TEMPEST: Porewater SO4/Cl

June (72-136) 2024 Samples

2025-10-20

Contents

##Add Required Packages

0.1 Run Information

```
###### Run information - PLEASE CHANGE
  Sample_Year = "2024"
  Date_Run = "2025-08-18"  #Date that instrument was run
  Run_by = "Zoe Read"  #Instrument user
  Script_run_by = "Zoe Read" #Code user
  run_notes = "All std 1's and one std 2 were lower than the expected concentration.
  The 5th dup had a high CV for Cl
  One sample ID is missing from metadata: TMP_FW_D5_20240617_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_202406_72-136_Cl.txt"
  raw_file_name_so4 = "Raw Data/COMPASS_TEMPEST_202406_72-136_SO4.txt"

#file path and name of processed data file
  processed_file_name = "Processed Data/COMPASS_TEMPEST_Processed_Cl_SO4_202406_72-136.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"
```

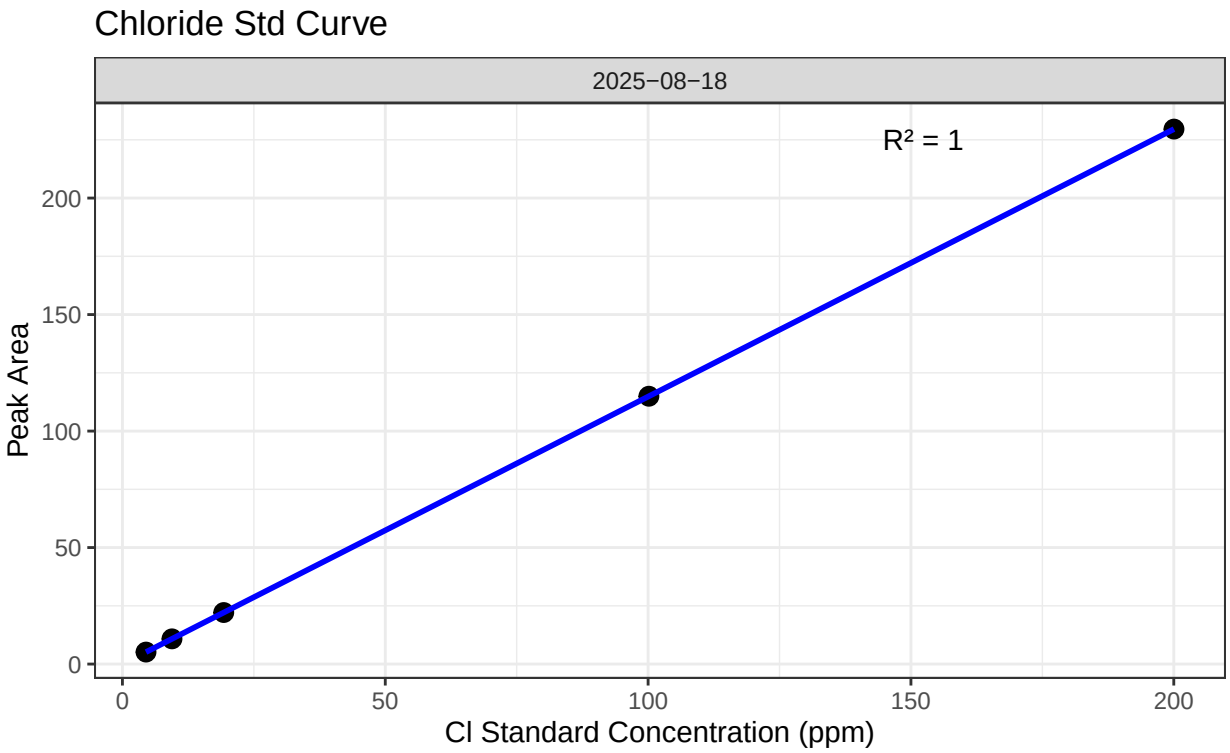
##Set Up Code - constants and QAQC cutoffs

