TEMPEST: Porewater SO4/Cl

Apr-Dec (No May or June) 2024 Samples

2025-09-25

Contents

##Add Required Packages

0.1 Run Information

```
###### Run information - PLEASE CHANGE
  Sample_Year = "2024"
  Date_Run = "2025-08-13"  #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.
  Some sample IDs are missing from metadata:
  TMP_SW_B4_20240426_15CM
  TMP_SW_B4_20240711_15CM
  TMP_SW_F6_20241111_15CM
  " #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_202404-202412_Cl.txt"
  raw_file_name_so4 = "Raw Data/COMPASS_TEMPEST_202404-202412_SO4.txt"

#file path and name of processed data file
  processed_file_name = "Processed Data/COMPASS_TEMPEST_Processed_Cl_SO4_202404-202412.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"
```

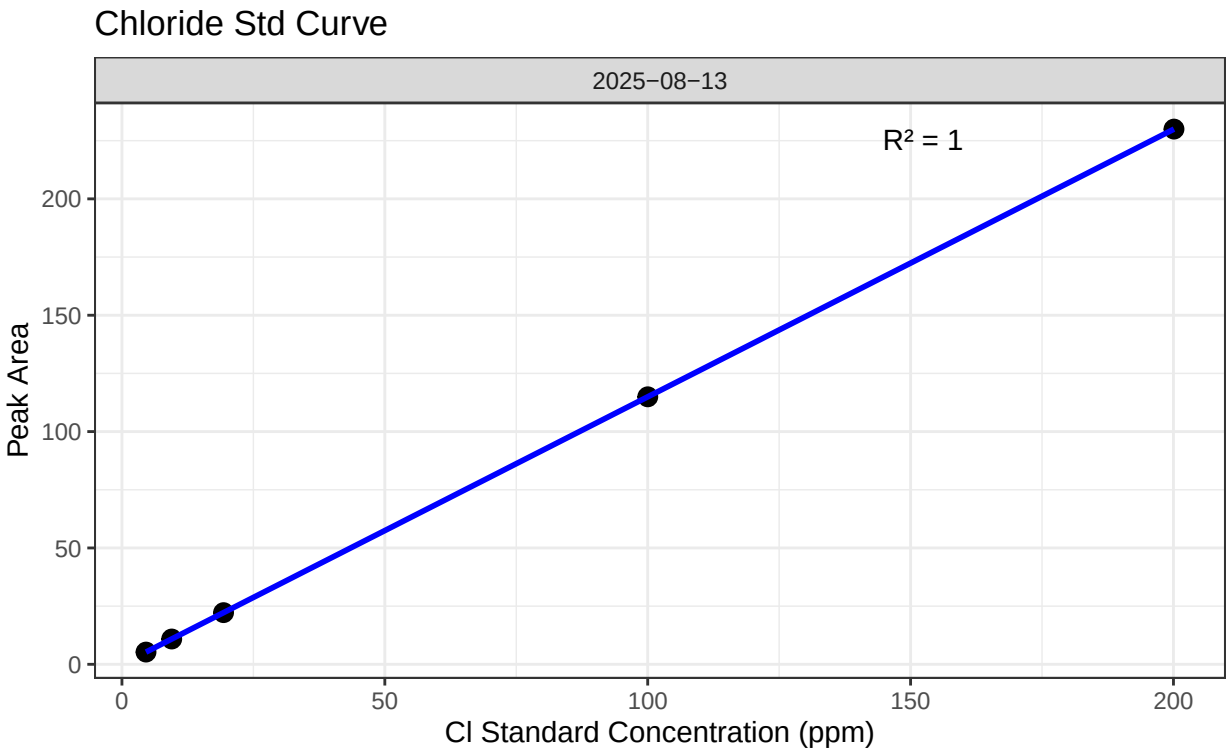
##Set Up Code - constants and QAQC cutoffs

