

TEMPEST: Porewater SO₄/Cl

June (1-71) 2024 Samples

2025-10-03

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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.
Some sample IDs are missing from metadata: TMP_C_H6_20240610_15CM, TMP_SW_H3_20240612_15CM_T3
" #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_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

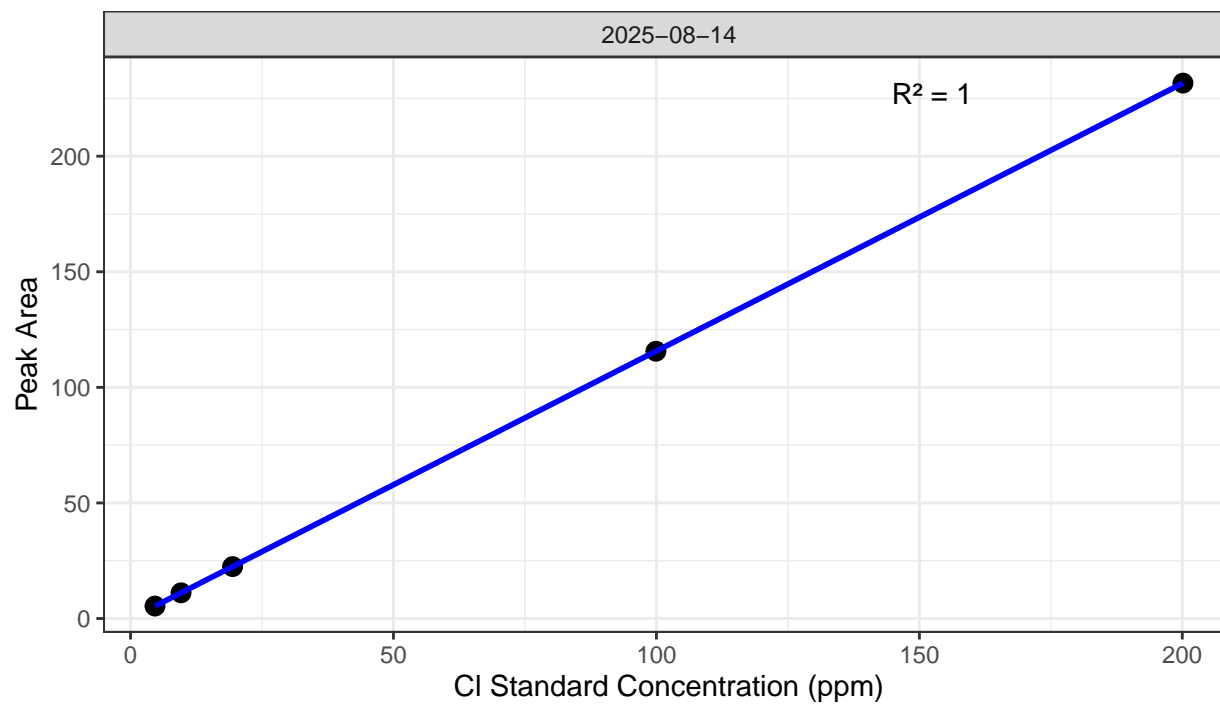
0.2 Pull in active porewater tracking inventory sheet from Google Drive:

##Create similar sample IDs to match with run samples

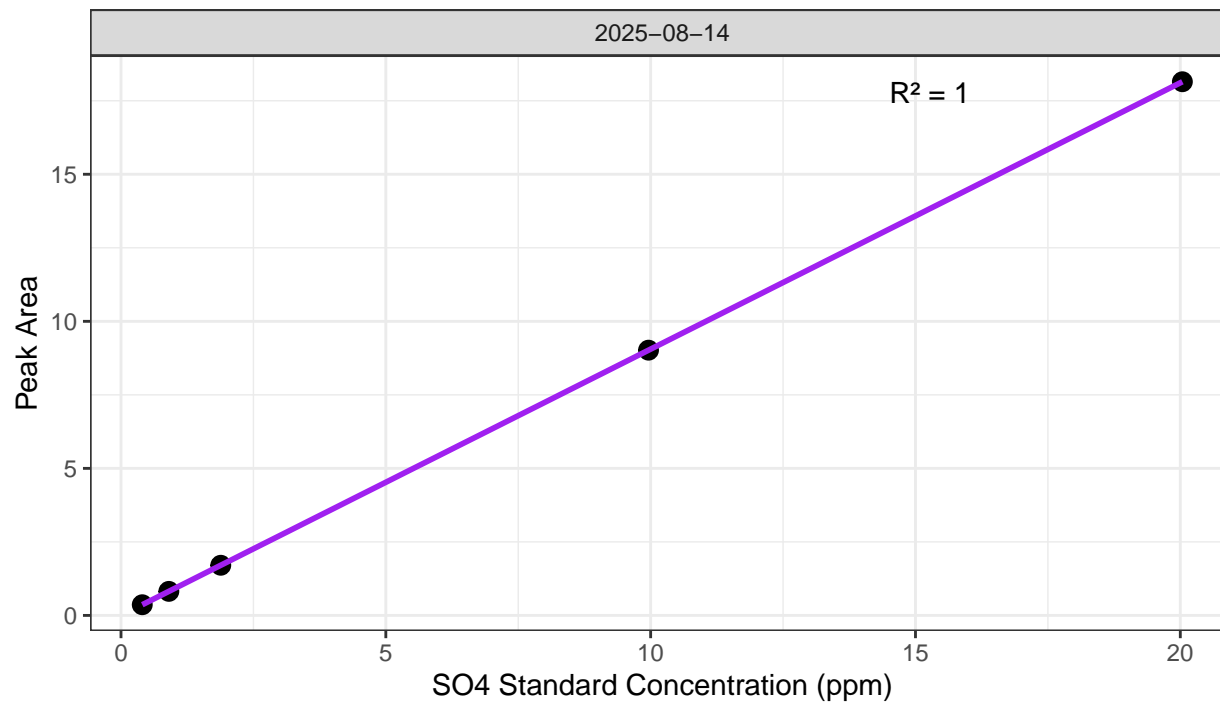
##Import Sample Data

0.3 Assess Standard Curves

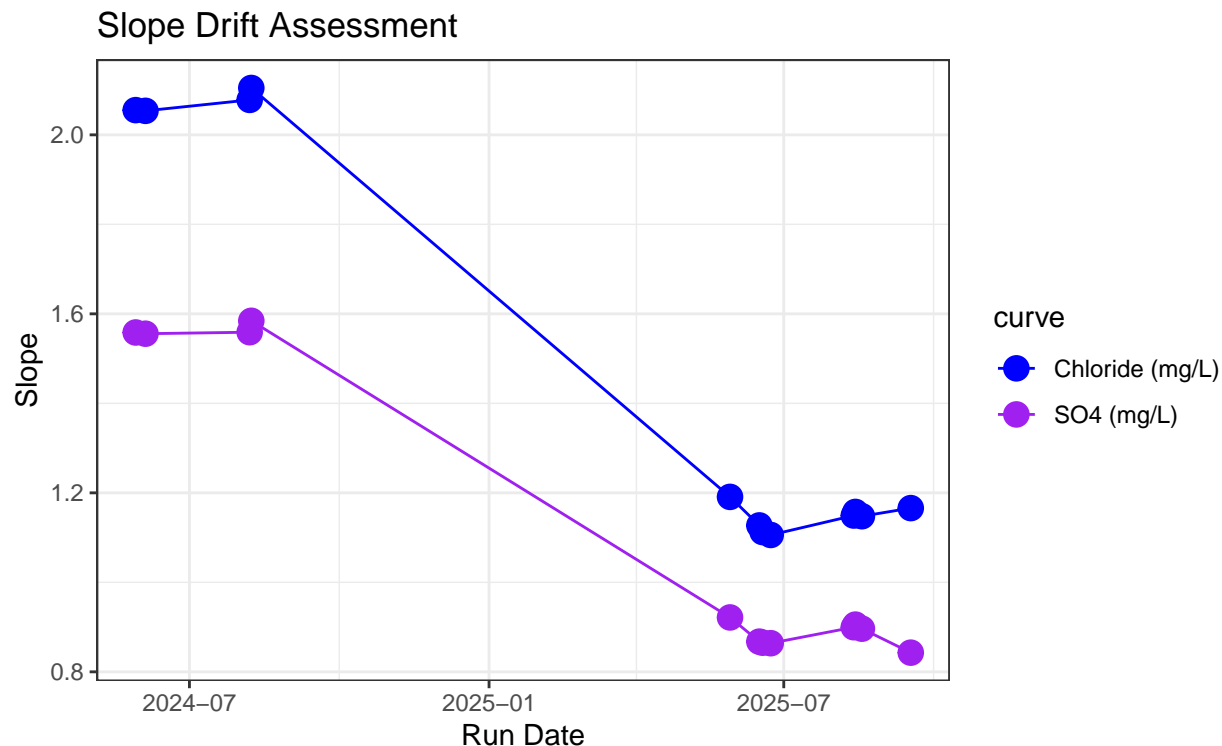
