

Synoptic CB: Porewater Nutrients

June 2023 Samples

2025-07-07

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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 <- "20240114"
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.
NOx duplicates are out of range due to sample concentrations bdl."

#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.  
## NOx duplicates are out of range due to sample concentrations bdl.
```

```
##Setup
```

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

0.1 Import Data & Clean

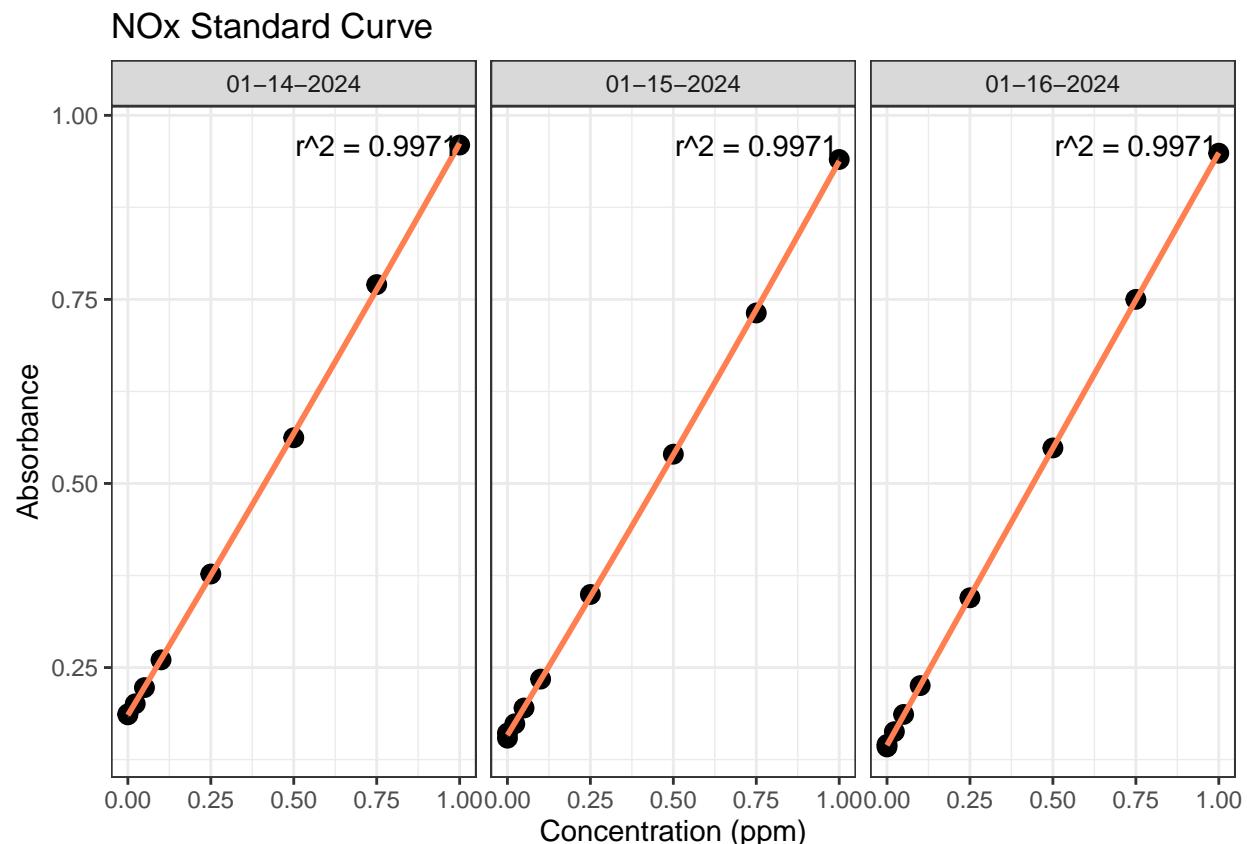
0.2 Assessing standard Curves

