

Synoptic CB: Porewater SO₄/Cl

May 2025 Samples

2025-10-03

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```
##Add Required Packages
```

0.1 Run Information

```
##### Run information - PLEASE CHANGE
Date_Run = "2025-09-24" #Date that instrument was run
Run_by = "Zoe Read" #Instrument user
Script_run_by = "Zoe Read" #Code user
run_notes = "Std 1 values are lower than the expected concentration - why is this?  
I have seen this with most of our recent runs.  
2 dups had high CV for Cl: 120_TEMPEST_AqWell_20250904_1225_C, 80_SWH_202505_UP_LysB_10cm  
1 spk had high recovery (122% compared to the 120% cutoff): 101_SWH_202505_TR_LysC_10cm  
Some sample IDs are missing from metadata:  
GCW_202505_TR_LYSC_45CM, TEMPEST_AQWELL_20250904_1300_B, TEMPEST_AQWELL_20250904_1225_B,  
TEMPEST_AQWELL_20250904_1400_B, TEMPEST_AQWELL_20250904_1400_A, TEMPEST_AQWELL_20250904_1225_C,  
TEMPEST_AQWELL_20250904_1400_C, TEMPEST_AQWELL_20250904_1225_A,  
TEMPEST_AQWELL_20250904_1300_A, TEMPEST_AQWELL_20250904_1300_C
" #any notes from the run
samples <- c("GCW", "GWI", "MSM", "SWH") #whatever identifies your samples within the same names
samples_pattern <- paste(samples, collapse = "|")
#samples_pattern <- "GCW" #use this instead of the line above if you have only one site code

##### File Names - PLEASE CHANGE
#file path and name for raw summary data file
raw_file_name_cl = "Raw Data/COMPASS_Synoptic_CB_MonMon_202505_Cl.txt"
raw_file_name_so4 = "Raw Data/COMPASS_Synoptic_CB_MonMon_202505_SO4.txt"

#file path and name of processed data file
processed_file_name = "Processed Data/COMPASS_SynopticCB_PW_Processed_Cl_SO4_202505.csv"

##### Log Files - PLEASE CHECK
#downloaded metadata csv - downloaded from Google drive as csv for this year
Raw_Metadata = "Raw Data/COMPASS_SynopticCB_PW_SampleLog_2025.csv"

#qaqc log file path for this year
Log_path = "Raw Data/COMPASS_Synoptic_Cl_SO4_QAQClog_2024.csv"
```

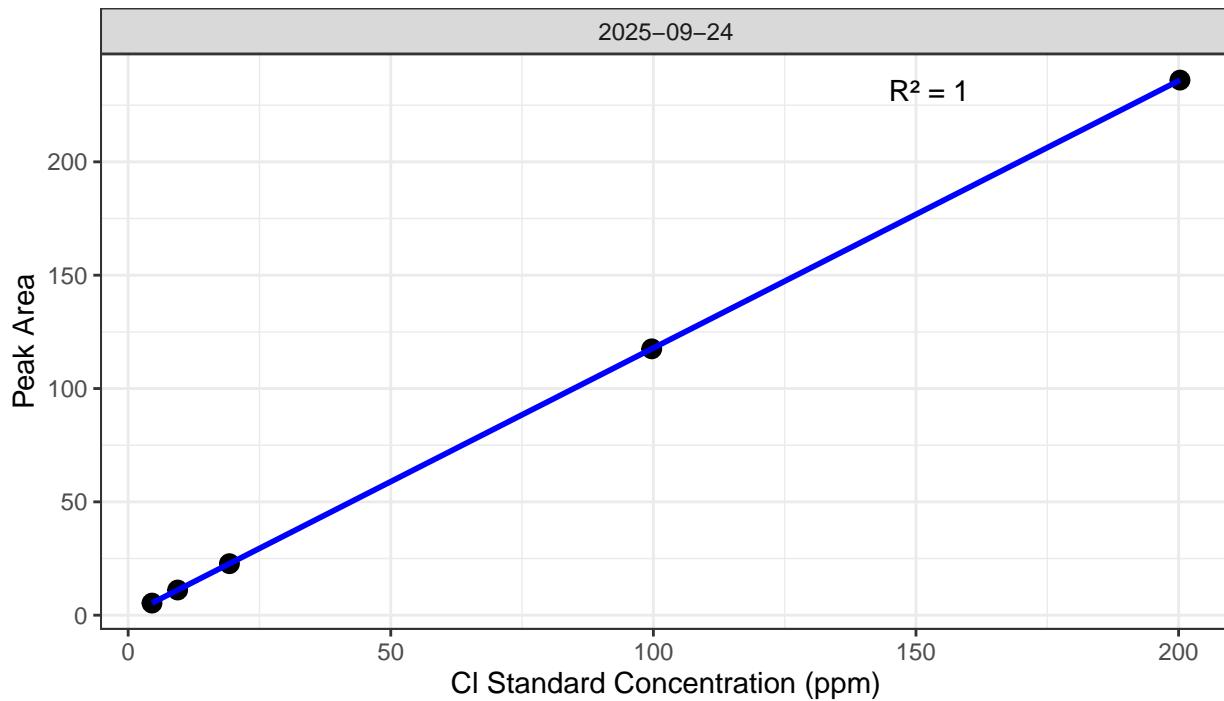
```
##Set Up Code - constants and QAQC cutoffs
```

