

Synoptic CB: Porewater Nutrients

June 2023 Samples

2025-07-08

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```

##Run Information

cat("Run Information: Input by User") #lets you know what section you're in

## Run Information: Input by User

#set the run date & user name
run_date <- "01/14/2024"
sample_year <- 2023
sample_month <- 06
user <- "Stephanie Wilson"

#identify the files you want to read in
#read in as a list to accomodate ultiple runs in a month
NOx_files <- c("Raw Data/SEAL_COMPASS_Synoptic_NOx_June2023_1.csv",
              "Raw Data/SEAL_COMPASS_Synoptic_NOx_June2023_2.csv",
              "Raw Data/SEAL_COMPASS_Synoptic_NOx_June2023_3.csv")
NH3_P04_files <- c("Raw Data/SEAL_COMPASS_Synoptic_NH3_P04_June2023_1.csv",
                    "Raw Data/SEAL_COMPASS_Synoptic_NH3_P04_June2023_2.csv",
                    "Raw Data/SEAL_COMPASS_Synoptic_NH3_P04_June2023_3.csv")

# Define the file path for QAQC log file - NO Need to change just check year
file_path <- "Raw Data/SEAL_COMPASS_Synoptic_QAQC_Log_2023.csv"
final_path <- "Processed Data/COMPASS_Synoptic_Nutrients_202306.csv"

#record any notes about the run or anything other info here:
run_notes <- "There are two sample names we suspect were input incorrectly,
they are listed below and have been checked against metadata."

#duplicate sample names to be changed
#list the sample IDs that are messed up and create a list
#with run number as well so that we can change them below
wrong_names <- c("GCW_202304_TR_LysC_45cm", "GCW_202304_TR_LysA_20cm_8",
                  "GWI_202304_UP_LysA_20cm", "GWI_202304_UP_LysA_20cm")
wrong_nums <- c(20, 16, 46, 44)
correct_names <- c("GCW_202304_TR_LysB_45cm", "GCW_202304_TR_LysA_20cm",
                   "GWI_202304_UP_LysA_10cm", "GWI_202304_UP_LysA_10cm")

#can't determine from metadata - for now unsure
remove_names <- c("GCW_202304_TR_LysA_20cm", "GCW_202304_TR_LysA_20cm",
                   "GCW_202304_TR_LysB_20cm_13", "GCW_202304_TR_LysB_20cm_13")
#couldn't tell which one this is from the metadata, no A_10cm which is what we thought
#marked on the sheet, need to check sample vials in freezer
#to see if we have a A_10cm from GCW_TR to be sure
remove_nums <- c(15, 13, 21, 19)

#Set up file path for metadata
#downloaded metadata csv - downloaded from Google drive as csv for this year
Raw_Metadata = "Raw Data/COMPASS_SynopticCB_PW_SampleLog_2023.csv"

cat(run_notes)

## There are two sample names we suspect were input incorrectly,
## they are listed below and have been checked against metadata.

```

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

0.1 Import Data & Clean

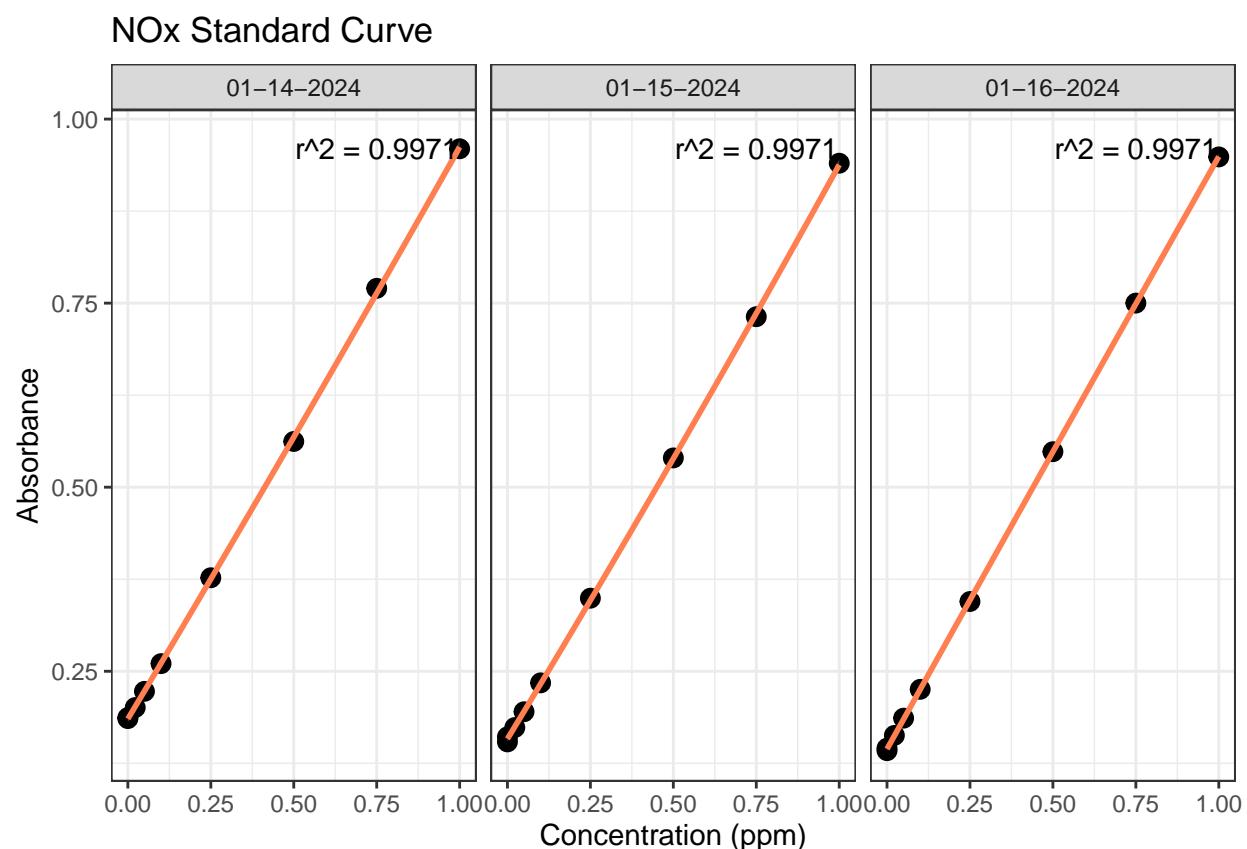
0.2 Assessing standard Curves

