TEMPEST: Porewater SO4/Cl

June (1-71) 2024 Samples

2025-12-19

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 Cl.
  " #any notes from the run

##Sample data that was entered incorrectly
# The Old ID is the original, incorrecly-entered ID and the New ID is the correct ID to change it to.
Old_ID_1 = "TMP_C_H6_20240610_15cm"
New_ID_1 = "TMP_C_H6_20240610_15cm_T0"

###### 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

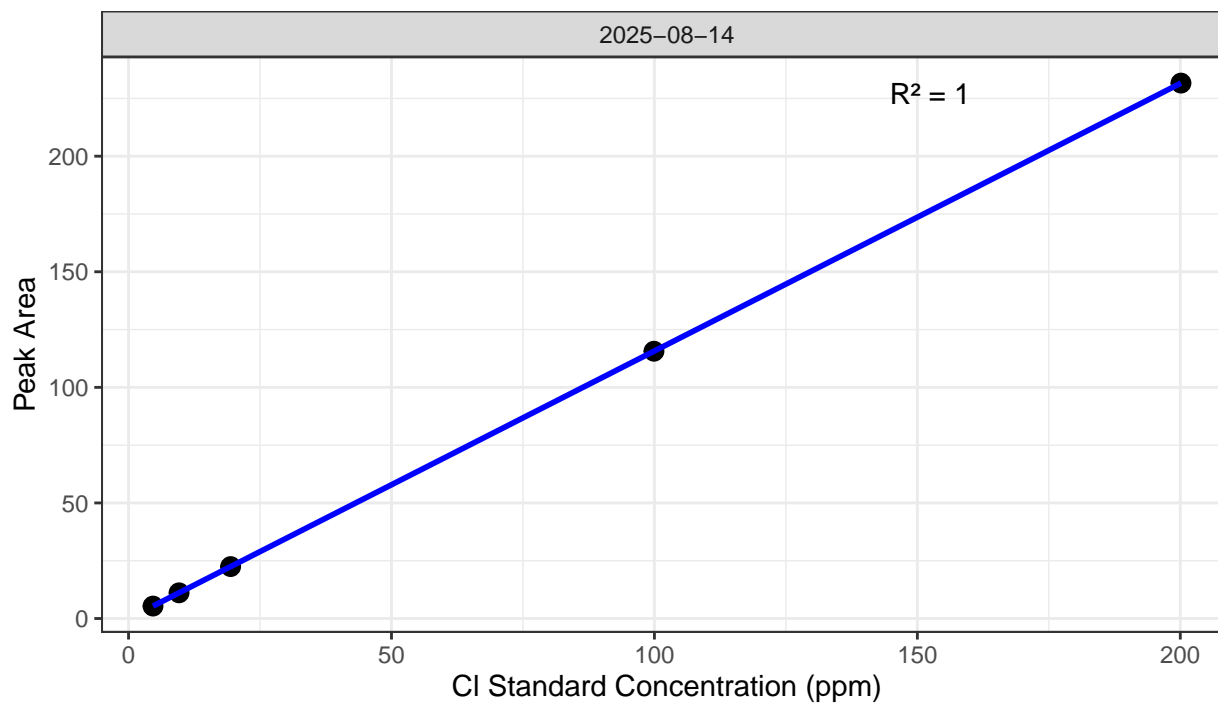## 0.2 Pull in active porewater tracking inventory sheet from Google Drive:

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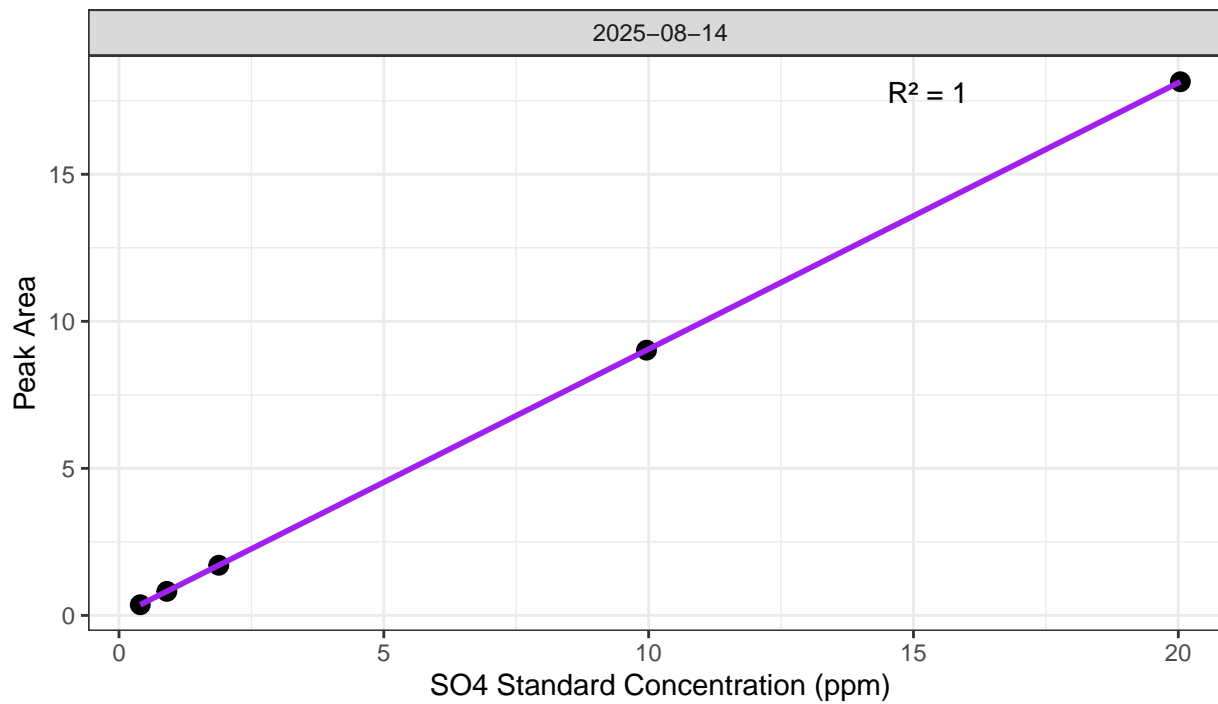
