

TEMPEST: Porewater SO₄/Cl

1-91 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 = "2025-12-05" #Date that instrument was run
Run_by = "Zoe Read" #Instrument user
Script_run_by = "Zoe Read" #Code user
run_notes = "
" #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_c1 = "Raw Data/COMPASS_TEMPEST_2025_1-91_C1.txt"
raw_file_name_so4 = "Raw Data/COMPASS_TEMPEST_2025_1-91_S04.txt"

#file path and name of processed data file
processed_file_name = "Processed Data/COMPASS_TEMPEST_Processed_C1_S04_2025_1-91.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"
```

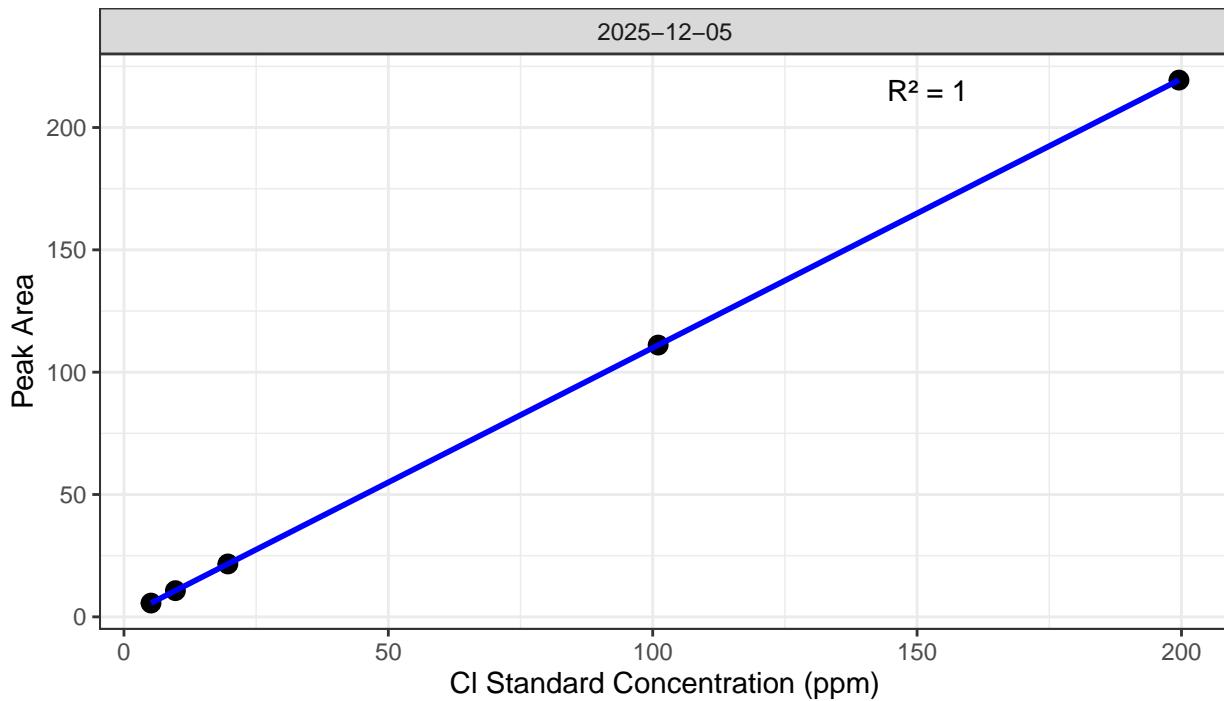
```
##Set Up Code - constants and QAQC cutoffs
```

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

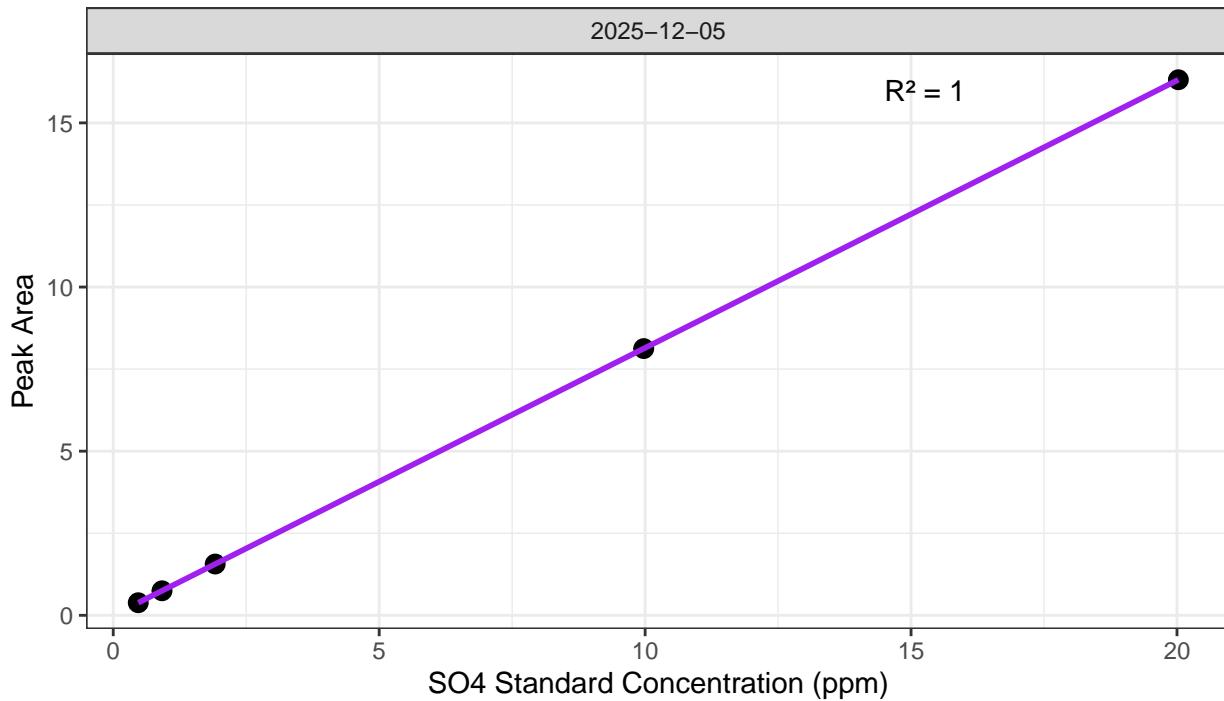
```
##Create similar sample IDs to match with run samples
##Import Sample Data
##Fix Sample IDs entered wrong
```

0.3 Assess Standard Curves

Chloride Std Curve

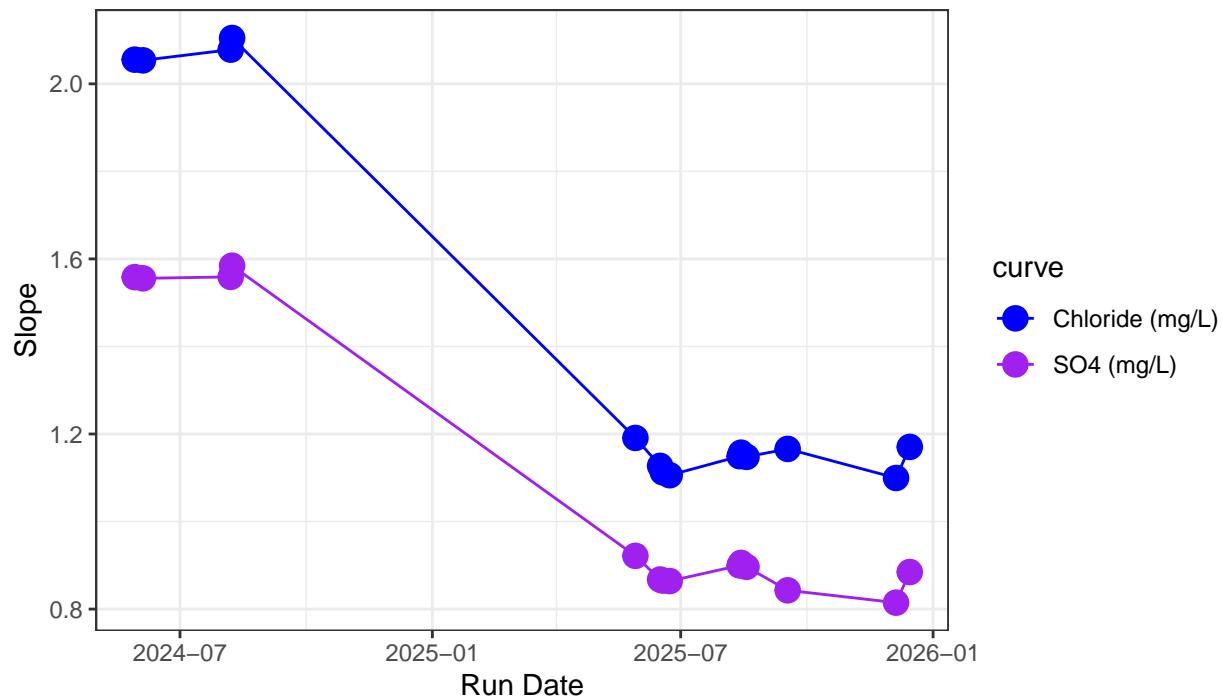


Sulfate Std Curve