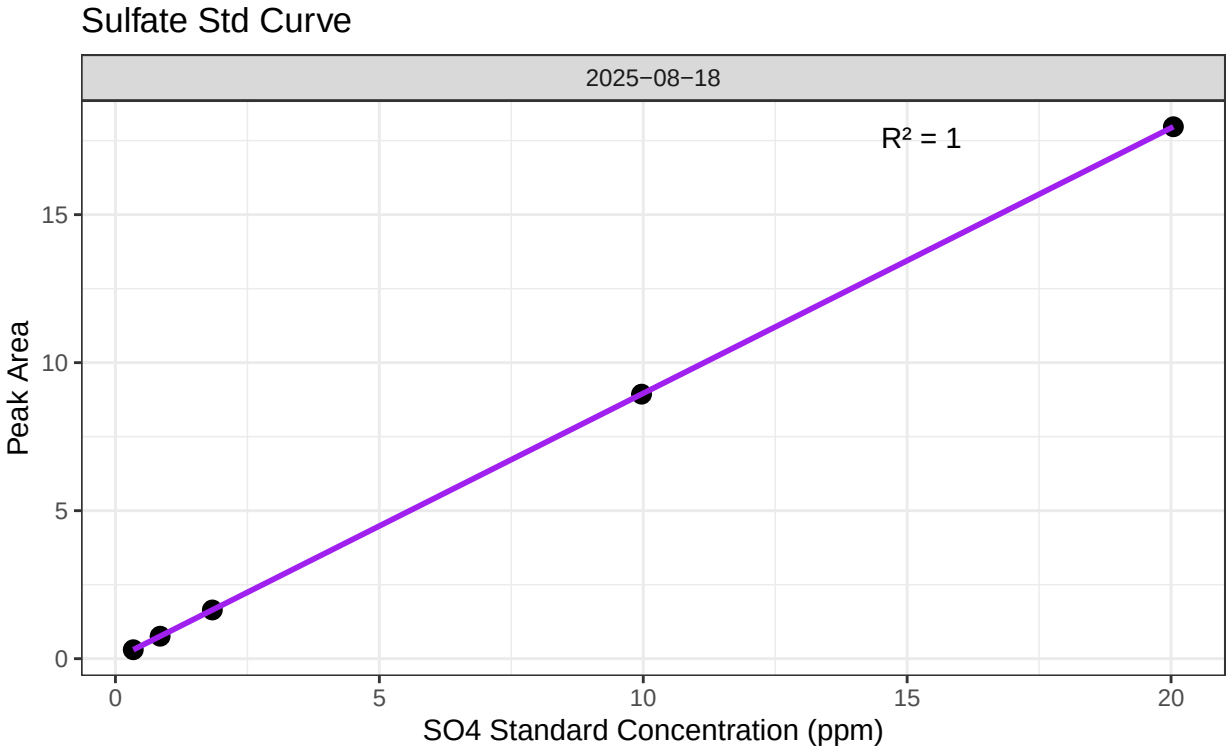
0.2 Pull in active porewater tracking inventory sheet from Google Drive:

##Create similar sample IDs to match with run samples

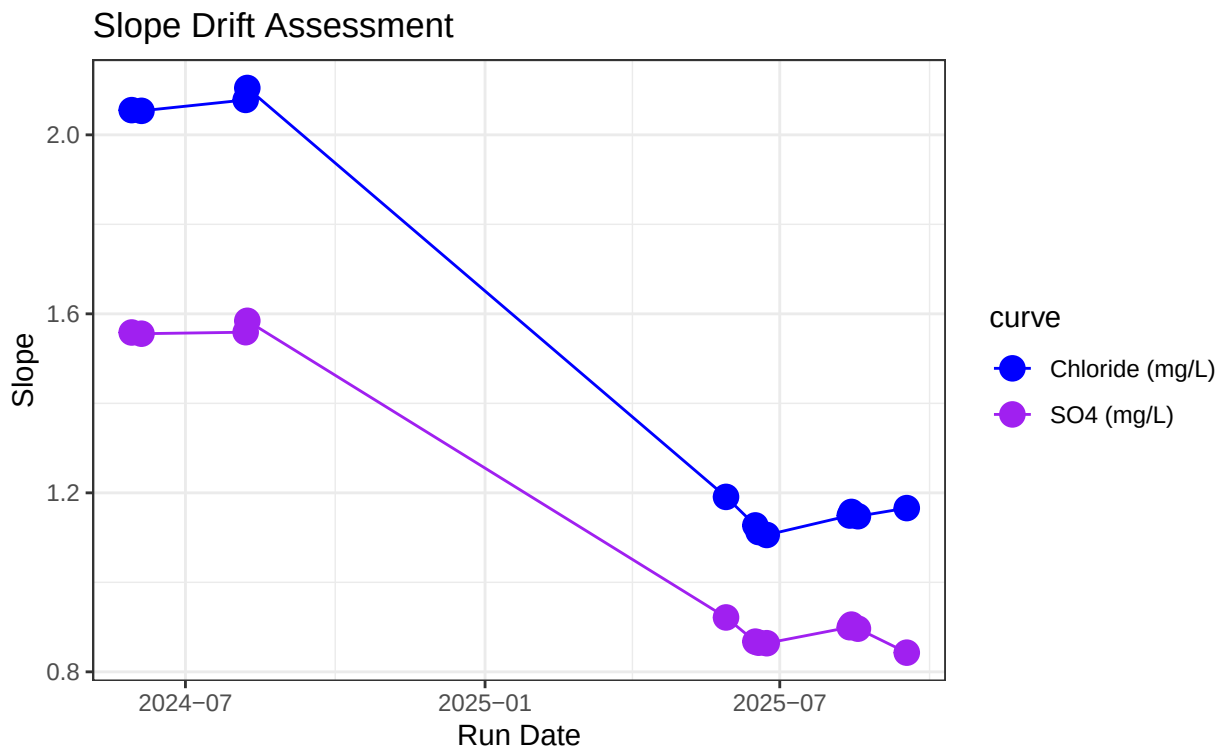
##Import Sample Data

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"
```

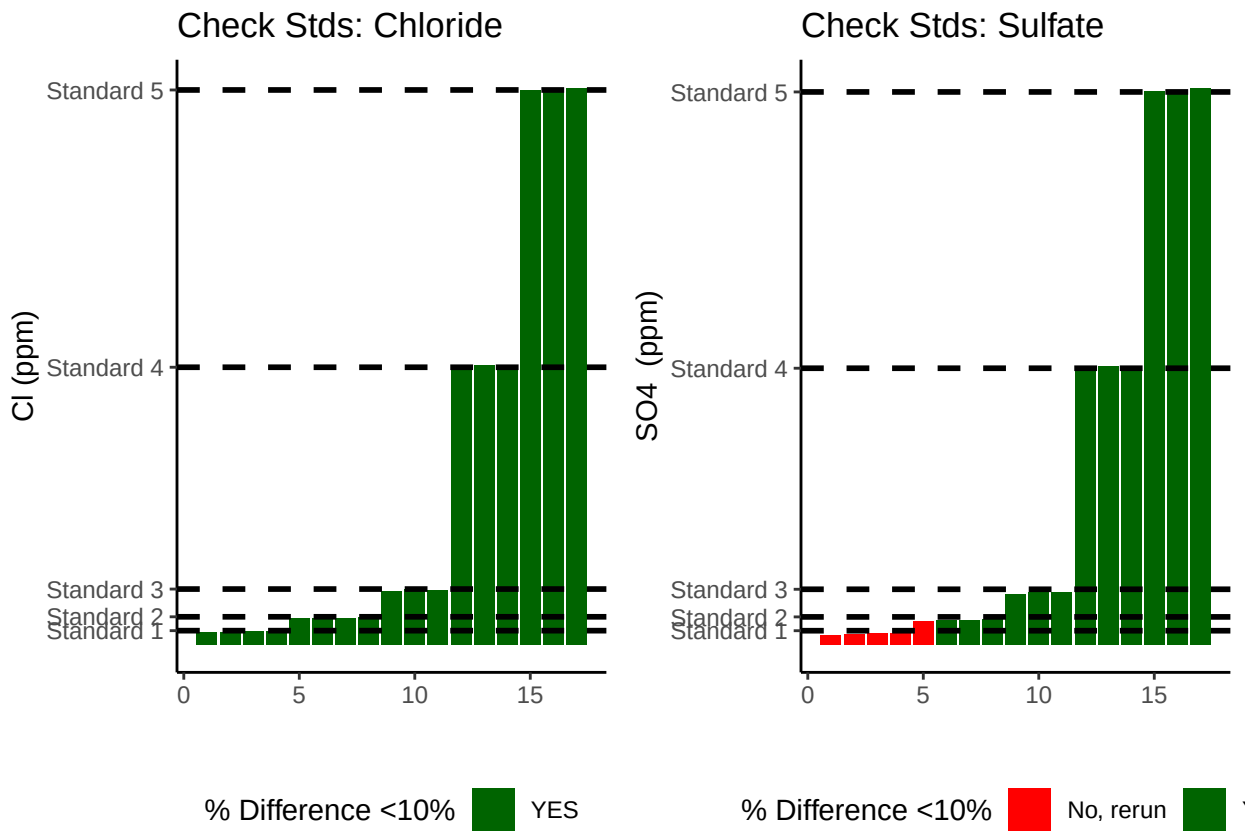
0.4 Assess Check Standards

