

TEMPEST: Porewater SO₄/Cl

Apr-Dec (No May or June) 2024 Samples

2025-12-19

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```
##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.
" #any notes from the run

##Sample data that was entered incorrectly
# The Old ID is the original, incorrectly-entered ID and the New ID is the correct ID to change it to.
Old_ID_1 = "TMP_SW_F6_20241111_15cm"
New_ID_1 = "TMP_SW_F6_20241104_15cm"

##### 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_QAAClog_2024.csv"
```

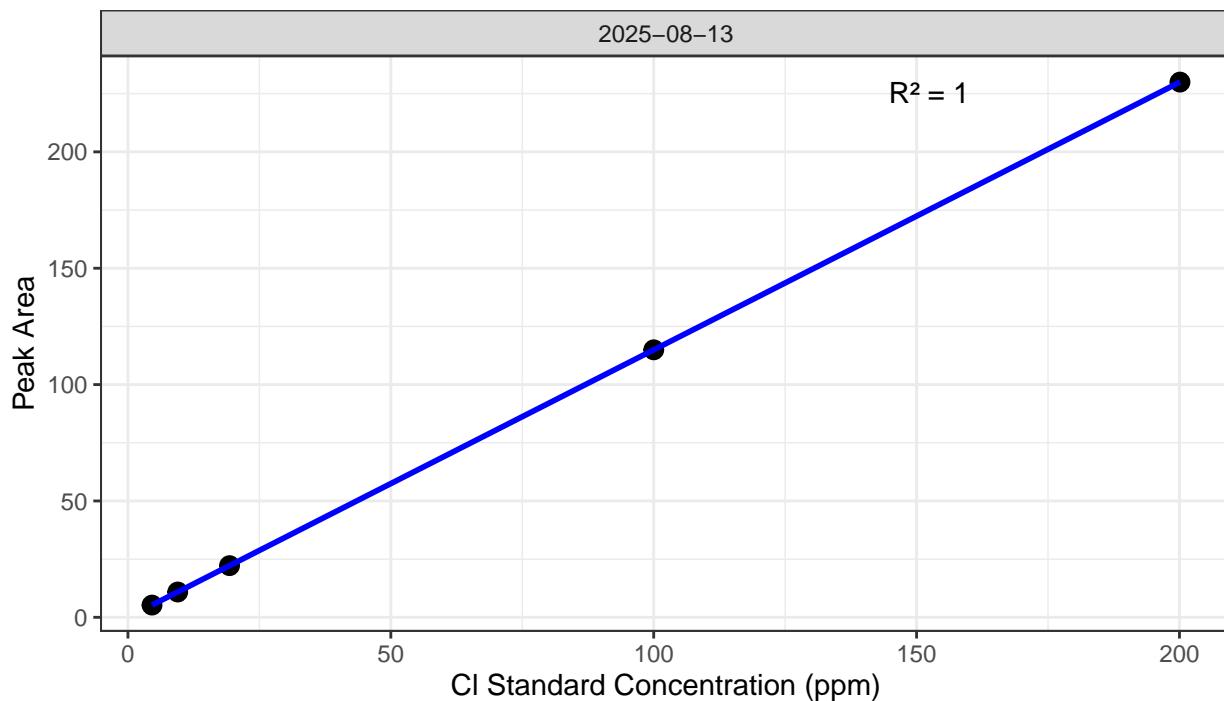
```
##Set Up Code - constants and QAQC cutoffs
```