```
##Read in metadata and create similar sample IDs for matching to samples
```

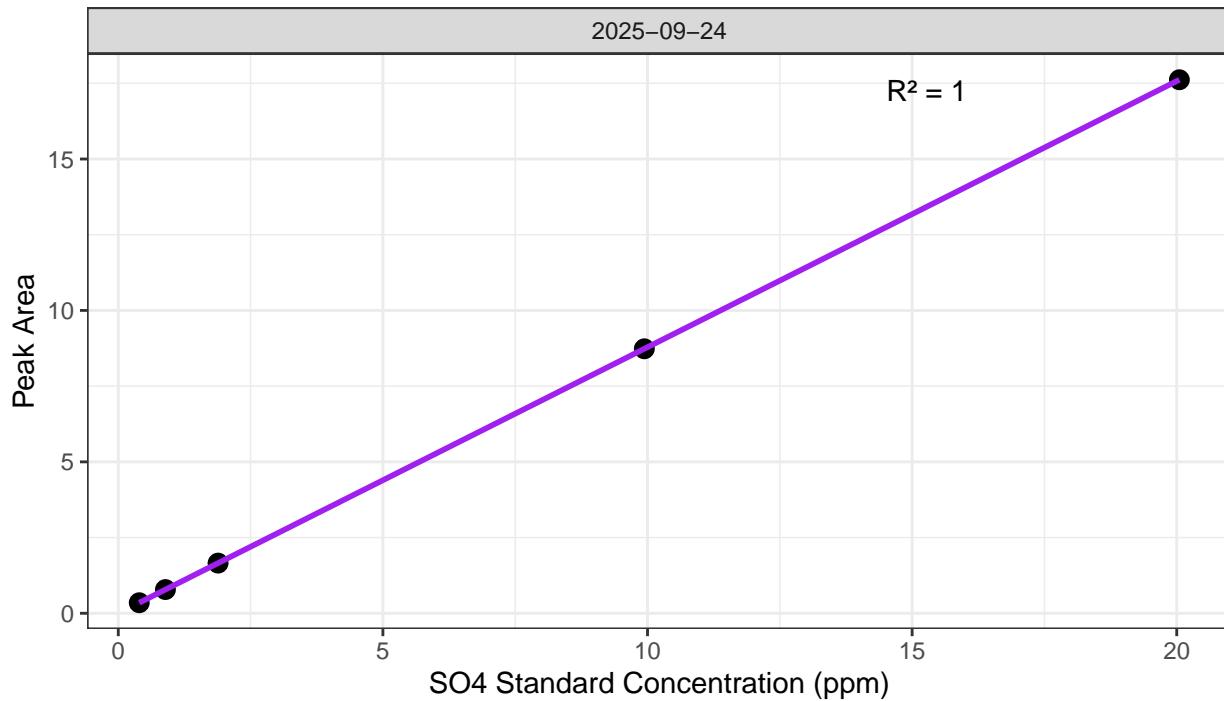
```
##Import Sample Data
```

0.2 Assess Standard Curves

Chloride Std Curve

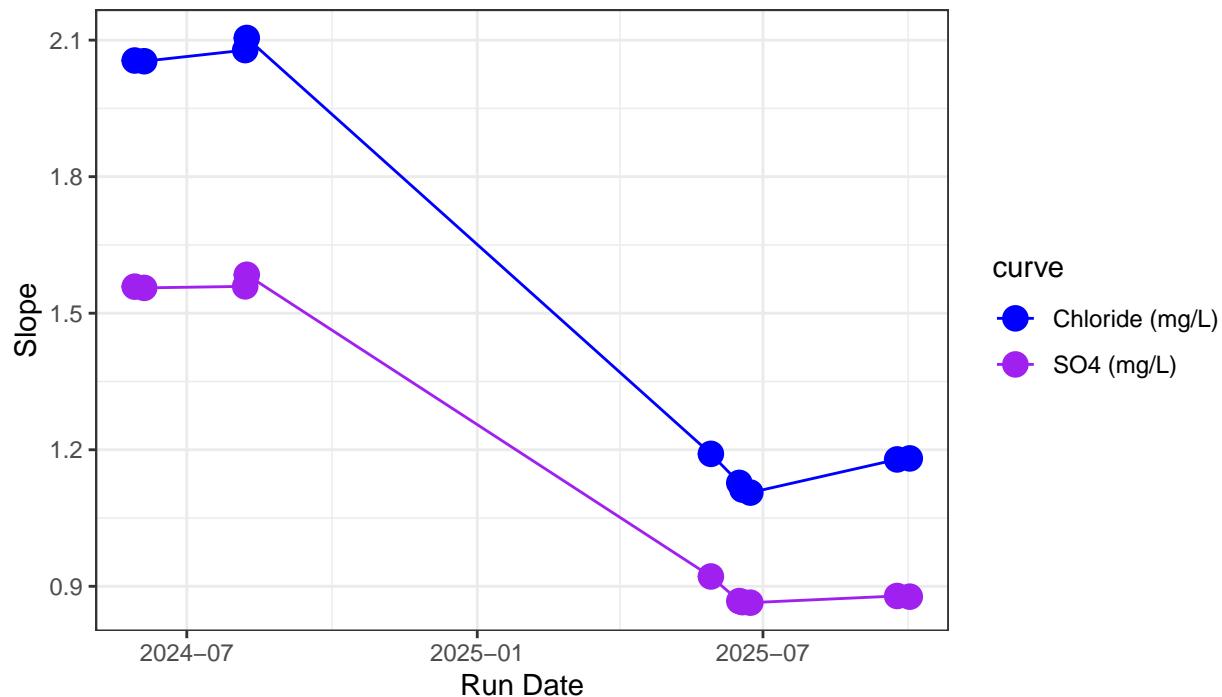


Sulfate Std Curve