```
## # A tibble: 5 x 5
##   sample_ID  mean_Cl sd_Cl   cv_Cl flag_Cl
##   <chr>        <dbl> <dbl>   <dbl> <chr>
## 1 Standard 1    4.68 0.166 0.0354  Chloride Check Standard RSD within Range - P~
## 2 Standard 2    9.62 0.159 0.0166  Chloride Check Standard RSD within Range - P~
## 3 Standard 3   19.6  0.313 0.0159  Chloride Check Standard RSD within Range - P~
## 4 Standard 4  101.   0.434 0.00432 Chloride Check Standard RSD within Range - P~
## 5 Standard 5  200.   0.610 0.00305 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    0.384 0.0314 0.0816  Sulfate Check Standard RSD within Range - ~
## 2 Standard 2    0.883 0.0266 0.0302  Sulfate Check Standard RSD within Range - ~
## 3 Standard 3    1.88  0.0368 0.0196  Sulfate Check Standard RSD within Range - ~
## 4 Standard 4   10.0   0.0555 0.00554 Sulfate Check Standard RSD within Range - ~
## 5 Standard 5   20.1   0.0913 0.00455 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"
```



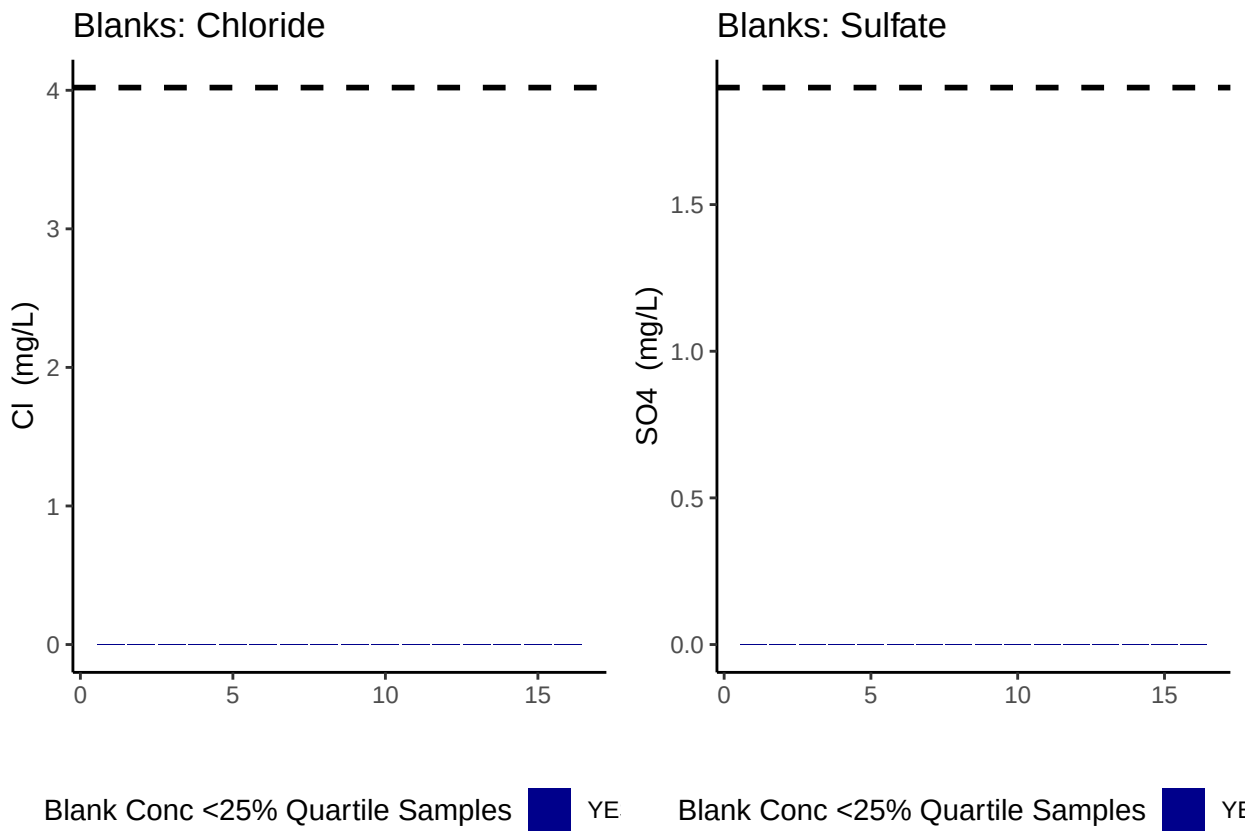