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

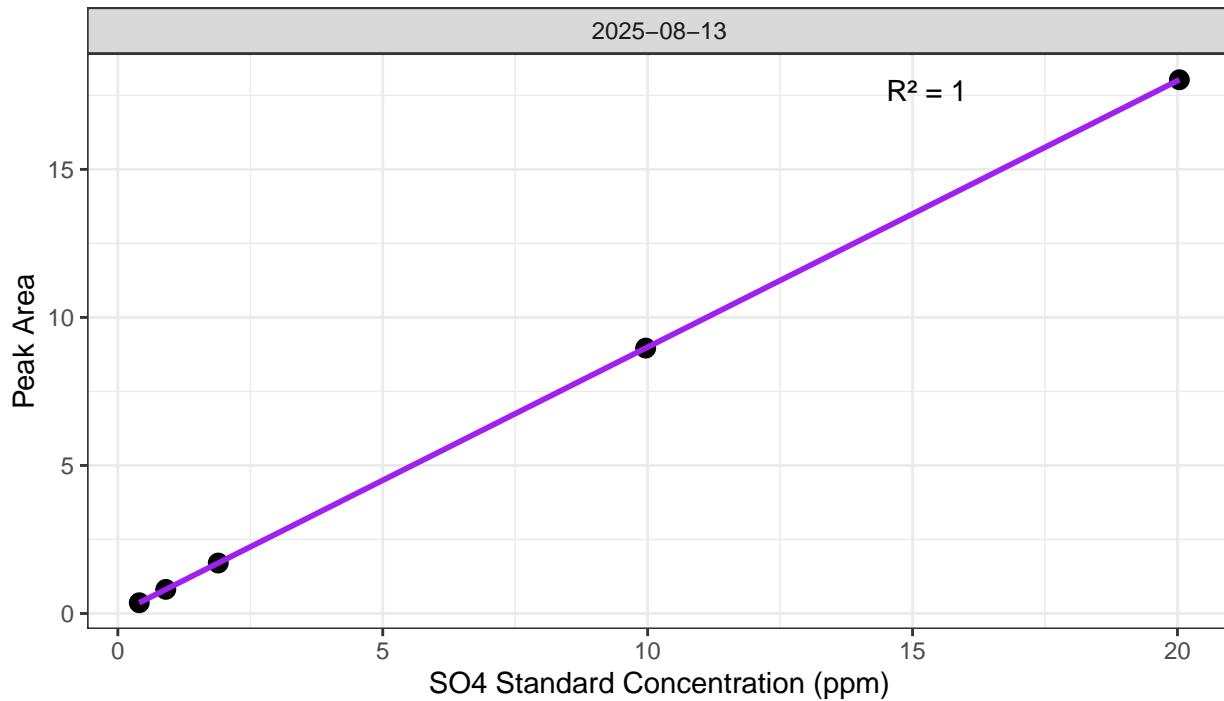
```
##Create similar sample IDs to match with run samples
##Import Sample Data
##Fix Sample IDs entered wrong
```

0.3 Assess Standard Curves

Chloride Std Curve

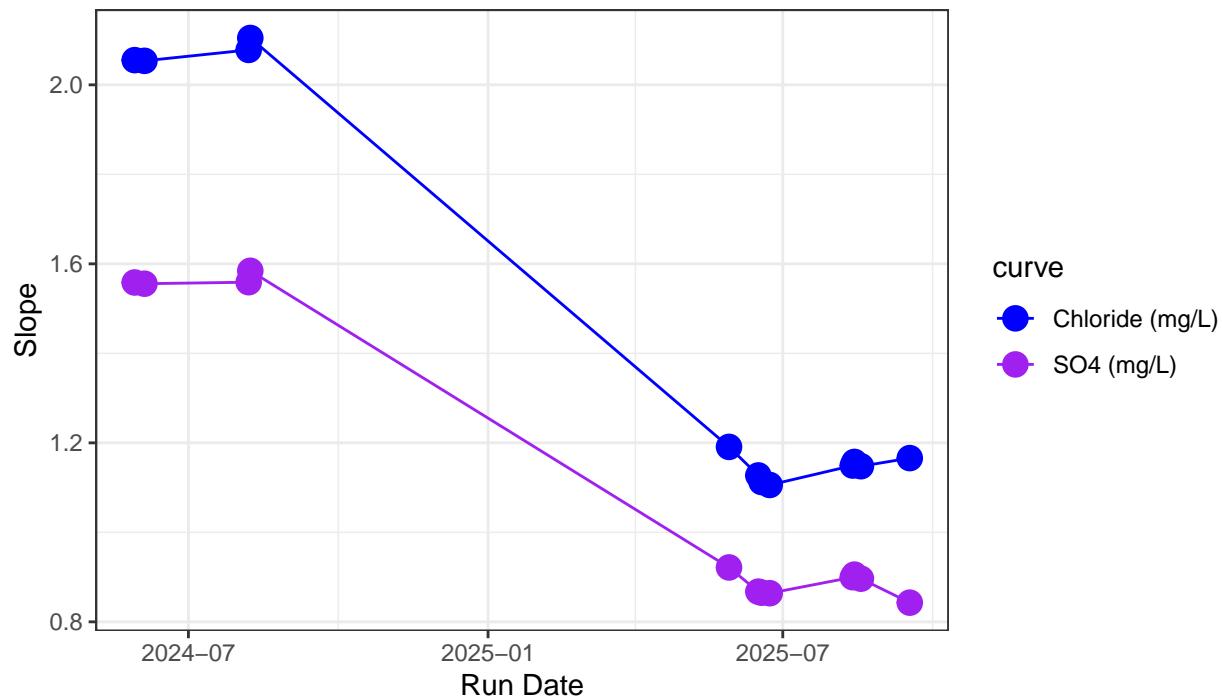


Sulfate Std Curve