```
#Pull out standards data
```

```
## Assess Standard Curves
```

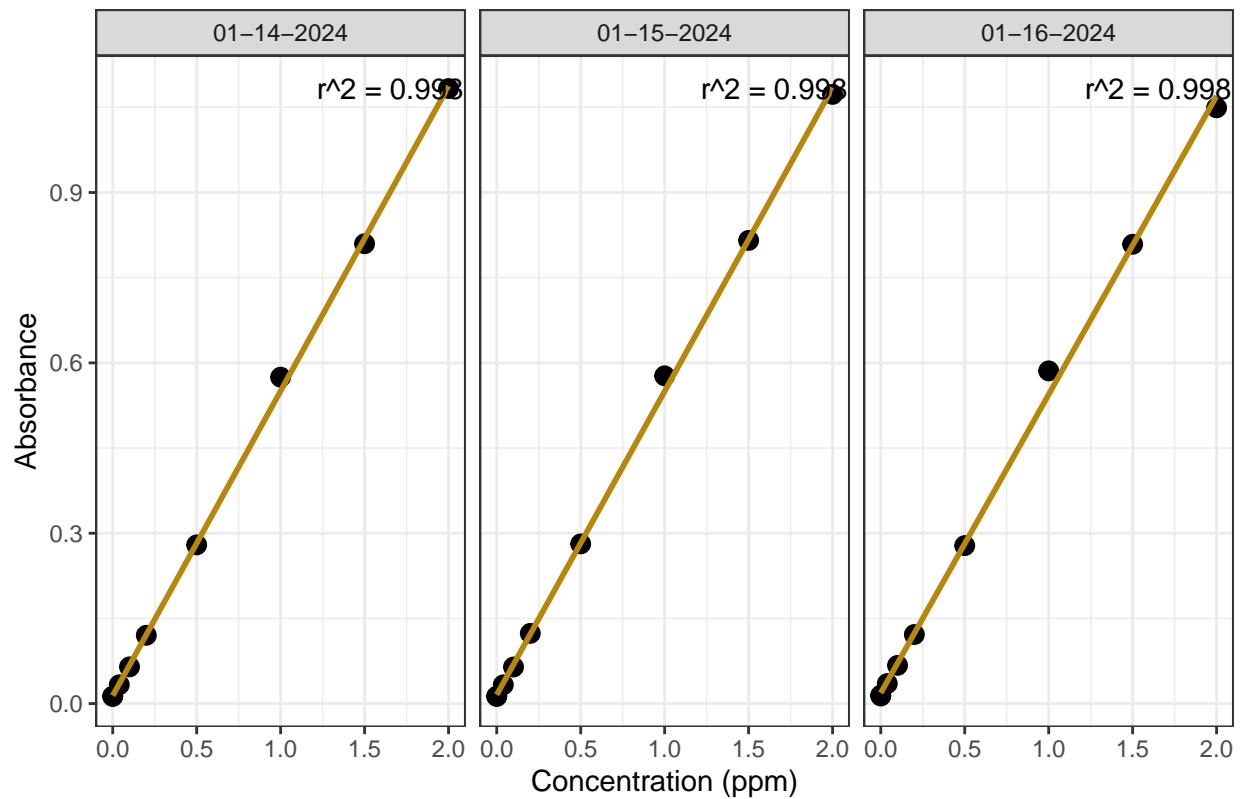
```
#Plot standards data
```

```
## Assess Standard Curves
```



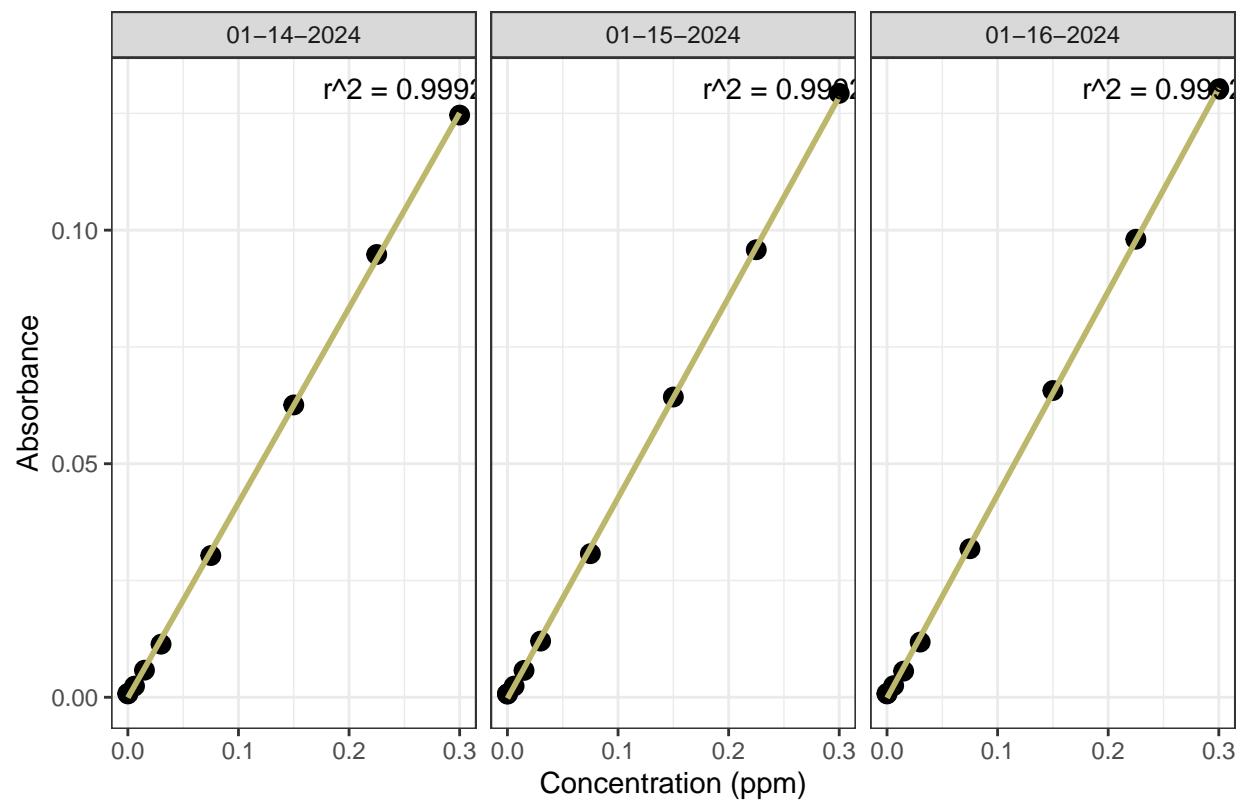
```
## `geom_smooth()` using formula = 'y ~ x'
```

NH3 Standard Curve



