

TEMPEST: Porewater SO₄/Cl

June (1-71) 2024 Samples

2025-10-20

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##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, incorrectly-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:

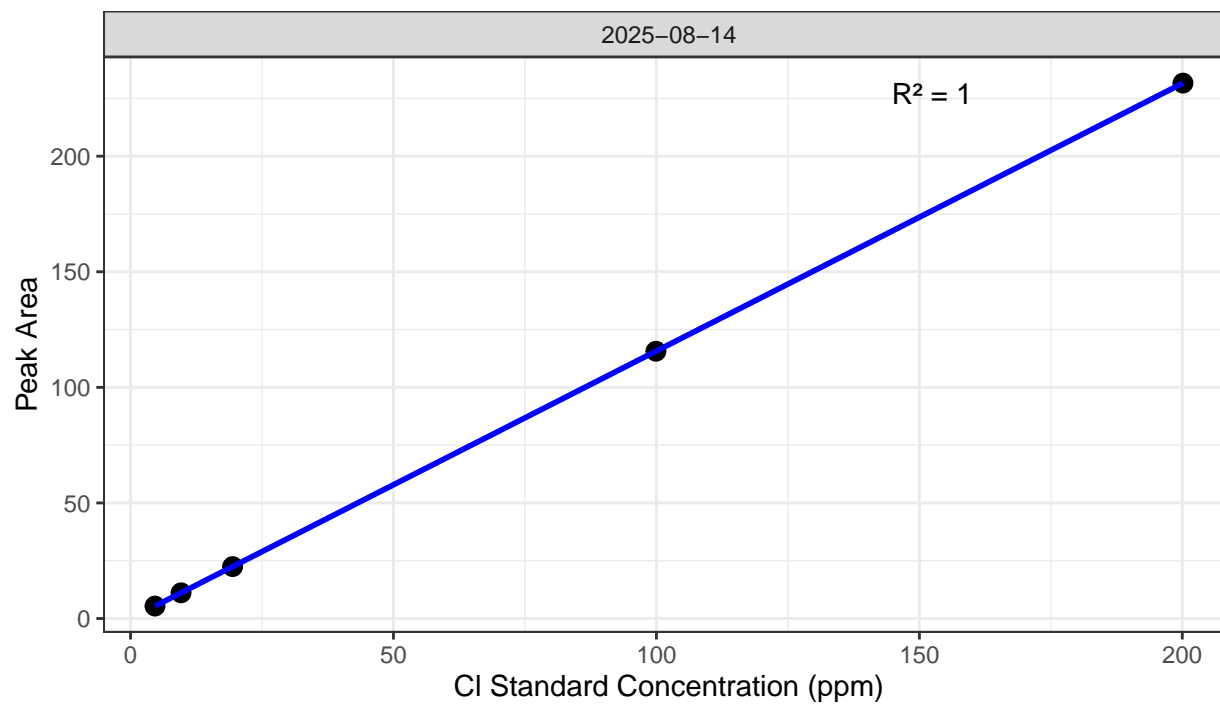
##Create similar sample IDs to match with run samples