```
## [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"
```

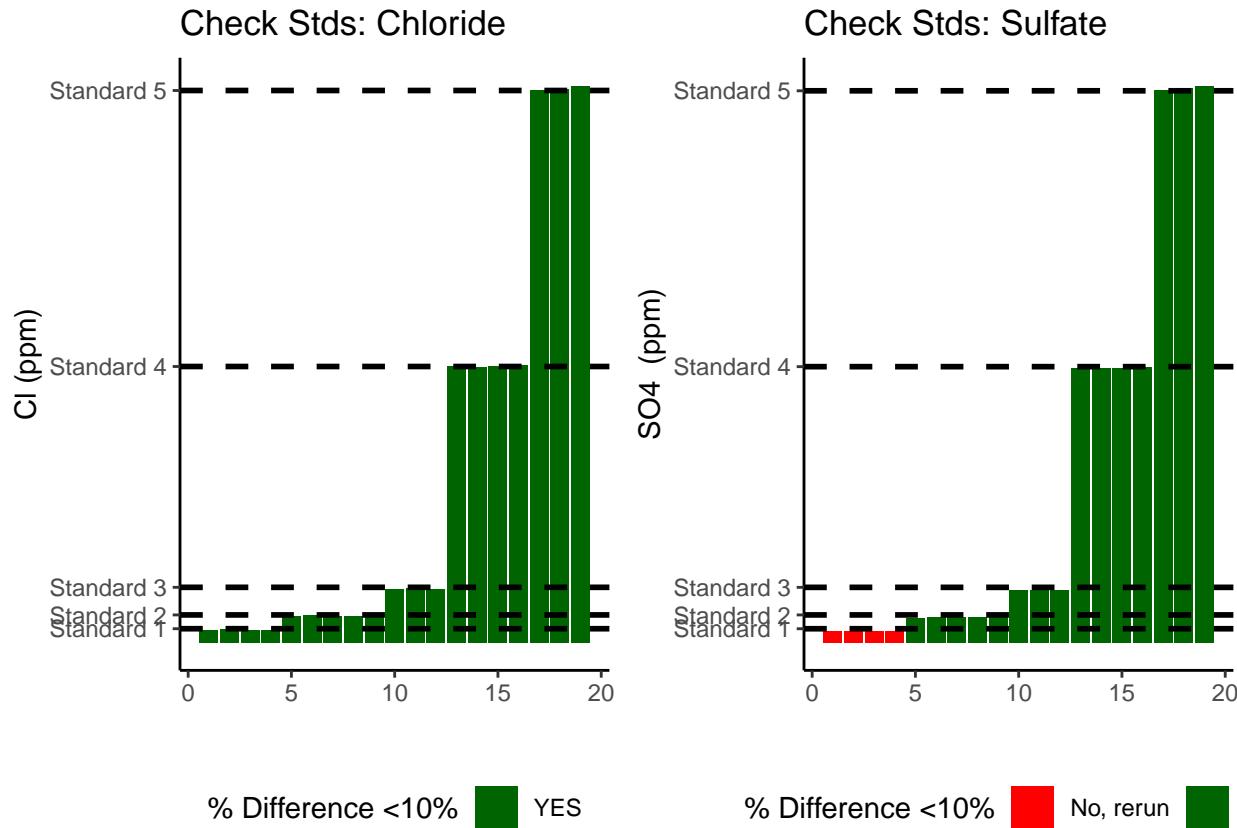
0.4 Assess Check Standards

```
## # 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  0.126  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"

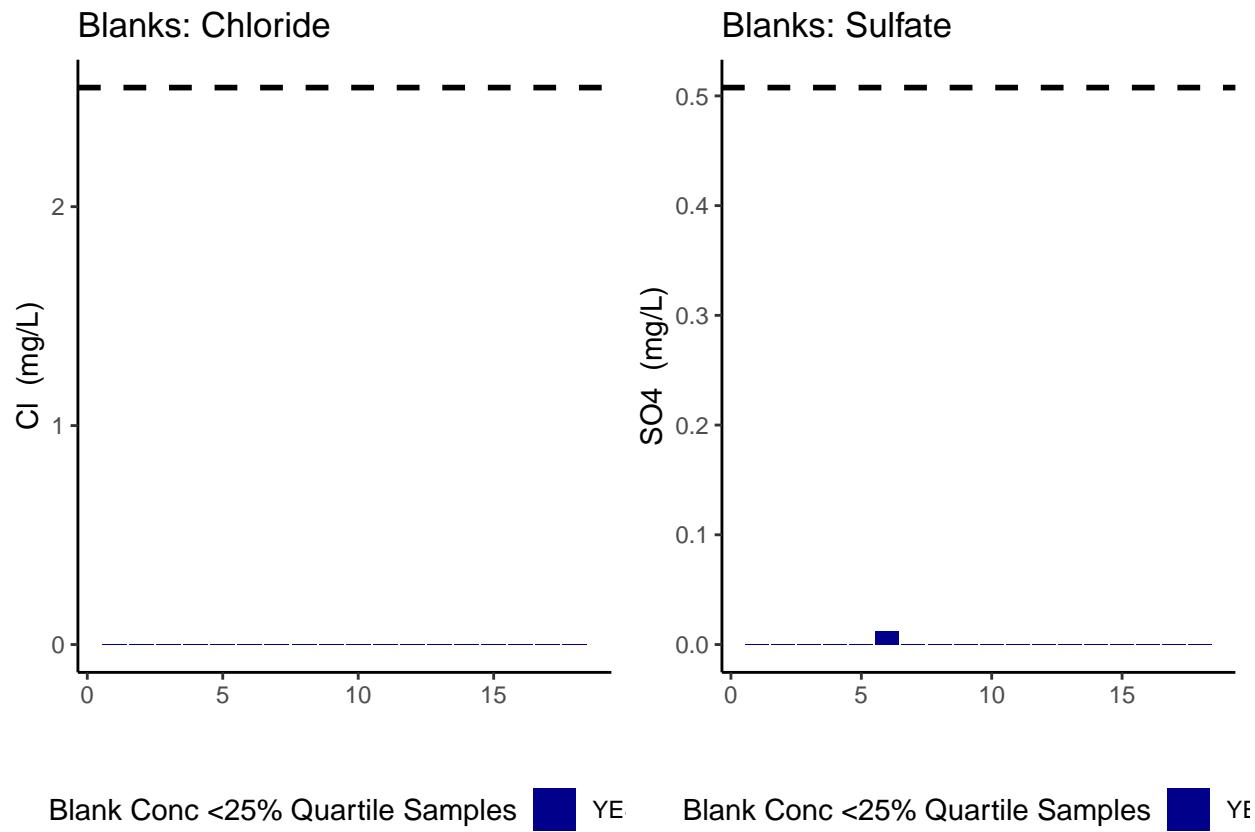
