TEMPEST: Porewater SO4/Cl

1-91 2025 Samples

2025-12-08

Contents

##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, incorrecly-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_1-91_Cl.txt"
  raw_file_name_so4 = "Raw Data/COMPASS_TEMPEST_2025_1-91_SO4.txt"

#file path and name of processed data file
  processed_file_name = "Processed Data/COMPASS_TEMPEST_Processed_Cl_SO4_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_Cl_SO4_QAQClog_2024.csv"
```

##Set Up Code - constants and QAQC cutoffs

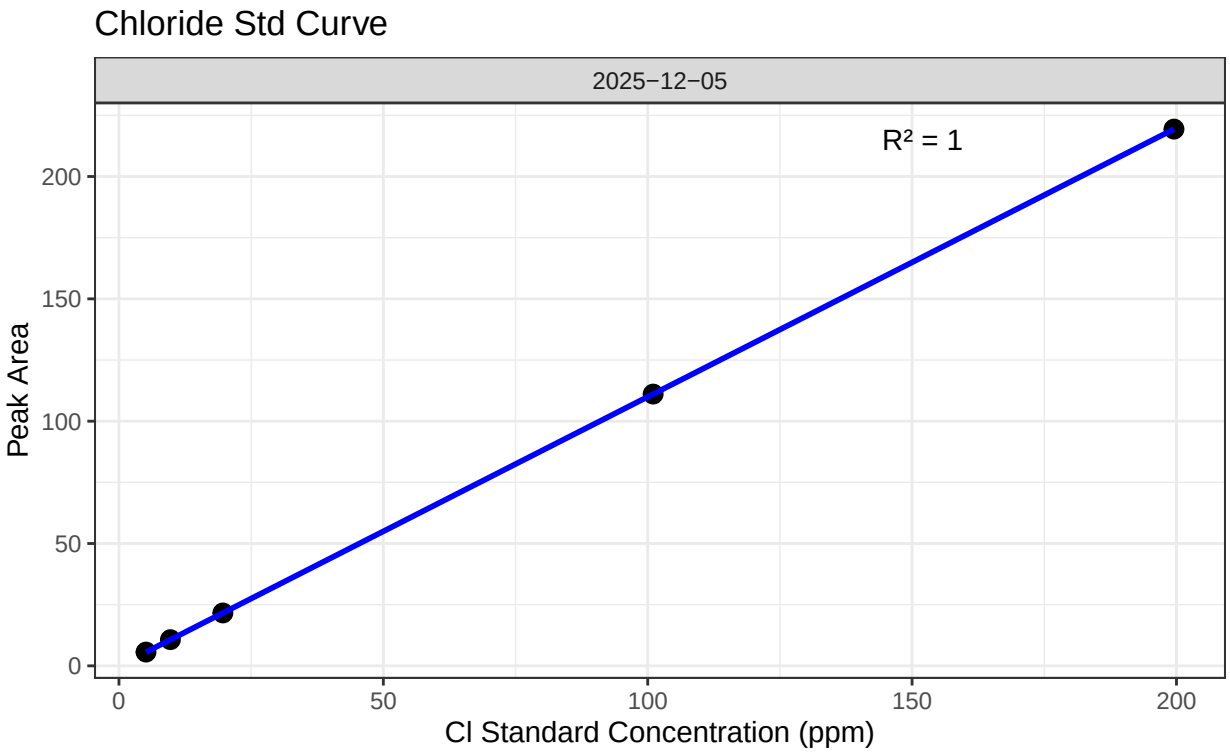
0.2 Pull in active porewater tracking inventory sheet from Google Drive:

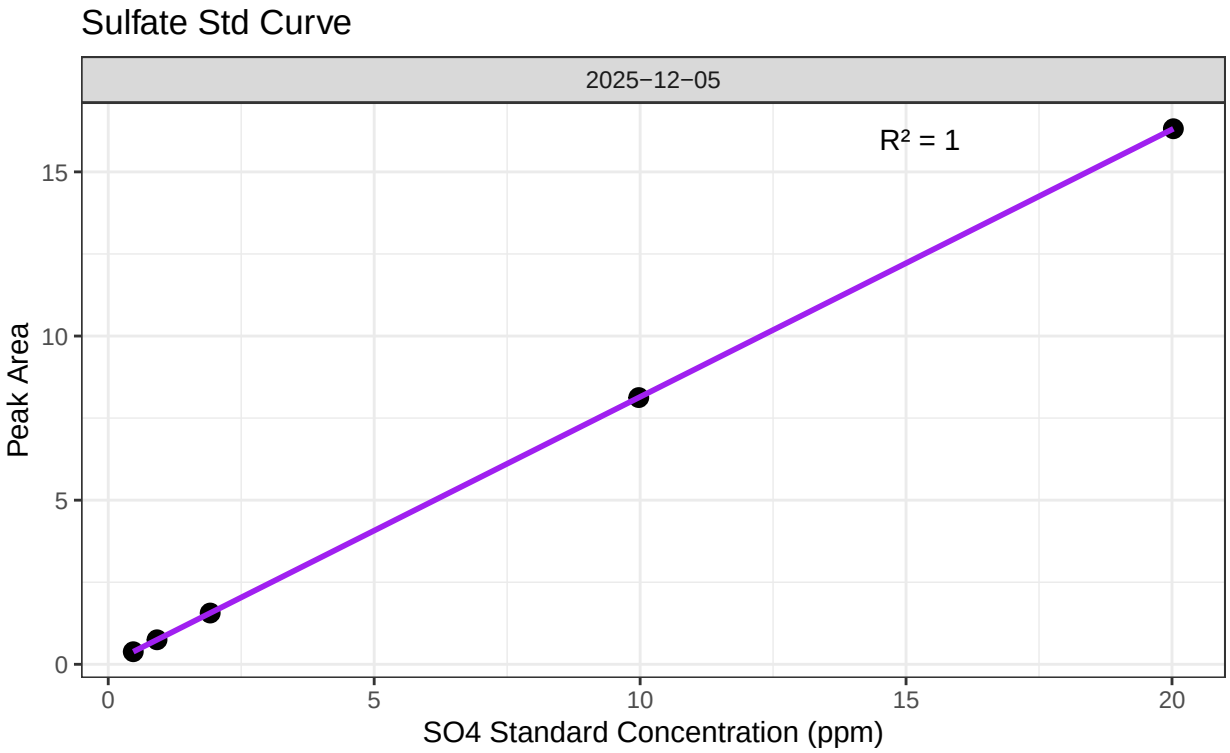
##Create similar sample IDs to match with run samples