##Import Sample Data

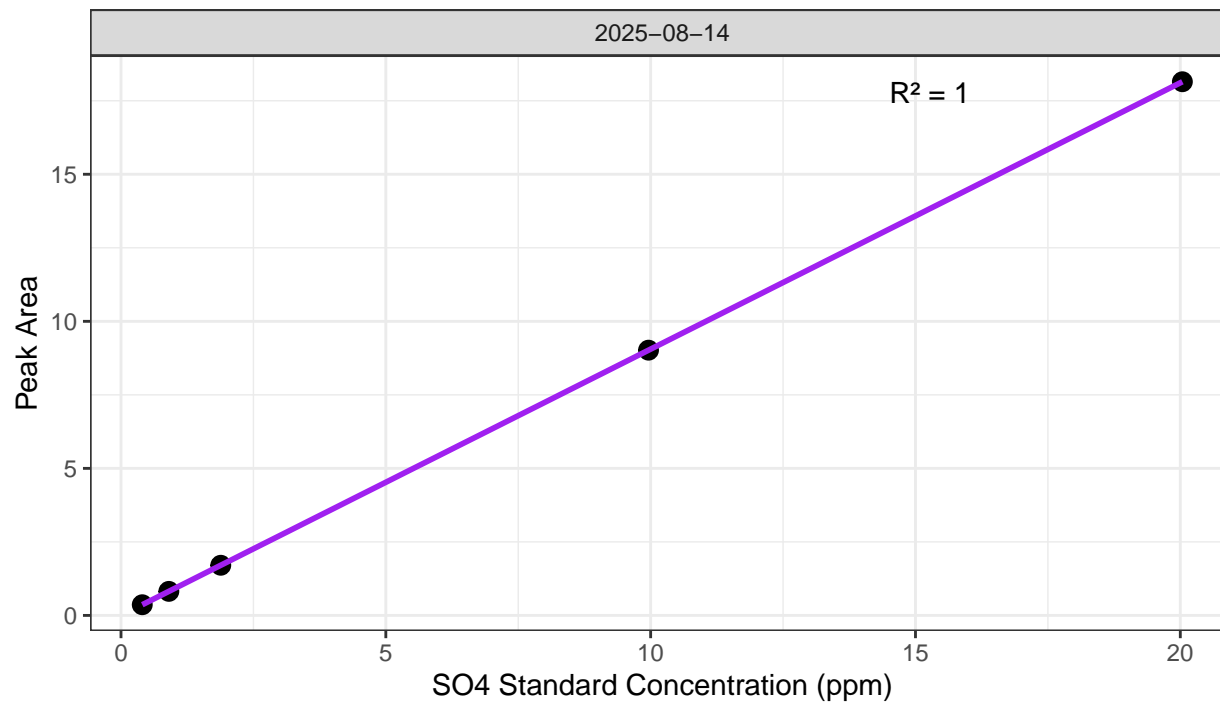
##Fix Sample IDs entered wrong

0.3 Assess Standard Curves

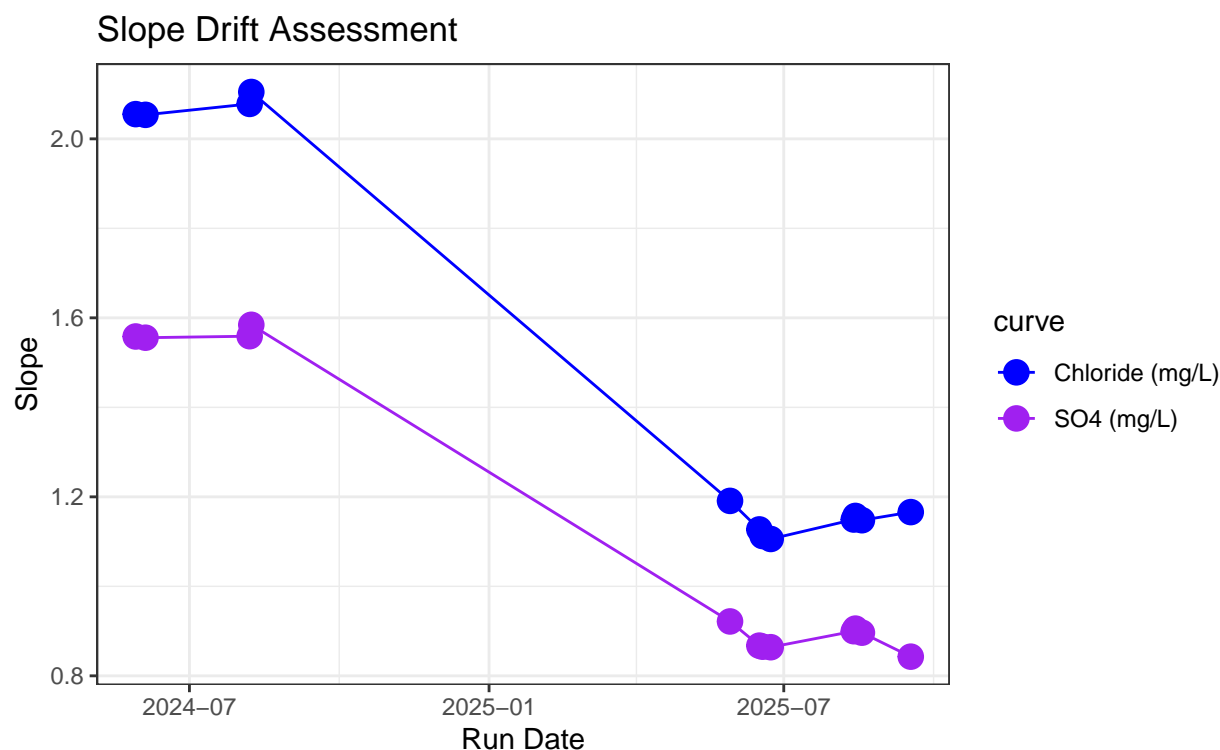
Chloride Std Curve



Sulfate Std Curve



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



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

