

TEMPEST: Porewater SO₄/Cl

92-142 2025 Samples

2025-12-19

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##Add Required Packages

0.1 Run Information

```
##### Run information - PLEASE CHANGE
Sample_Year = "2025"
Date_Run = "2025-12-15" #Date that instrument was run
Run_by = "Zoe Read" #Instrument user
Script_run_by = "Zoe Read" #Code user
run_notes = "Some sample IDs are missing from metadata: TMP_SW_H6_20250926_15CM.
One bad dup and one bad spk.
" #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 = NA
New_ID_1 = NA

##### File Names - PLEASE CHANGE
#file path and name for raw summary data file
raw_file_name_cl = "Raw Data/COMPASS_TEMPEST_2025_92-142_and_FATE_C1.txt"
raw_file_name_so4 = "Raw Data/COMPASS_TEMPEST_2025_92-142_and_FATE_S04.txt"

#file path and name of processed data file
processed_file_name = "Processed Data/COMPASS_TEMPEST_Processed_C1_S04_2025_92-142.csv"

##### Log Files - PLEASE CHECK

#qaqc log file path for this year copied over from COMPASS GitHub
Log_path = "Raw Data/COMPASS_Synoptic_C1_S04_QAQClog_2024.csv"
```

##Set Up Code - constants and QAQC cutoffs

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

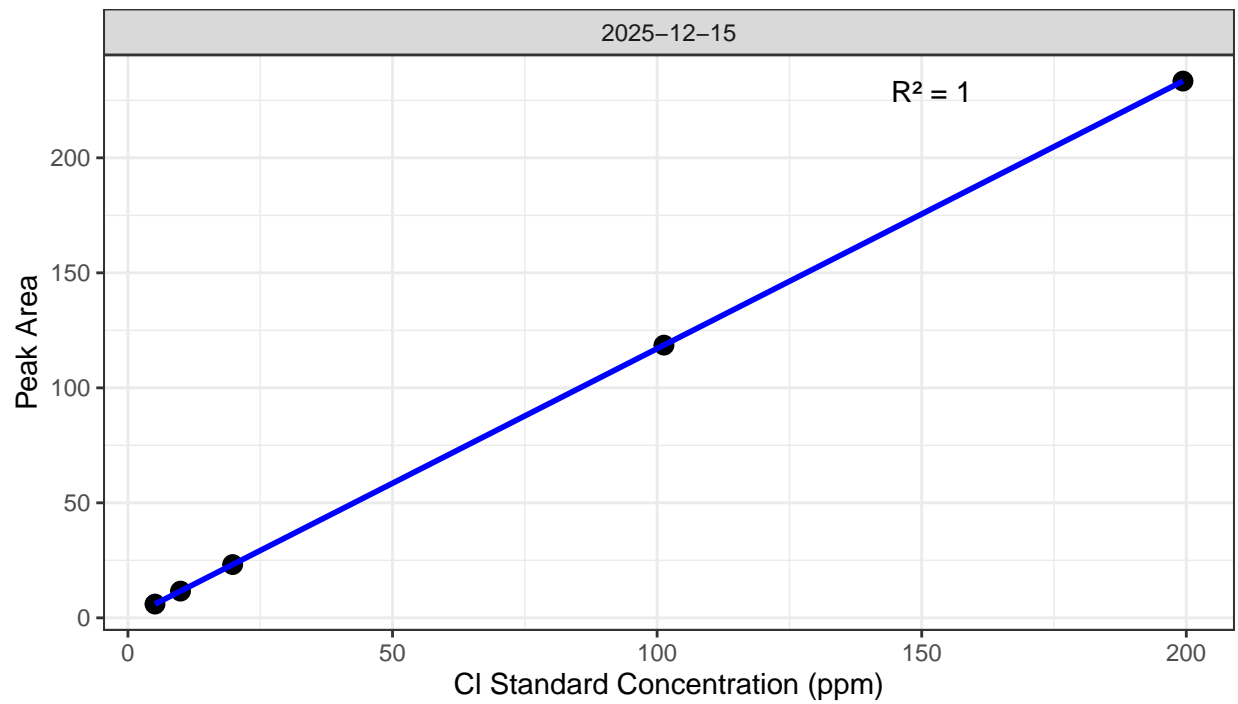
##Create similar sample IDs to match with run samples