```
## [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"
```

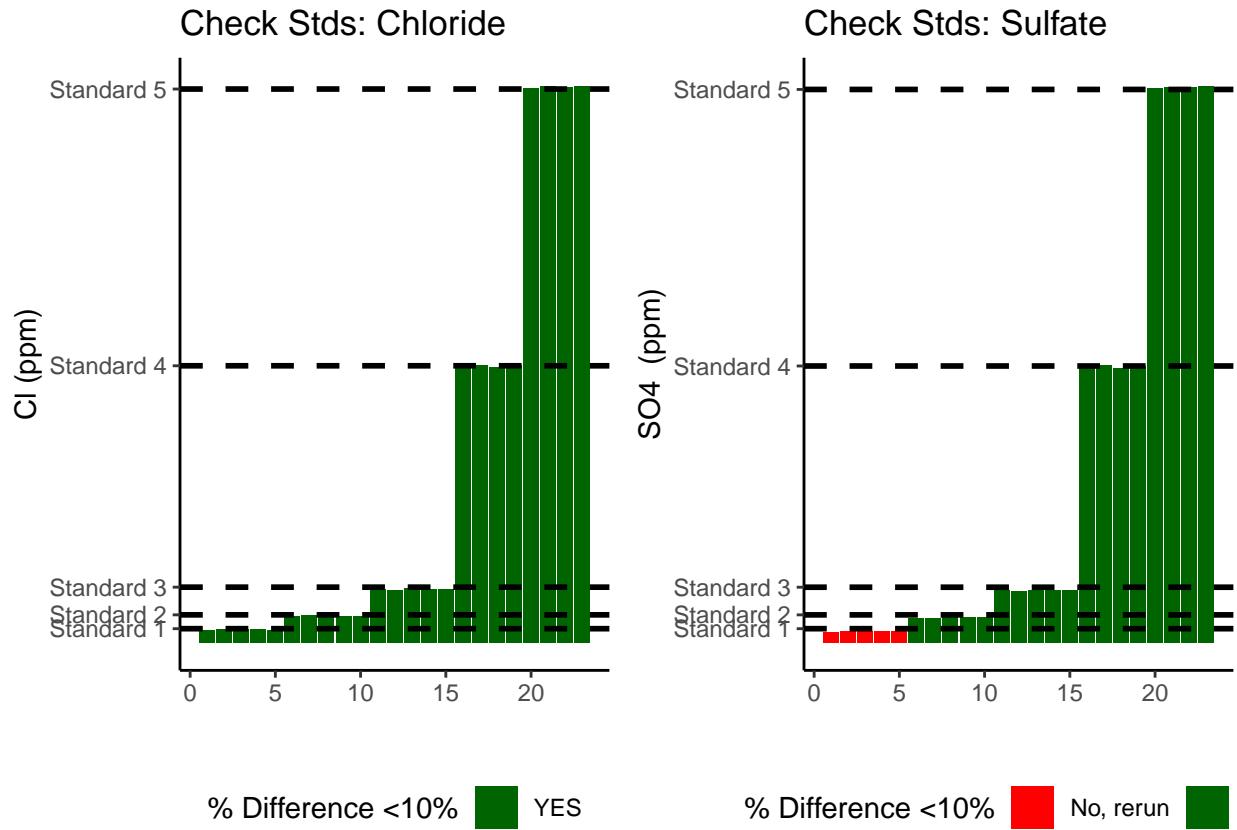
0.3 Assess Check Standards