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

Slope Drift Assessment



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

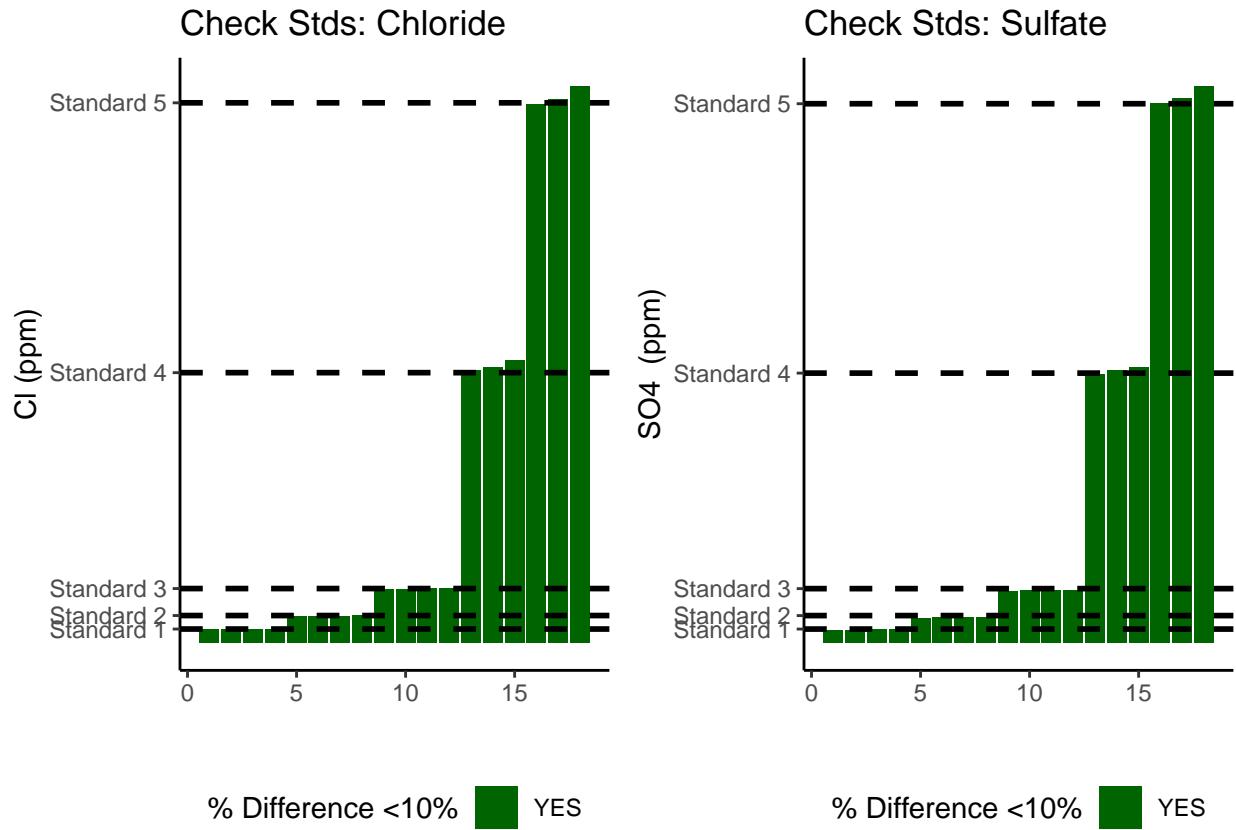
```
## [1] "SO4 Curve r2 GOOD"
```

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  5.14  0.0398  0.00774 Chloride Check Standard RSD within Range - ~
## 2 Standard 2  9.88  0.137   0.0139  Chloride Check Standard RSD within Range - ~
## 3 Standard 3  20.0   0.324   0.0162  Chloride Check Standard RSD within Range - ~
## 4 Standard 4  103.    