##Import Sample Data

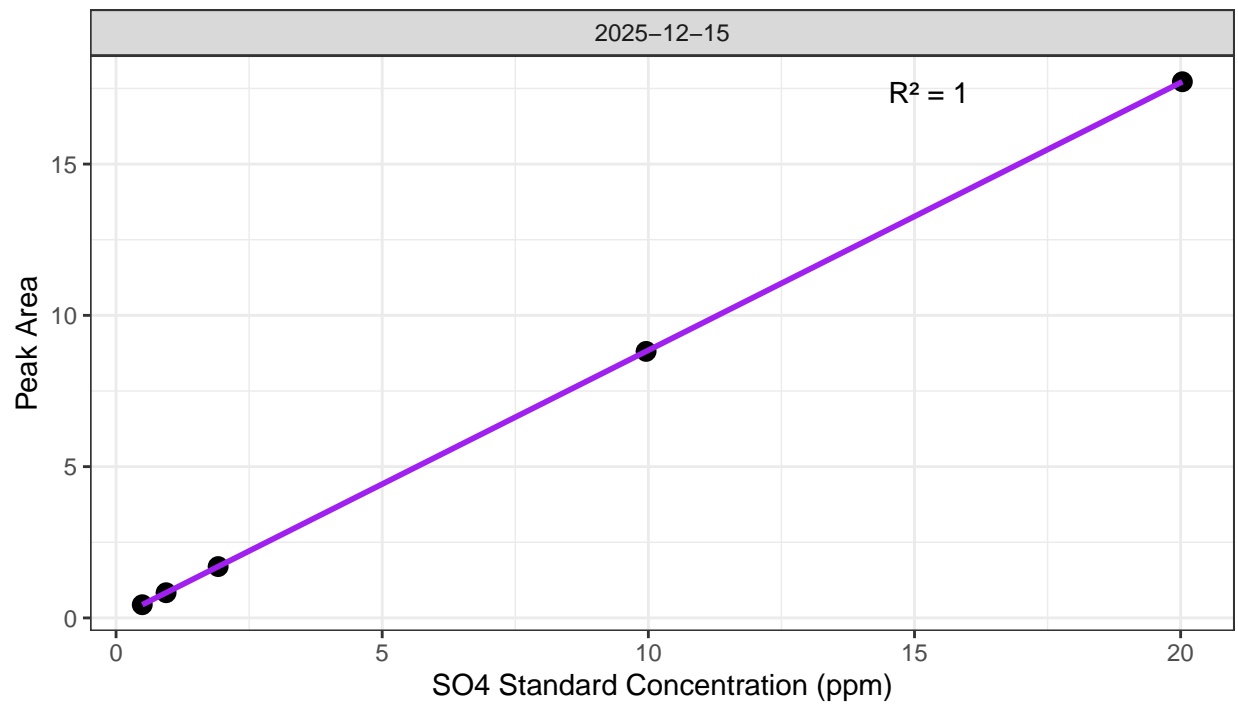
##Fix Sample IDs entered wrong

0.3 Assess Standard Curves

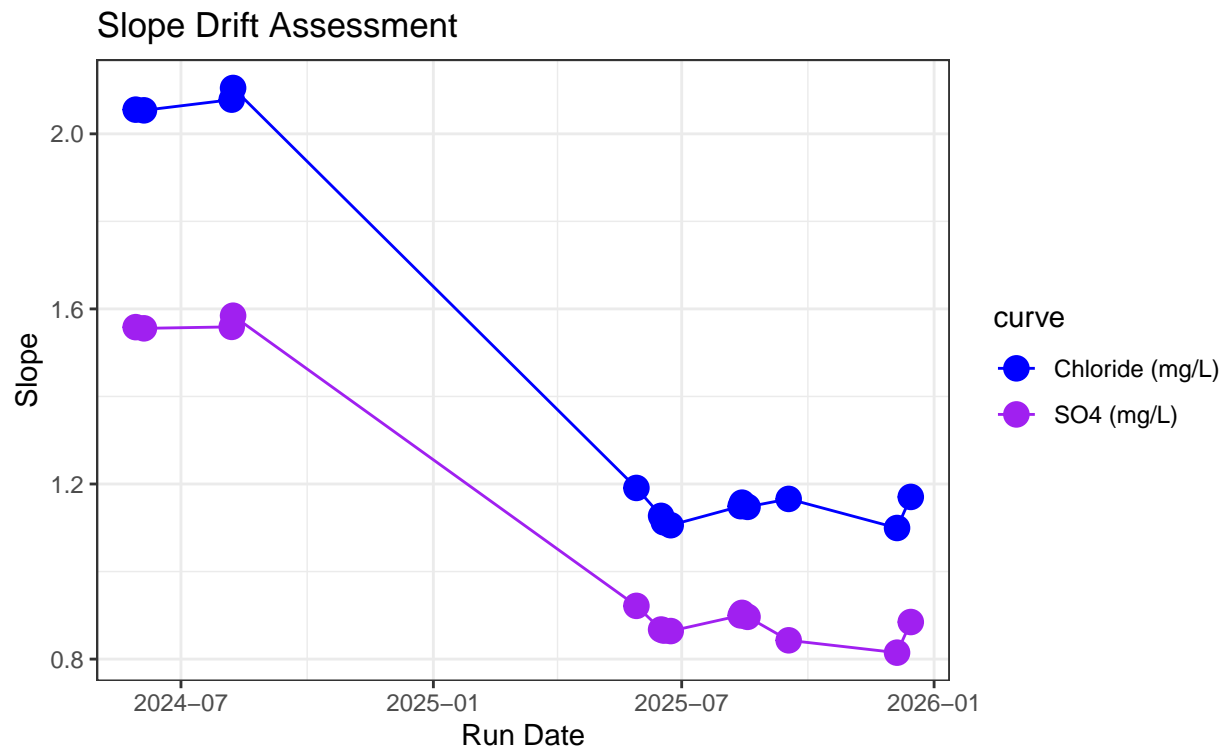