Chloride Std Curve



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"
```

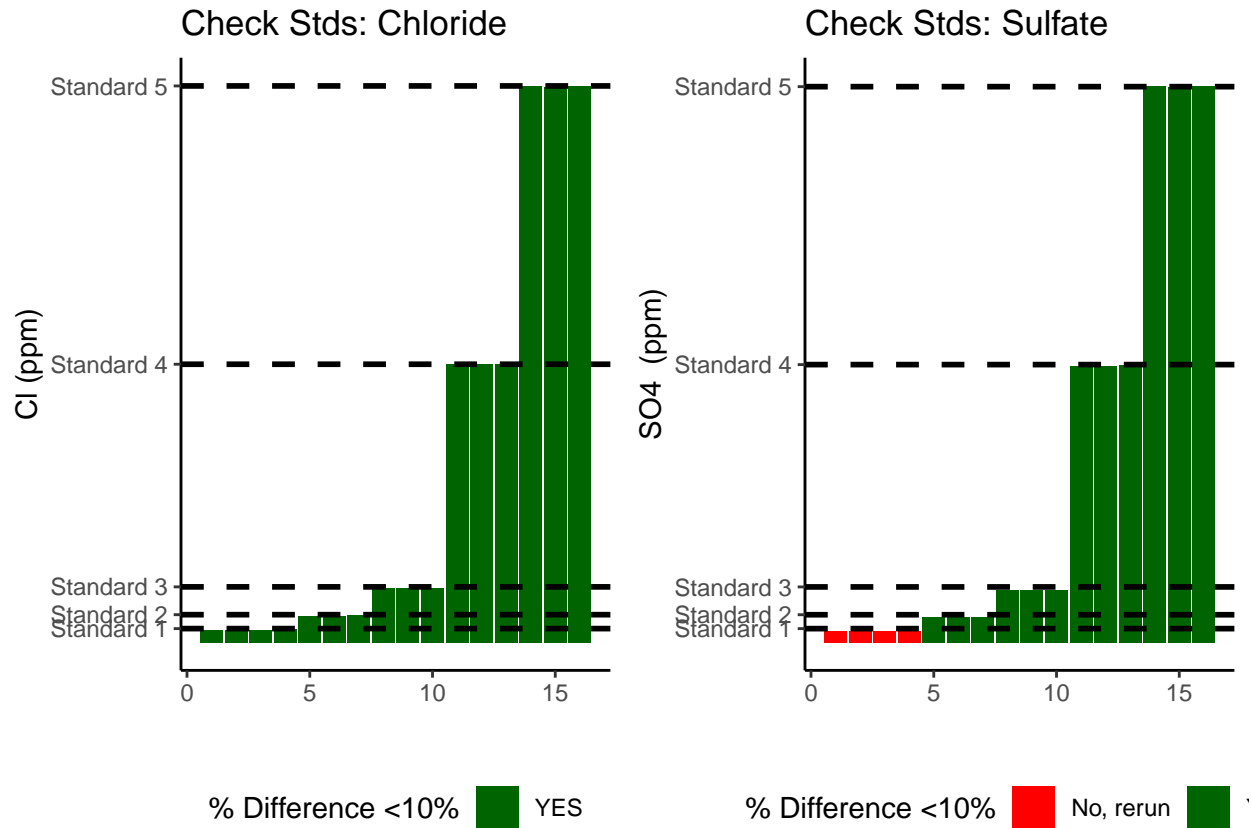
0.4 Assess Check Standards