```
## `geom_smooth()` using formula = 'y ~ x'
```

PO4 Standard Curve



```
## [1] "NOx Curve r2 GOOD - PROCEED"  
## [1] "NH3 Curve r2 GOOD - PROCEED"  
## [1] "PO4 Curve r2 GOOD - PROCEED"  
## [1] "QAQC log file exists and has been read into the code."
```

Slope Drift Assessment

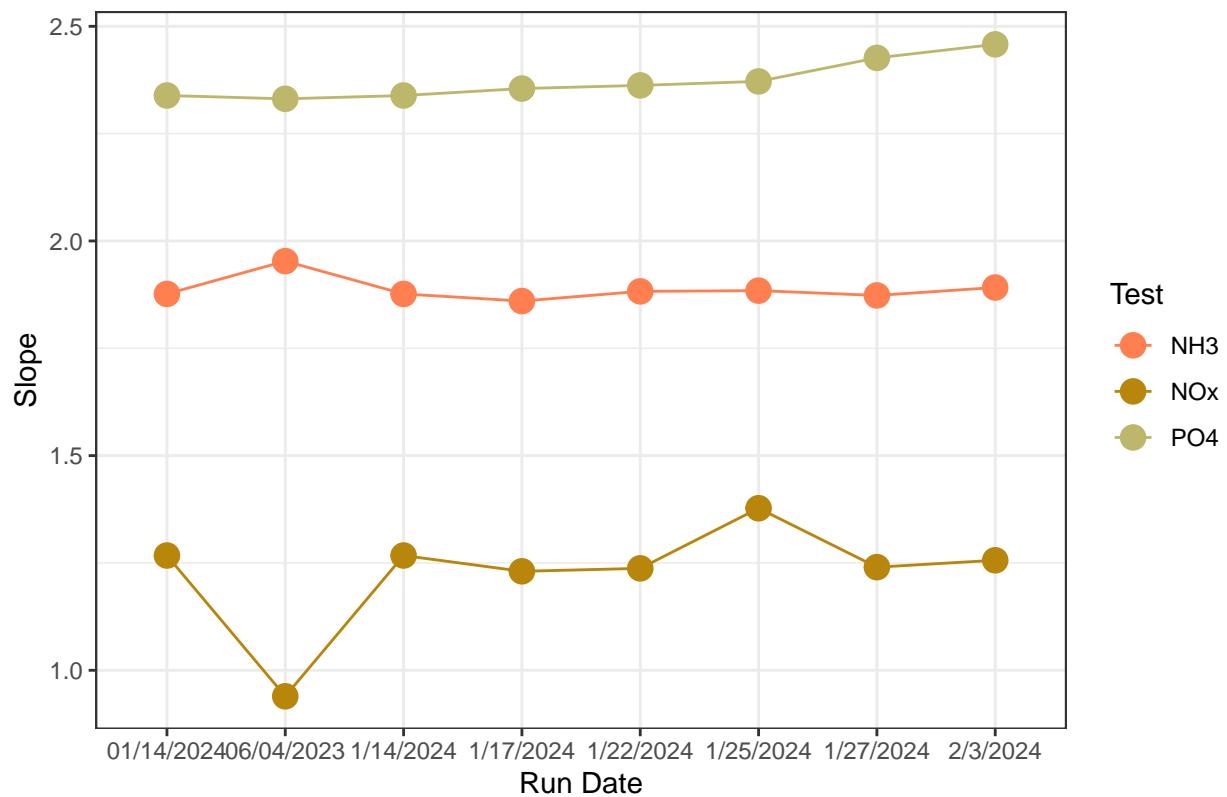


Table 1: Average Slope by Analyte

Test	avg_slope
NH3	1.887
NOx	1.227
PO4	2.373

0.3 Dilution Corrections - ensure the latest dilution is kept

```
## Dilution Corrections

## Duplicated samples: MSM_202306_TR_LysB_20cm, GCW_202306_WC_LysA_45cm, SWH_202306_TR_LysB_45cm, SWH_202306_WC_LysA_20cm

## All duplicated samples have valid dilutions. No naming issues detected.
```

0.4 Performance Check

```
## [1] "NOx pe Check has a % Difference <25% - PROCEED"