```
#Pull out standards data
```

```
## Assess Standard Curves
```

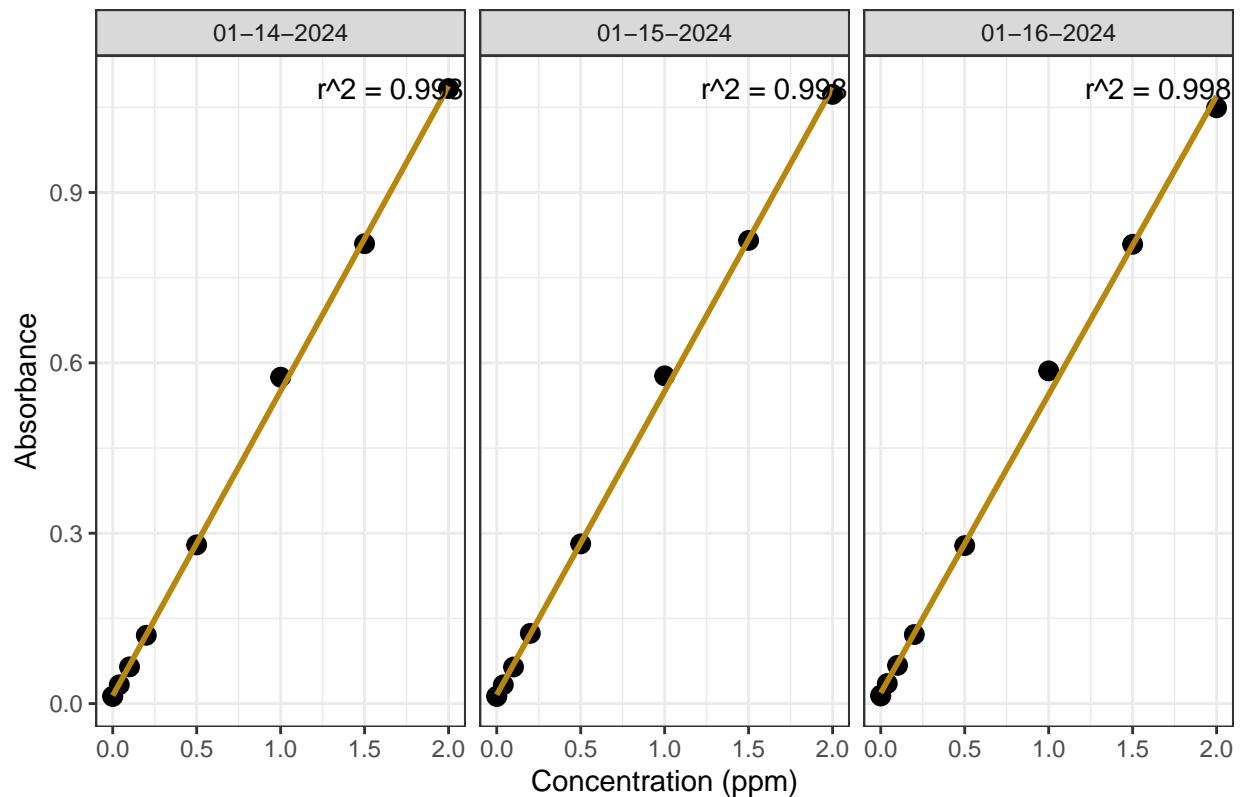
```
#Plot standards data
```