```
## [1] ">80% of Chloride Check Standards are within range of expected concentration - PROCEED"
```

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

0.5 Assess Blanks

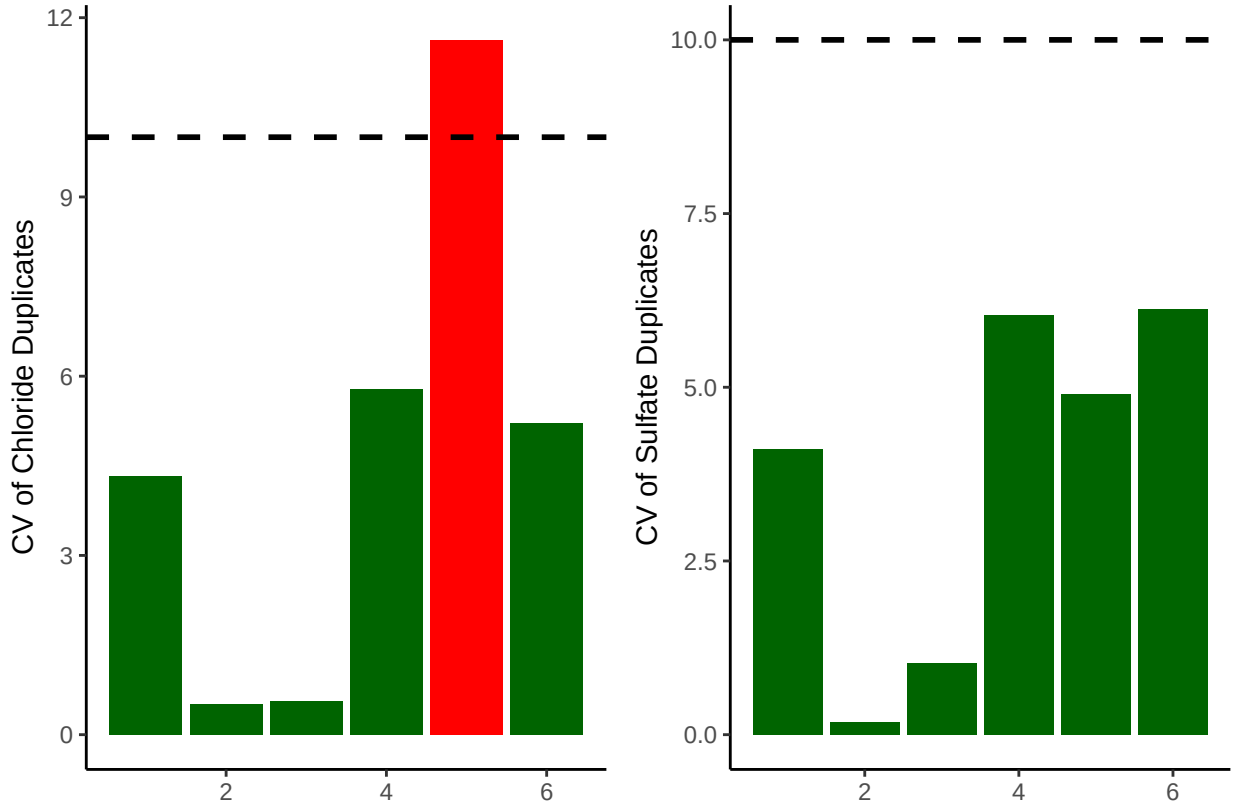
```
## [1] ">80% of Chloride Blank concentrations are lower 25% quartile of samples"
```

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



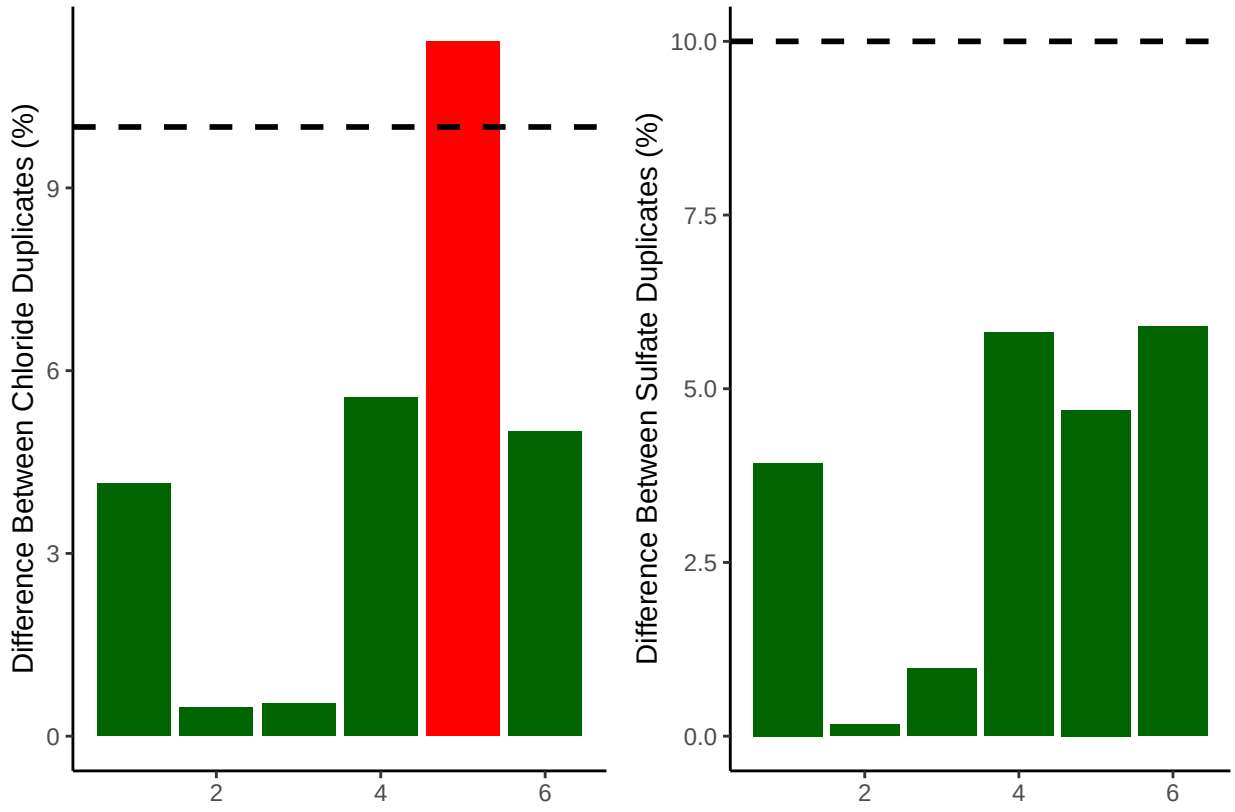