##Import Sample Data

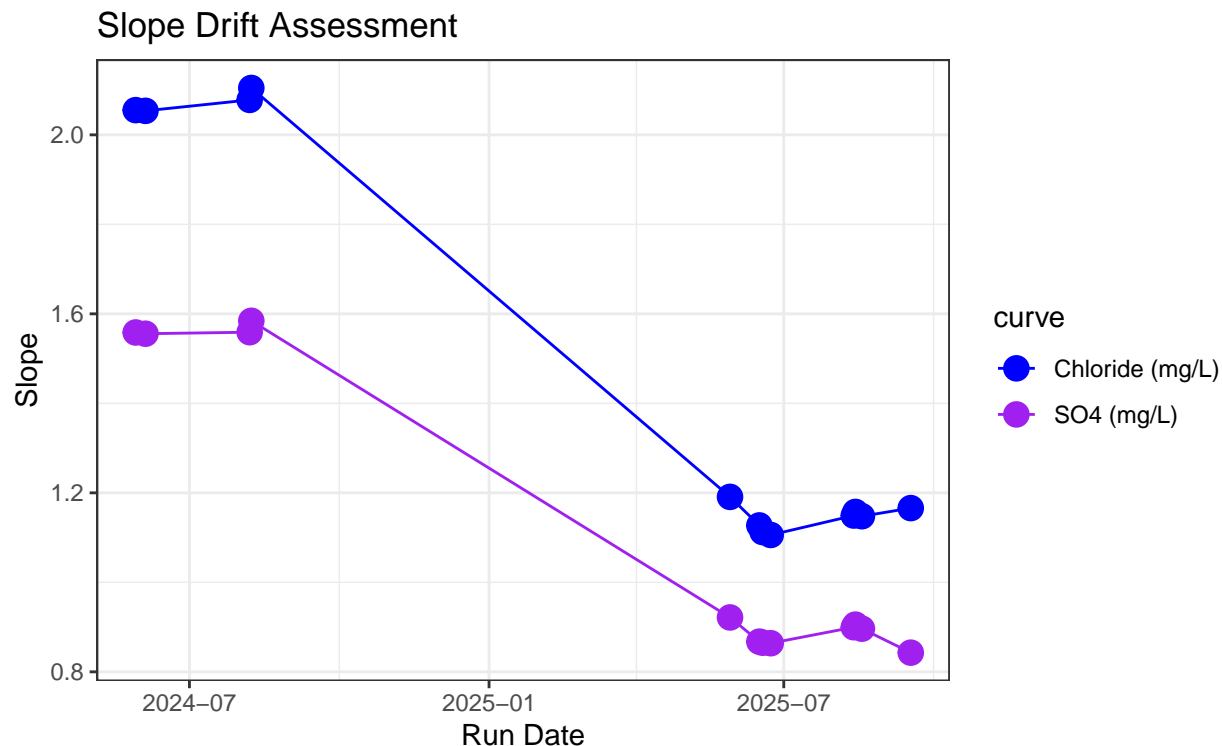##Fix Sample IDs entered wrong

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"
```
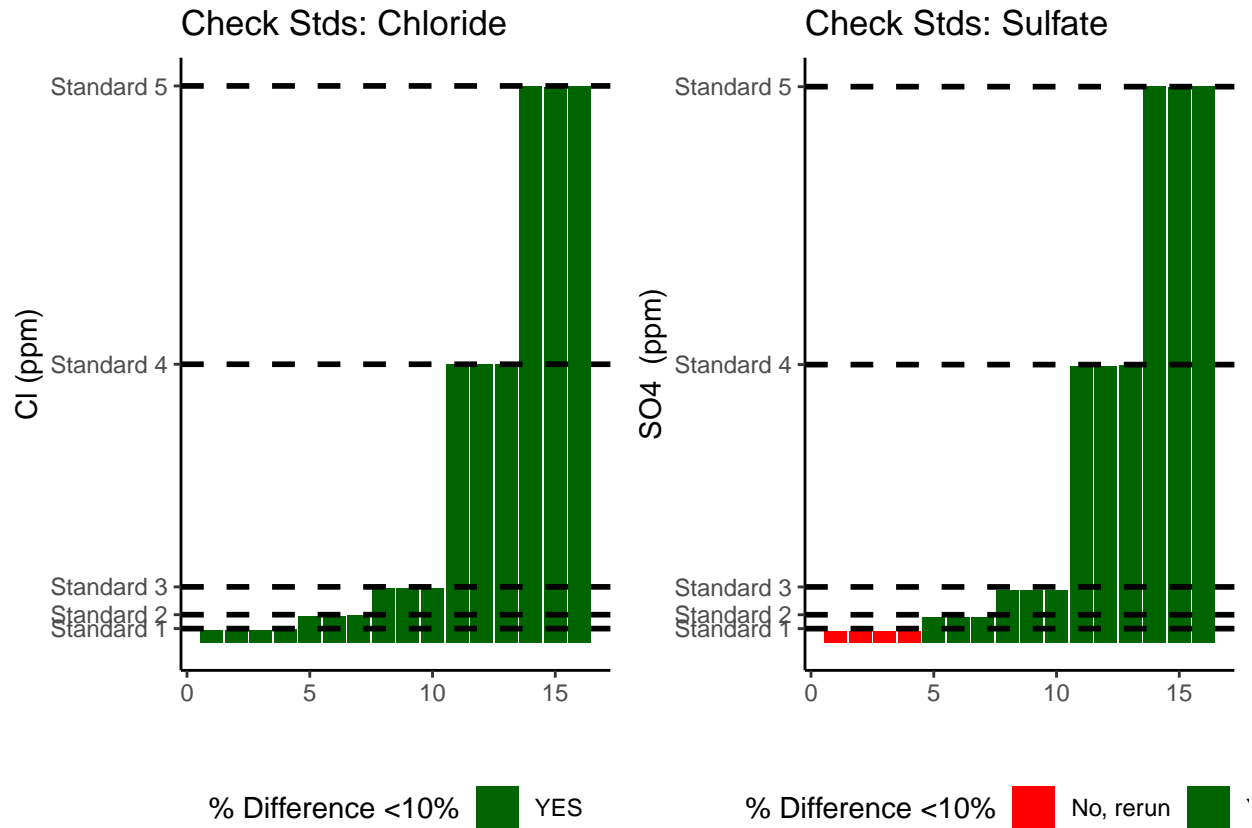
0.4 Assess Check Standards

```
## # 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"
```