```
## Assess Standard Curves
```



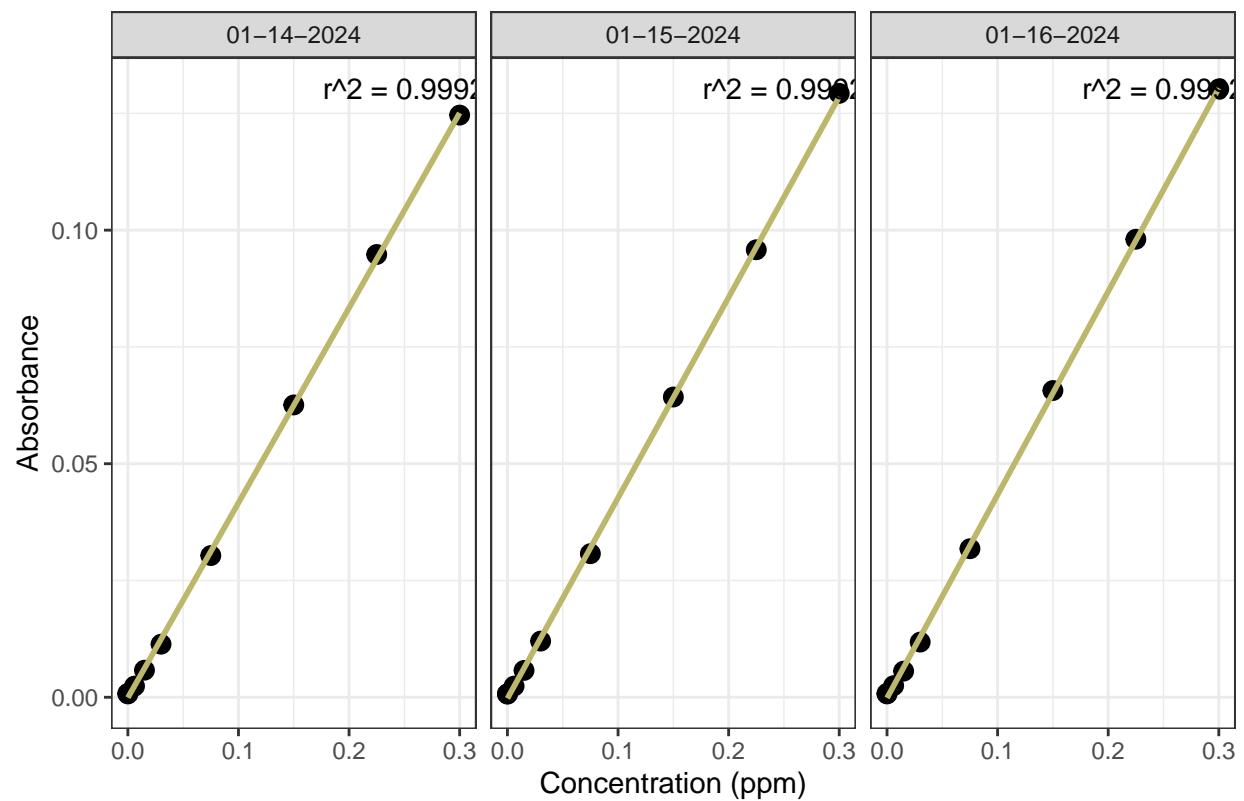
```
## `geom_smooth()` using formula = 'y ~ x'
```

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

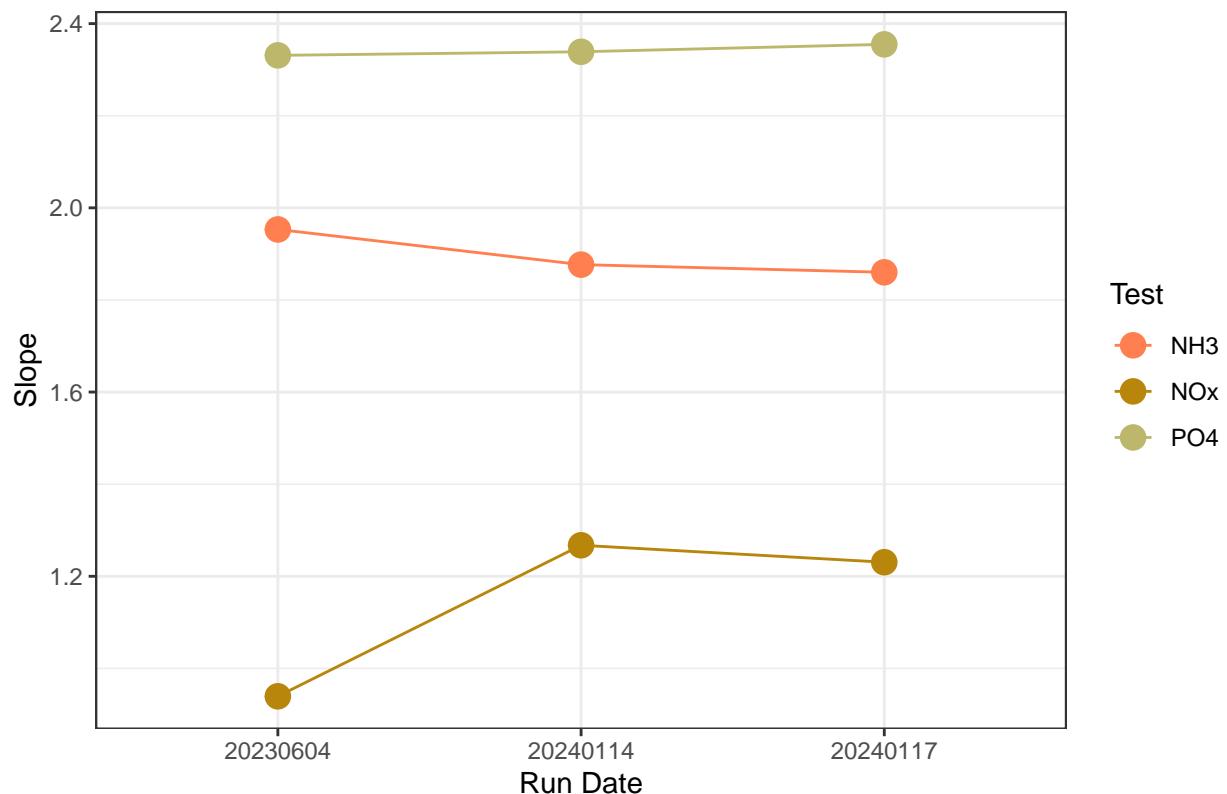


Table 1: Average Slope by Analyte

Test	avg_slope
NH3	1.897
NOx	1.146
PO4	2.342

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 <10% - PROCEED"