## [1] ">80% of Sulfate Check Standards have RSD within range - PROCEED"
```



```
## [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"
```



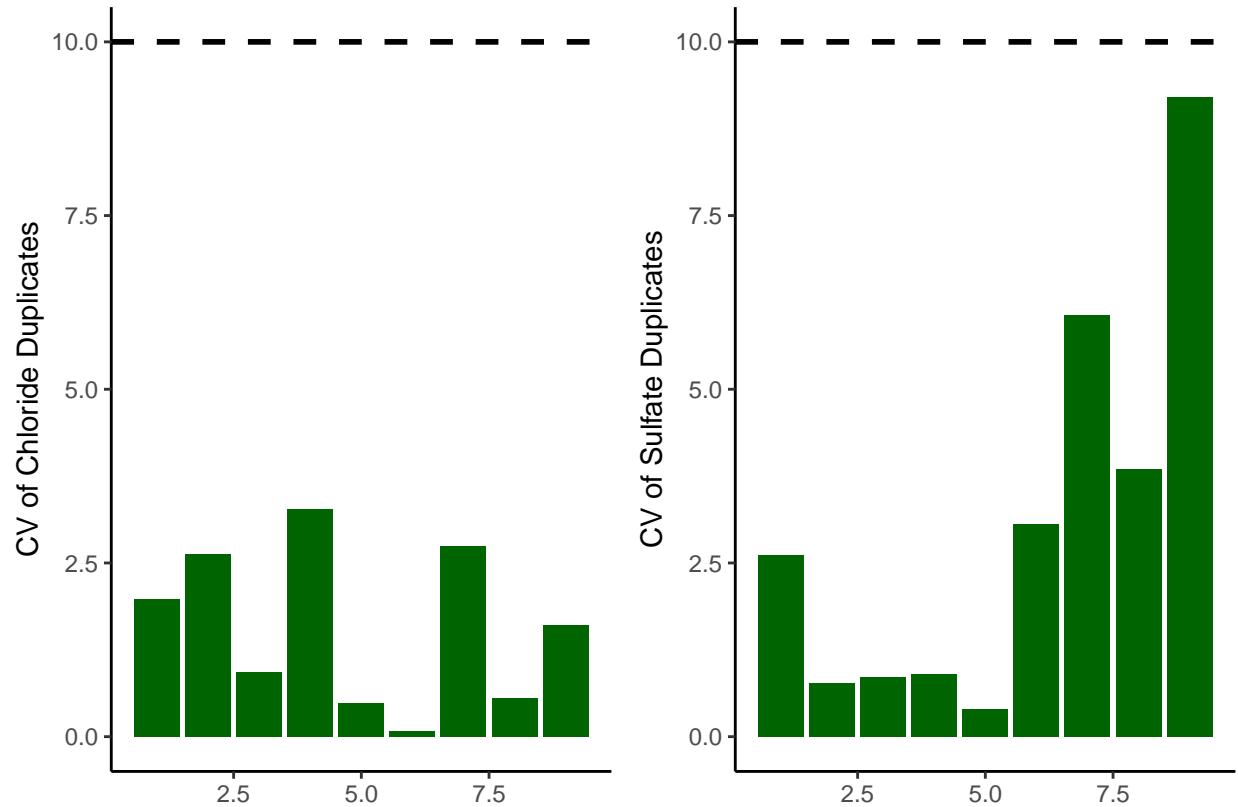
```
## Chloride blanks mean ppm:
```

```
## [1] 0
```

```
## Sulfate blanks mean ppm:
```

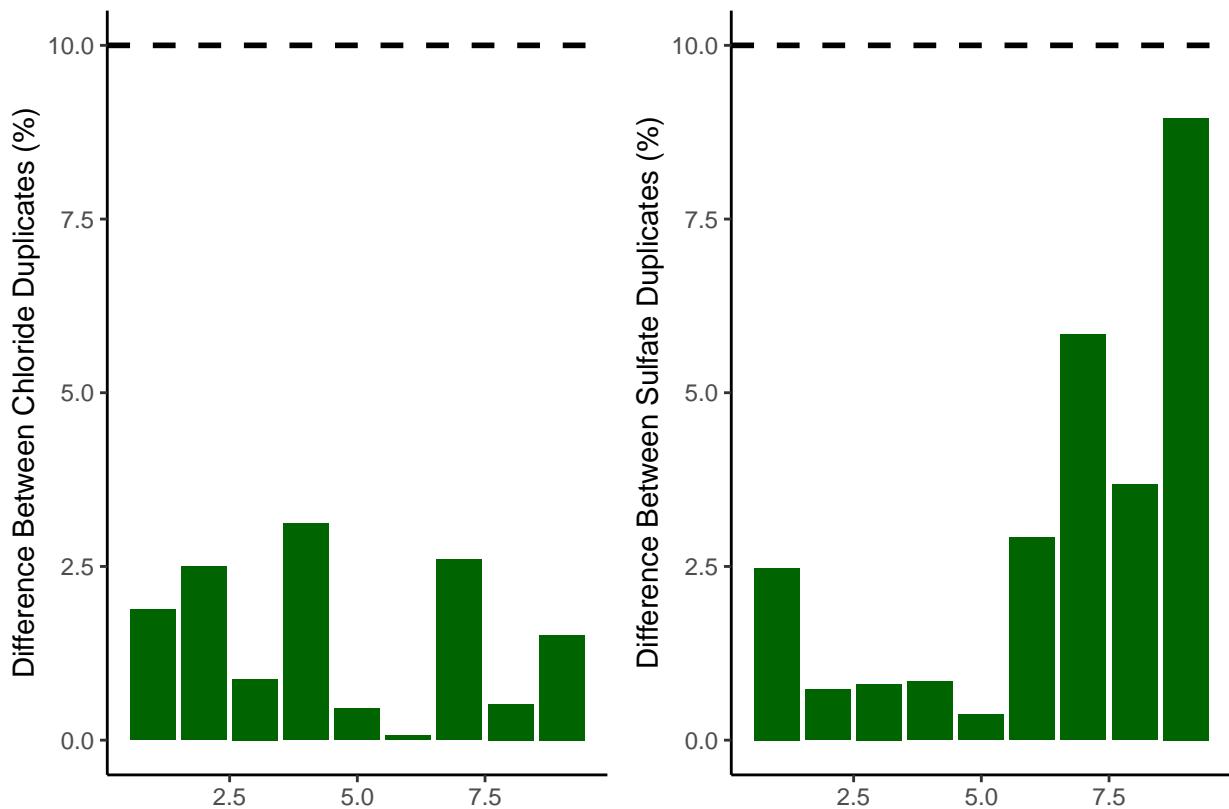