```
## # A tibble: 5 x 5
##   sample_ID  mean_Cl    sd_Cl    cv_Cl flag_Cl
##   <chr>       <dbl>     <dbl>     <dbl> <chr>
## 1 Standard 1  4.68  0.125  0.0267 Chloride Check Standard RSD within Range - P~
## 2 Standard 2  9.59  0.206  0.0215 Chloride Check Standard RSD within Range - P~
## 3 Standard 3 19.3   0.236  0.0122 Chloride Check Standard RSD within Range - P~
## 4 Standard 4 100.    0.453  0.00454 Chloride Check Standard RSD within Range - P~
## 5 Standard 5 201.    0.450  0.00224 Chloride Check Standard RSD within Range - P~

## # A tibble: 5 x 5
##   sample_ID  mean_SO4    sd_SO4    cv_SO4 flag_SO4
##   <chr>       <dbl>     <dbl>     <dbl> <chr>
## 1 Standard 1  0.407  0.00769  0.0189 Sulfate Check Standard RSD within Range --
## 2 Standard 2  0.904  0.00754  0.00834 Sulfate Check Standard RSD within Range --
## 3 Standard 3  1.89   0.0107   0.00566 Sulfate Check Standard RSD within Range --
## 4 Standard 4  9.98   0.0454   0.00455 Sulfate Check Standard RSD within Range --
## 5 Standard 5 20.1    0.0378   0.00188 Sulfate Check Standard RSD within Range --

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

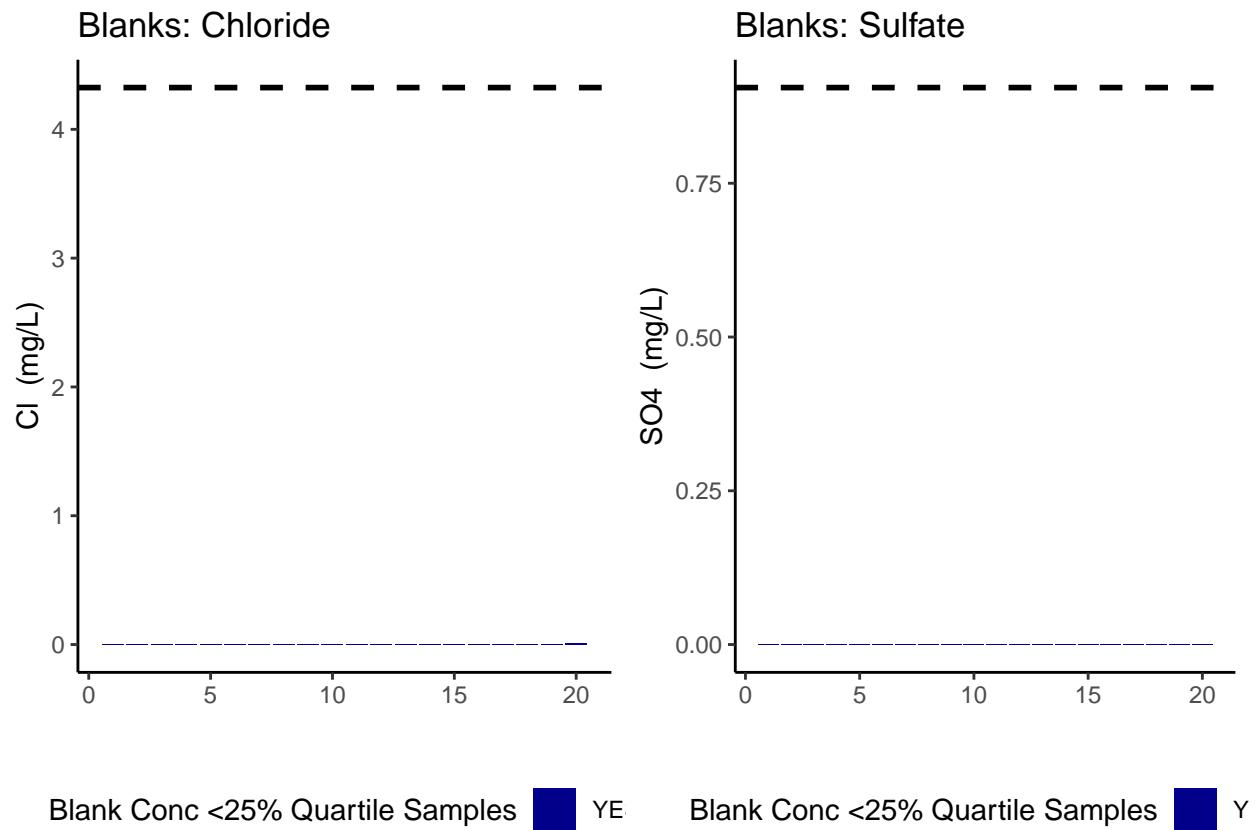
## [1] ">80% of Sulfate Check Standards have RSD within range - PROCEED"
```