##Import Sample Data

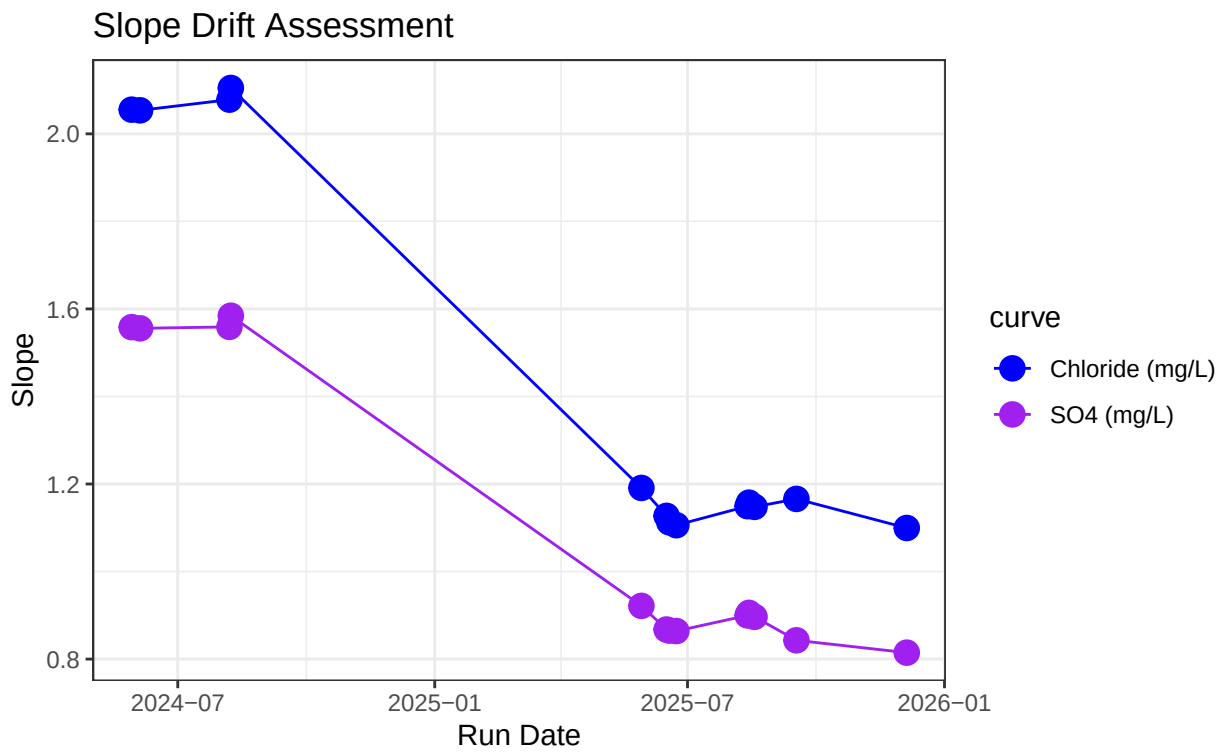
##Fix Sample IDs entered wrong

0.3 Assess Standard Curves






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




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

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

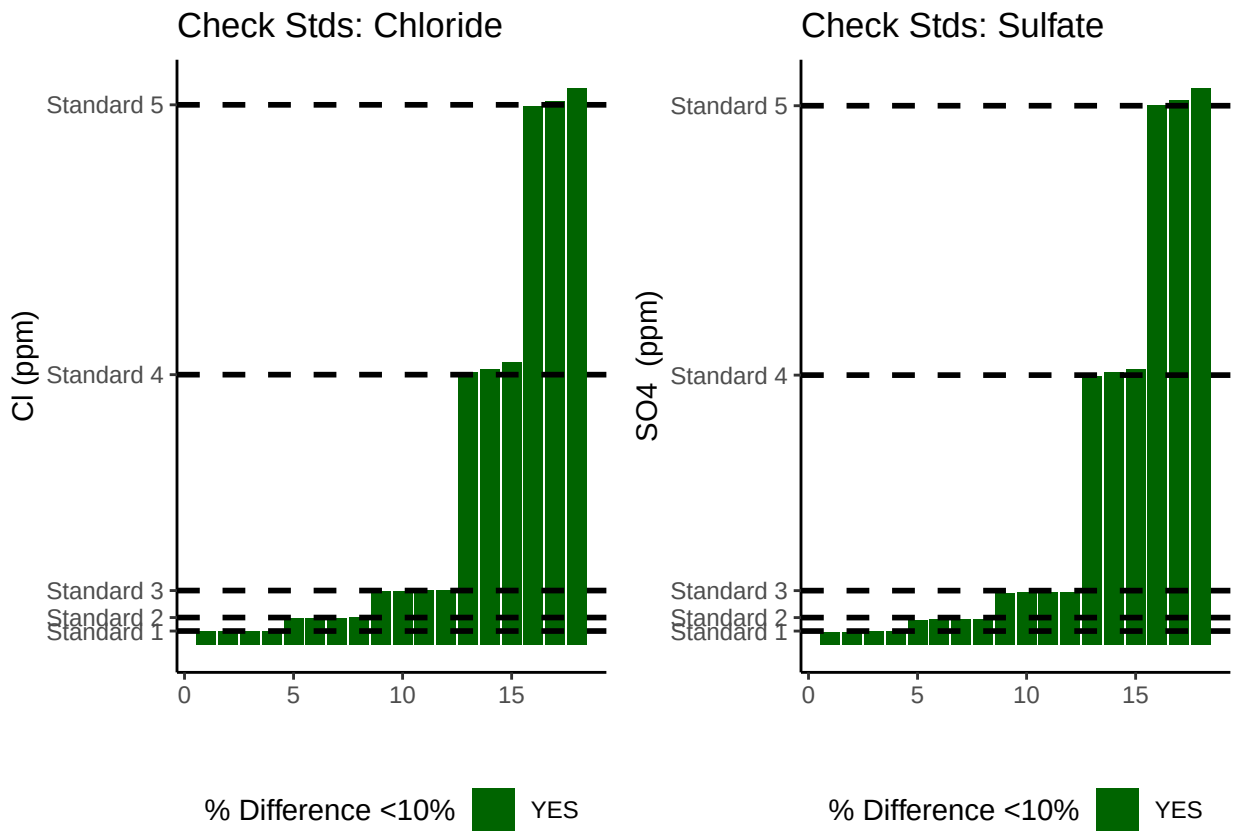
0.4 Assess Check Standards