```
## [1] 0.0006722222
```

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

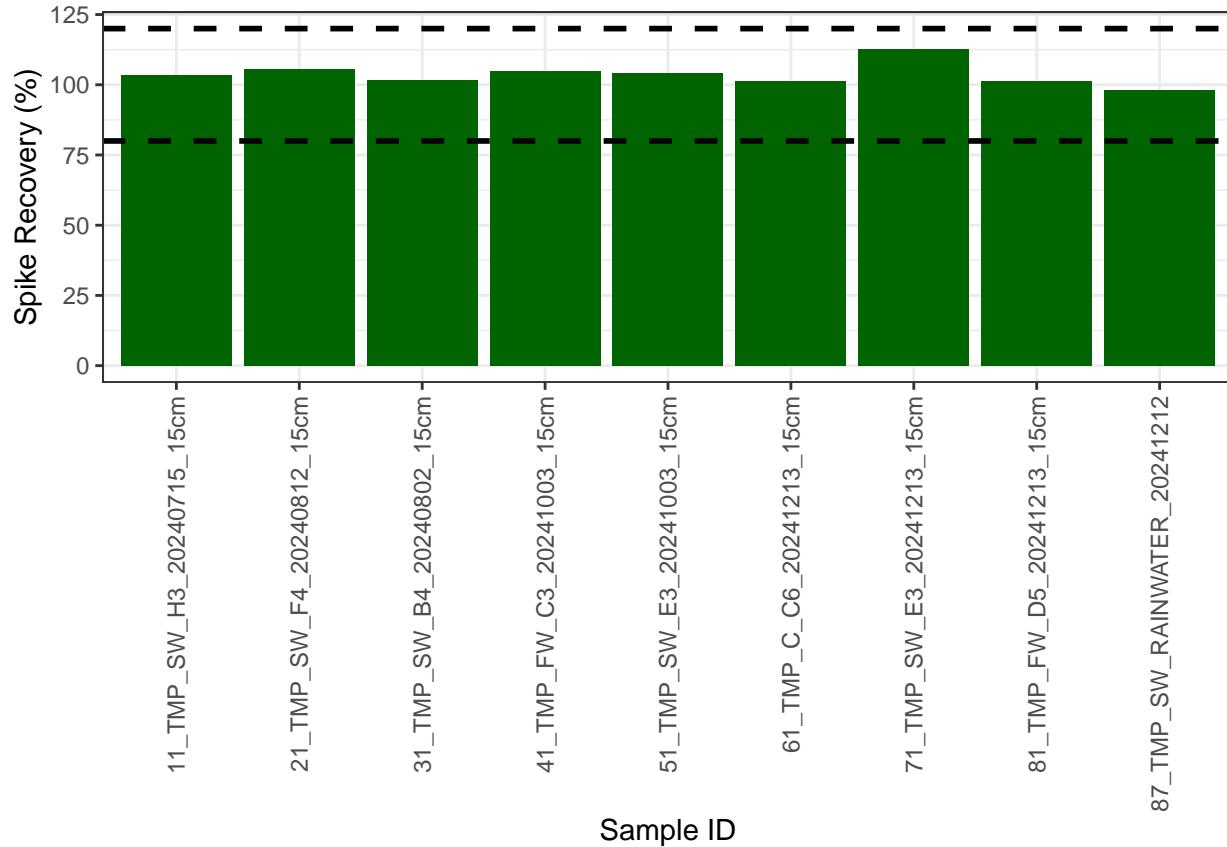
```
# Convert ppm to mmol/L
all_dat$SO4_Conc_mM <- (all_dat$SO4_ppm / s_mw)
all_dat$Cl_Conc_mM <- (all_dat$Cl_ppm / cl_mw)

# 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$salinity <- ((1.807 * all_dat$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 S04 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
```

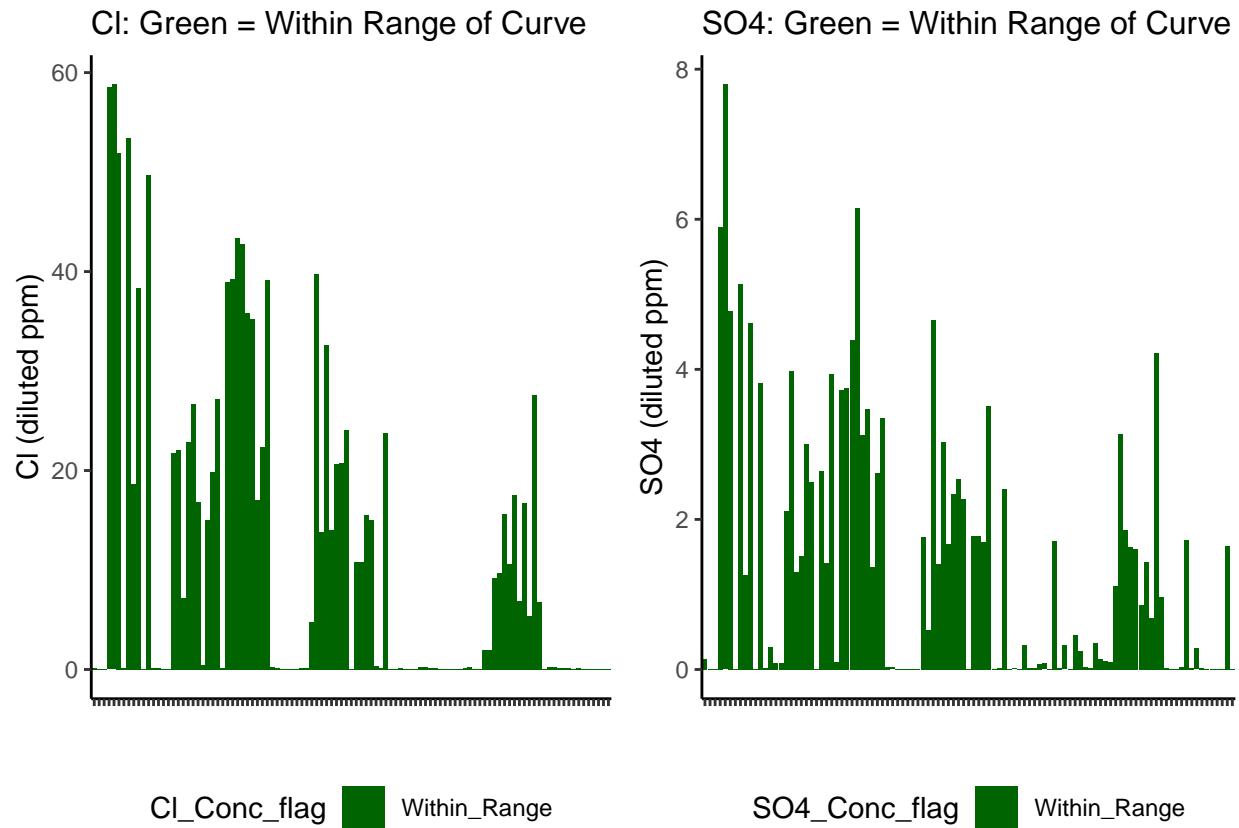


Table 1: SO4 samples

SO4_Conc_flag	Percent_samples
Within_Range	100

Table 2: Cl samples

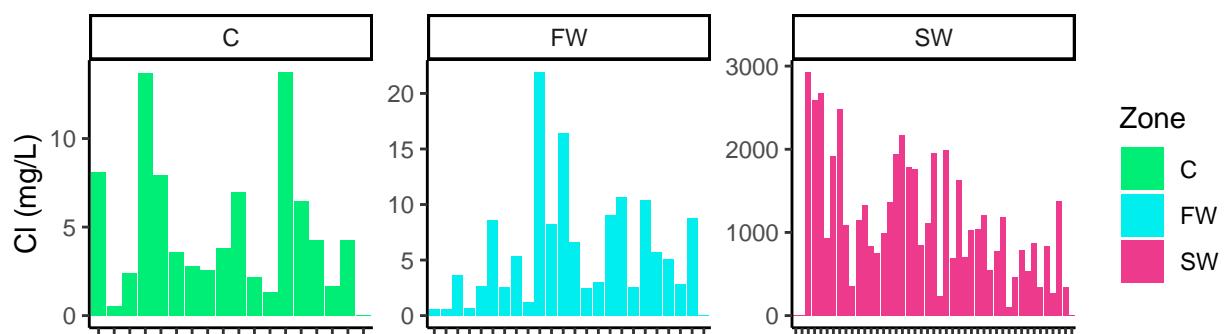
