

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_C1.txt"
raw_file_name_so4 = "Raw Data/COMPASS_Synoptic_CB_MonMon_202505_S04.txt"

#file path and name of processed data file
processed_file_name = "Processed Data/COMPASS_SynopticCB_PW_Processed_C1_S04_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_C1_S04_QAQClog_2024.csv"
```

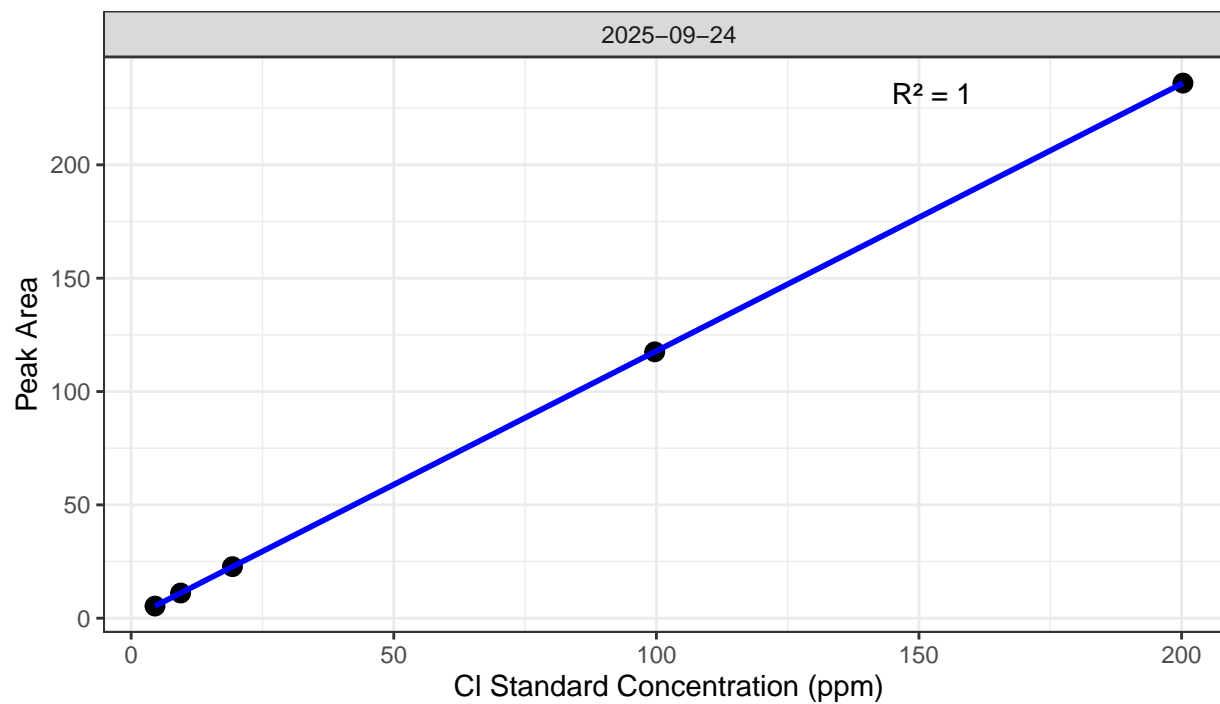