Chloride Std Curve



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"
```

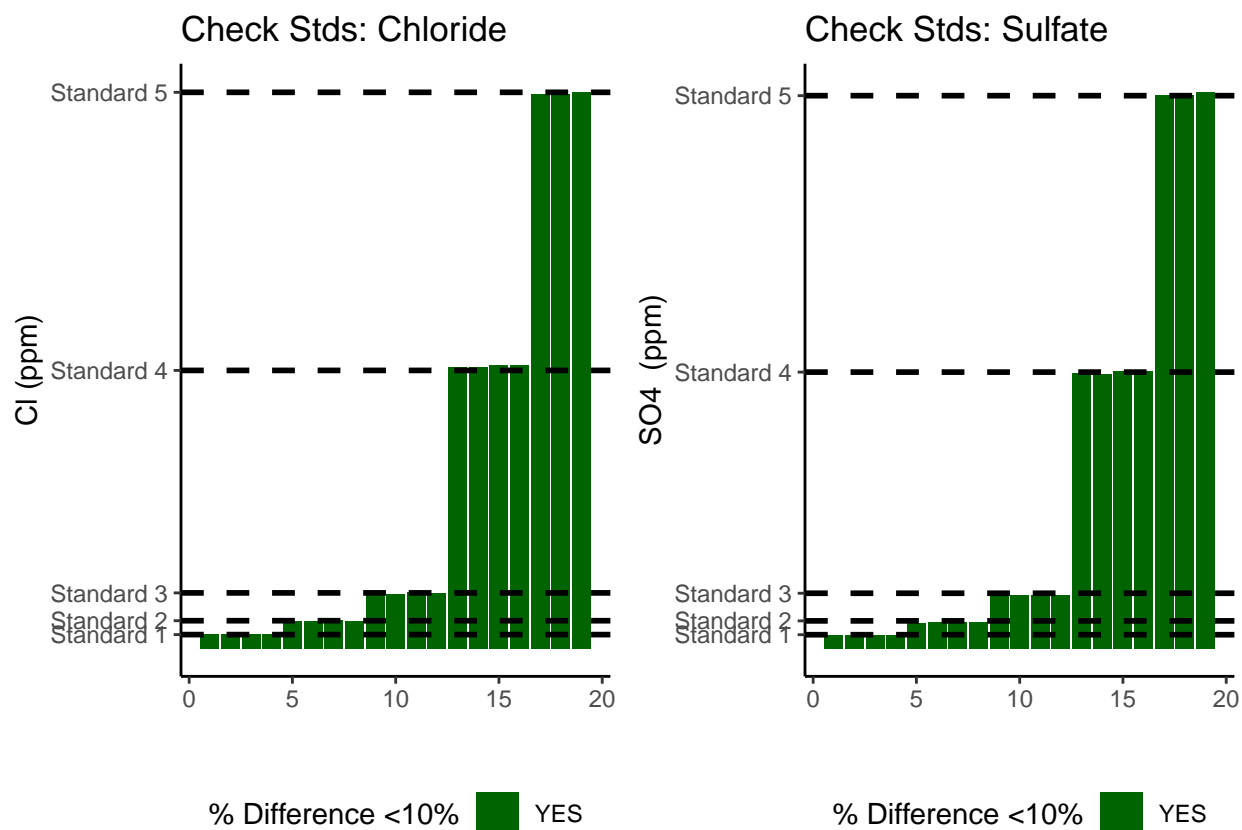
0.4 Assess Check Standards