```
## # A tibble: 5 x 5
##   sample_ID  mean_Cl  sd_Cl   cv_Cl flag_Cl
##   <chr>        <dbl>  <dbl>   <dbl> <chr>
## 1 Standard 1    5.14 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"
```



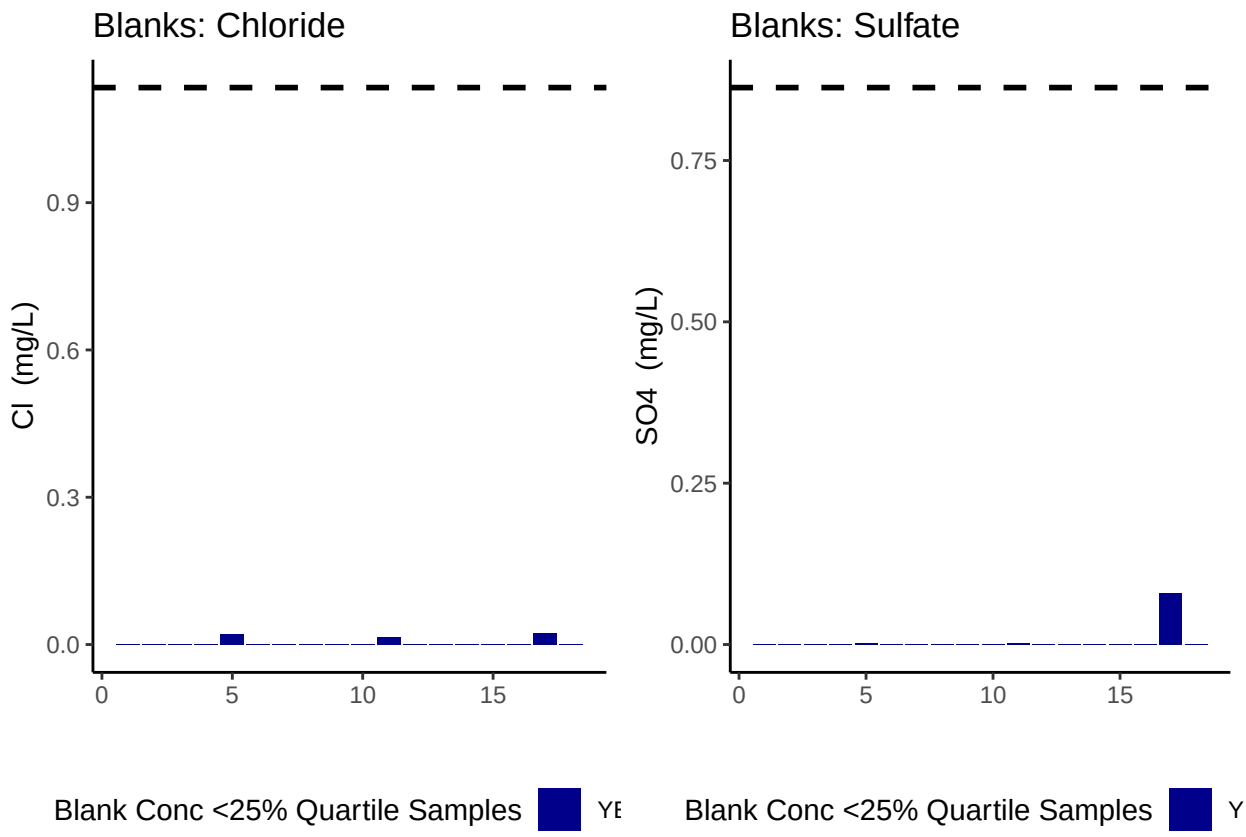