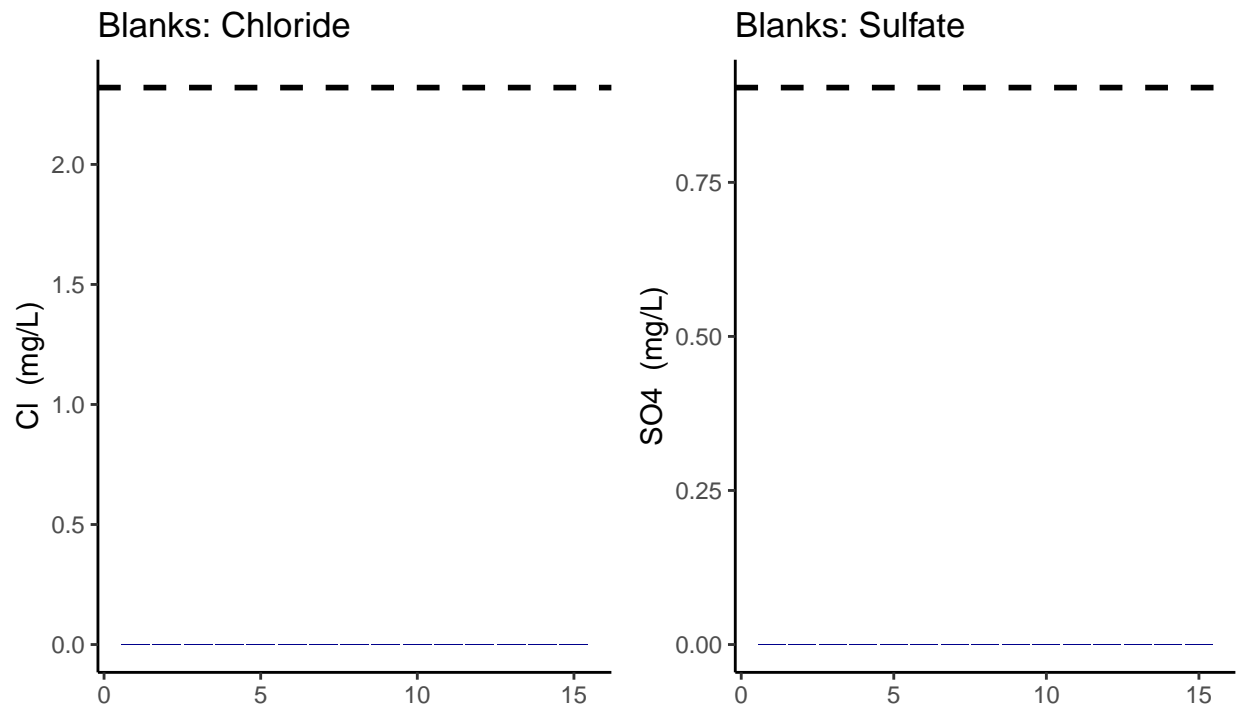
Check Stds: Chloride

Check Stds: Sulfate

% Difference <10% ▮ YES

% Difference <10% ▮ No, rerun ▮ 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

CI (mg/L)

Blanks: Sulfate

SO4 (mg/L)

Blank Conc <25% Quartile Samples   YE

Blank Conc <25% Quartile Samples   Y