## Run mean = 0.714342

## Expected = 0.706

## [1] "NH3 pe Check has a % Difference >25% - REASSESS"

## Run mean = 1.20727

## Expected = 0.948

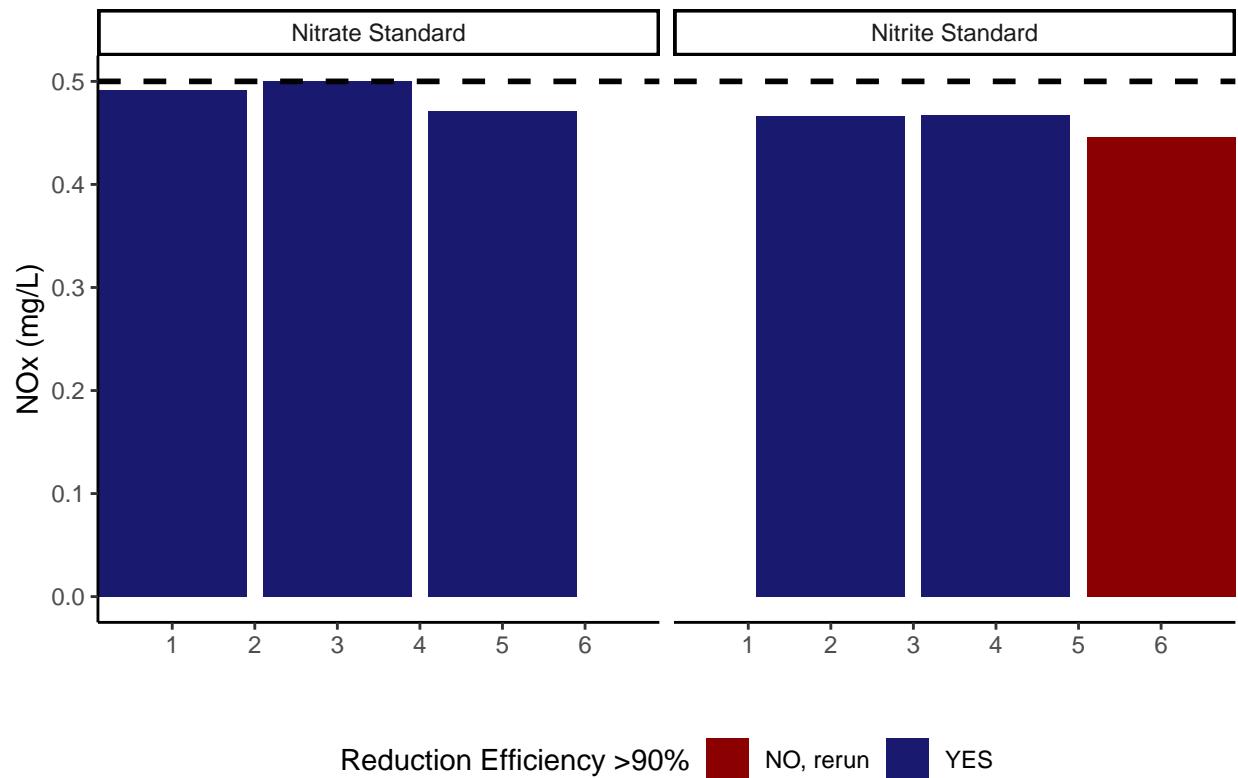
## [1] "PO4 pe Check has a % Difference >25% - REASSESS"

## Run mean = 0.5901153

## Expected = 0.818

#Check NOx Reduction Efficiency

## Assess Reduction Efficiency
```



```
## [1] "Mean NOx Reduction Efficiency <95% - REASSESS"
```

```
## [1] 94.7757
```

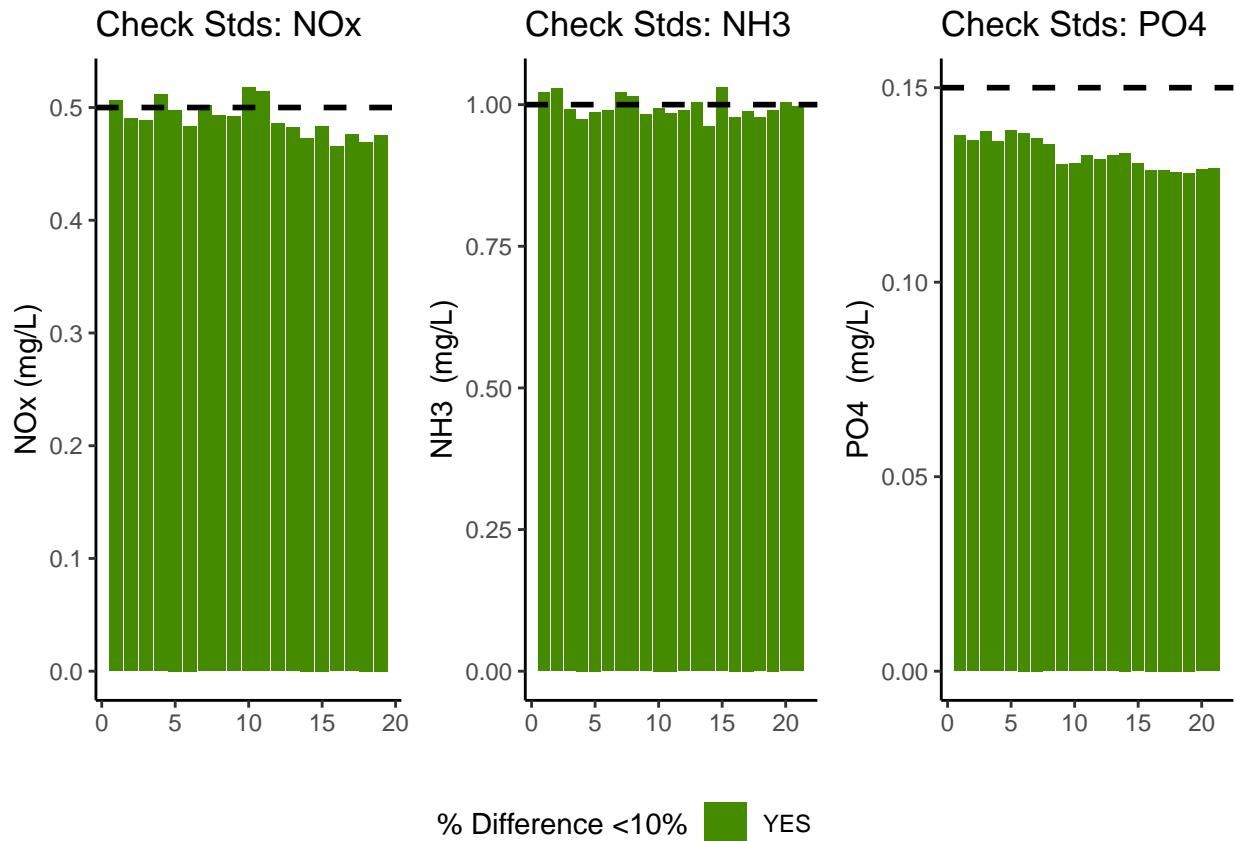
0.5 Analyze the Check Standards