1.89    0.0184  Chloride Check Standard RSD within Range - ~
## 5 Standard 5  202.    3.56    0.0176  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  0.479  0.00950  0.0198 Sulfate Check Standard RSD within Range -- 
## 2 Standard 2  0.935  0.0147   0.0157 Sulfate Check Standard RSD within Range -- 
## 3 Standard 3  1.94   0.0161   0.00828 Sulfate Check Standard RSD within Range -- 
## 4 Standard 4  10.1   0.125    0.0123 Sulfate Check Standard RSD within Range -- 
## 5 Standard 5  20.3   0.334    0.0164 Sulfate Check Standard RSD within Range -- 

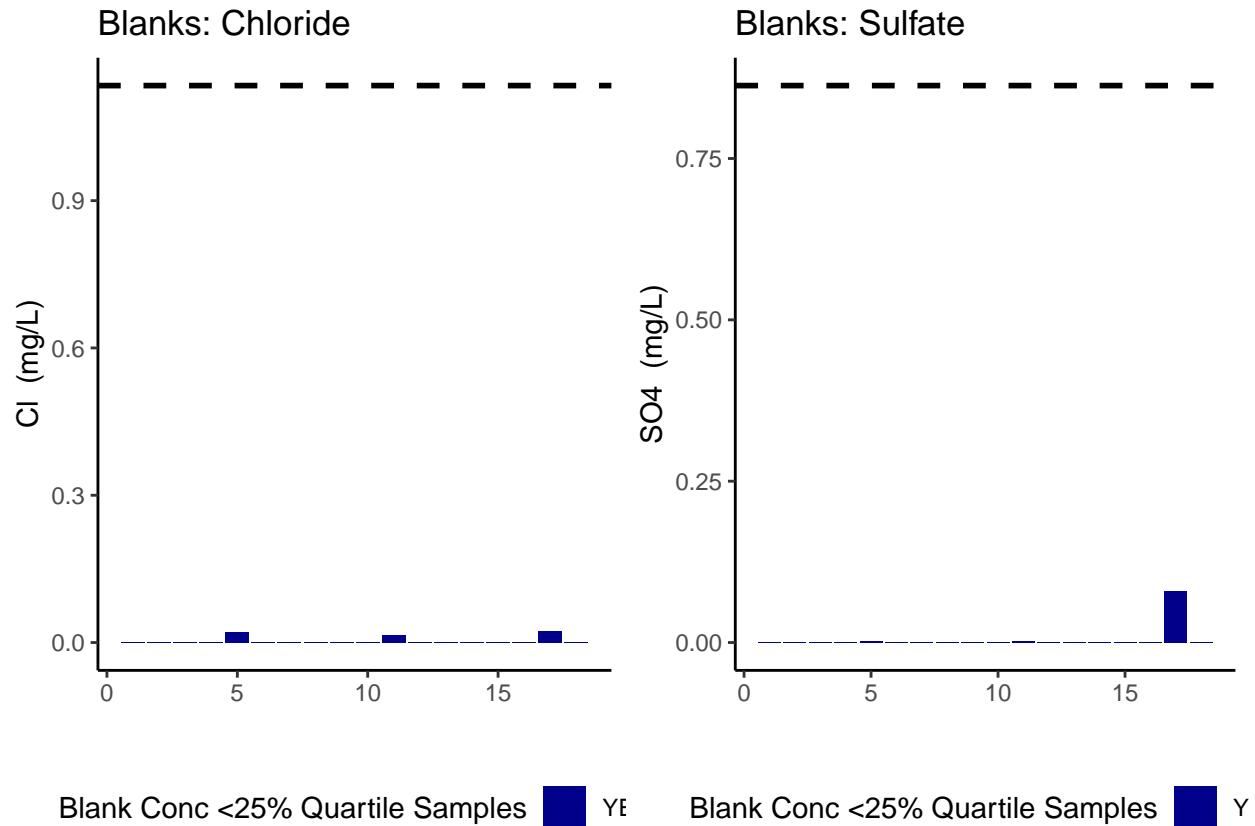
## [1] ">80% of Chloride Check Standards have RSD within range - PROCEED"
## [1] ">80% of Sulfate Check Standards have RSD within range - PROCEED"
```



```
## [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:
```

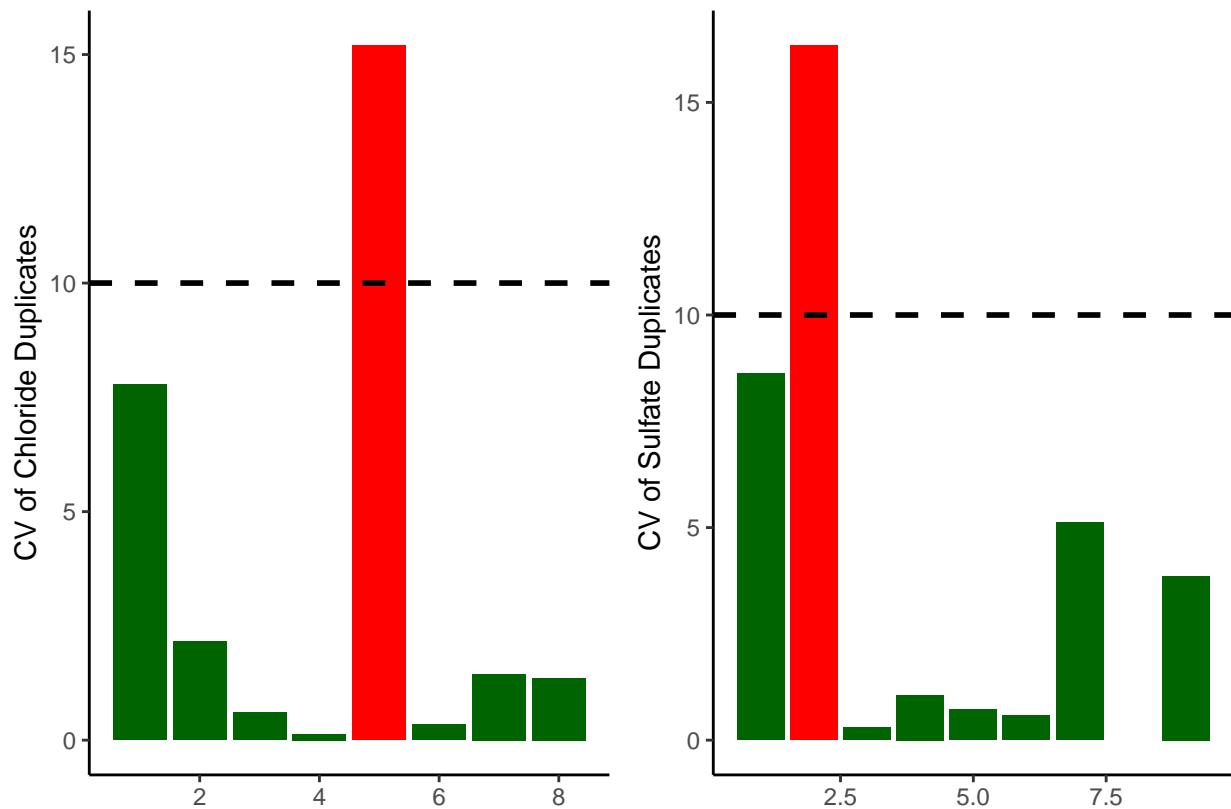
```
## [1] 0.003311111
```

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

```
## [1] 0.0047
```

0.6 Assess Duplicates