##Set Up Code - constants and QAQC cutoffs

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

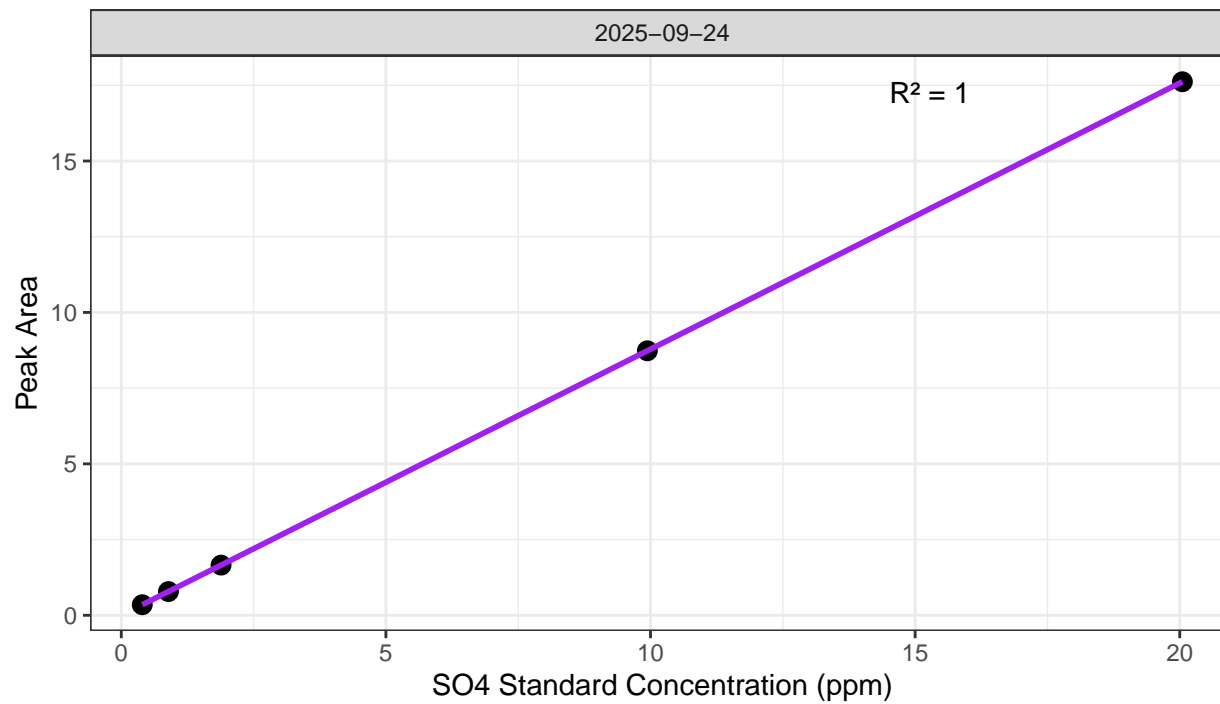
##Import Sample Data

0.2 Assess Standard Curves

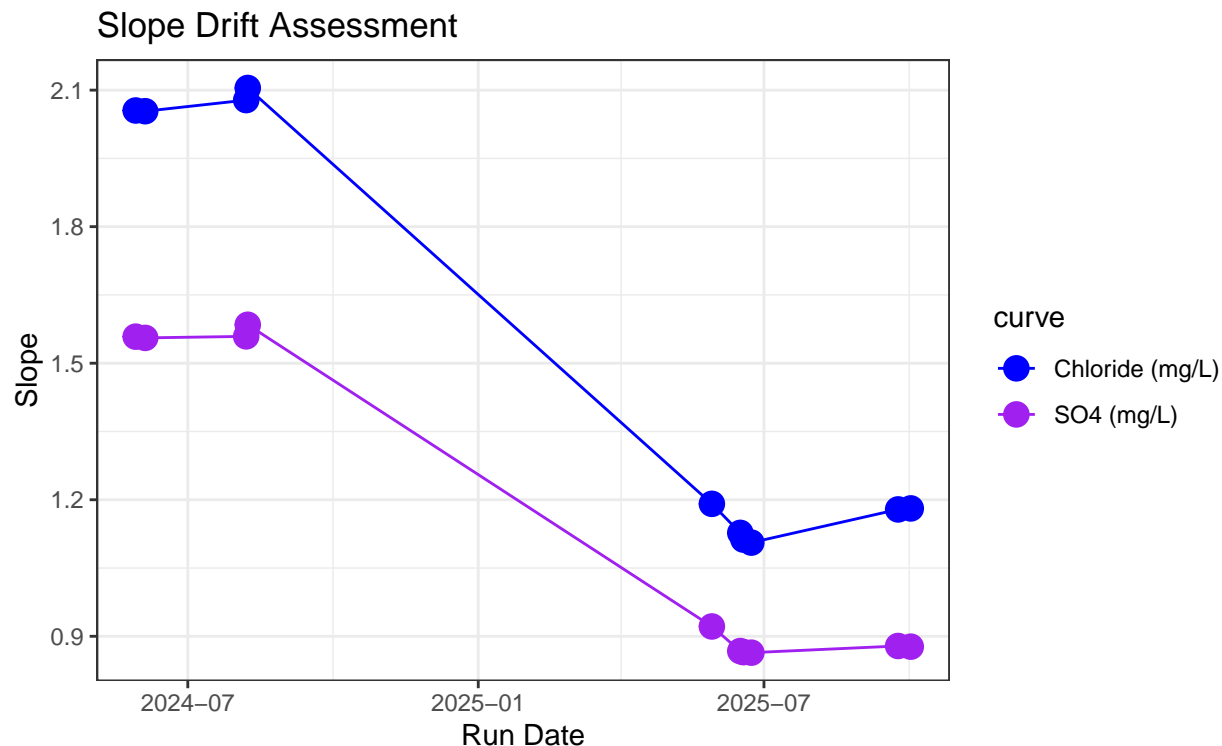
Chloride Std Curve



Sulfate Std Curve



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



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