```
## Analyze Check Standards

## [1] "NOx Check Standard RSD within Range - PROCEED"

## [1] "NH3 Check Standard RSD within Range - PROCEED"

## [1] "PO4 Check Standard RSD within Range - PROCEED"
```



```
## [1] ">60% of NOx Check Standards are within range of expected concentration - PROCEED"

## [1] ">60% of NH3 Check Standards are within range of expected concentration - PROCEED"

## [1] ">60% of PO4 Check Standards are within range of expected concentration - PROCEED"
```

0.6 Analyze Blanks

```
## Assess Blanks
```

```
## [1] ">60% of NOx Blanks are below the lower 25% quartile of samples or 1/2 detection limit - PROCEED"
## [1] ">60% of NH3 Blanks are below the lower 25% quartile of samples - PROCEED"
## [1] ">60% of PO4 Blanks are below the lower 25% quartile of samples- PROCEED"
```

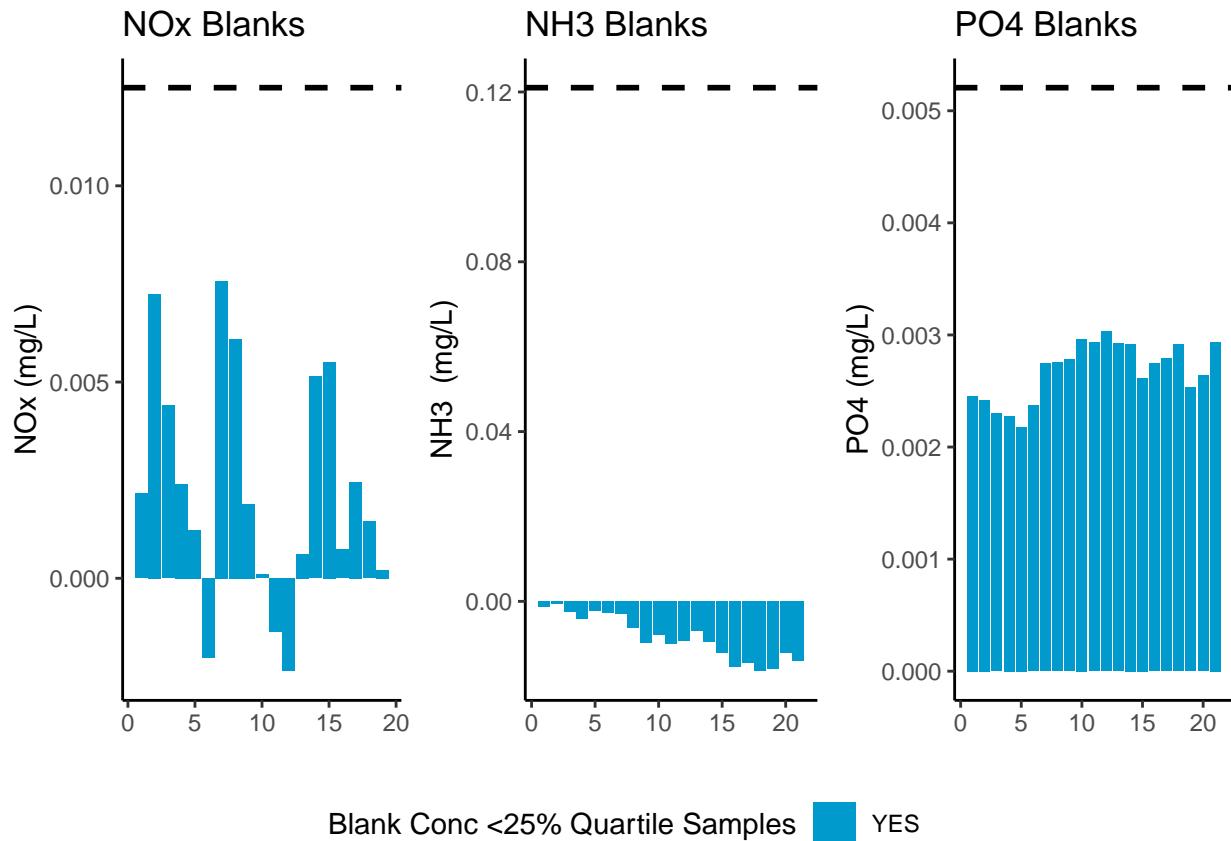


Table 2: Mean Concentration of Blanks

Test	Blank_Mean_Conc
NOx	0.0023
NH3	-0.0084
PO4	0.0027

0.7 Analyze Duplicates