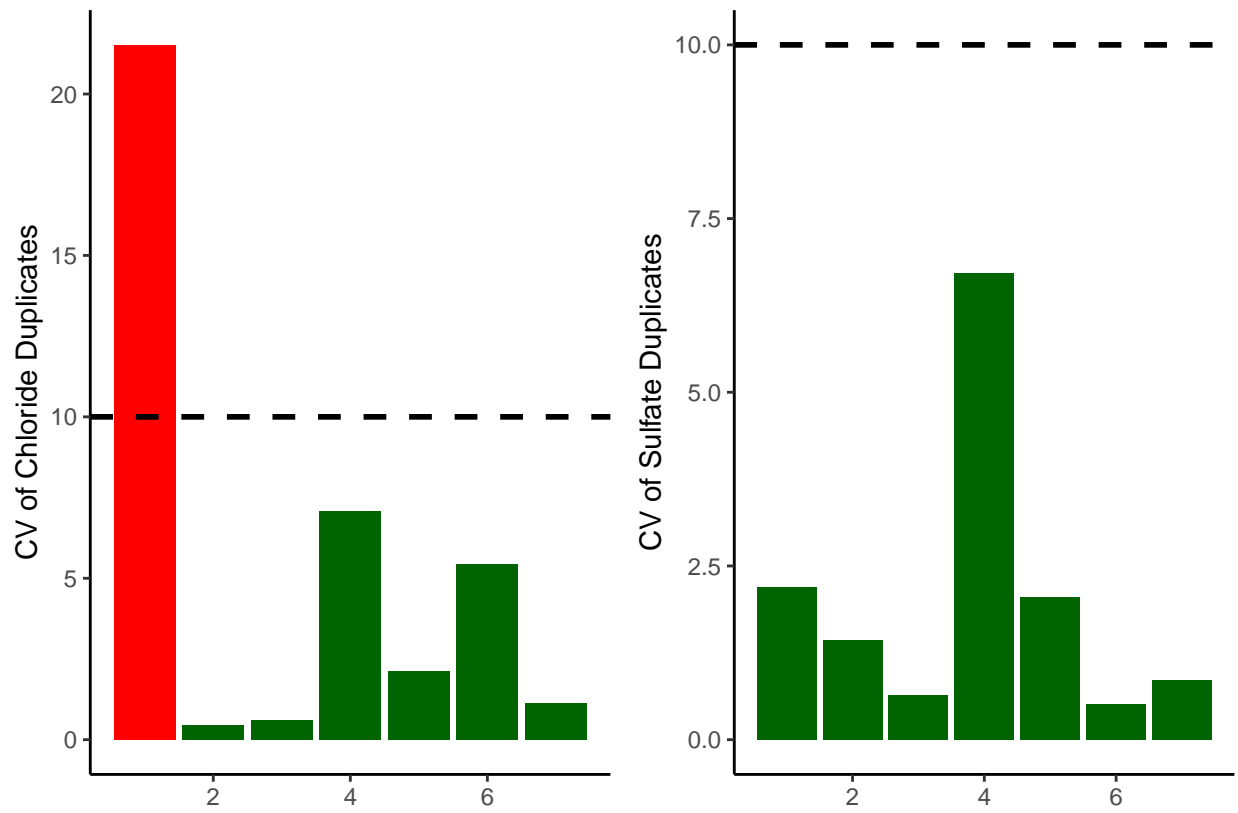```
Chloride blanks mean ppm:

[1] 0

Sulfate blanks mean ppm:

[1] 0
```
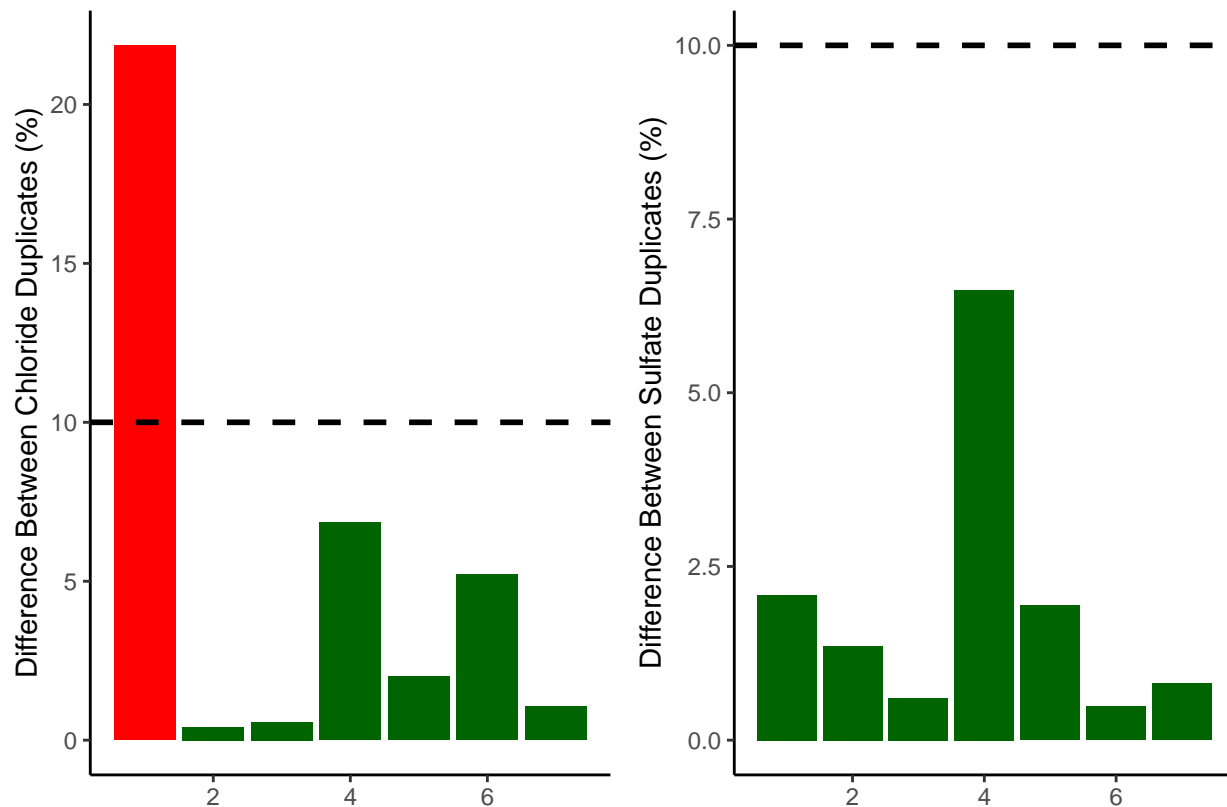
## 0.6    Assess Duplicates



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

0.7 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)
```