```
## # A tibble: 5 x 5
##   sample_ID mean_Cl sd_Cl cv_Cl flag_Cl
##   <chr>      <dbl> <dbl> <dbl> <chr>
## 1 Standard 1    5.18 0.0723 0.0139 Chloride Check Standard RSD within Range - ~
## 2 Standard 2   10.0 0.139 0.0138 Chloride Check Standard RSD within Range - ~
## 3 Standard 3   19.9 0.178 0.00891 Chloride Check Standard RSD within Range - ~
## 4 Standard 4  102. 0.418 0.00411 Chloride Check Standard RSD within Range - ~
## 5 Standard 5  200. 0.506 0.00254 Chloride Check Standard RSD within Range - ~
```

```
## # A tibble: 5 x 5
##   sample_ID mean_SO4 sd_SO4 cv_SO4 flag_SO4
##   <chr>      <dbl> <dbl> <dbl> <chr>
## 1 Standard 1    0.502 0.00629 0.0125 Sulfate Check Standard RSD within Range --
## 2 Standard 2    0.950 0.00703 0.00740 Sulfate Check Standard RSD within Range --
## 3 Standard 3    1.93 0.0106 0.00548 Sulfate Check Standard RSD within Range --
## 4 Standard 4    9.99 0.0456 0.00456 Sulfate Check Standard RSD within Range --
## 5 Standard 5   20.1 0.0721 0.00359 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"
```



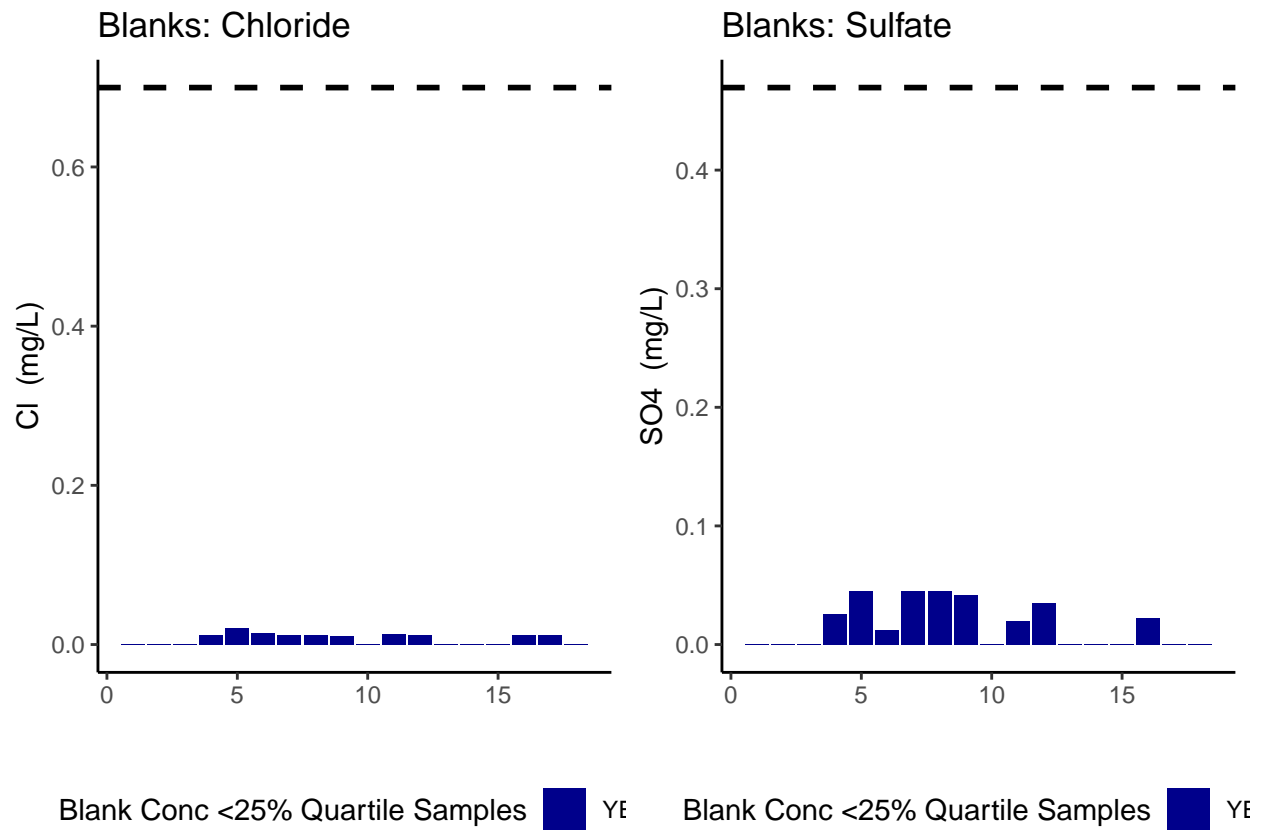
```
## [1] ">80% of Chloride Check Standards are within range of expected concentration - PROCEED"
```

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

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"
```