```

## Analyze Duplicates

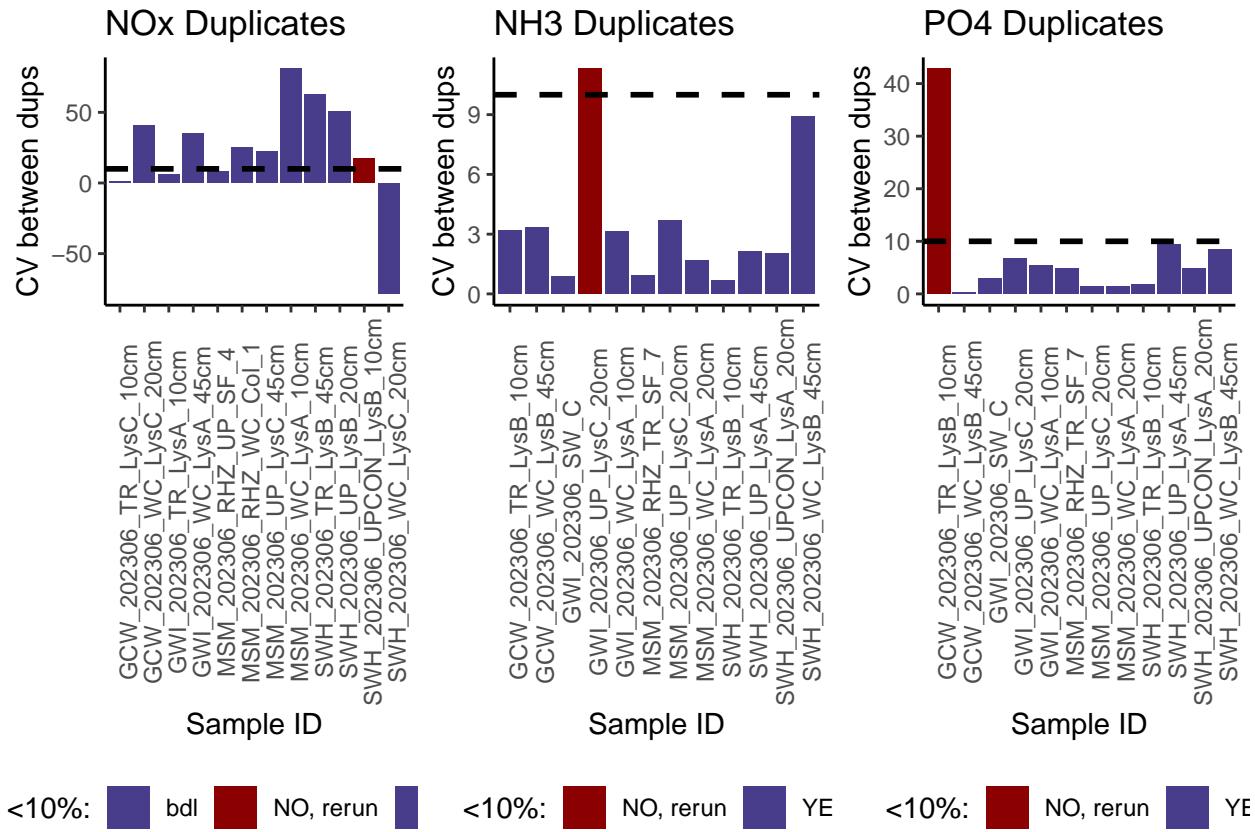
## [1] ">60% of NOx Duplicates have a CV <10% - PROCEED"

## [1] ">60% of NH3 Duplicates have a CV <10% - PROCEED"

## [1] ">60% of PO4 Duplicates have a CV <10% - PROCEED"

## Warning: Using 'size' aesthetic for lines was deprecated in ggplot2 3.4.0.
## i Please use 'linewidth' instead.
## This warning is displayed once every 8 hours.
## Call 'lifecycle::last_lifecycle_warnings()' to see where this warning was
## generated.

```

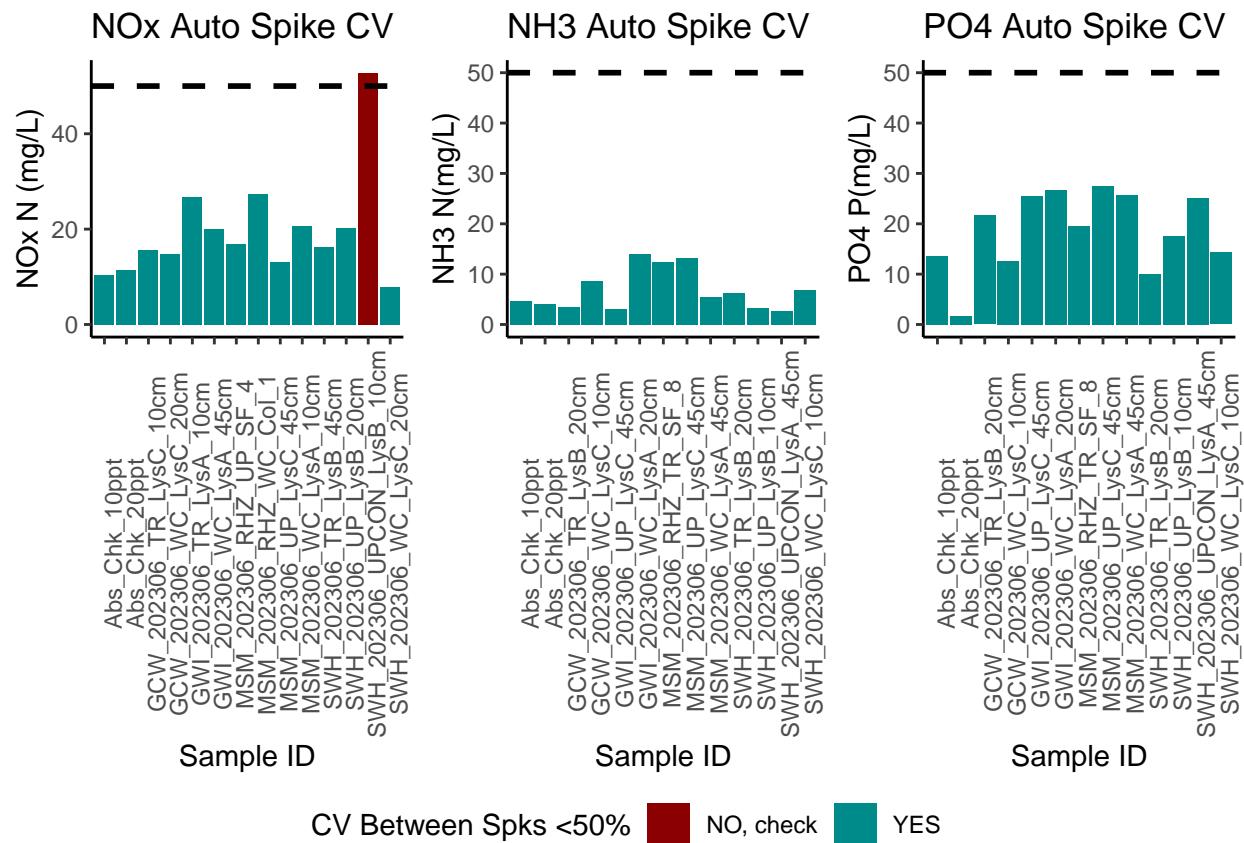


0.8 Spikes