```
## [1] ">80% of Chloride Check Standards are within range of expected concentration - PROCEED"
```

```
## [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"
```

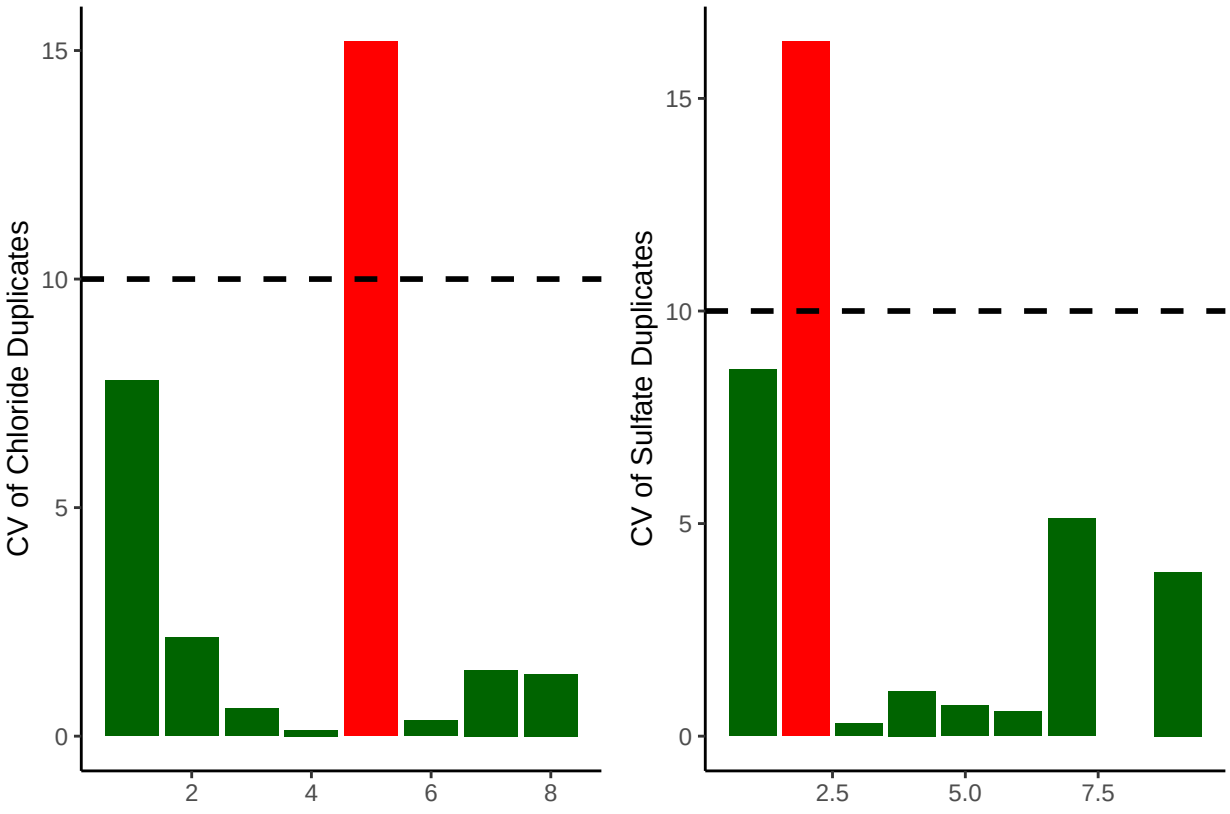
```
## [1] ">80% of Sulfate Blank concentrations are lower 25% quartile of samples"
```




```
## Chloride blanks mean ppm:

## [1] 0.003311111

## Sulfate blanks mean ppm:

## [1] 0.0047
```

0.6 Assess Duplicates

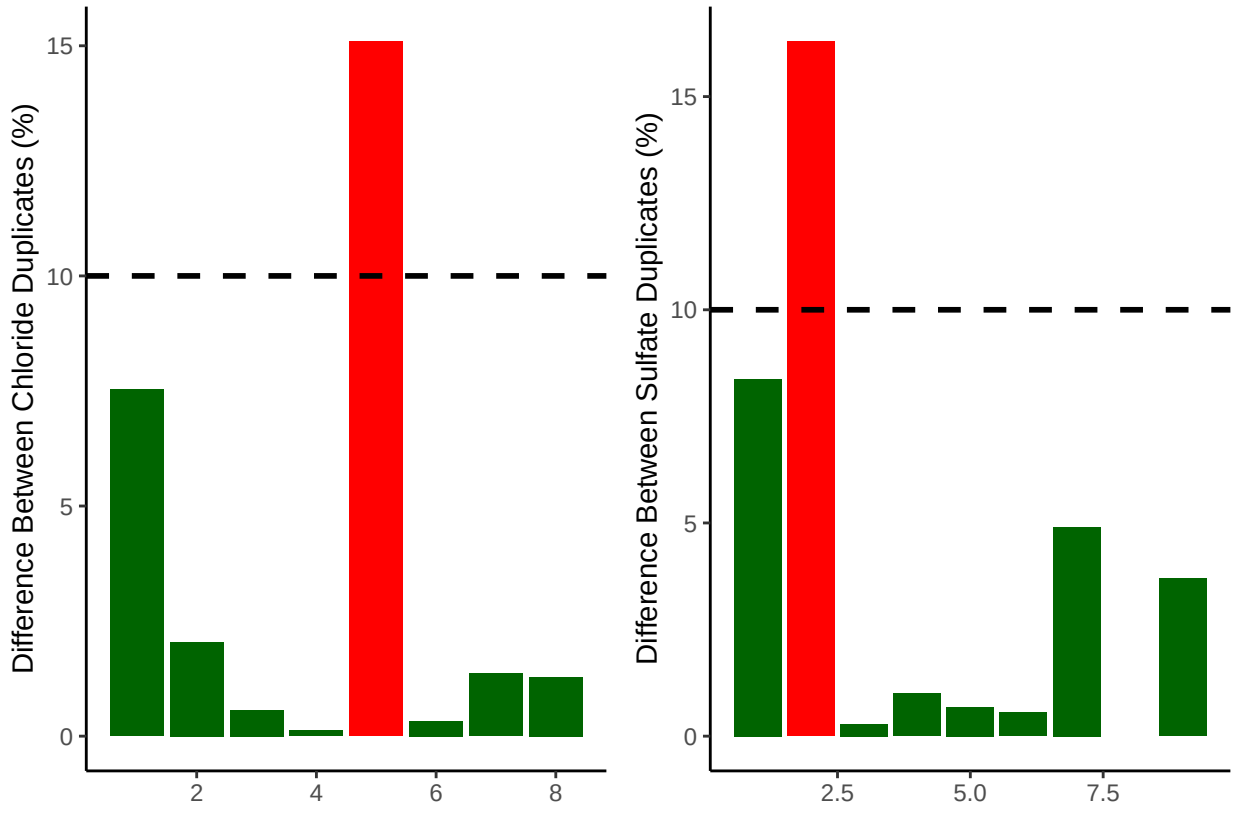
```
## Warning: Removed 1 row containing missing values or values outside the scale range
## (`geom_bar()`).
## Removed 1 row containing missing values or values outside the scale range
## (`geom_bar()`).
```




```