```
## Warning: Removed 1 row containing missing values or values outside the scale range
## ('geom_bar()').
## Removed 1 row containing missing values or values outside the scale range
## ('geom_bar()').
```



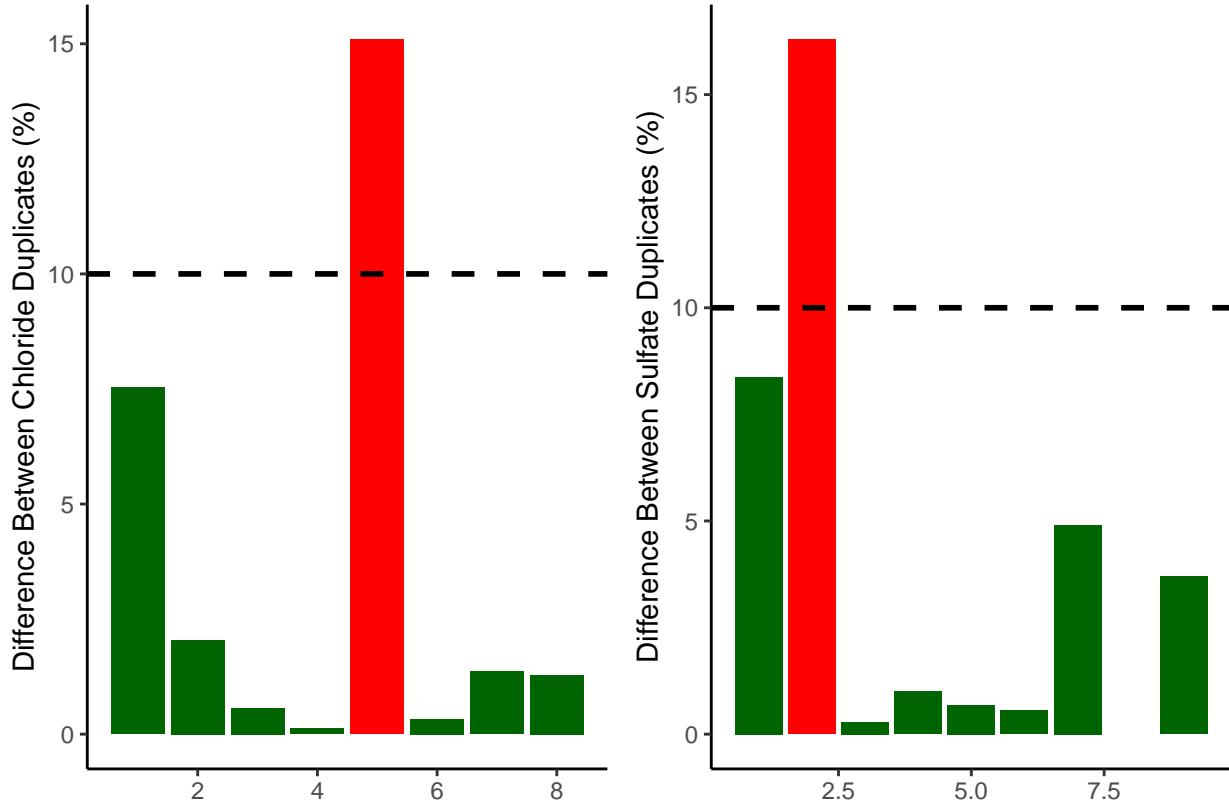
```

## [1] ">80% of Chloride Duplicates have a CV <10% - PROCEED"

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

## Warning: Removed 1 row containing missing values or values outside the scale range
## ('geom_bar()').