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

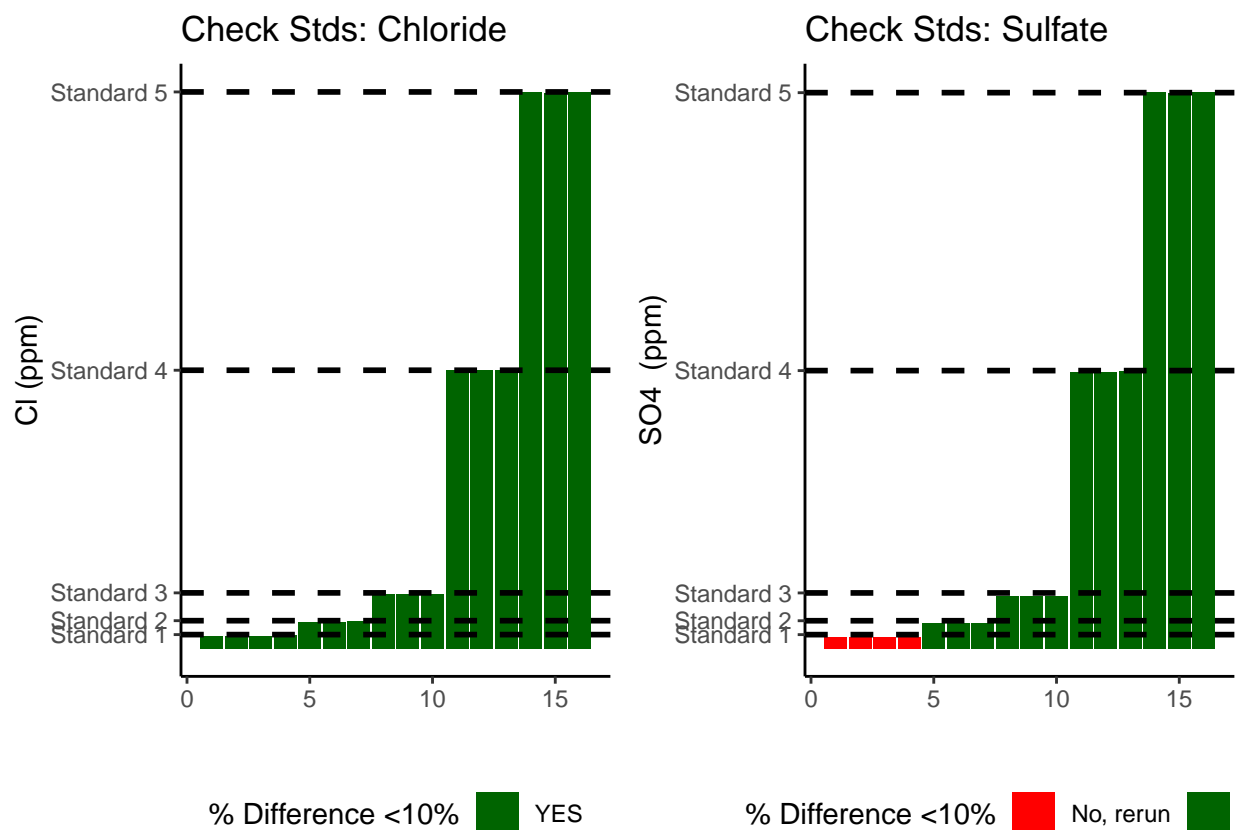
0.4 Assess Check Standards

```
## # 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_S04 sd_S04 cv_S04 flag_S04
##   <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"
```