```
## Chloride blanks mean ppm:

## [1] 0

## Sulfate blanks mean ppm:

## [1] 1.875e-05
```

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"
```

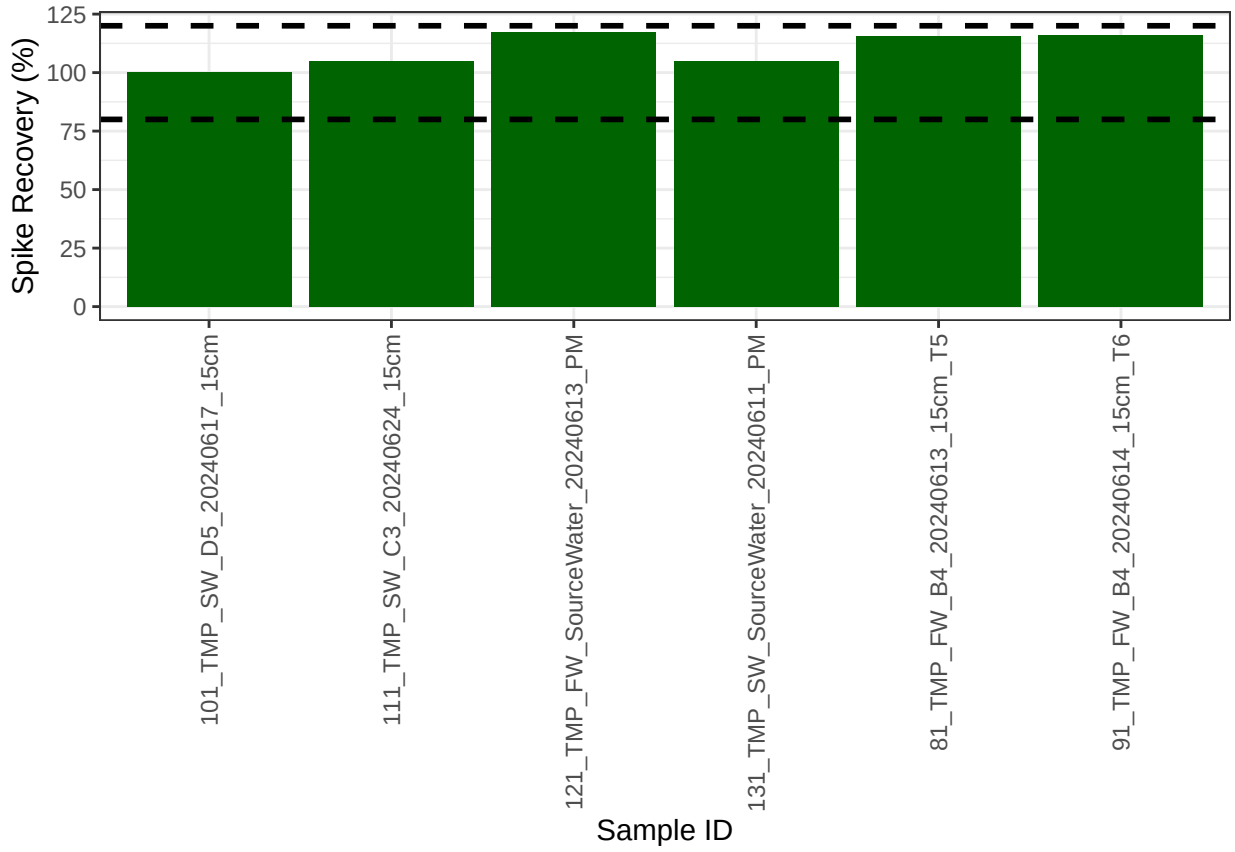
```
## [1] ">80% of Sulfate Duplicates have a percent difference <10% - PROCEED"
```