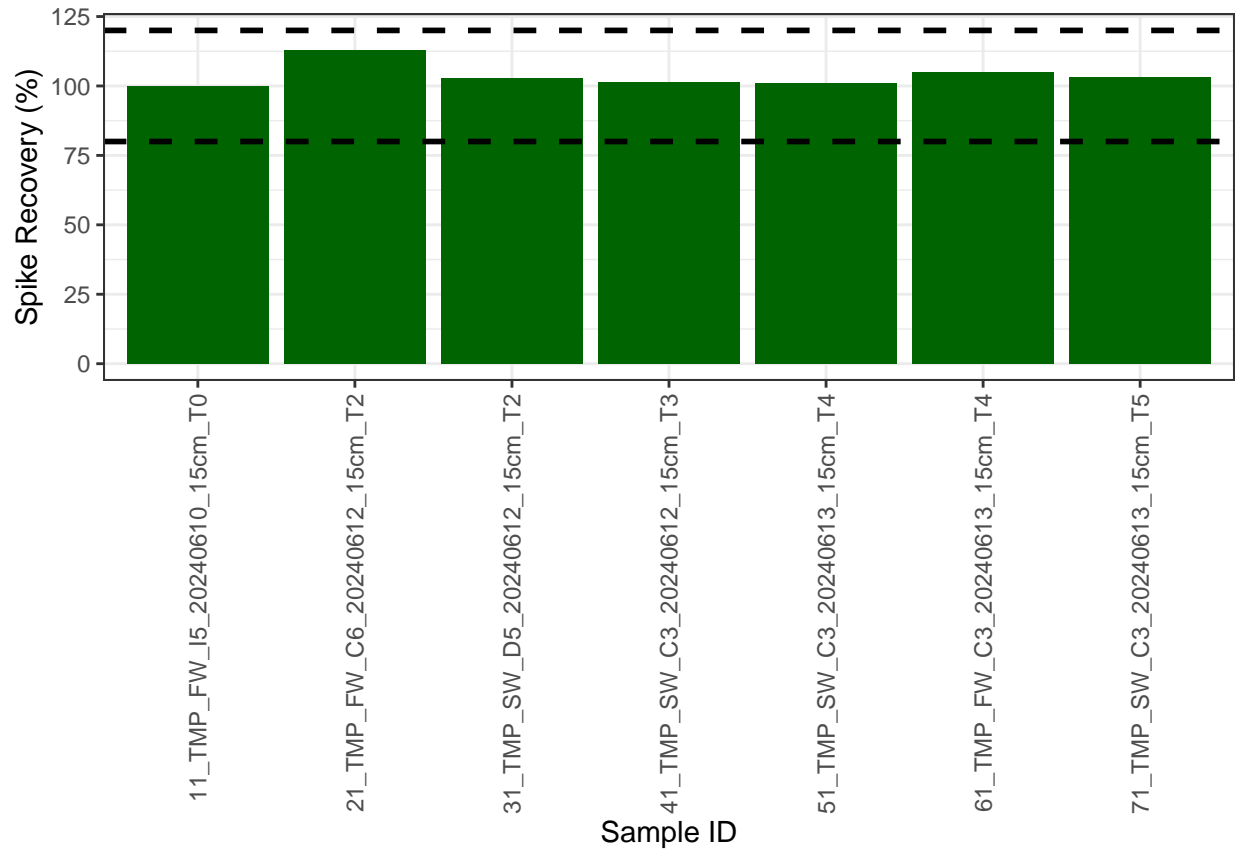
```
# head(all_dat)
```

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
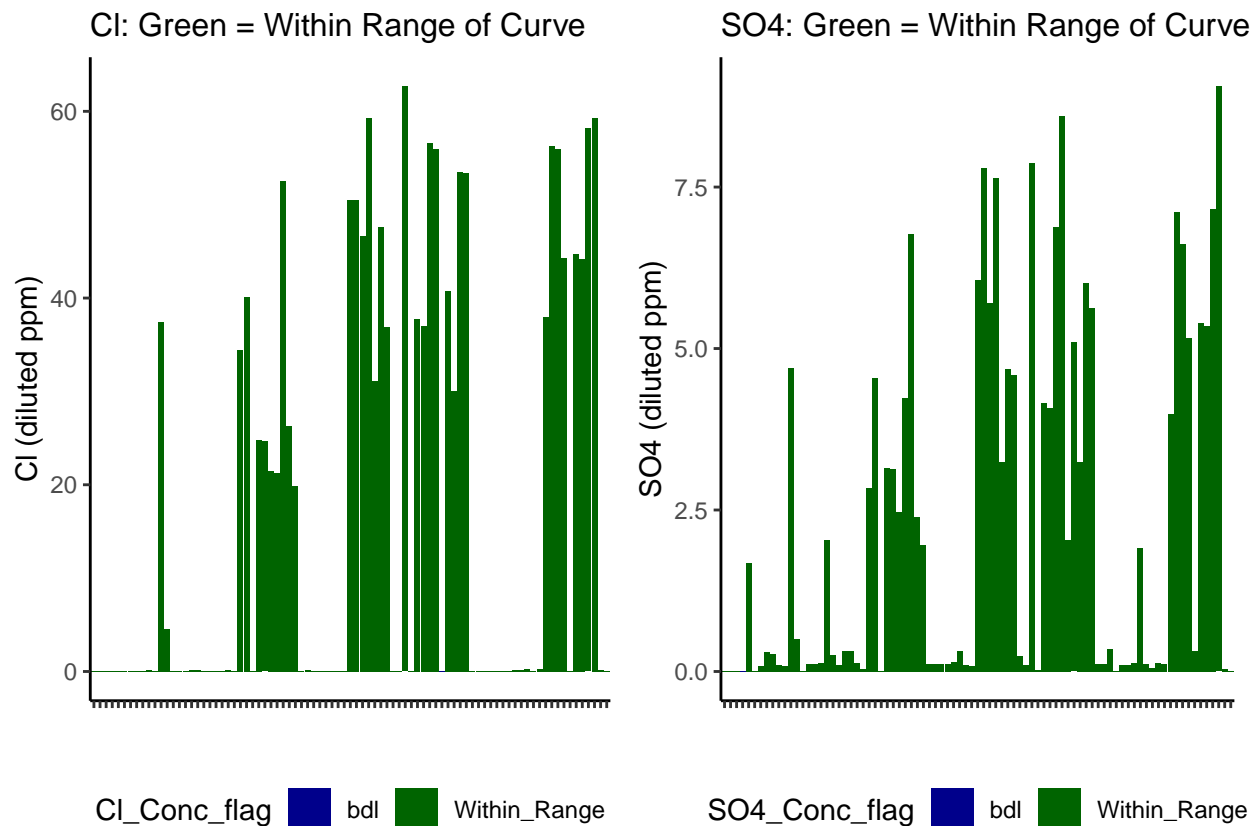
```
## Sample Flagging
```

Cl: Green = Within Range of Curve   SO4: Green = Within Range of Curve

Cl_Conc_flag ■ bdl ■ Within_Range

SO4_Conc_flag ■ bdl ■ Within_Range

Table 1: SO4 samples

SO4_Conc_flag	Percent_samples
Within_Range	98.823529
bdl	1.176471

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

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

0.11   Visualize Data by Plot

Samples: Chloride

Samples: SO4

0.12   Export Processed Data

#end