```
## [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"
```

0.4 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:
```

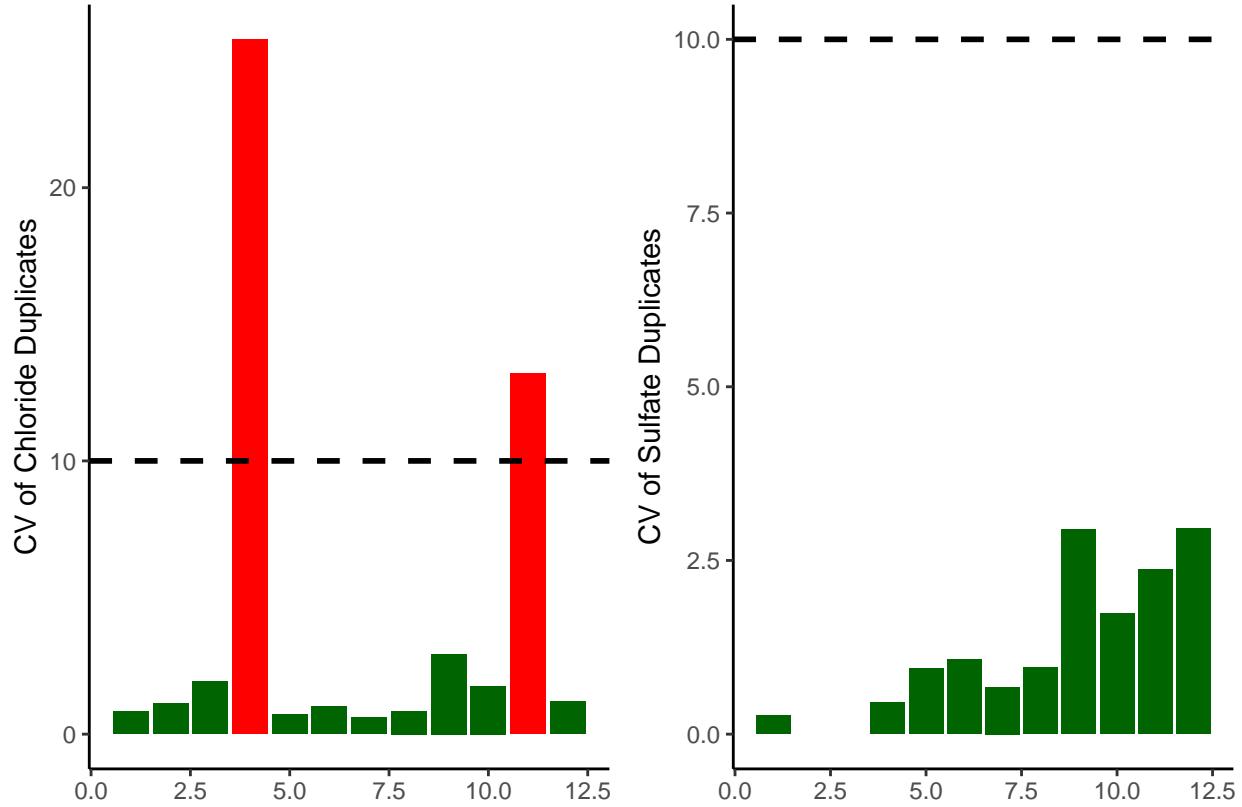
```
## [1] 0.000495
```

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

```
## [1] 3e-05
```

0.5 Assess Duplicates

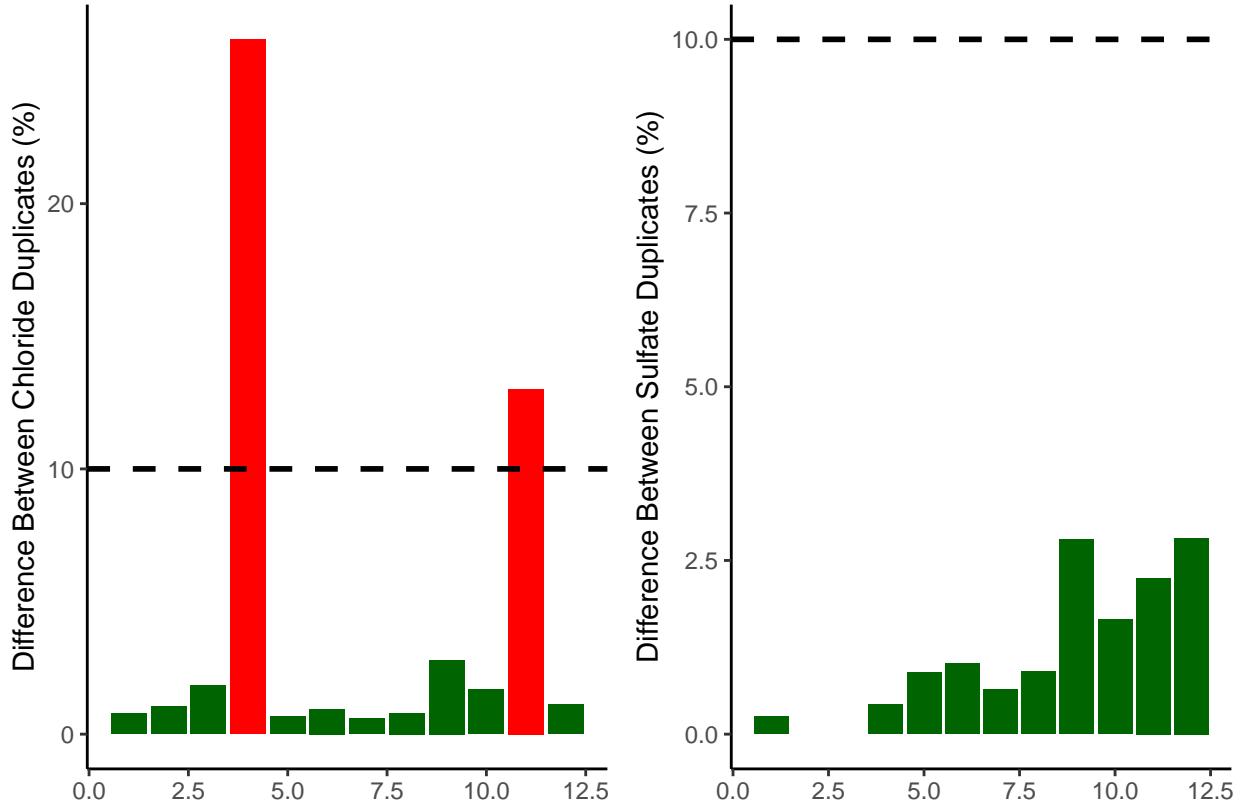
```
## Warning: Removed 2 rows containing missing values or values outside the scale range
## ('geom_bar()').
```



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

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