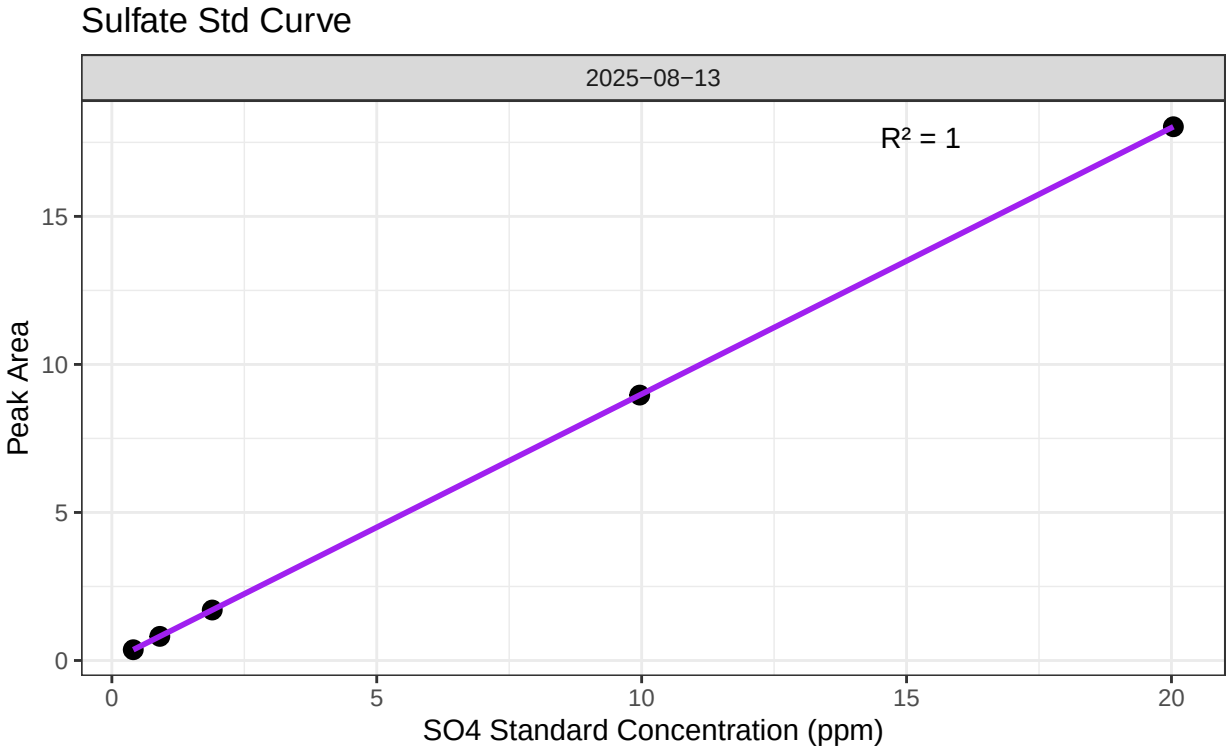
0.2 Pull in active porewater tracking inventory sheet from Google Drive:

##Create similar sample IDs to match with run samples

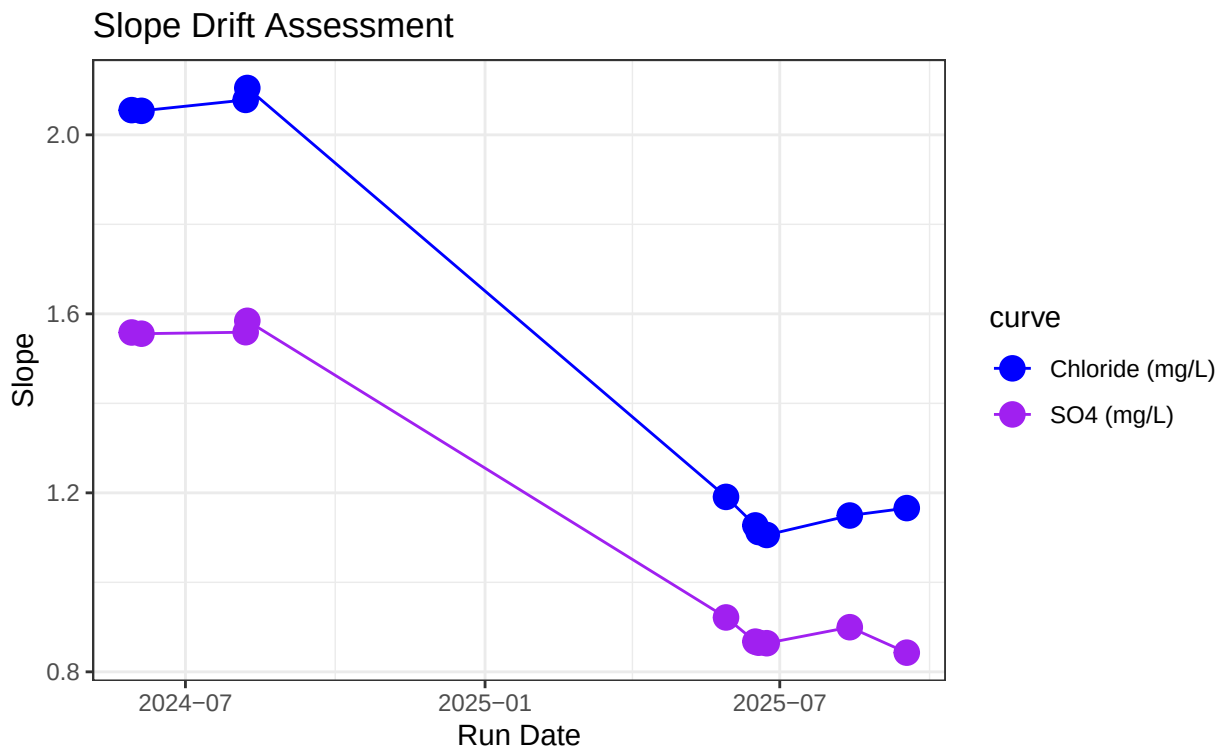
##Import Sample Data

0.3 Assess Standard Curves






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




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

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

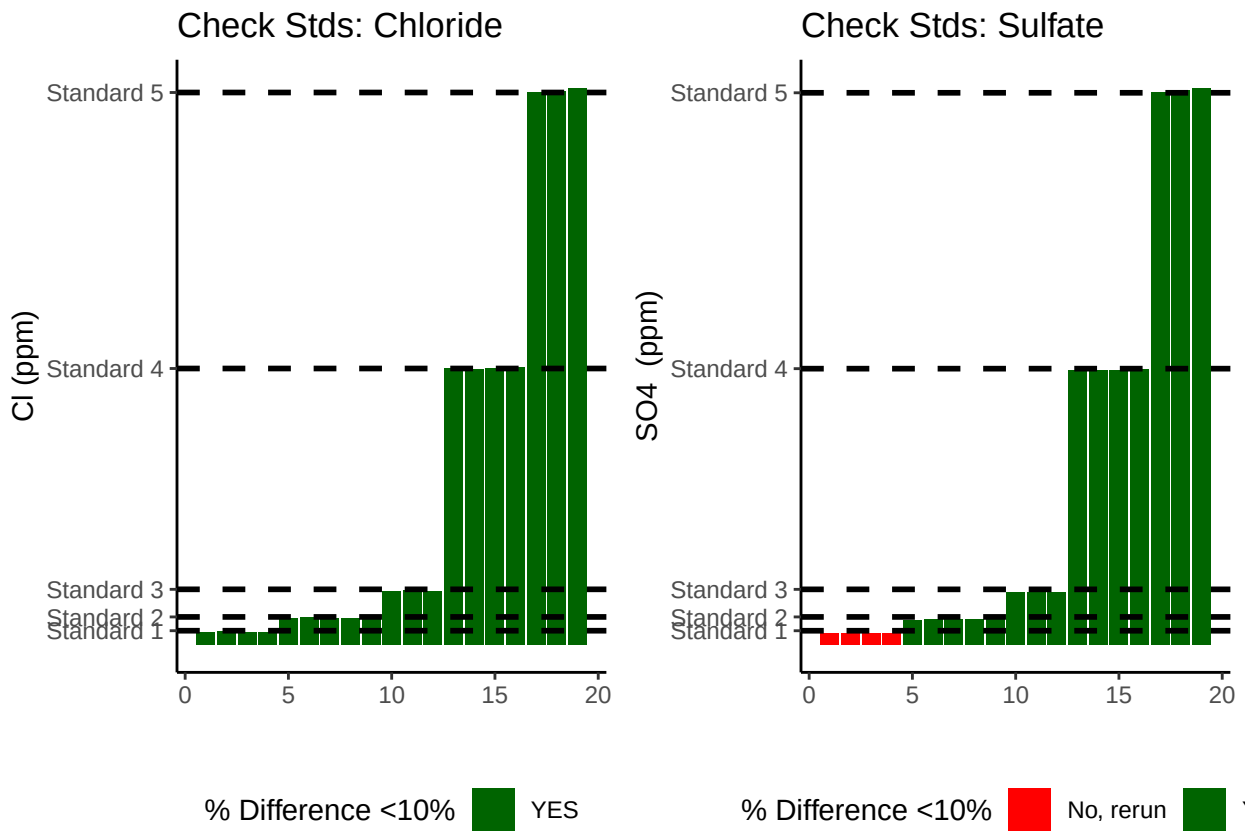
0.4 Assess Check Standards

```
## # 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 0.126 0.0270  Chloride Check Standard RSD within Range - P~
## 2 Standard 2    9.60 0.153 0.0159  Chloride Check Standard RSD within Range - P~
## 3 Standard 3   19.5  0.296 0.0152  Chloride Check Standard RSD within Range - P~
## 4 Standard 4  100.   0.188 0.00188 Chloride Check Standard RSD within Range - P~
## 5 Standard 5  201.   0.852 0.00424 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    0.409 0.00380 0.00929 Sulfate Check Standard RSD within Range -~
## 2 Standard 2    0.910 0.00386 0.00424 Sulfate Check Standard RSD within Range -~
## 3 Standard 3    1.90  0.00779 0.00409 Sulfate Check Standard RSD within Range -~
## 4 Standard 4    9.96  0.0194  0.00195 Sulfate Check Standard RSD within Range -~
## 5 Standard 5   20.1   0.0776  0.00386 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"
```