```
## # 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"
```



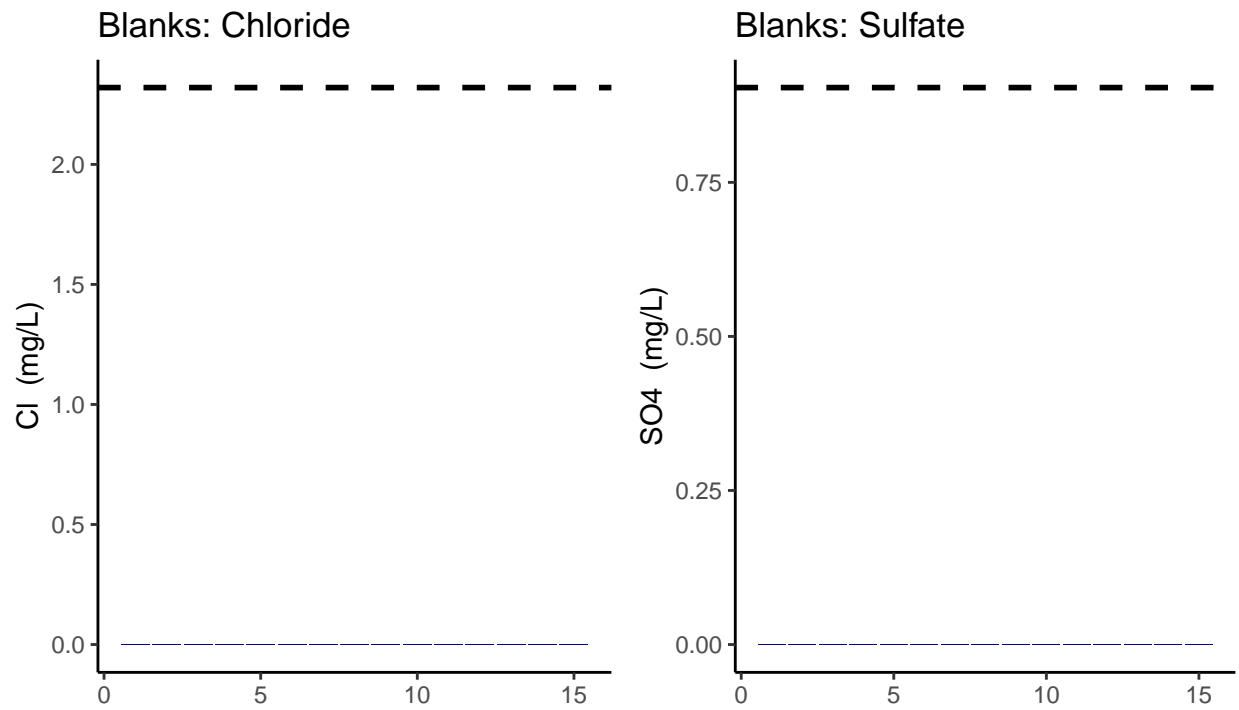
```
## [1] ">80% of Chloride Check Standards are within range of expected concentration - PROCEED"
```