```
## Warning: Removed 2 rows 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"
```

0.6 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 Steph / COMPASS this depends on the site so...
all_dat$Dilution <- 1
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "MSM") & str_detect(all_dat$sample_ID, "UP"),
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "MSM") & str_detect(all_dat$sample_ID, "TR"),
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "MSM") & str_detect(all_dat$sample_ID, "WC"),
```

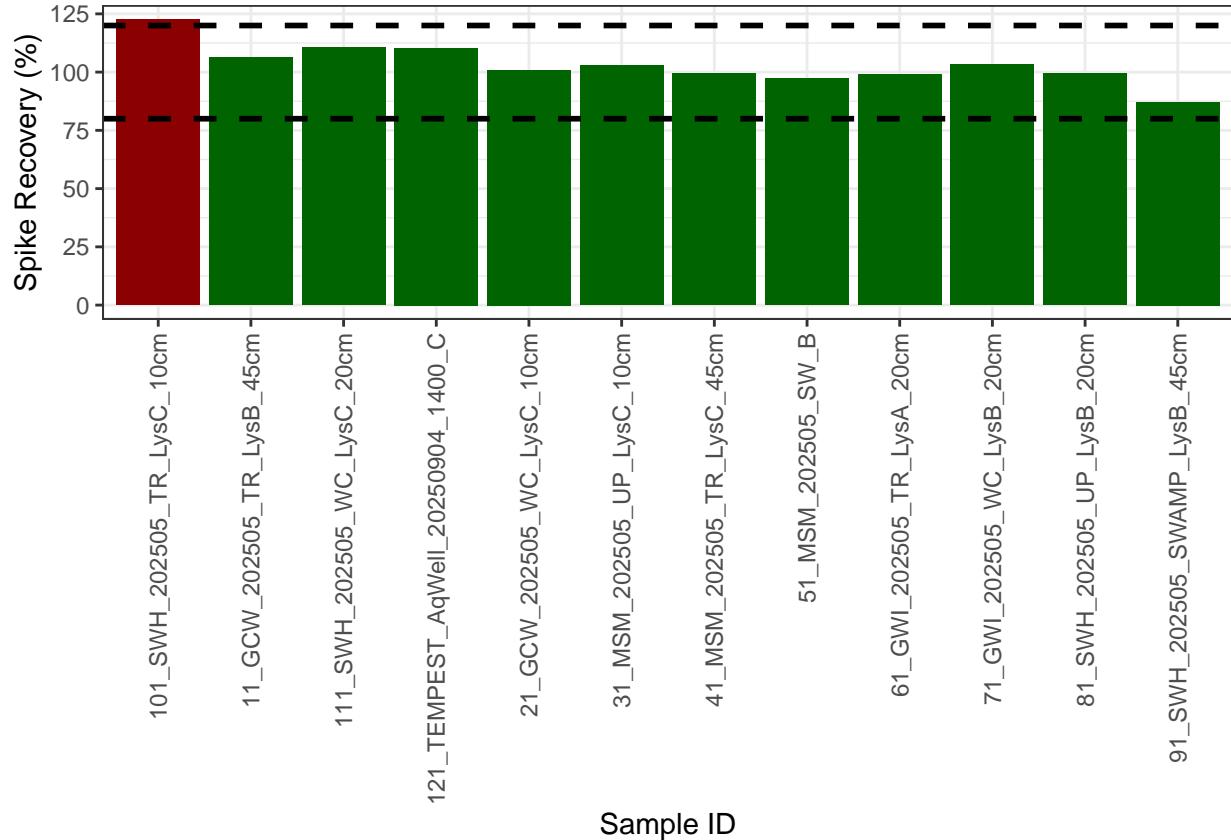
```