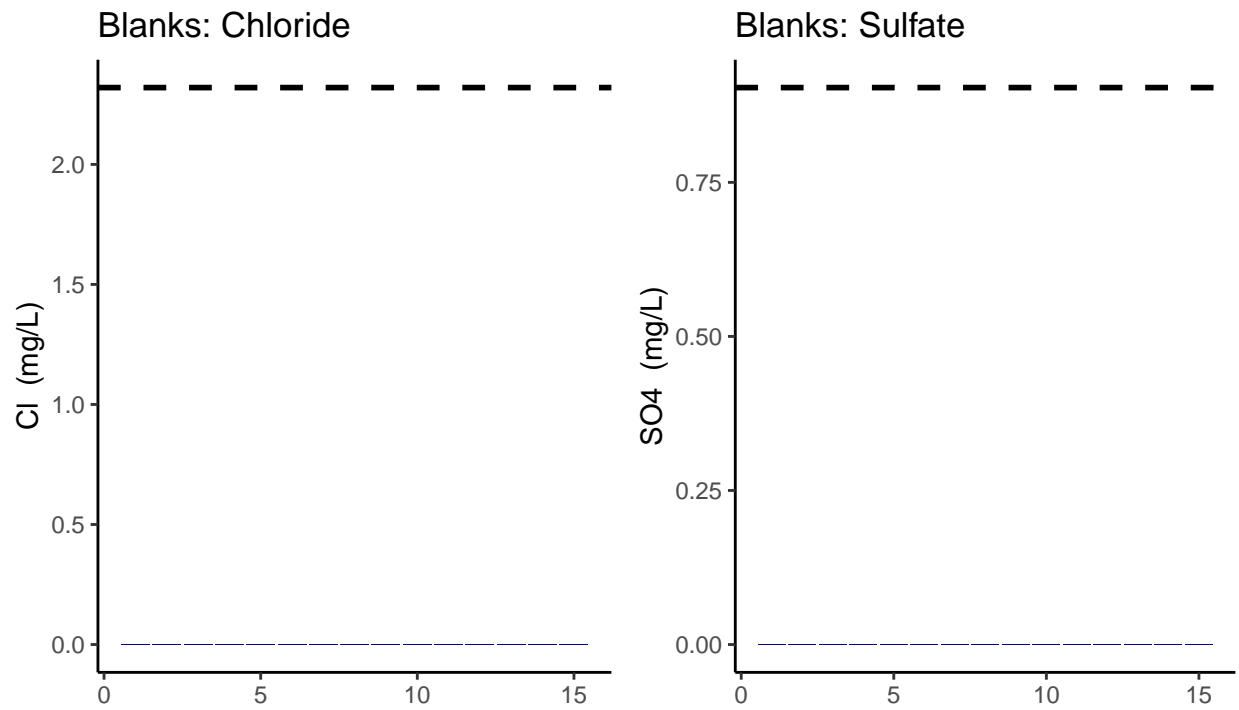
```
## [1] ">80% of Chloride Check Standards are within range of expected concentration - PROCEED"
```

```
## [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"
```