```
## [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

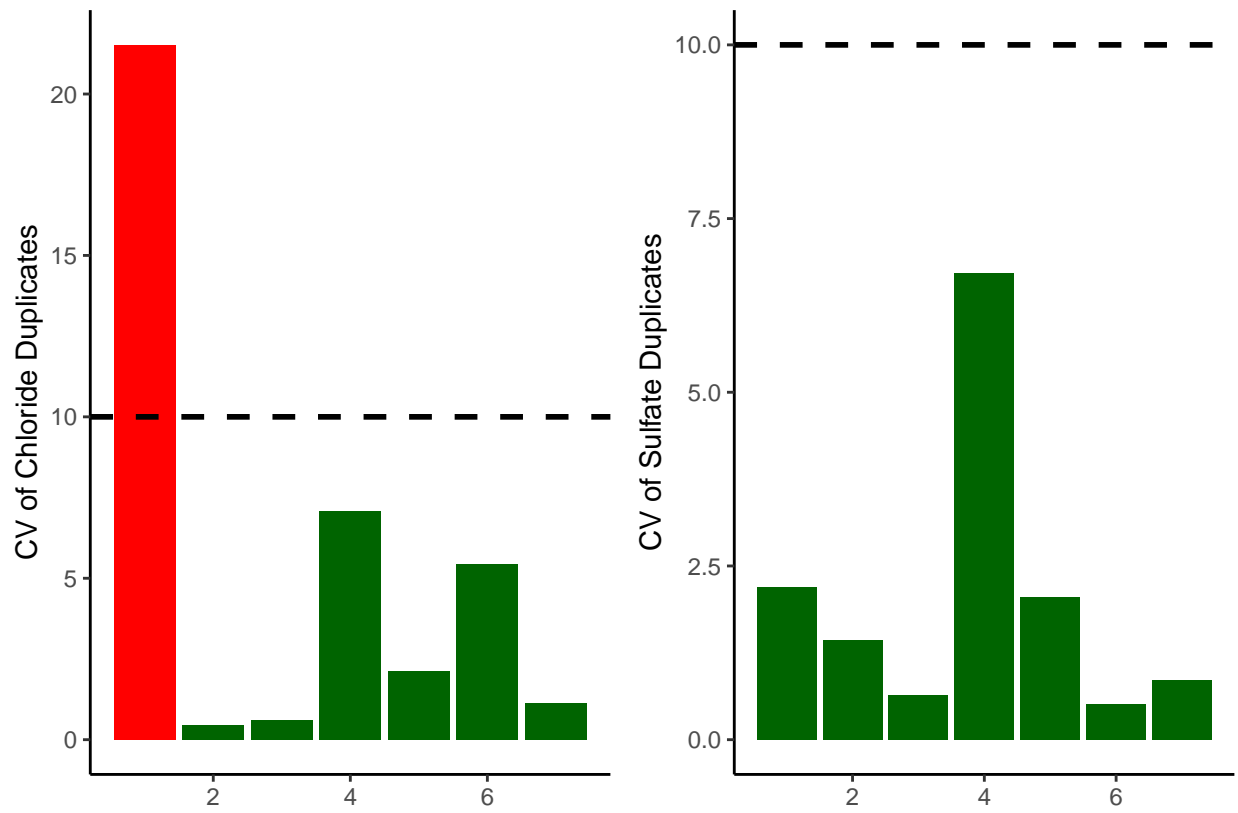
```
## Chloride blanks mean ppm:
```

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

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

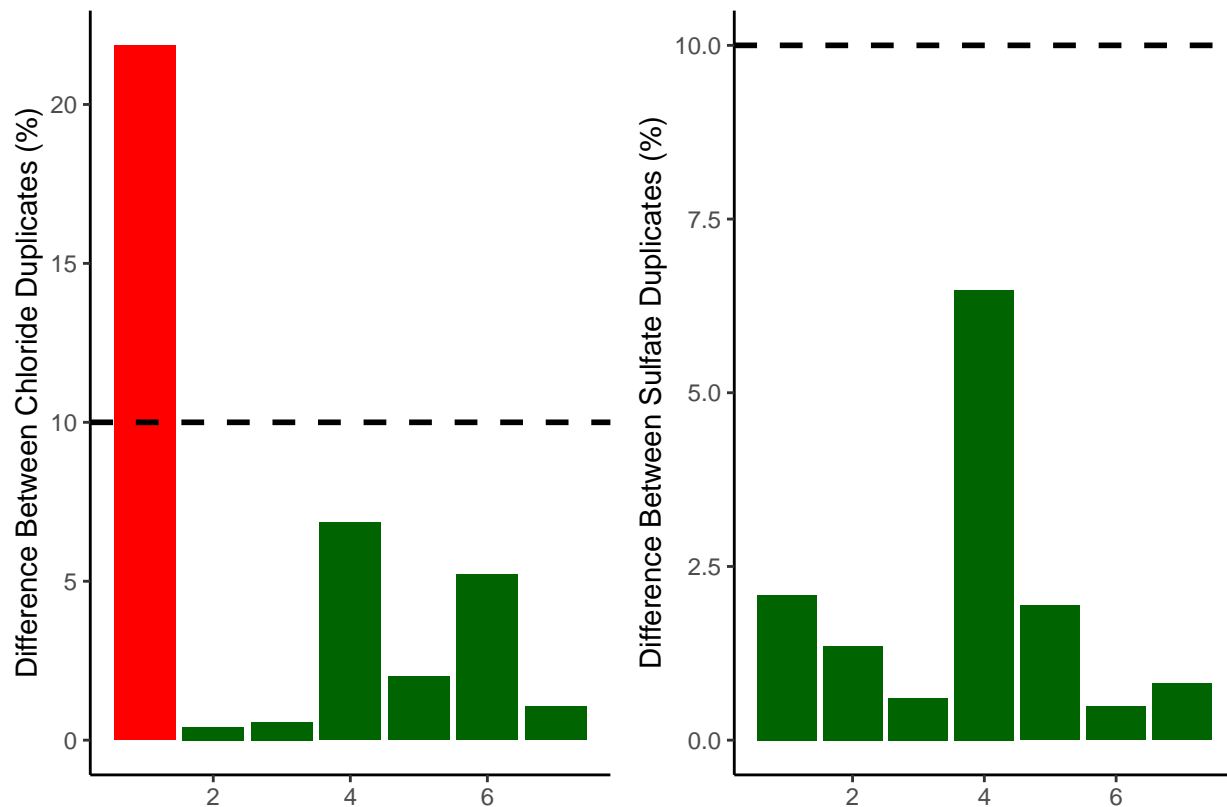
```
## [1] 0
```

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$SO4_Conc_mM <- (all_dat$SO4_ppm / s_mw)