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
```

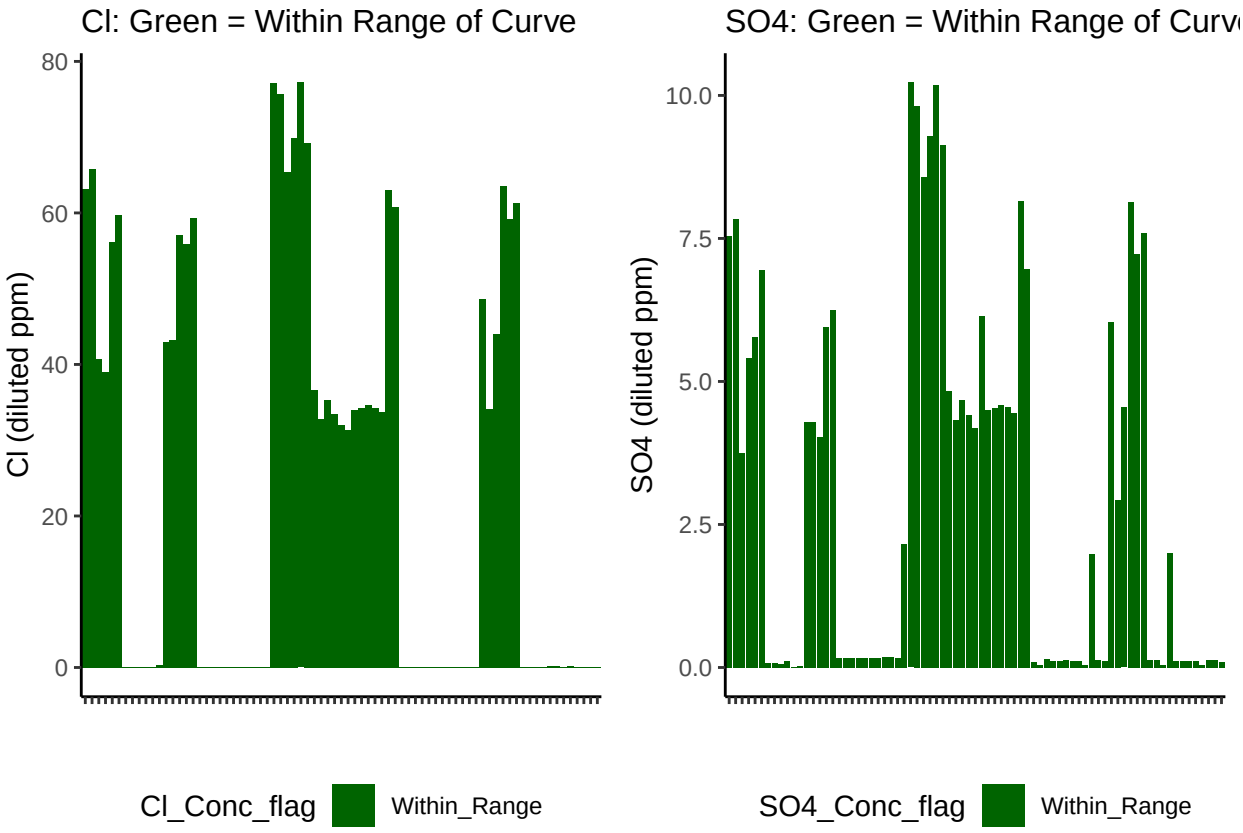


Table 1: SO4 samples

SO4_Conc_flag	Percent_samples
Within_Range	100

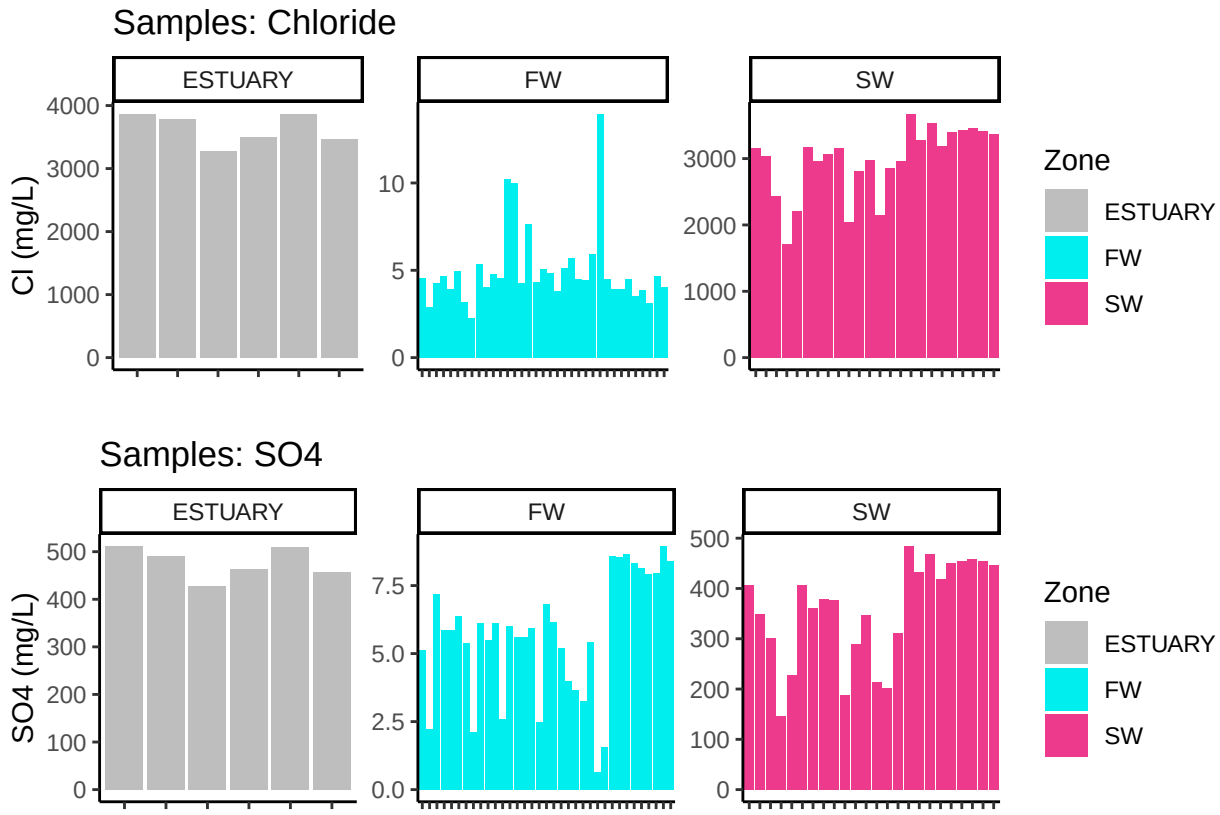
Table 2: Cl samples

Cl_Conc_flag	Percent_samples
Within_Range	100

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

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

0.11 Visualize Data by Plot



0.12 Export Processed Data

#end