```
## [1] ">60% of Spikes have a CV <50% - PROCEED"
```

```
## [1] ">60% of Spikes have a CV <50% - PROCEED"
```

```
## [1] ">60% of Spikes have a CV <50% - PROCEED"
```



0.9 Matrix Effects

```
## [1] "NO NOx Matrix Effect, PROCEED"  
  
## [1] "NO NH3 Matrix Effect, PROCEED"  
  
## [1] "NO PO4 Matrix Effect, PROCEED"
```

0.10 Unit Converted Data Column Added (mg/L to uM)

0.11 Sample Flagging - Within range of standard curve

```
## Sample Flagging
```

0.12 Pull out sample id information

```
## Sample Processing
```

```
## Warning: Expected 5 pieces. Missing pieces filled with 'NA' in 36 rows [22, 23, 24, 49,  
## 50, 51, 87, 88, 89, 115, 116, 117, 139, 140, 141, 181, 182, 183, 209, 210,  
## ...].
```

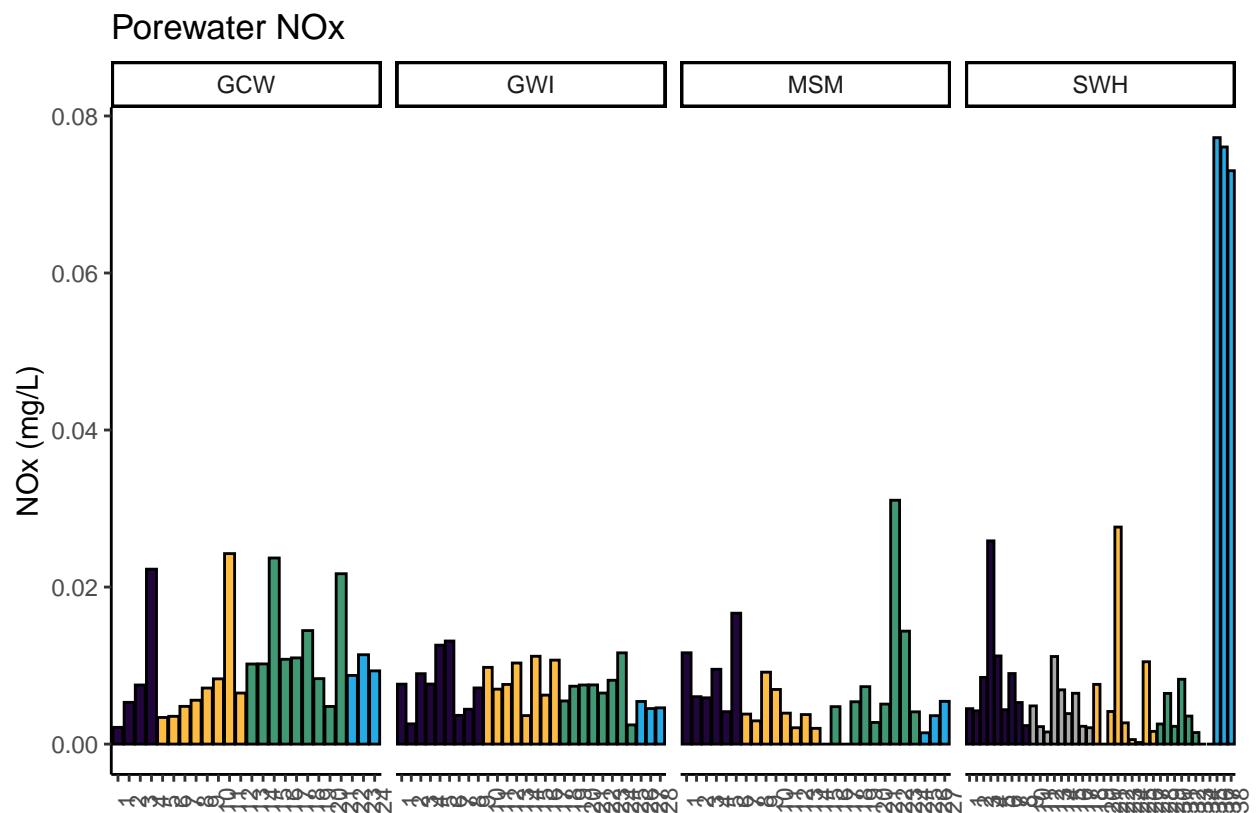
0.13 Pulling Out Rhizon Samples

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

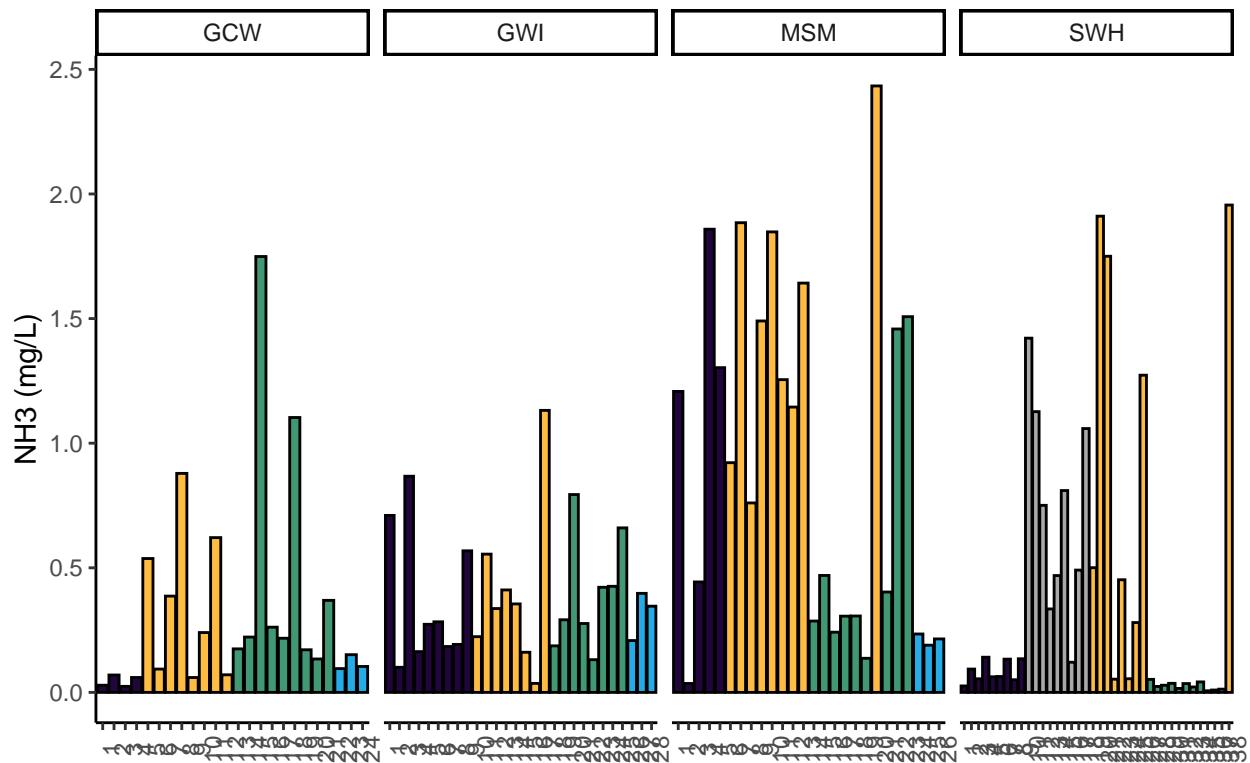
```
## Check Sample IDs with Metadata  
  
