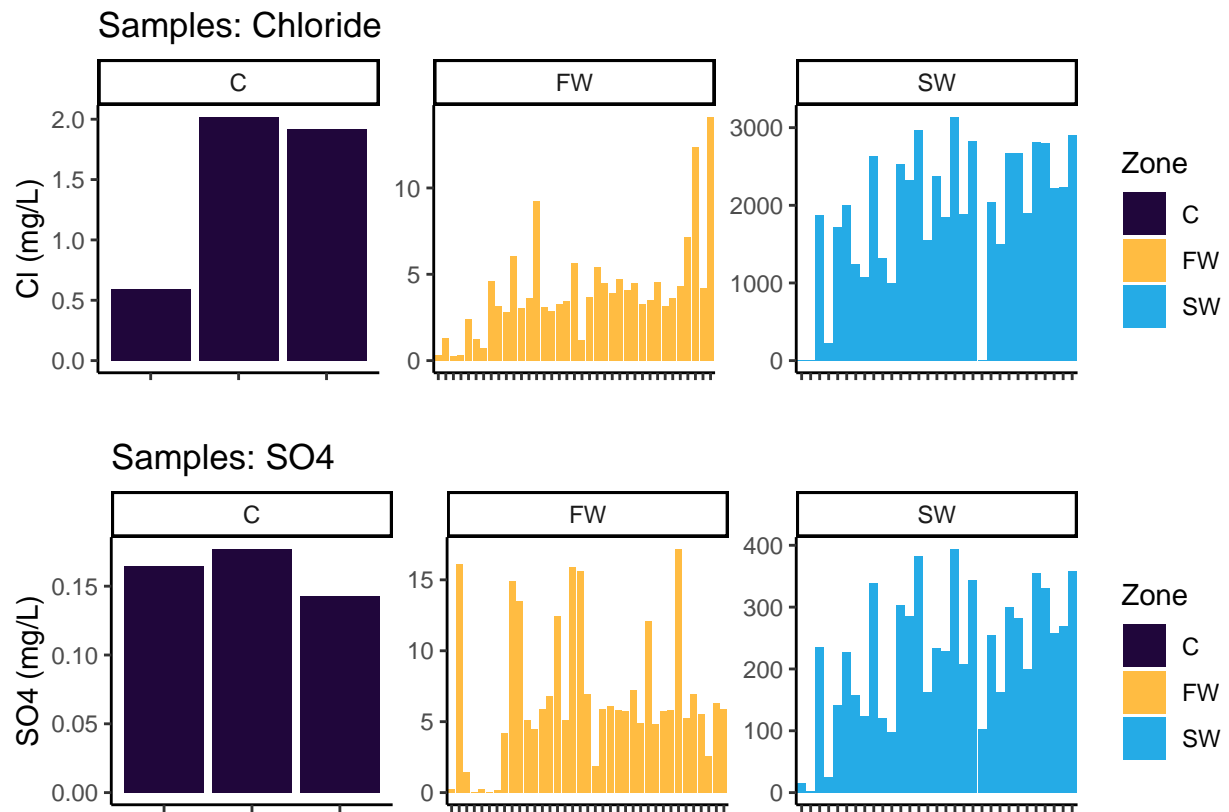| SO4_Conc_flag	Percent_samples
Within_Range	100

Table 2: Cl samples

Cl_Conc_flag	Percent_samples
Within_Range	98.823529
bdl	1.176471

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

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

```
## [1] "TMP_C_H6_20240610_15CM"      "TMP_SW_H3_20240612_15CM_T3"
```

0.11 Visualize Data by Plot

Samples: Chloride

Samples: SO4

0.12 Export Processed Data

#end