Blank Conc <25% Quartile Samples ☒ YE

Blank Conc <25% Quartile Samples ☒ Y

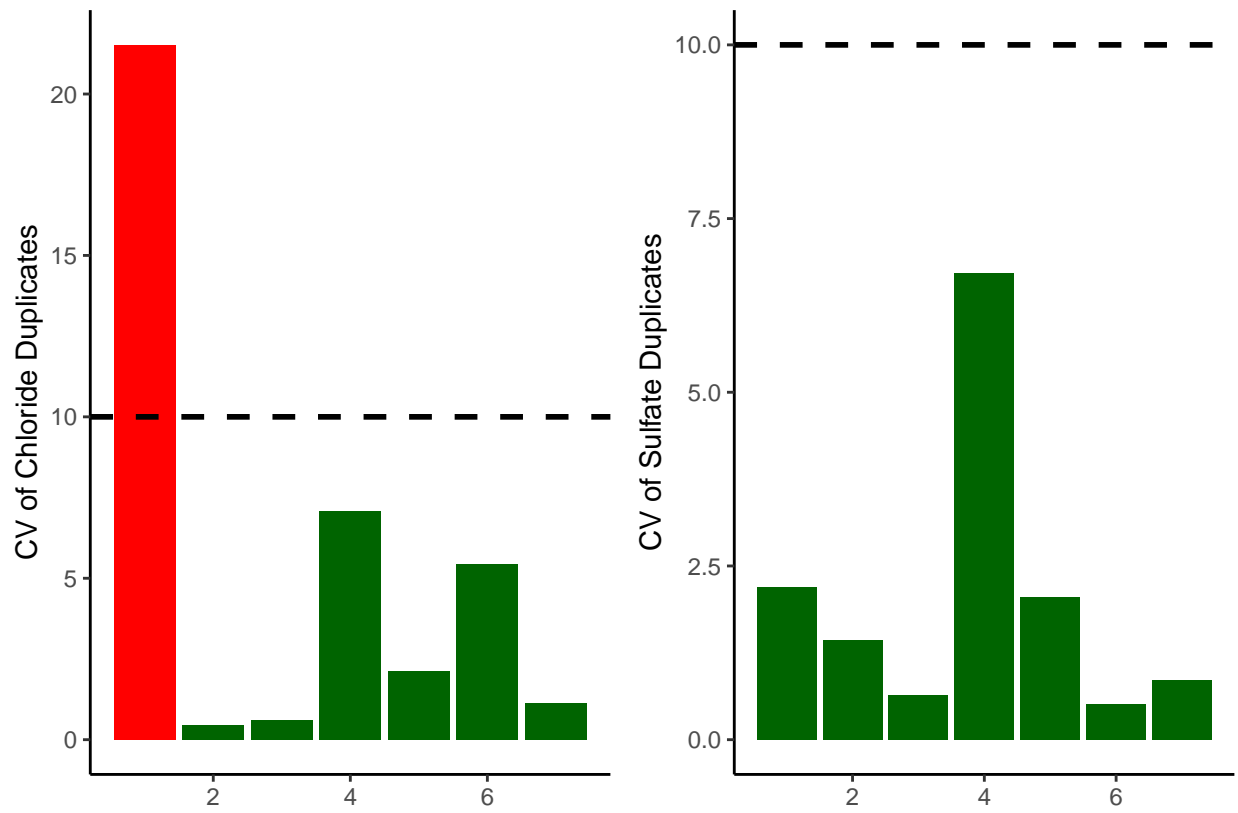
```
## Chloride blanks mean ppm:
```

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

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

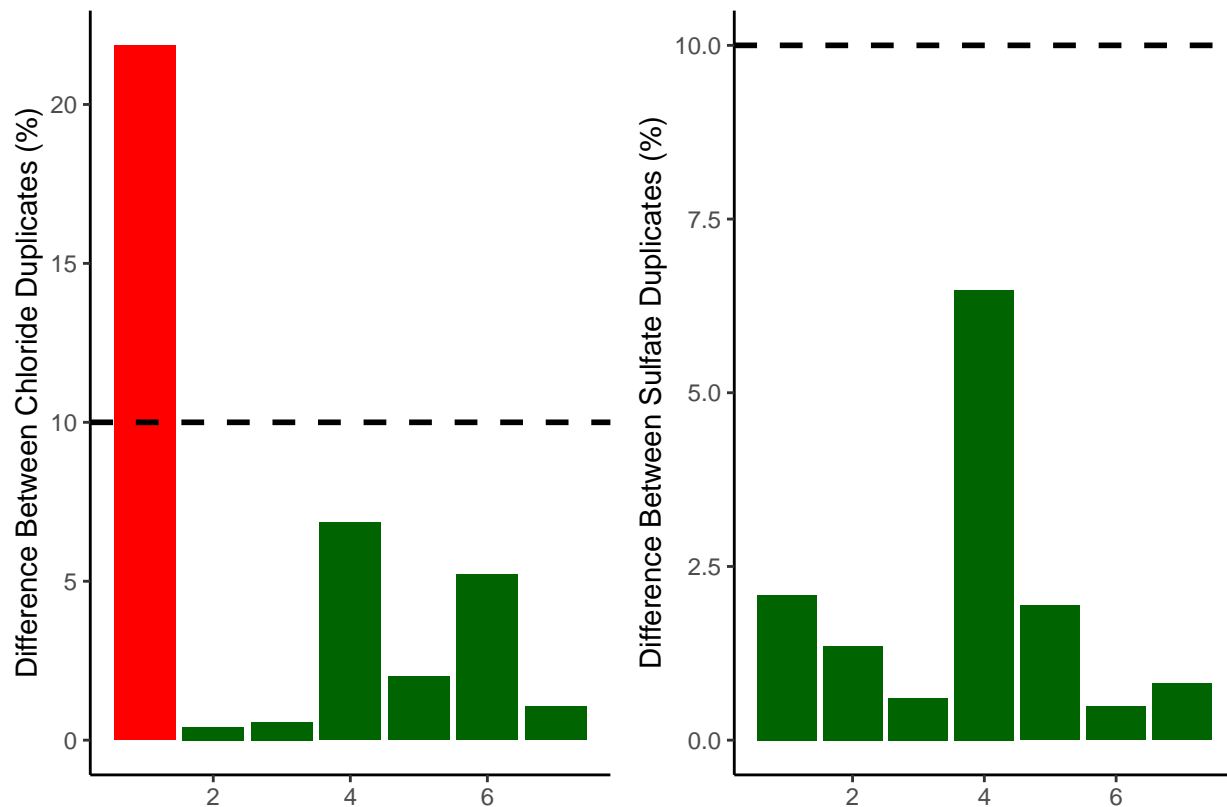
```
## [1] 0
```

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

```
# Convert ppm to mmol/L
all_dat$S04_Conc_mM <- (all_dat$S04_ppm / s_mw)