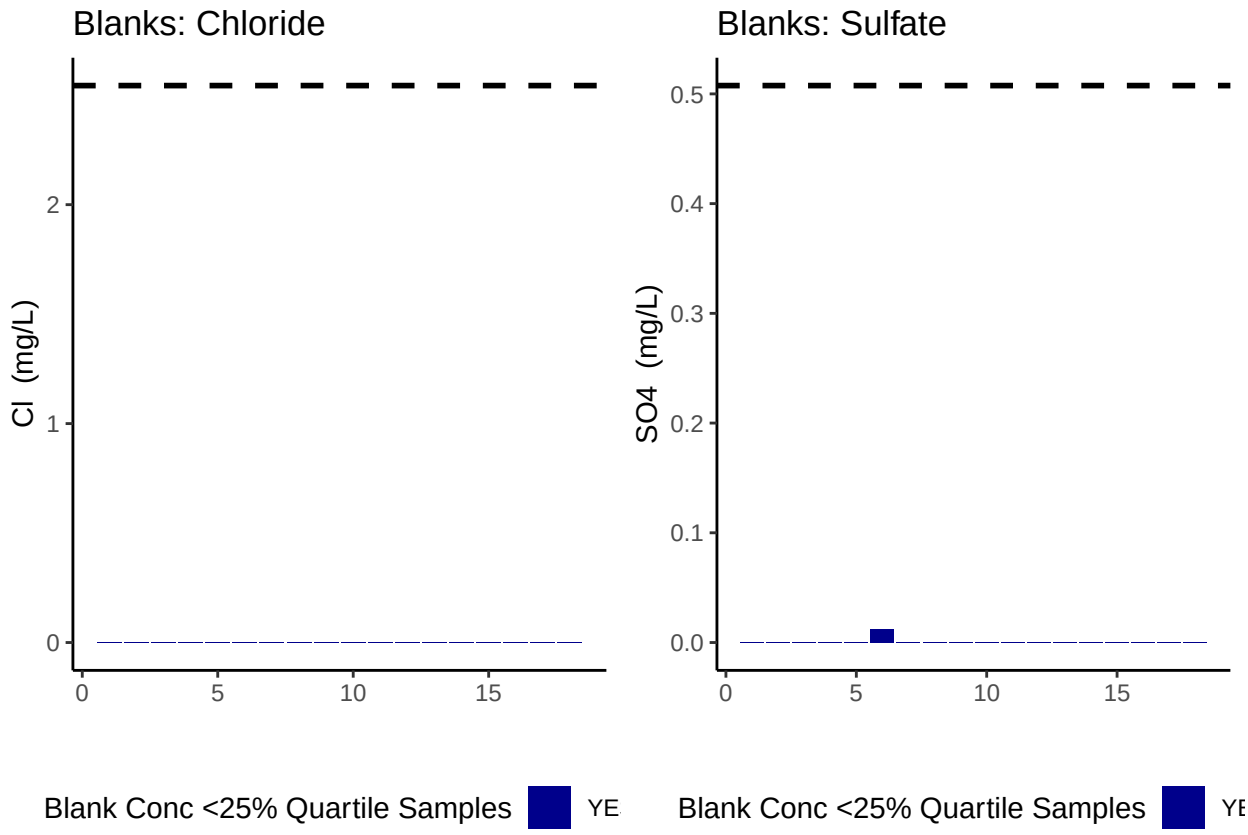

```
## [1] ">80% of Chloride Check Standards are within range of expected concentration - PROCEED"
```