## Removed 1 row containing missing values or values outside the scale range
## ('geom_bar()').

```



```
## [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

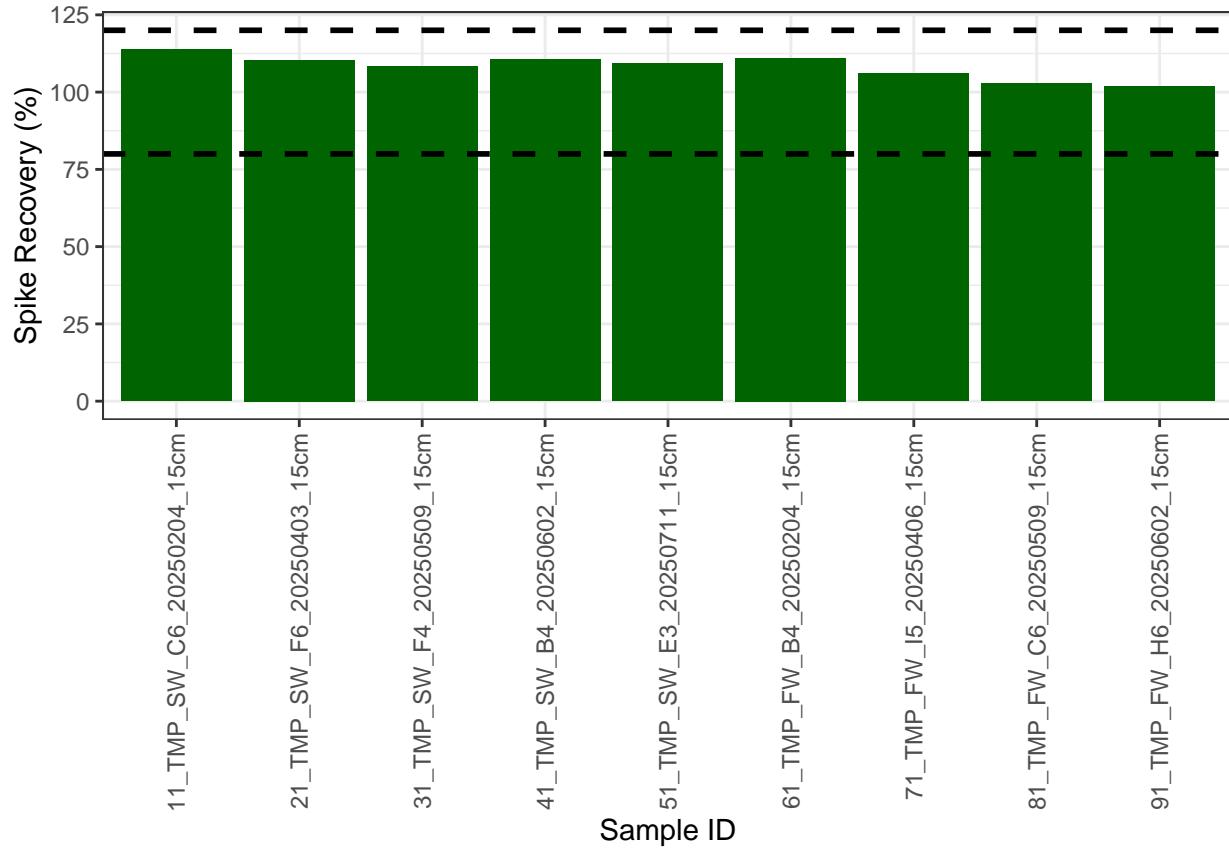
```
# Convert ppm to mmol/L
all_dat$SO4_Conc_mM <- (all_dat$SO4_ppm / s_mw)
all_dat$Cl_Conc_mM <- (all_dat$Cl_ppm / cl_mw)

# 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
```

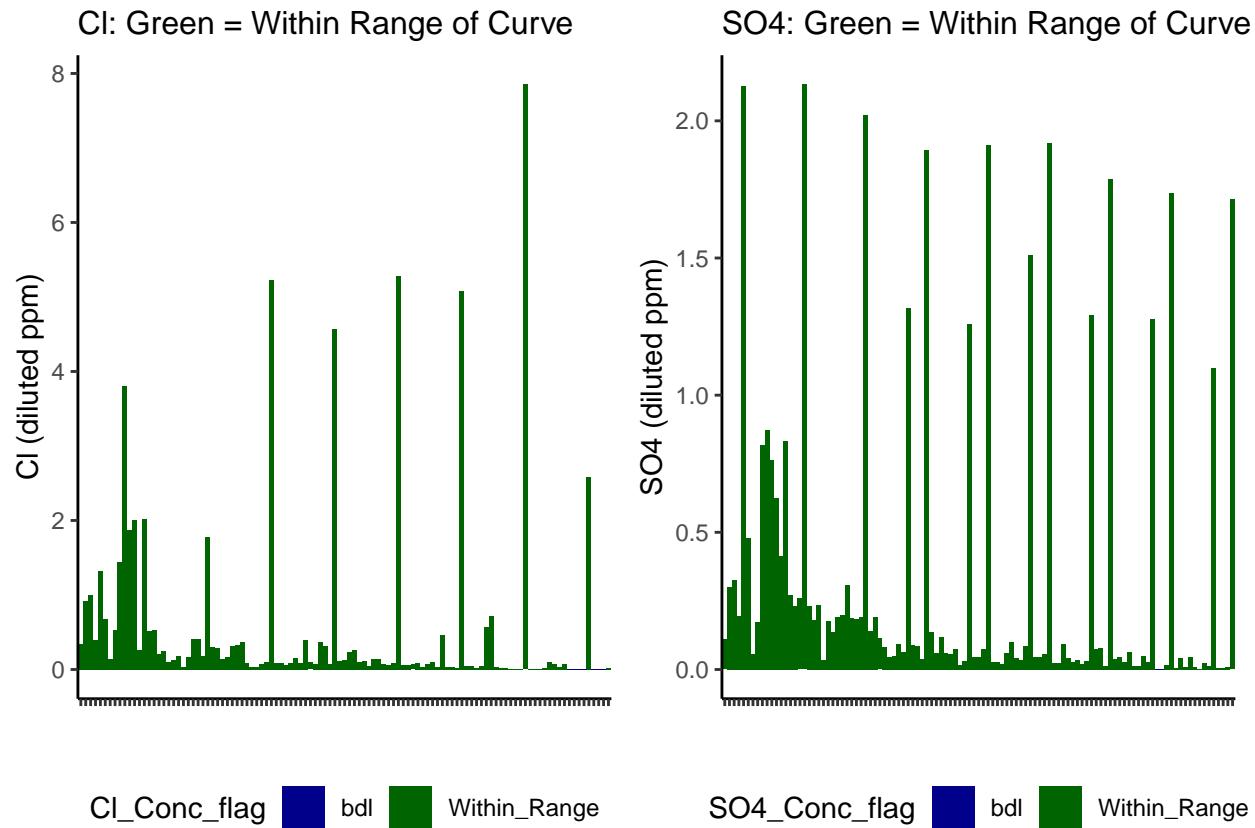