all_dat$Cl_Conc_mM <- (all_dat$Cl_ppm / cl_mw)

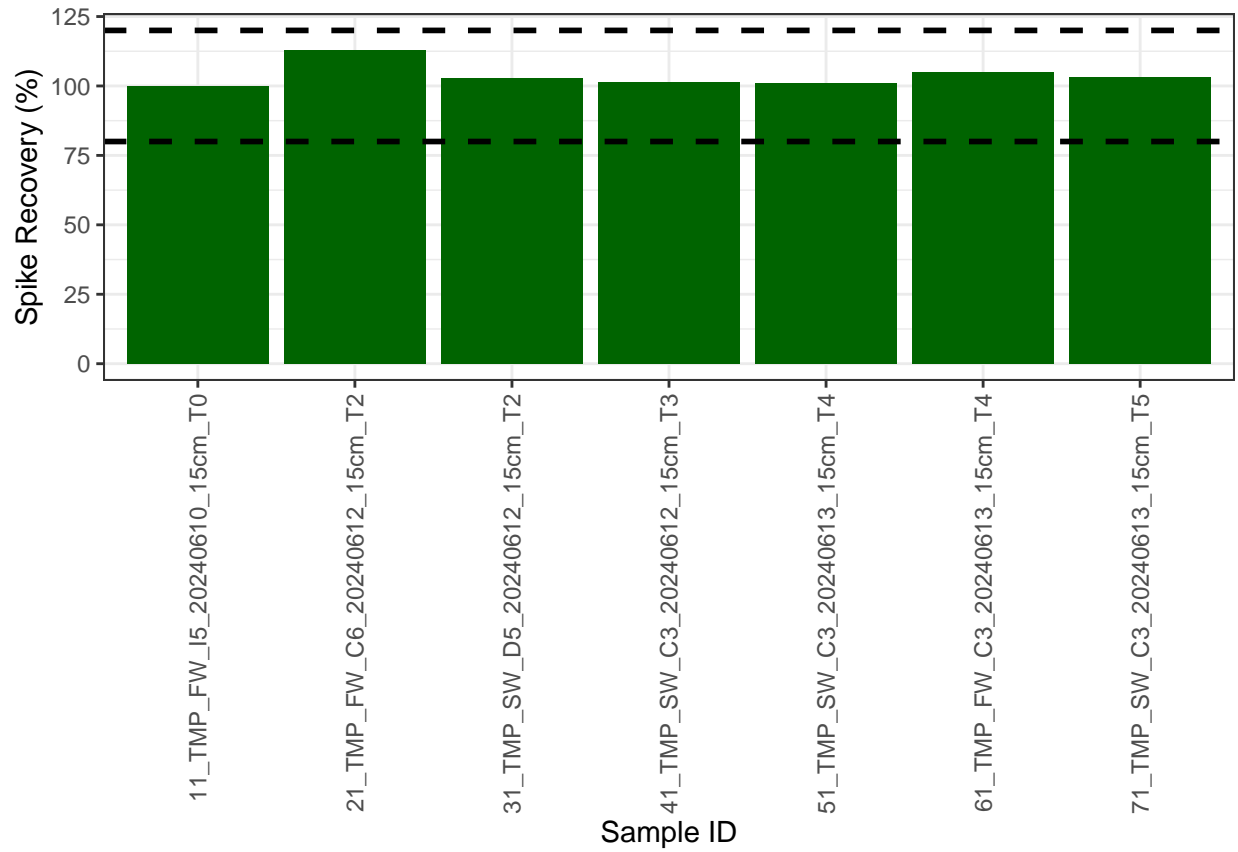
# Calculate Salinity
# calculated using the Knudsen equation
# Salinity = 0.03 + 1.8050 * Chlorinity
# Ref: A Practical Handbook of Seawater Analysis by Strickland & Parsons (P. 11)
# = ((1.807*Cl_ppm)+0.026)/1000
all_dat$salinity <- ((1.8070 * all_dat$Cl_ppm) + 0.026) / 1000

#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 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
```