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

0.5 Assess Blanks

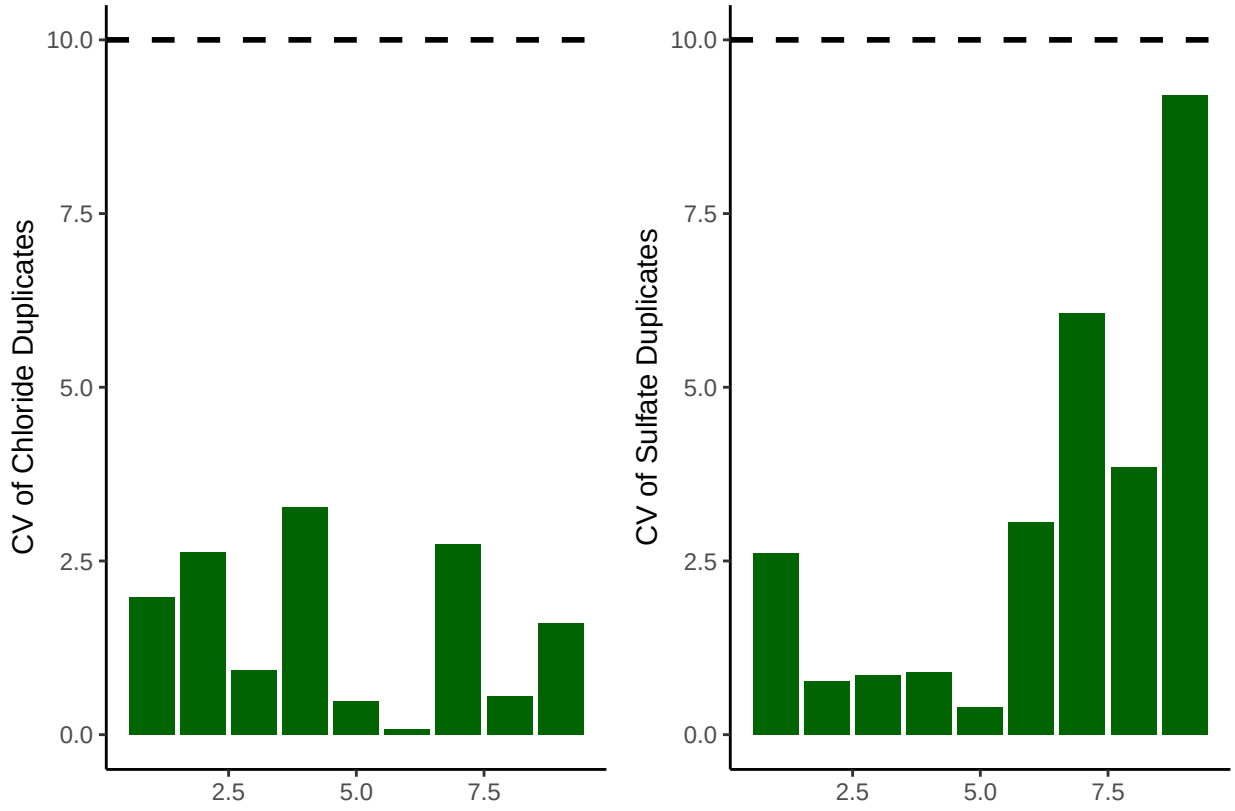
```
## [1] ">80% of Chloride Blank concentrations are lower 25% quartile of samples"
```