## All sample IDs are present in metadata.  
  
## Warning: Expected 5 pieces. Missing pieces filled with 'NA' in 36 rows [22, 23, 24, 49,  
## 50, 51, 87, 88, 89, 115, 116, 117, 139, 140, 141, 181, 182, 183, 209, 210,  
## ...].
```

0.15 Visualize Data

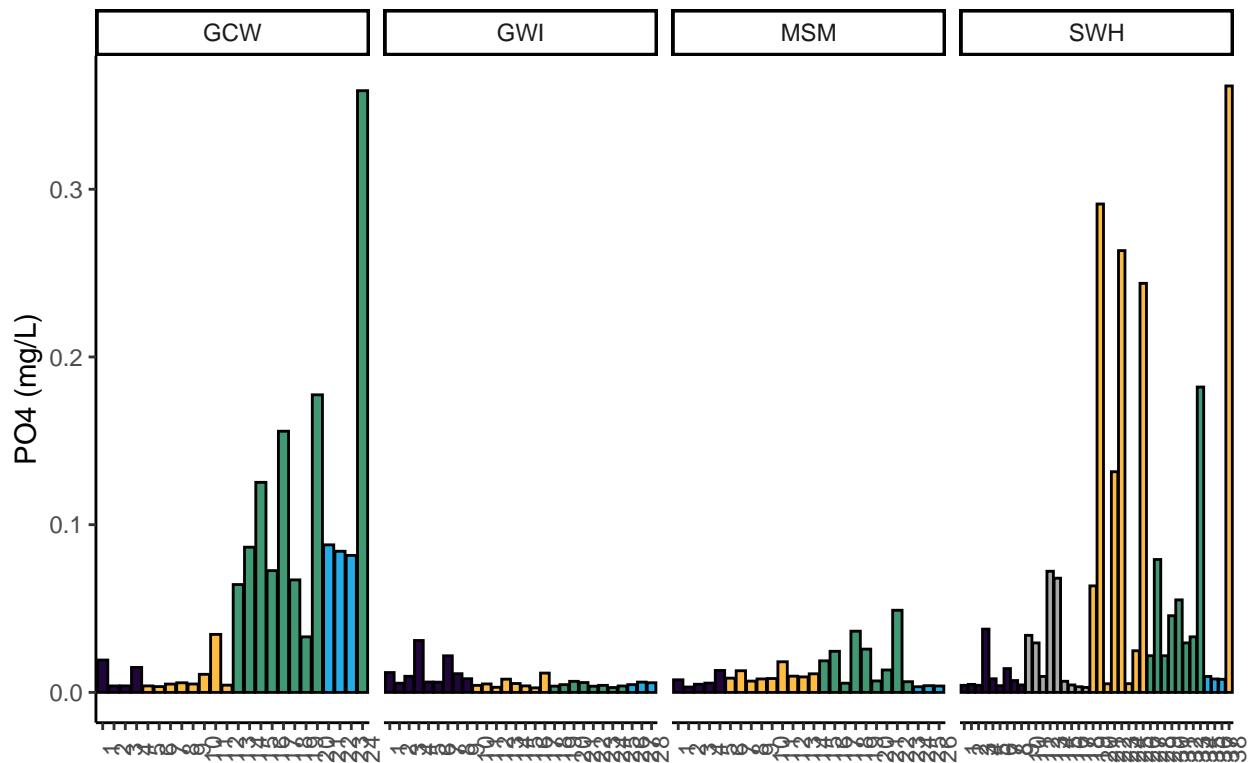
```
## Visualize Data
```



Porewater NH₃



Porewater PO4



0.16 Export Processed Data

```
#end
```