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

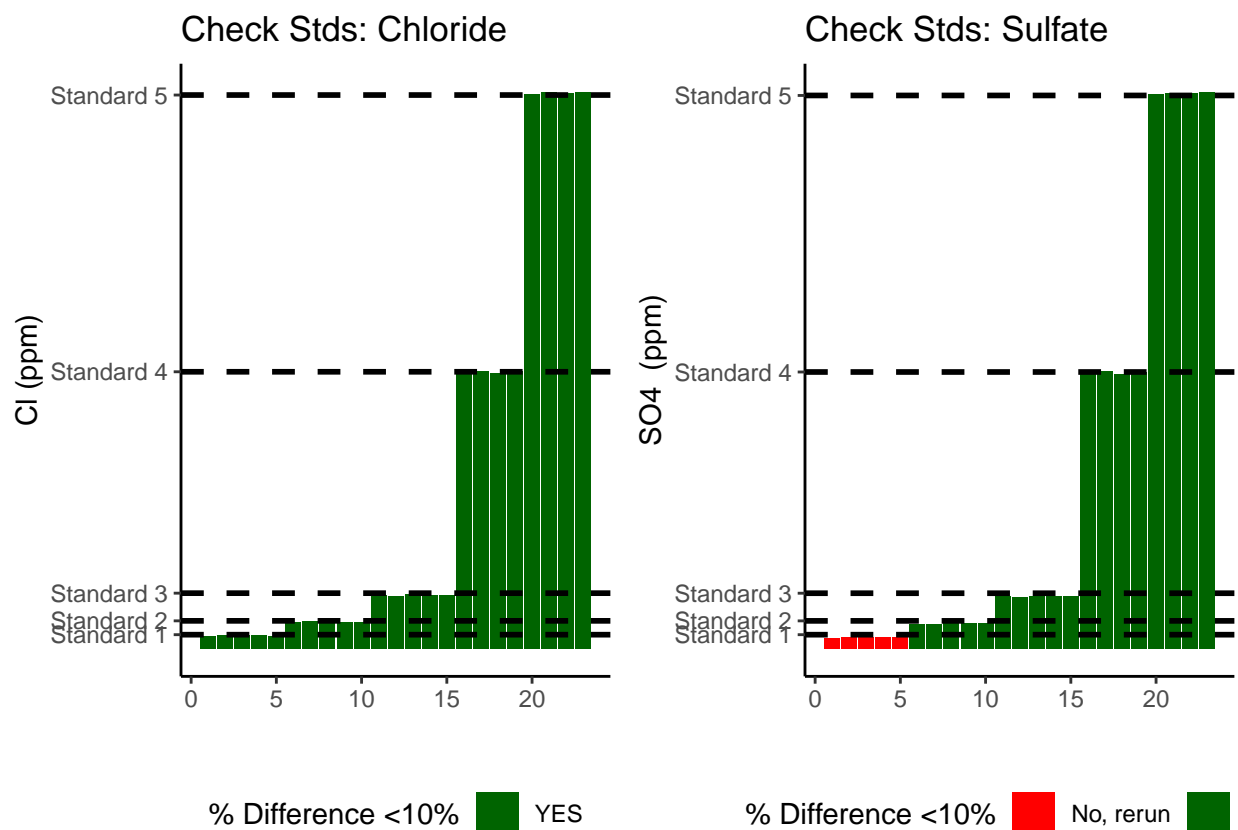
0.3 Assess Check Standards

```
## # 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"
```



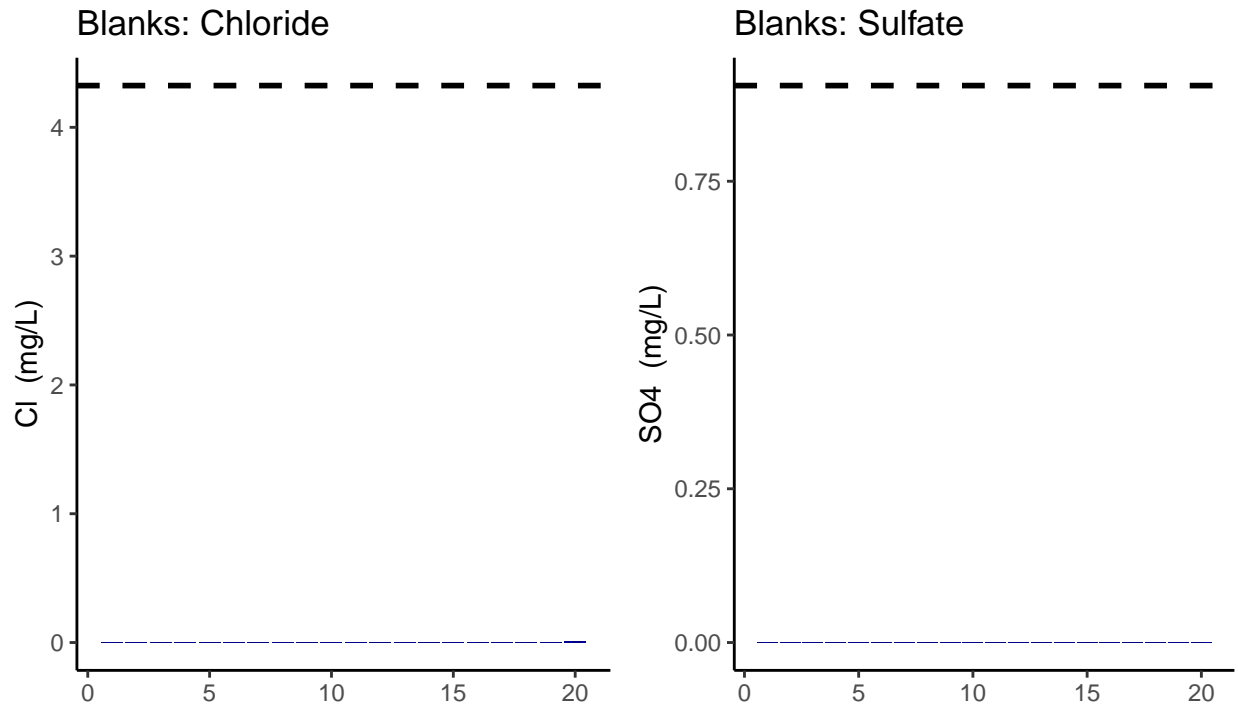
[1] ">80% of Chloride Check Standards are within range of expected concentration - PROCEED"

[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"