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



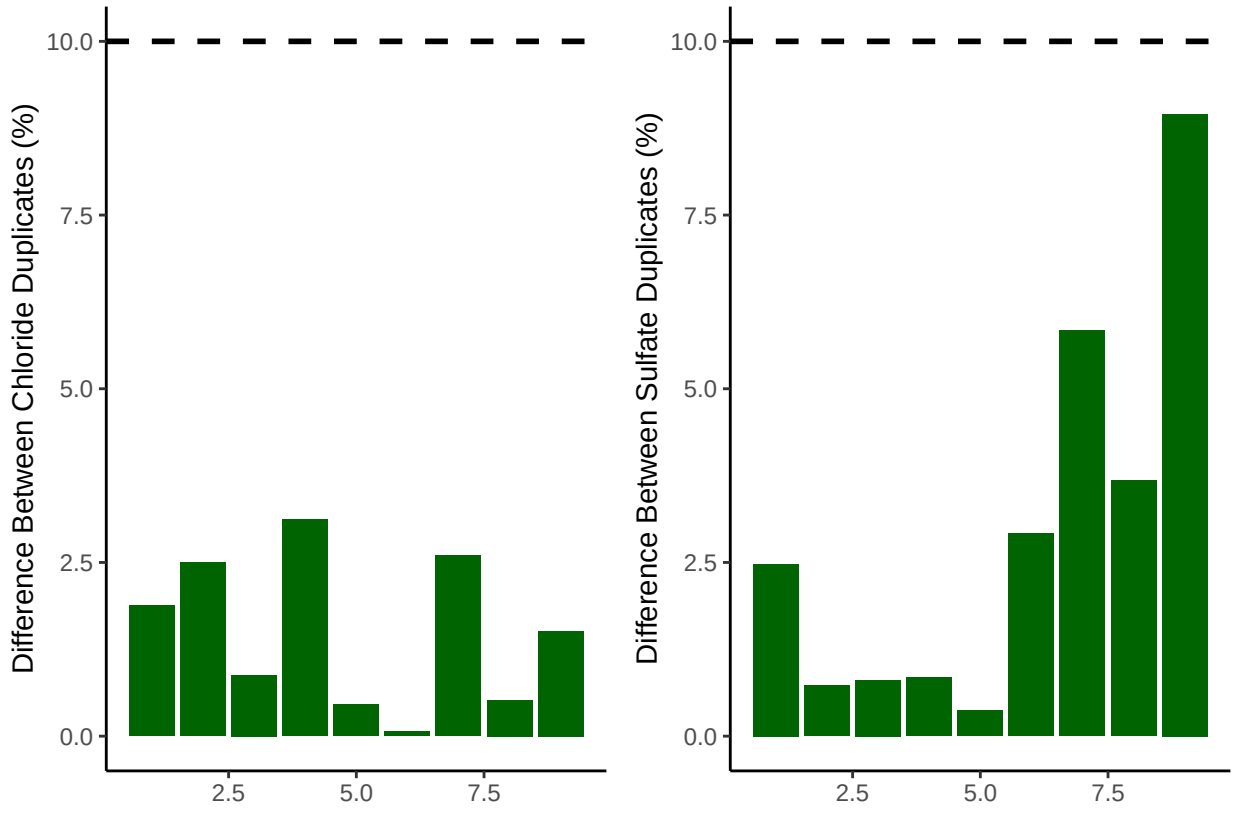

```
## Chloride blanks mean ppm:

## [1] 0

## Sulfate blanks mean ppm:

## [1] 0.0006722222
```

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"
```

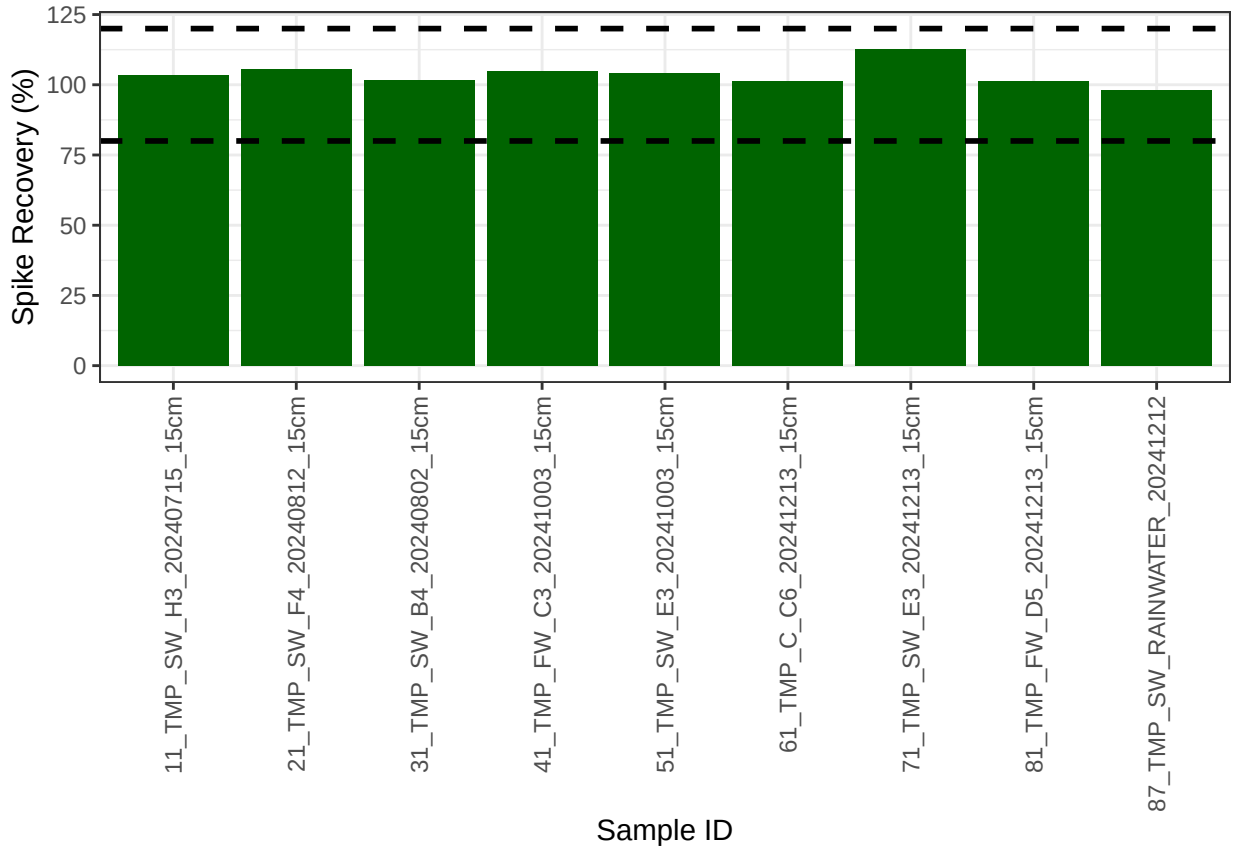
```
## [1] ">80% of Sulfate Duplicates have a percent difference <10% - PROCEED"
```

0.7 Calculate mmol/L concentrations & salinity, add dilutions