all_dat$Cl_Conc_mM <- (all_dat$Cl_ppm / cl_mw)

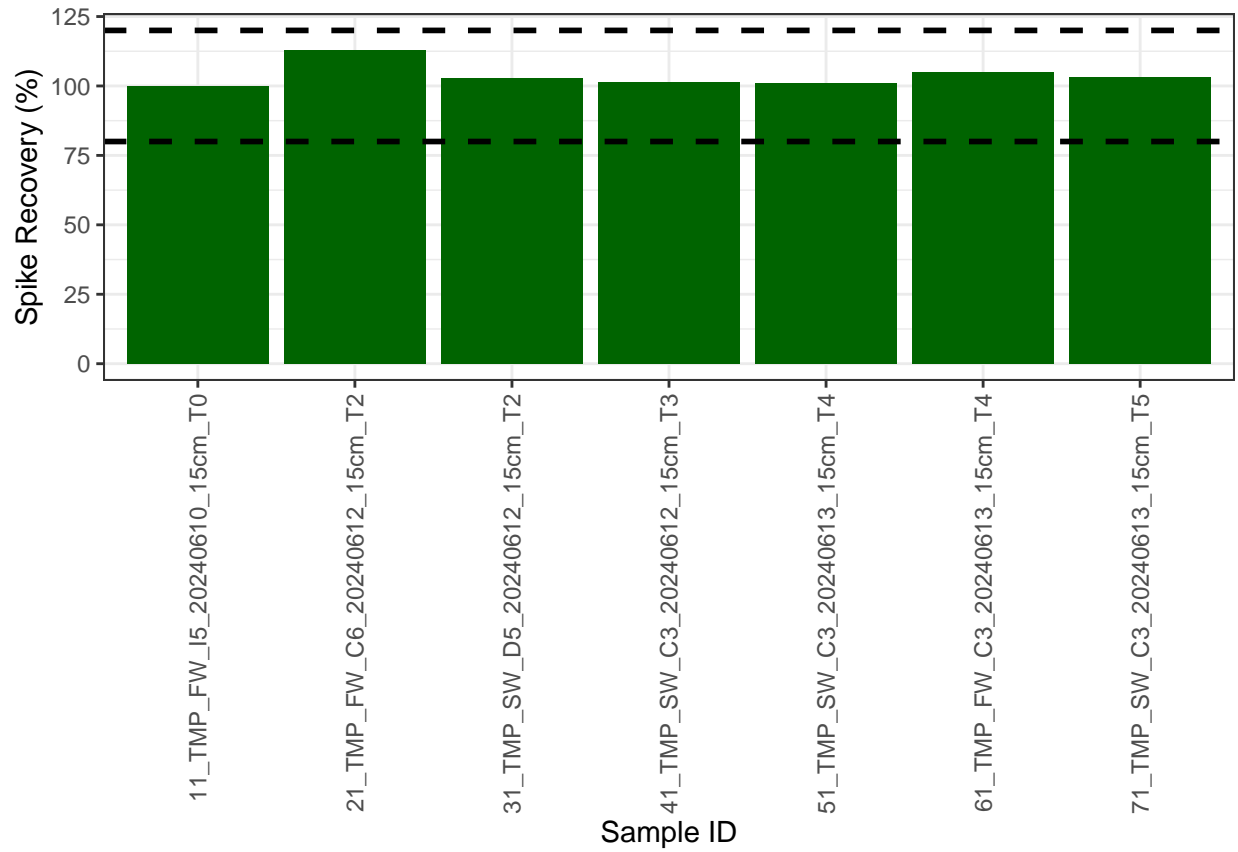
# Calculate Salinity
# calculated using the Knudsen equation
# Salinity = 0.03 + 1.8050 * Chlorinity
# Ref: A Practical Handbook of Seawater Analysis by Strickland & Parsons (P. 11)
# = ((1.807*Cl_ppm)+0.026)/1000
all_dat$salinity <- ((1.8070 * all_dat$Cl_ppm) + 0.026) / 1000