## [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"
```

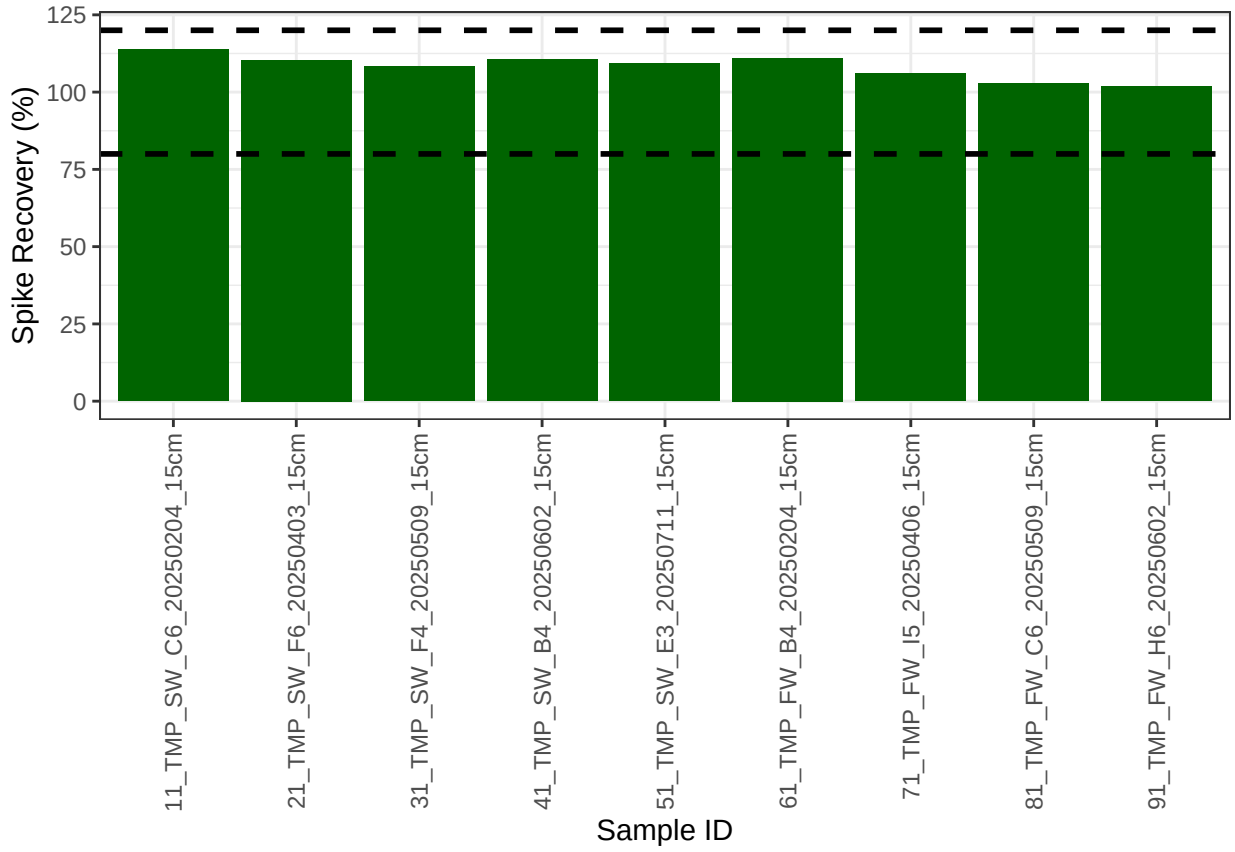
```
## [1] ">80% of Sulfate Duplicates have a percent difference <10% - PROCEED"
```

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$salinity <- ((1.8070 * all_dat$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 SO4 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
```