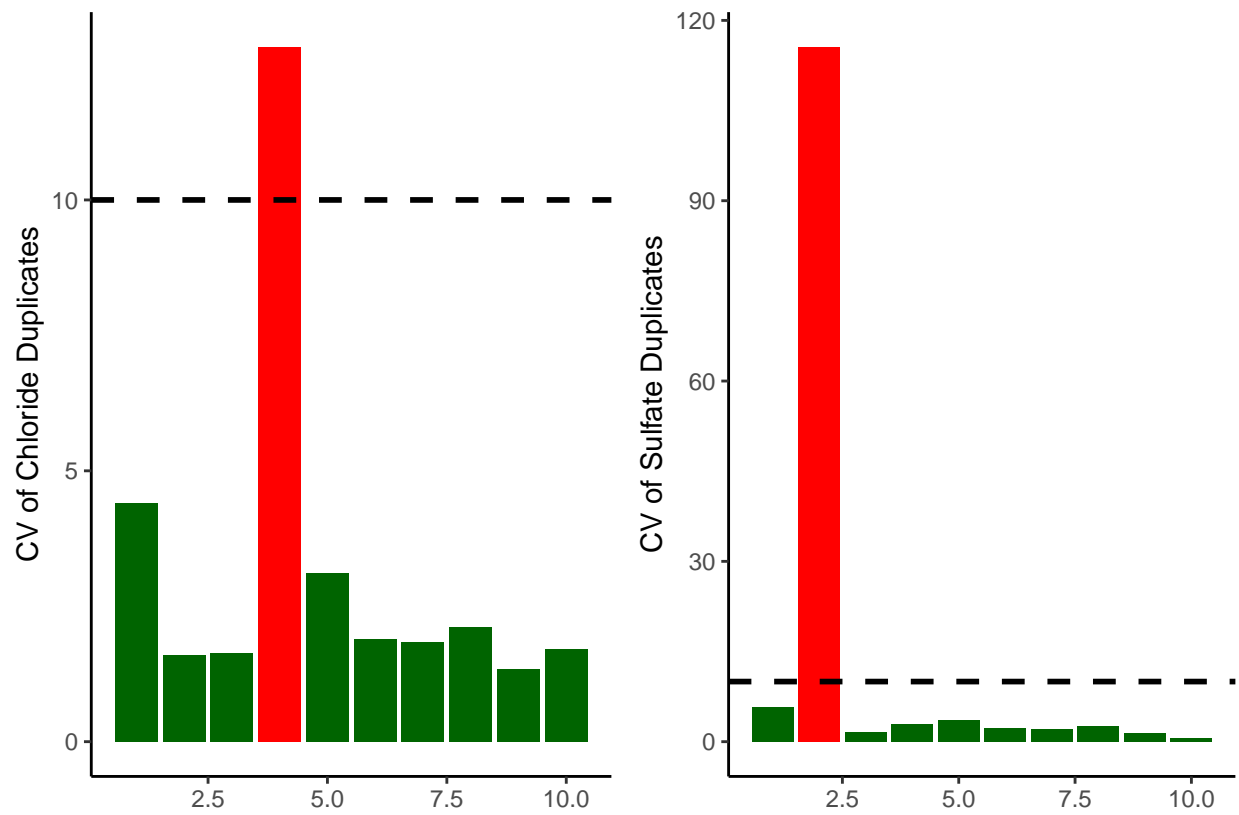
```
## Chloride blanks mean ppm:
```

```
## [1] 0.007288889
```