Cl_Conc_flag	Percent_samples
Within_Range	100

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

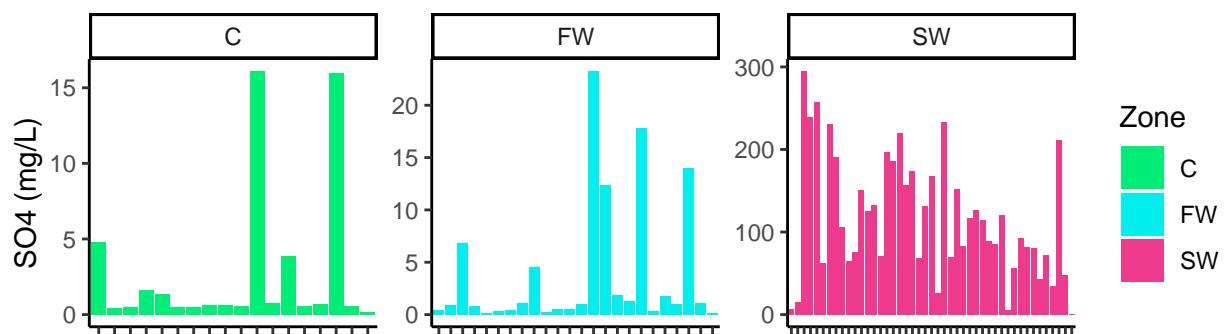
```
## All sample IDs are present in metadata.
```

0.11 Visualize Data by Plot

Samples: Chloride



Samples: SO4



0.12 Export Processed Data

```
#end
```