Table 1: SO4 samples

SO4_Conc_flag	Percent_samples
Within_Range	98.165138
bdl	1.834862

Table 2: Cl samples

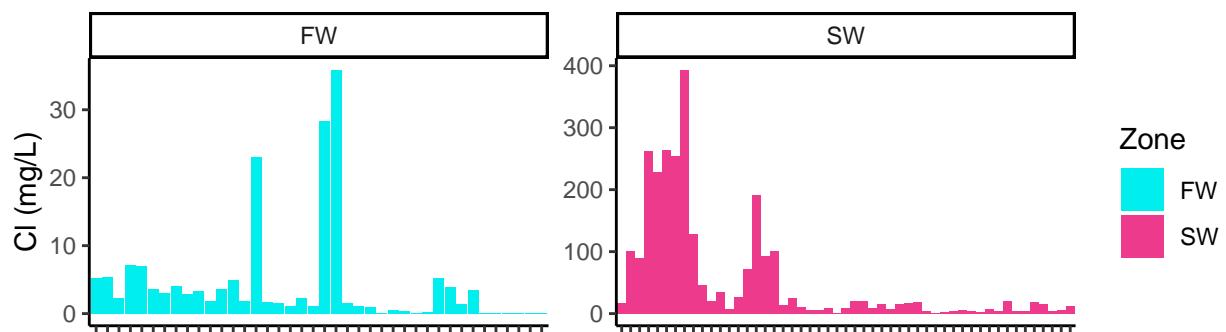
Cl_Conc_flag	Percent_samples
Within_Range	93.577982
bdl	6.422018

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

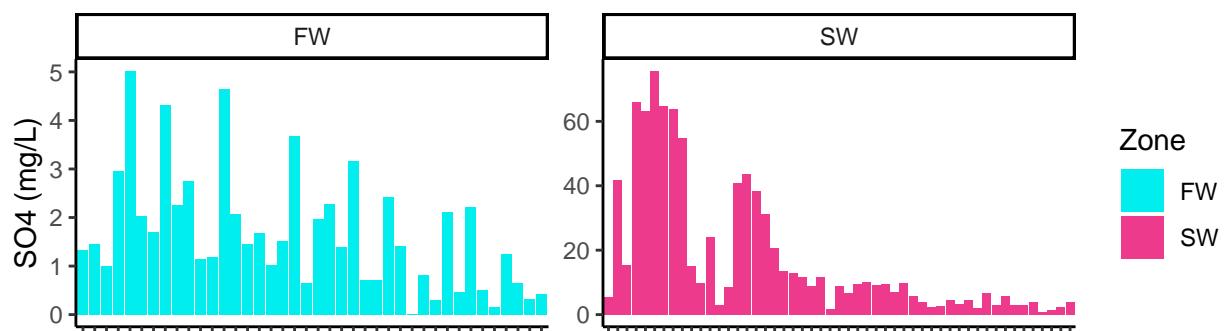
```
## All sample IDs are present in metadata.
```

0.11 Visualize Data by Plot

Samples: Chloride



Samples: SO4



0.12 Export Processed Data

```
#end
```