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

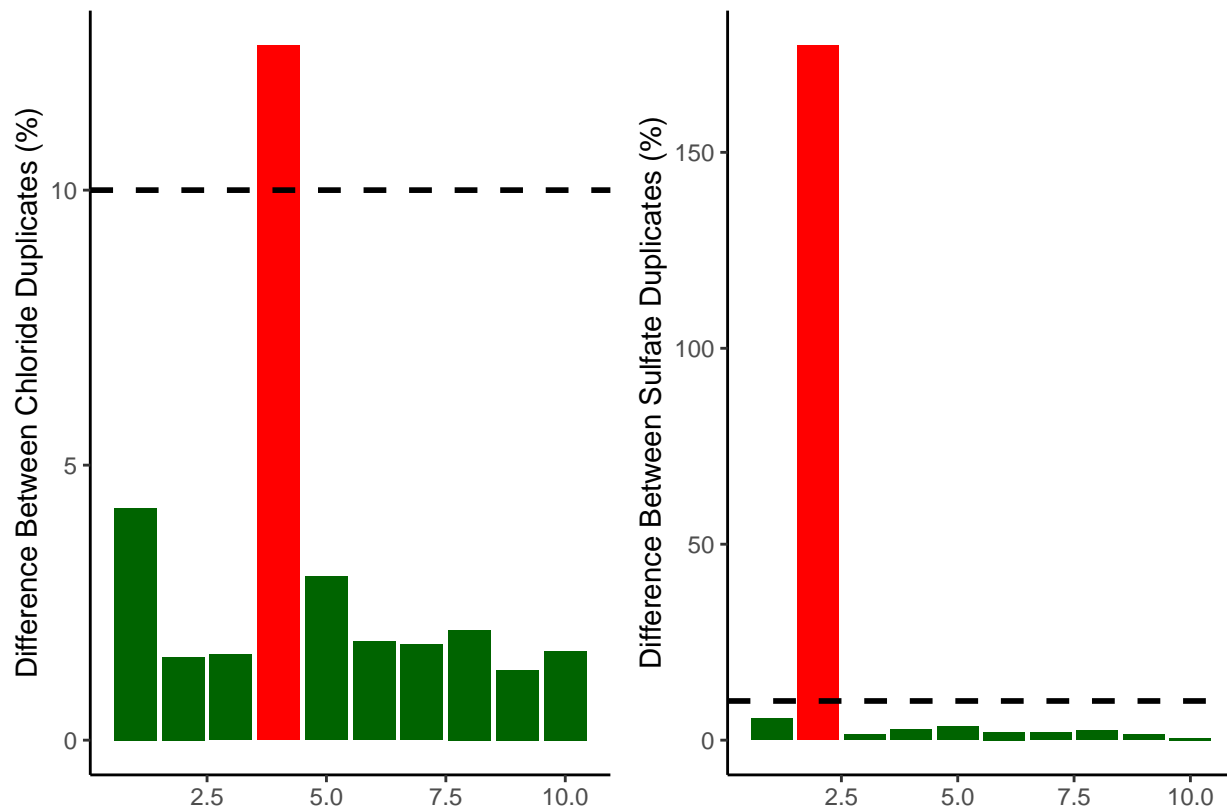
```
## [1] 0.01626111
```

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

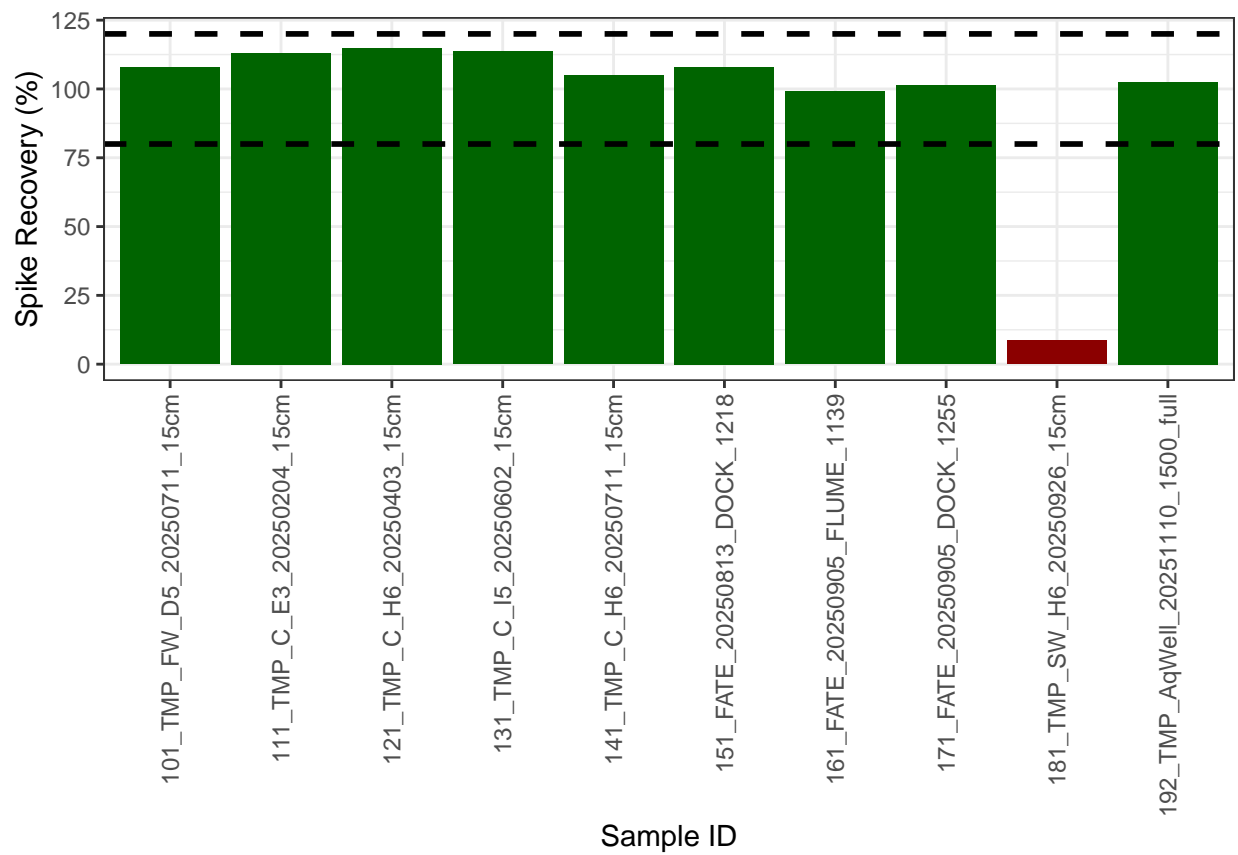
#Need to determine dilution factors for your samples
#for TEMPEST this depends on the sample so...
all_dat$Dilution <- 1
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "TMP"), 50, all_dat$Dilution)
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "EST_SourceWater"), 100, all_dat$Dilution)
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "SW_SourceWater"), 100, all_dat$Dilution)
```