#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 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
```

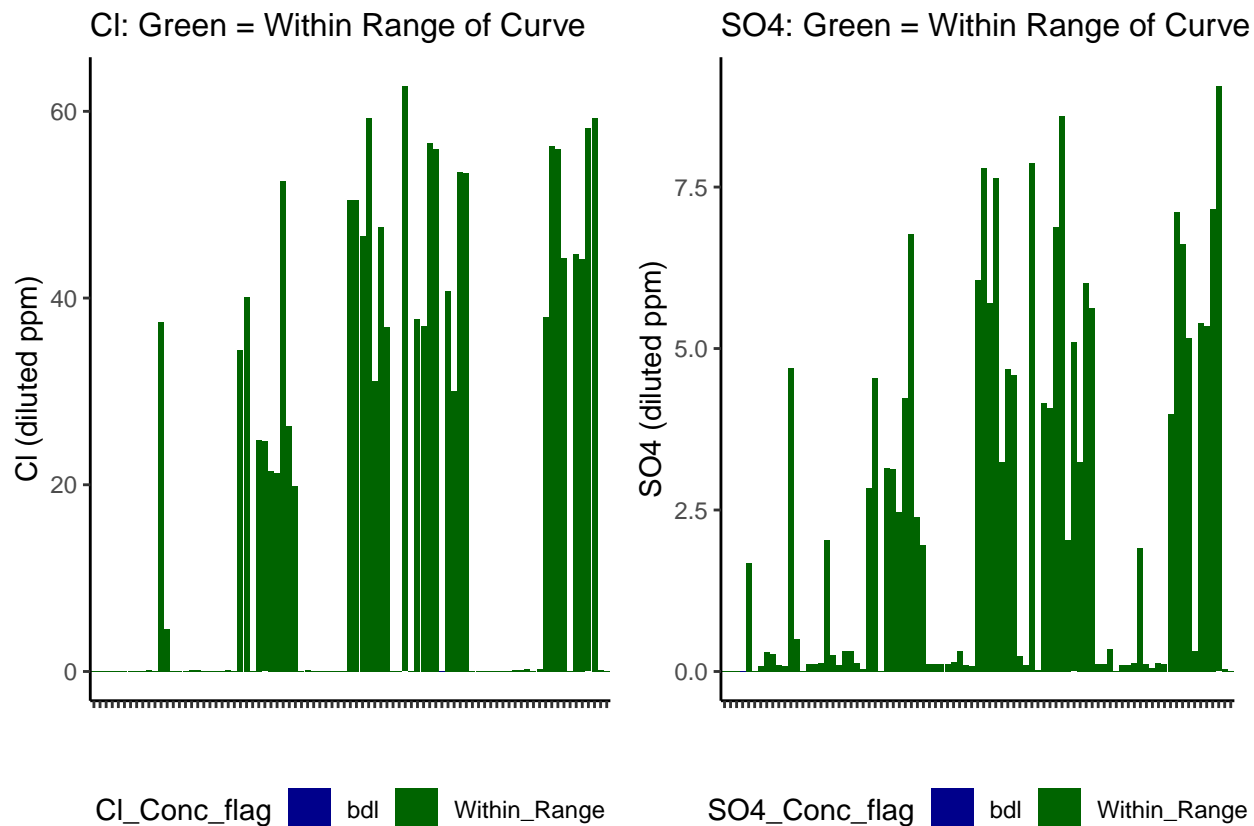


Table 1: SO4 samples

SO4_Conc_flag	Percent_samples
Within_Range	98.823529
bdl	1.176471

Table 2: Cl samples

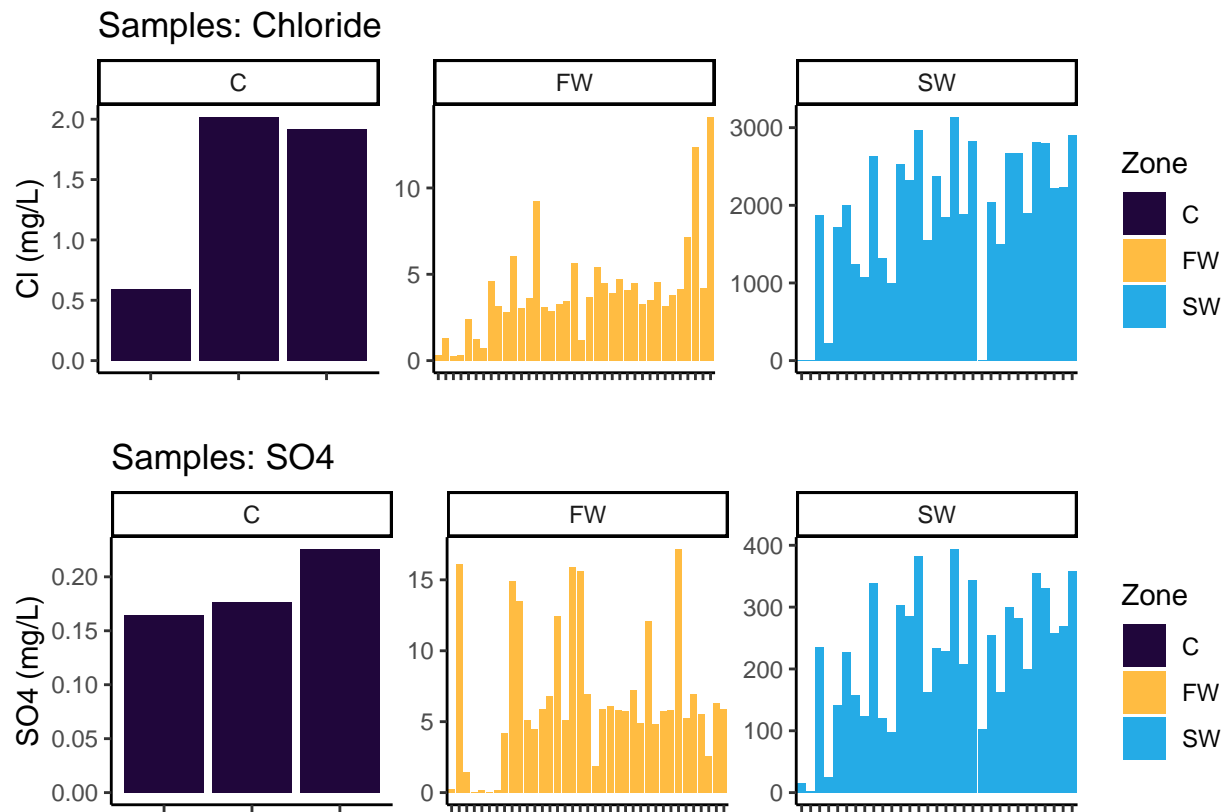
Cl_Conc_flag	Percent_samples
Within_Range	98.823529
bdl	1.176471

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

Some sample IDs are missing from metadata.

[1] "TMP_C_H6_20240610_15CM" "TMP_SW_H3_20240612_15CM_T3"

0.11 Visualize Data by Plot



0.12 Export Processed Data

#end