all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "MSM") & str_detect(all_dat$sample_ID, "SW"), 50,
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GCW") & str_detect(all_dat$sample_ID, "UP"), 50,
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GCW") & str_detect(all_dat$sample_ID, "TR"), 50,
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GCW") & str_detect(all_dat$sample_ID, "WC"), 50,
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GCW") & str_detect(all_dat$sample_ID, "SW"), 50,
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GWI") & str_detect(all_dat$sample_ID, "UP"), 50,
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GWI") & str_detect(all_dat$sample_ID, "TR"), 50,
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GWI") & str_detect(all_dat$sample_ID, "WC"), 50,
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GWI") & str_detect(all_dat$sample_ID, "SW"), 50,
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "SWH"), 50, all_dat$Dilution)
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "TEMPEST"), 50, all_dat$Dilution)

# head(all_dat)

```

0.7 Assess Analytical Spikes



```
## [1] ">80% of S04 spikes have a recovery between the high and low cutoff - PROCEED"
```

0.8 Check if samples within the range of the standard curve

```
## Sample Flagging
```

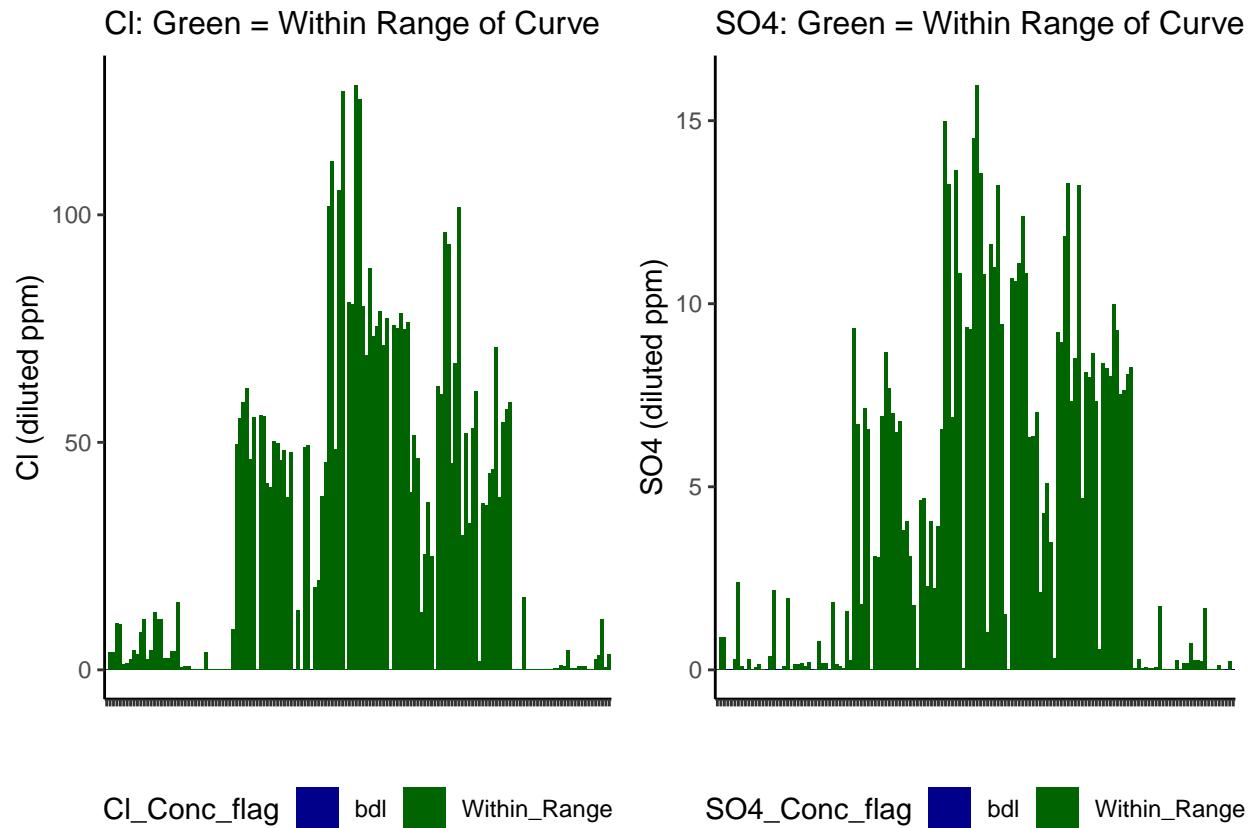


Table 1: SO4 samples

SO4_Conc_flag	Percent_samples
Within_Range	93.243243
bdl	6.756757

Table 2: Cl samples

Cl_Conc_flag	Percent_samples
Within_Range	98.648649
bdl	1.351351

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

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

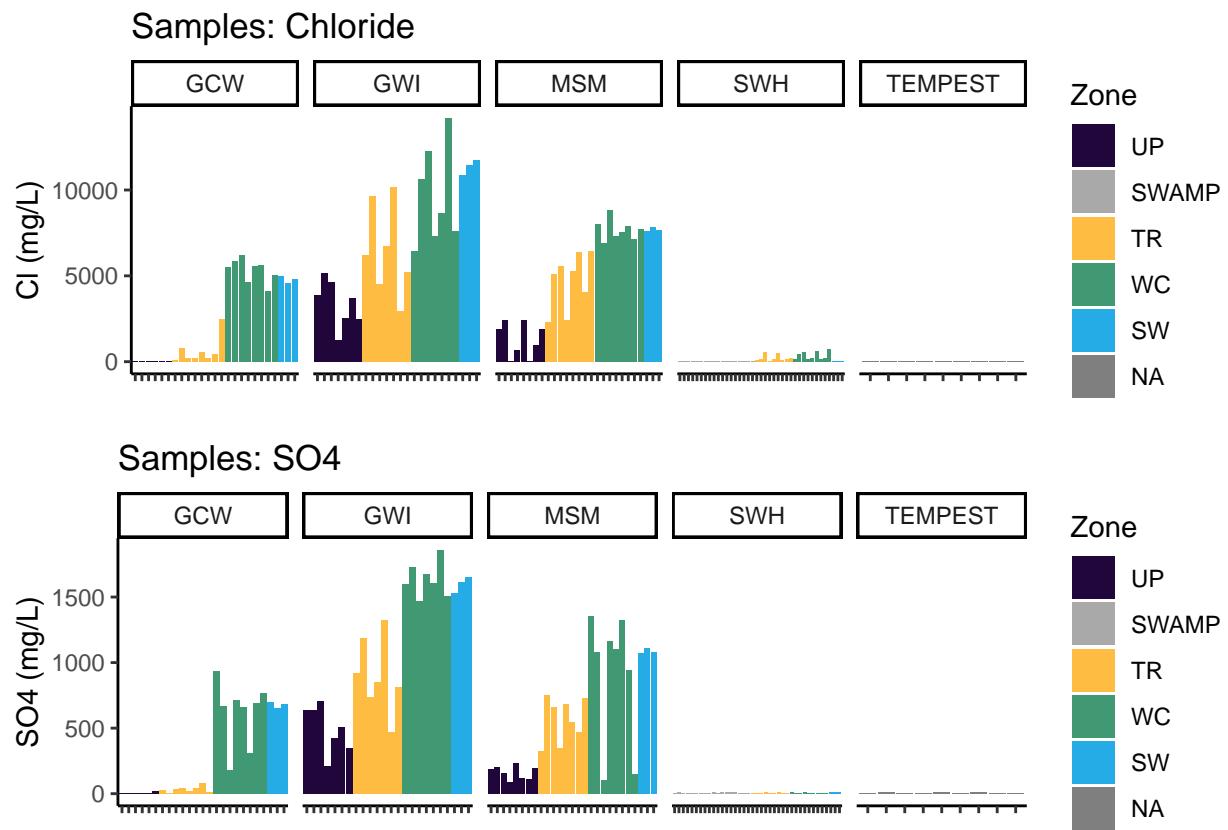
```
## [1] "GCW_202505_TR_LYSC_45CM"      "TEMPEST_AQWELL_20250904_1300_B"
## [3] "TEMPEST_AQWELL_20250904_1225_B" "TEMPEST_AQWELL_20250904_1400_B"
```

```

## [5] "TEMPEST_AQWELL_20250904_1400_A" "TEMPEST_AQWELL_20250904_1225_C"
## [7] "TEMPEST_AQWELL_20250904_1400_C" "TEMPEST_AQWELL_20250904_1225_A"
## [9] "TEMPEST_AQWELL_20250904_1300_A" "TEMPEST_AQWELL_20250904_1300_C"

```

0.10 Visualize Data by Plot



0.11 Export Processed Data

```
#end
```