Blank Conc <25% Quartile Samples ■ YE

Blank Conc <25% Quartile Samples ■ Y

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

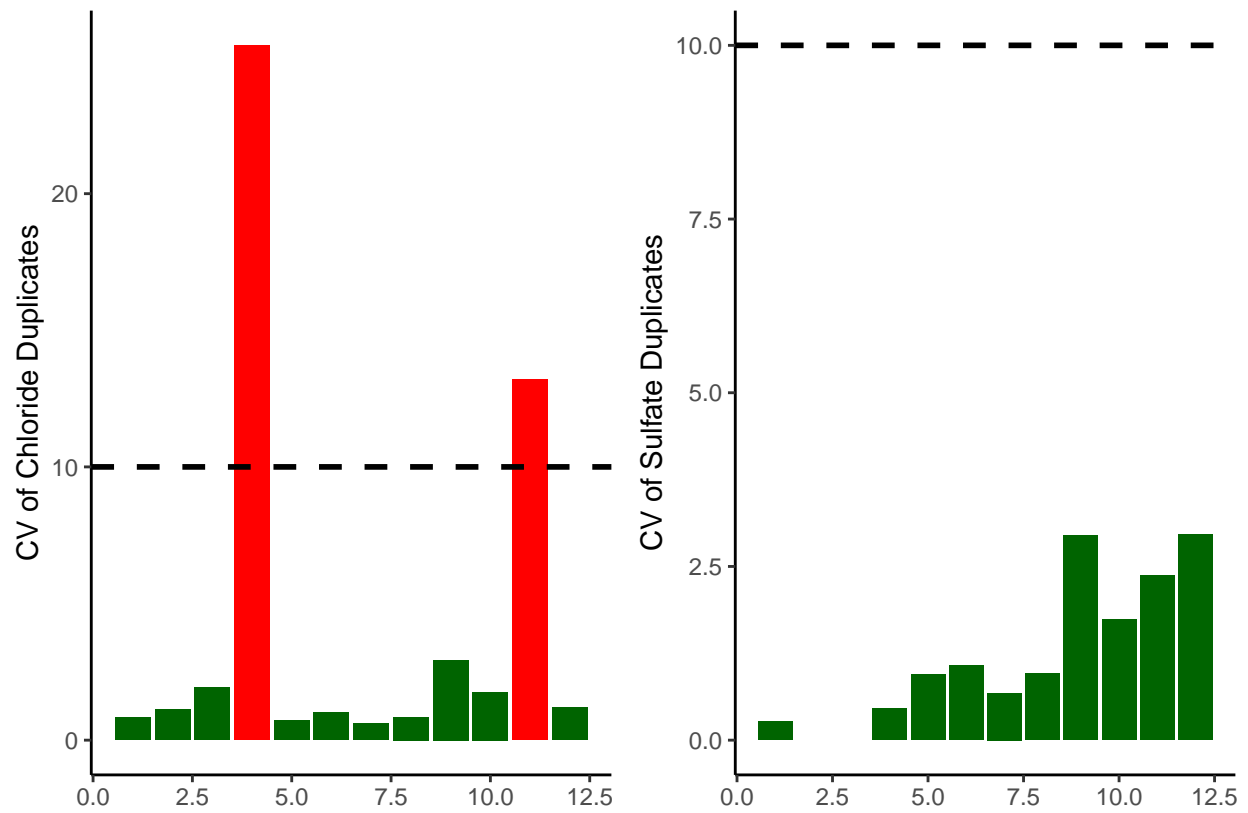
```
## [1] 0.000495
```

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

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

0.5 Assess Duplicates

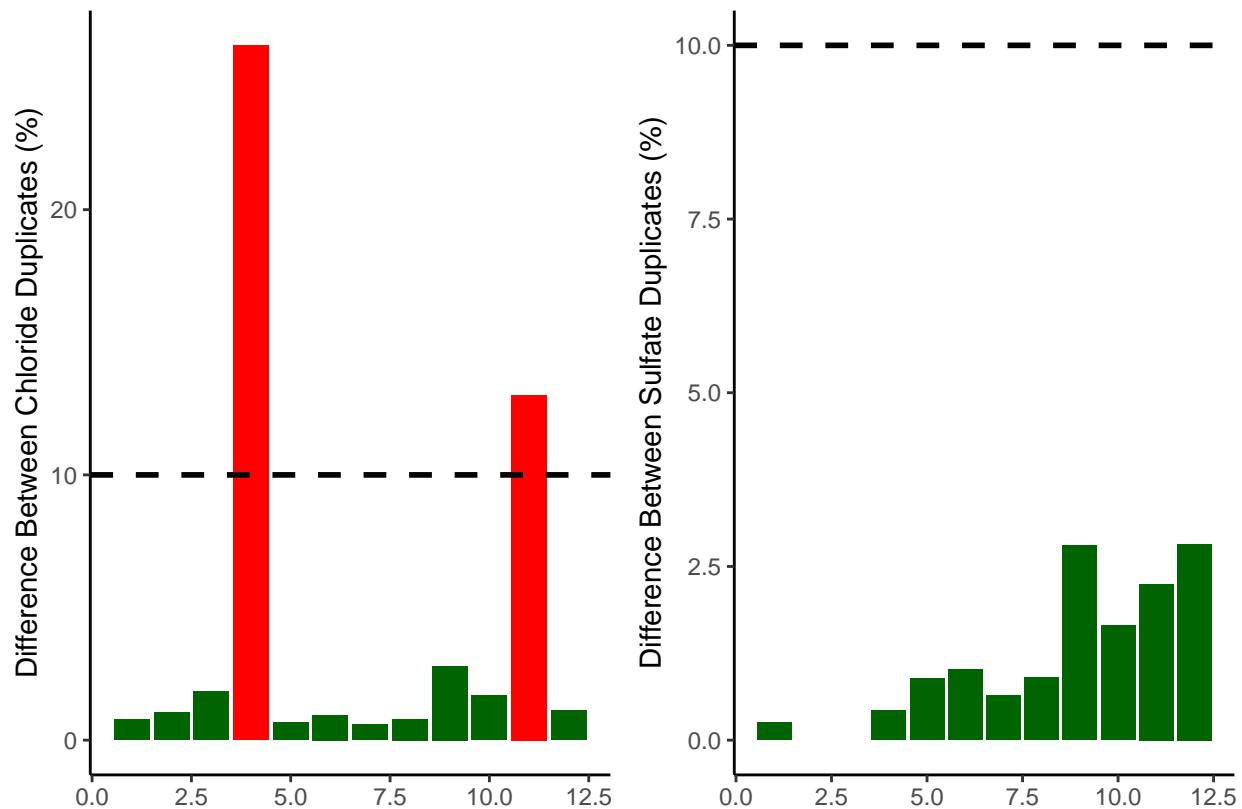
```