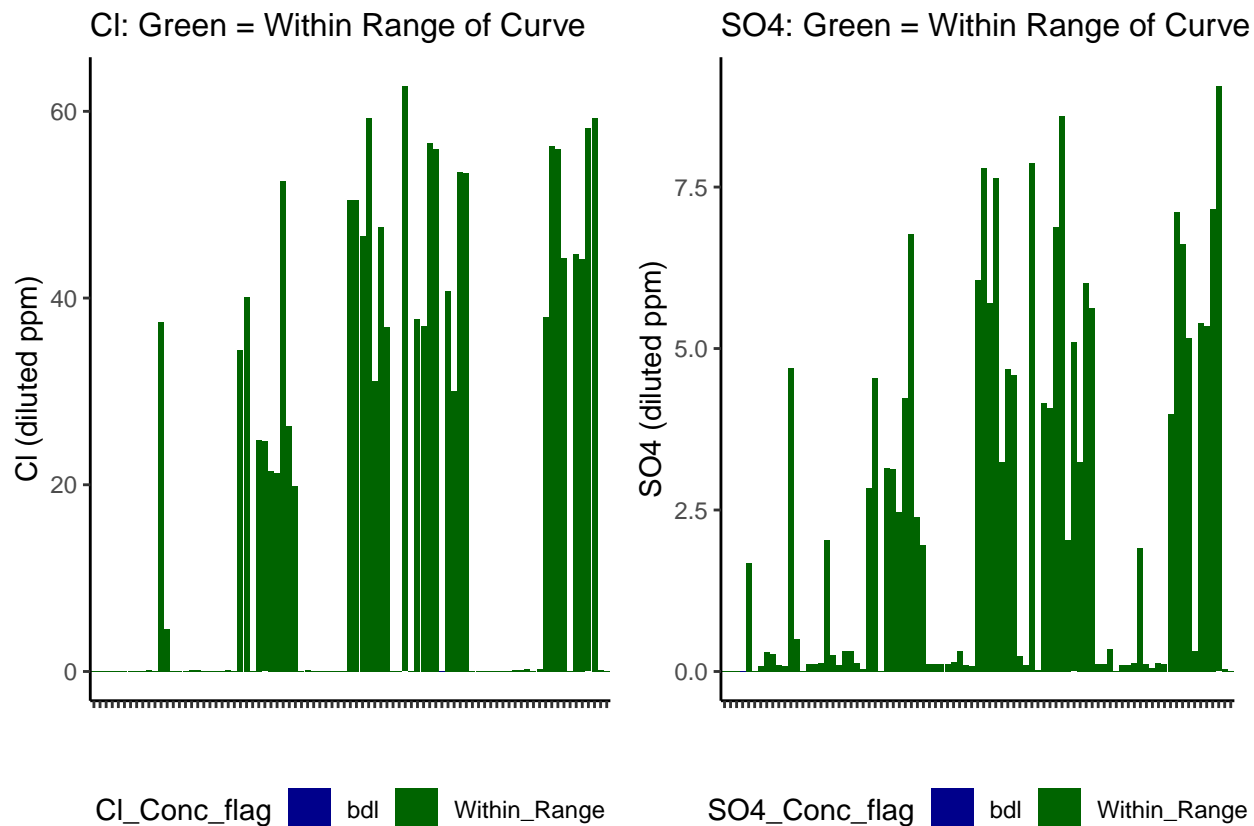


Table 1: SO4 samples

SO4_Conc_flag	Percent_samples
Within_Range	98.823529
bdl	1.176471