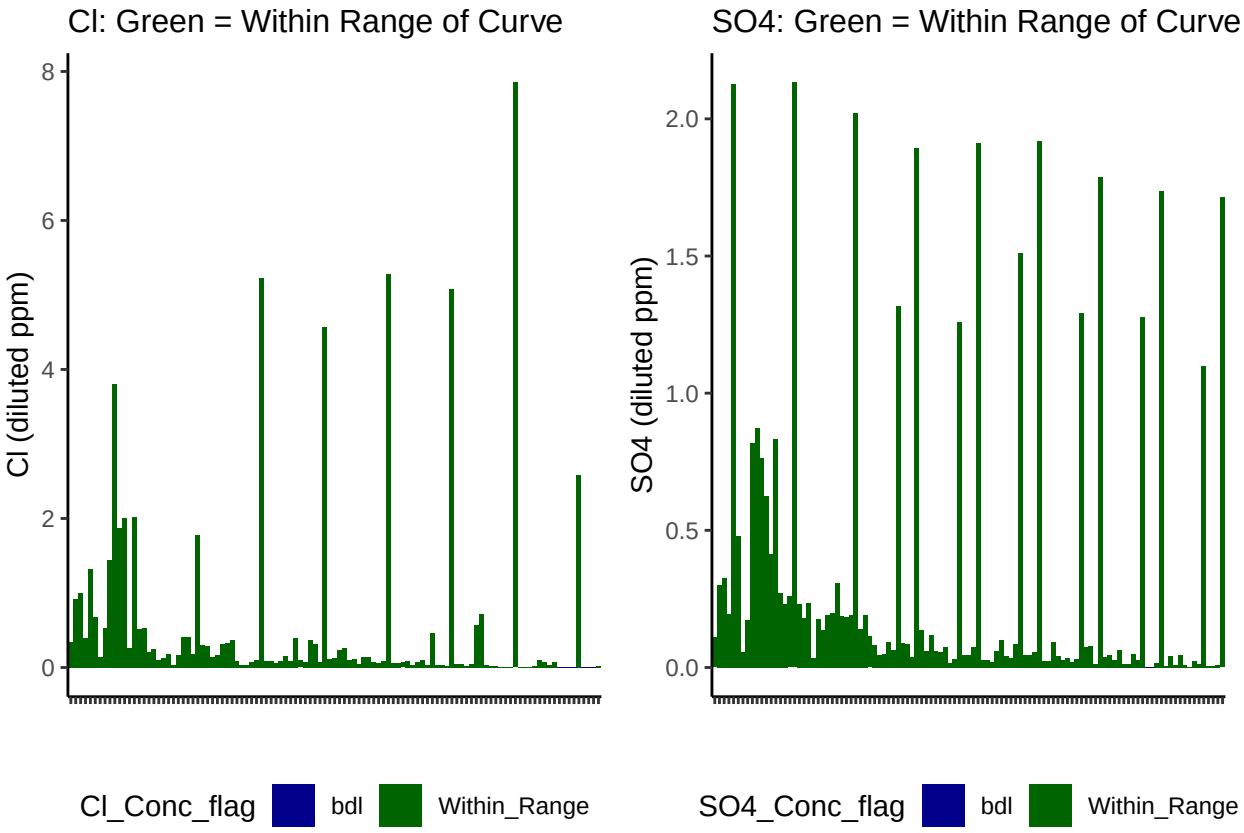


Table 1: SO4 samples

SO4_Conc_flag	Percent_samples
Within_Range	98.165138
bdl	1.834862

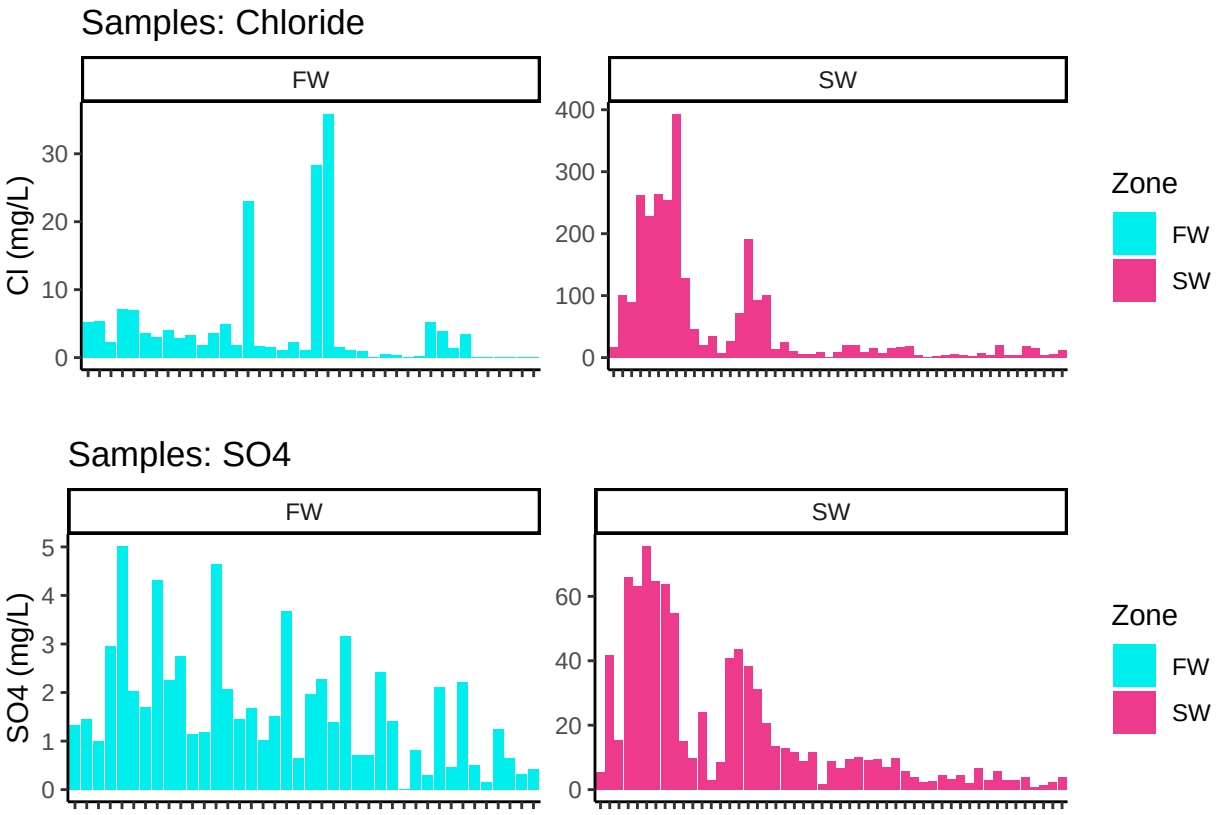
Table 2: Cl samples

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



0.12 Export Processed Data

#end