```
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "FATE"), 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
```

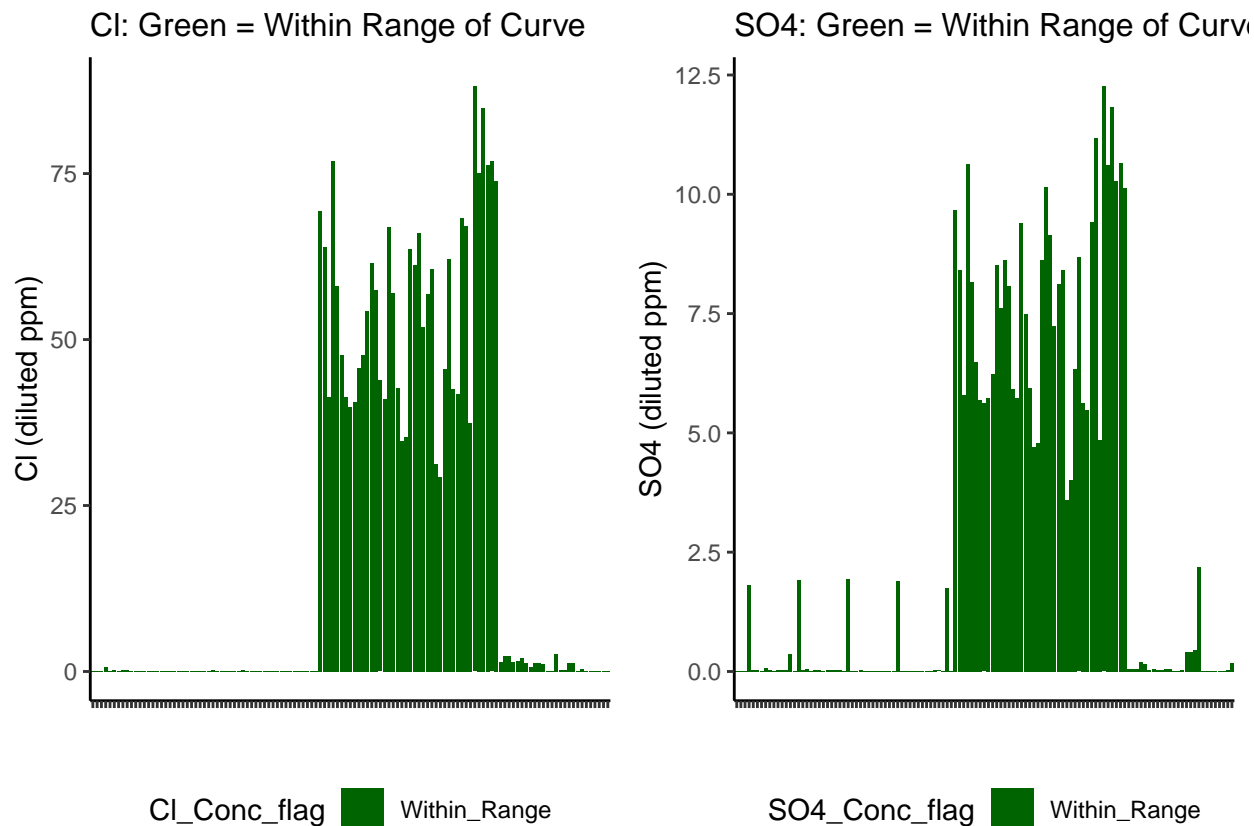


Table 1: SO4 samples

SO4_Conc_flag	Percent_samples
Within_Range	100

Table 2: Cl samples

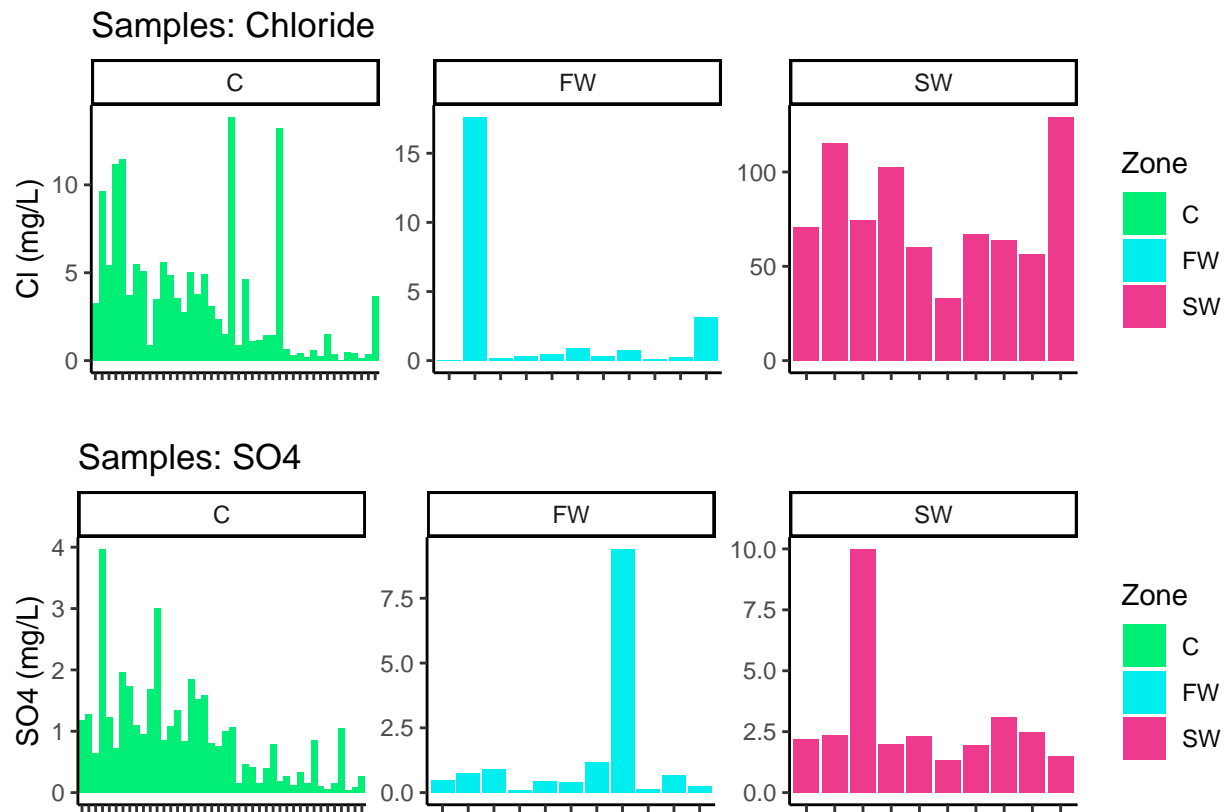
Cl_Conc_flag	Percent_samples
Within_Range	100

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

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

```
## [1] "TMP_SW_H6_20250926_15CM"
```

0.11 Visualize Data by Plot



0.12 Export Processed Data

#end