```
# 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
```

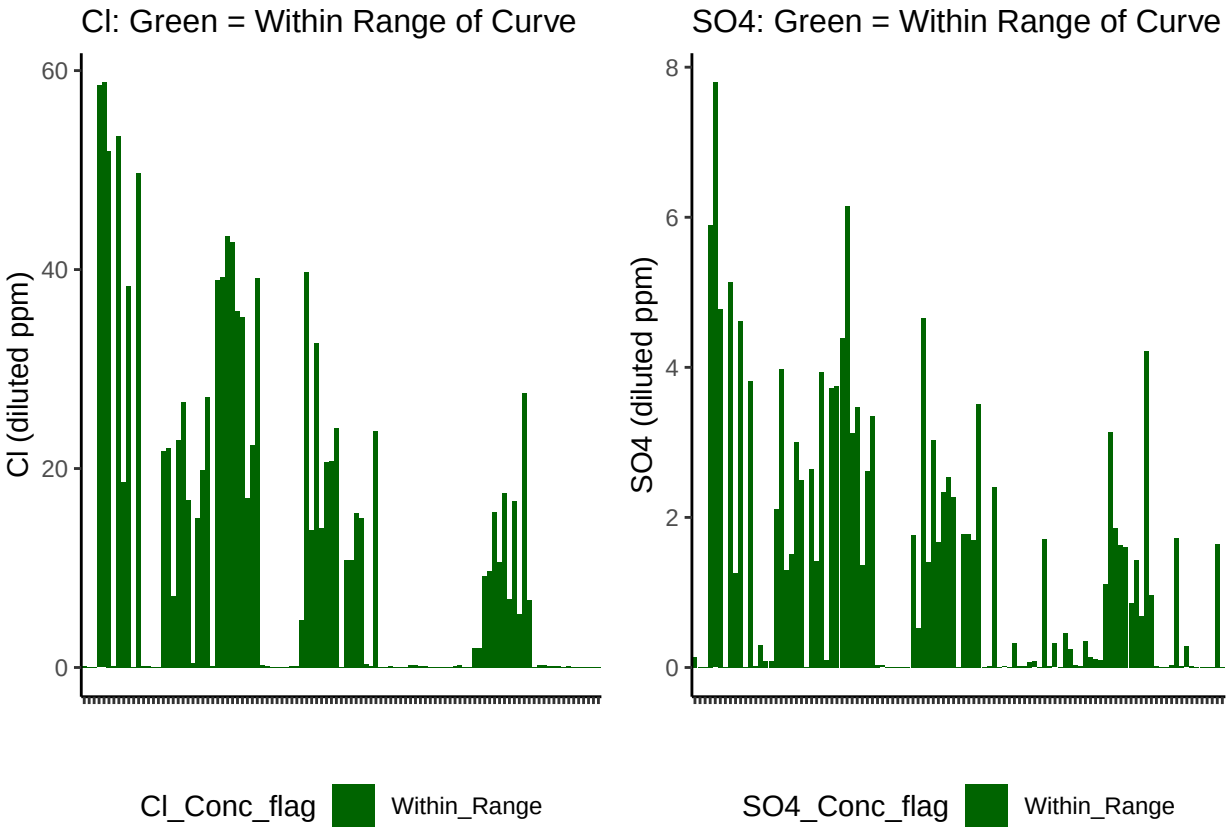


Table 1: SO4 samples

SO4_Conc_flag	Percent_samples
Within_Range	100

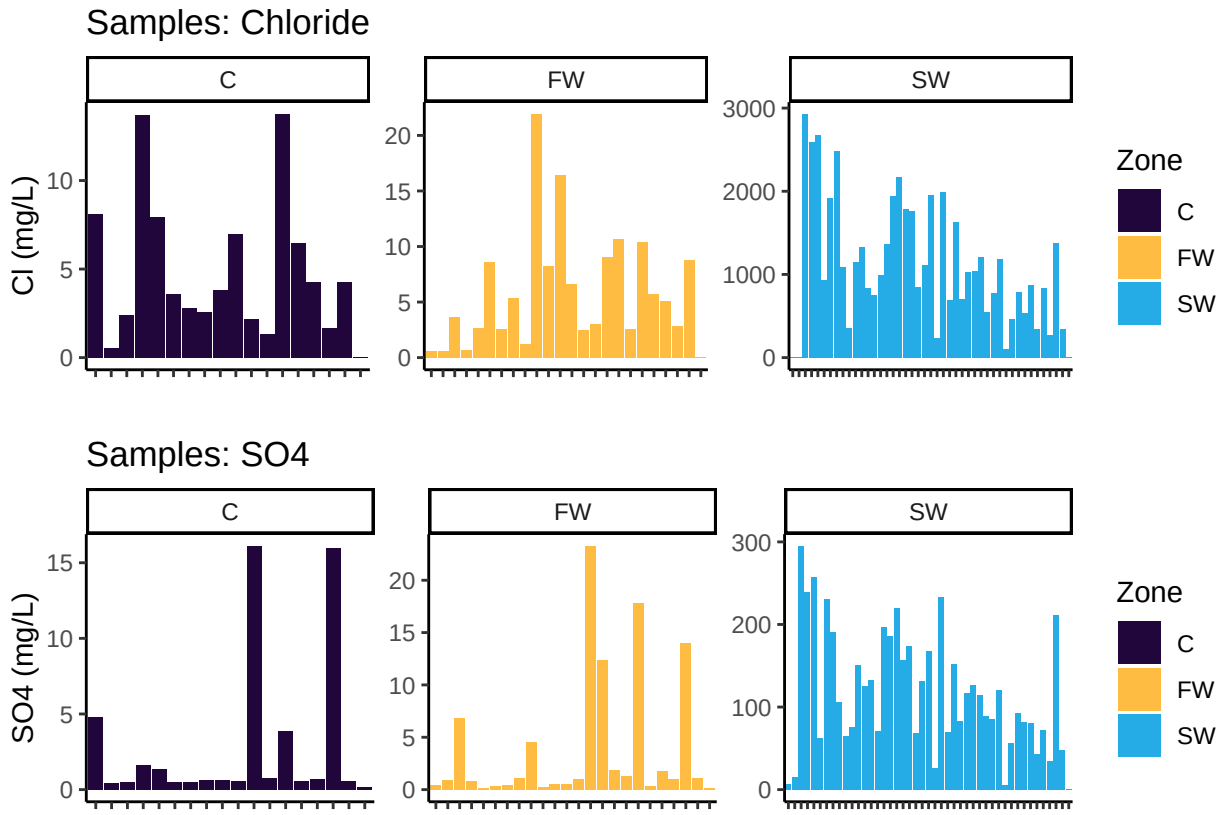
Table 2: Cl samples

Cl_Conc_flag	Percent_samples
Within_Range	100

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

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

## [1] "TMP_SW_B4_20240426_15CM" "TMP_SW_B4_20240711_15CM"
## [3] "TMP_SW_F6_20241111_15CM"
```

0.11 Visualize Data by Plot



0.12 Export Processed Data

#end