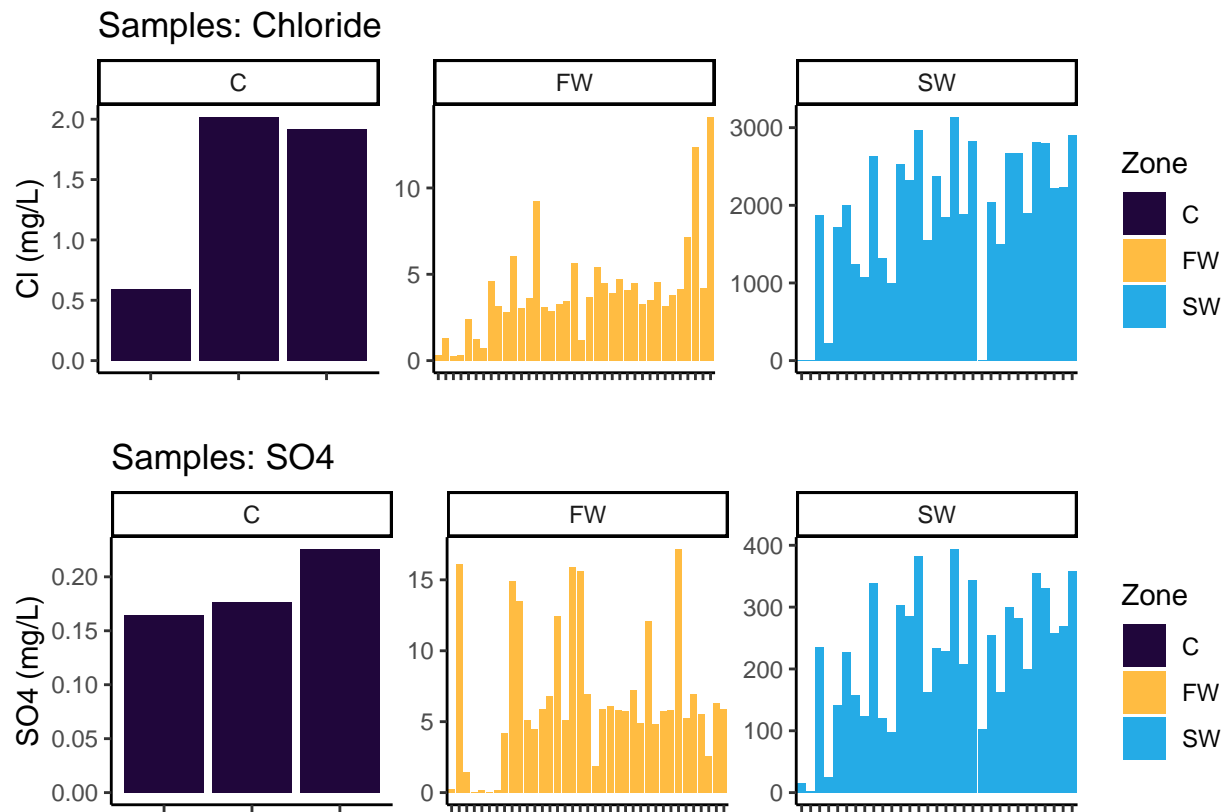
Table 2: Cl samples

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



0.12 Export Processed Data

#end