## Warning: Removed 2 rows containing missing values or values outside the scale range
## ('geom_bar()').
```



```
## [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$S04_Conc_mM <- (all_dat$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 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$sample_ID, "SW"),
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GCW") & str_detect(all_dat$sample_ID, "UP"),
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GCW") & str_detect(all_dat$sample_ID, "TR"),
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GCW") & str_detect(all_dat$sample_ID, "WC"),
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GCW") & str_detect(all_dat$sample_ID, "SW"),

all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GWI") & str_detect(all_dat$sample_ID, "UP"),
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GWI") & str_detect(all_dat$sample_ID, "TR"),
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GWI") & str_detect(all_dat$sample_ID, "WC"),
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "GWI") & str_detect(all_dat$sample_ID, "SW"),

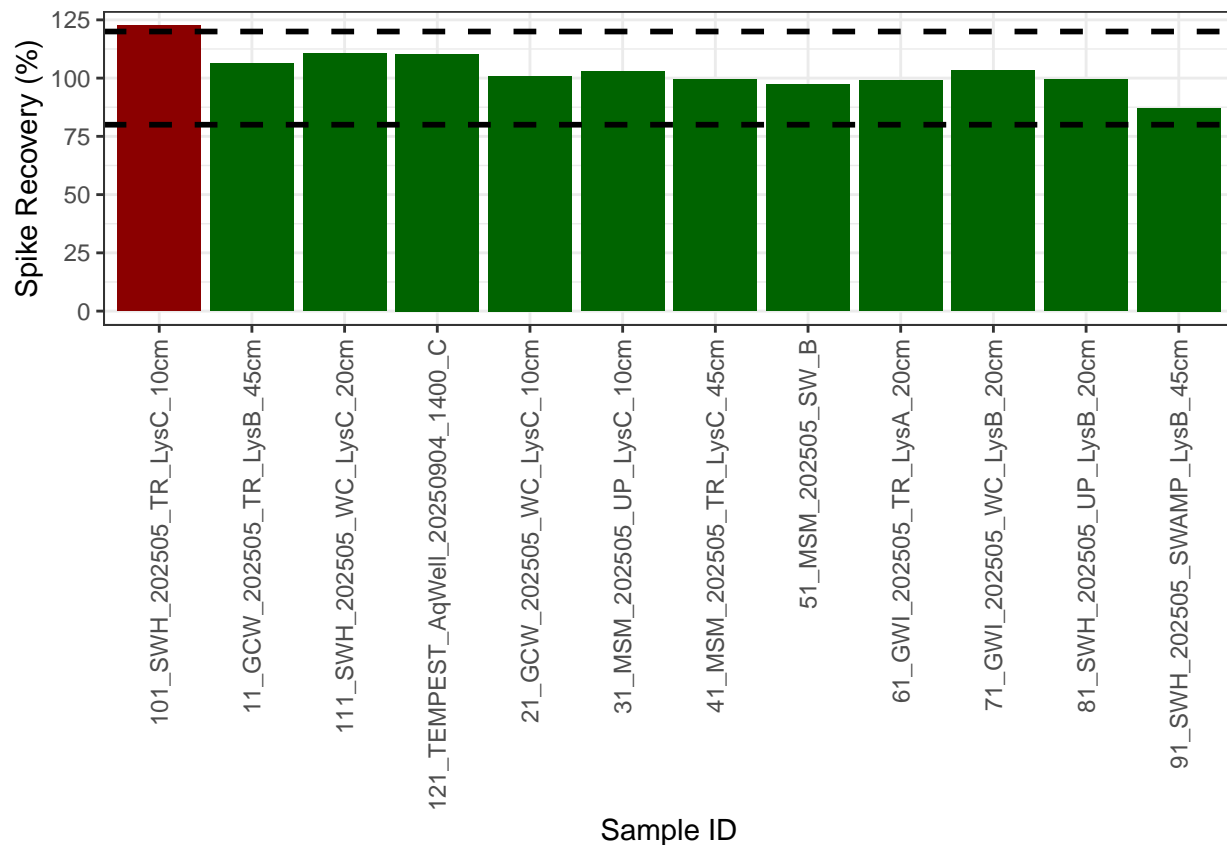
all_dat$Dilution <- ifelse(str_detect(all_dat$sample_ID, "SWH"), 50, all_dat$Dilution)

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

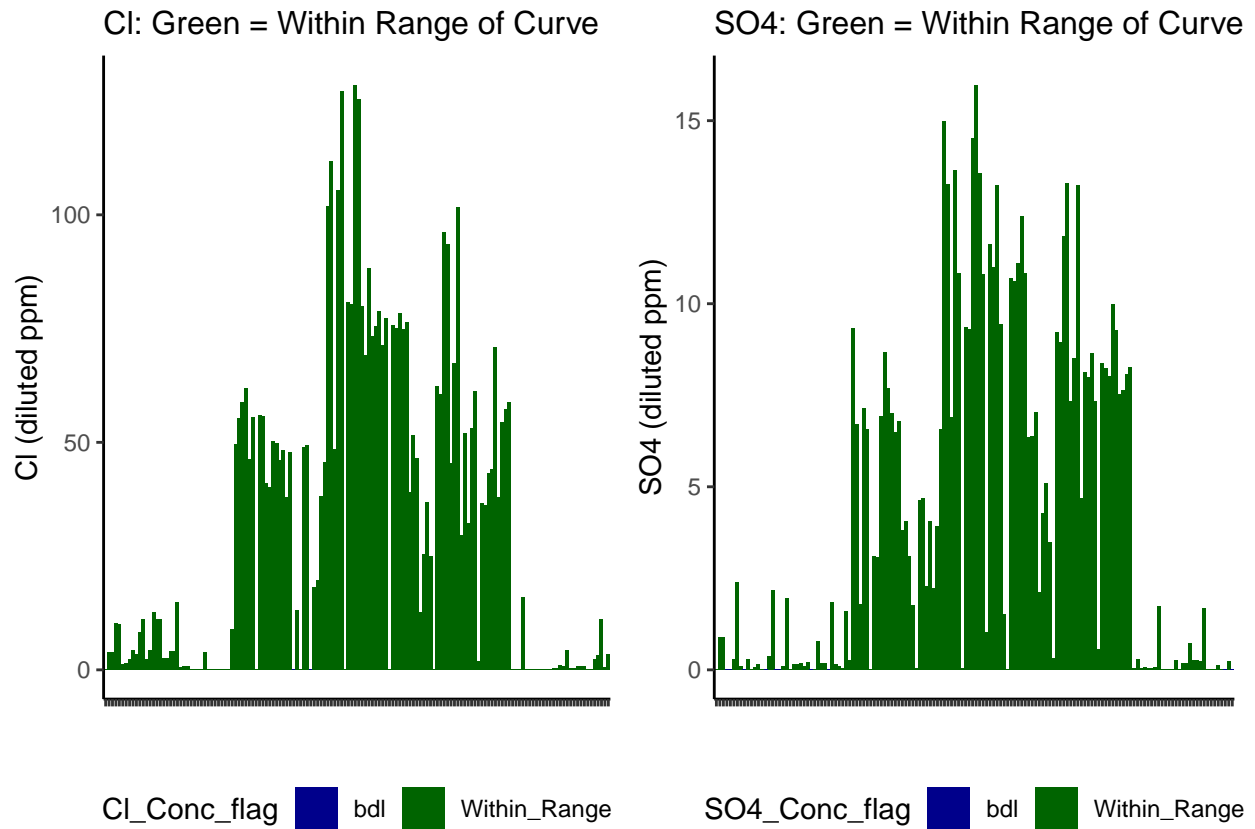


Table 1: SO4 samples

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

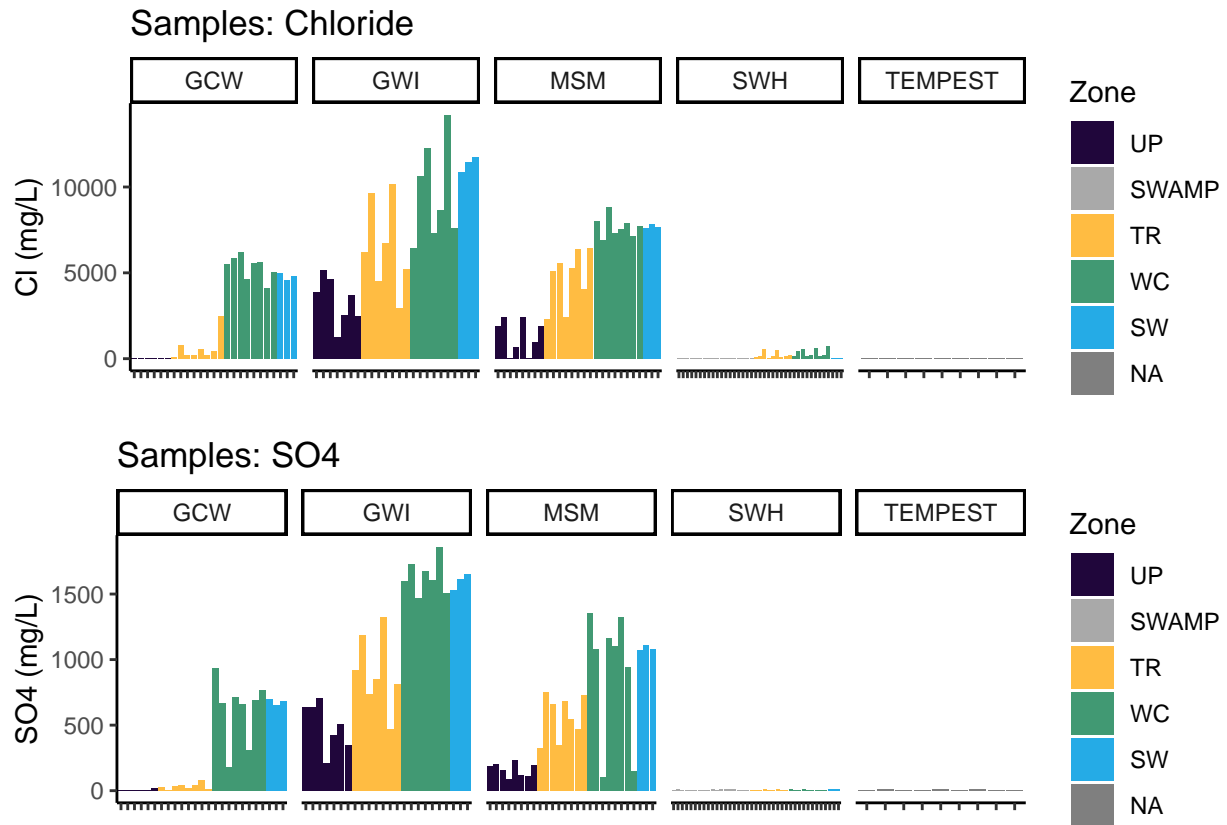
0.9 Check to see if samples run match metadata & merge info

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