## Run mean = 0.714342

## Expected = 0.706

## [1] "NH3 pe Check has a % Difference >10% - REASSESS"

## Run mean = 1.20727

## Expected = 0.948

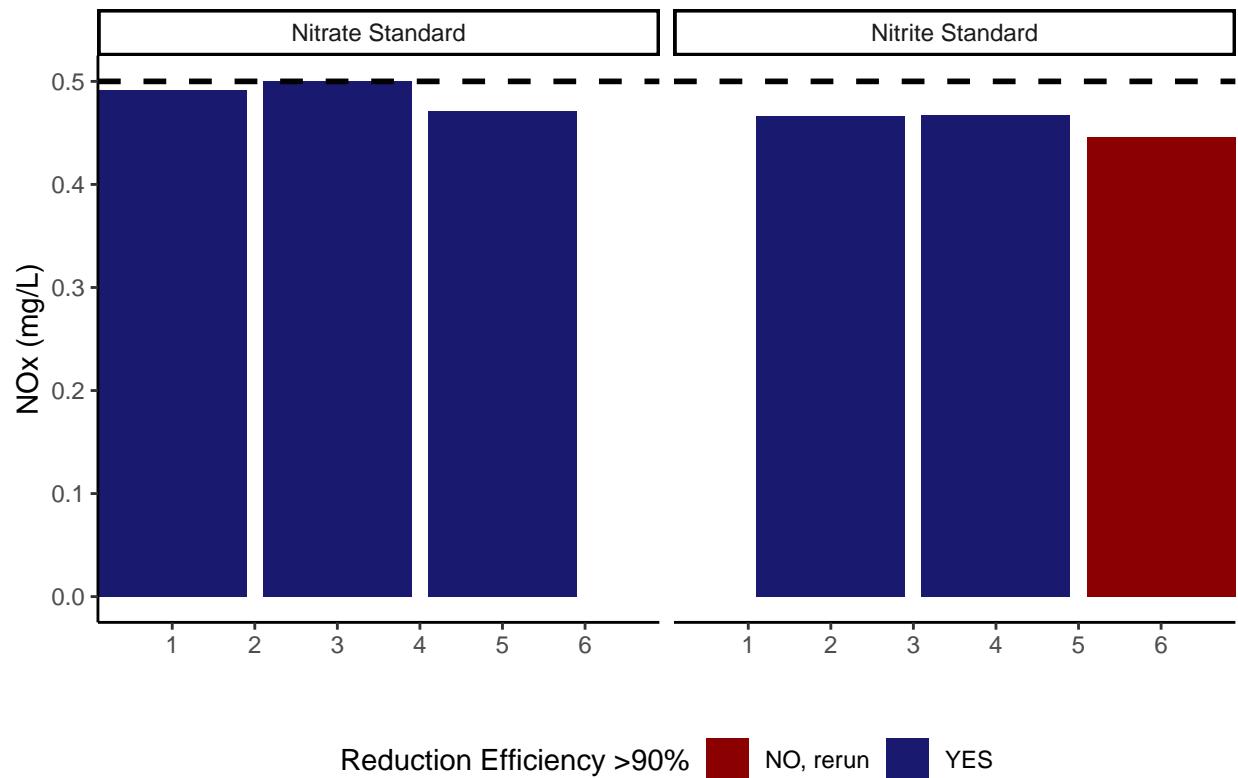
## [1] "PO4 pe Check has a % Difference >10% - REASSESS"

## Run mean = 0.5901153

## Expected = 0.818

#Check NOx Reduction Efficiency

## Assess Reduction Efficiency
```



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

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

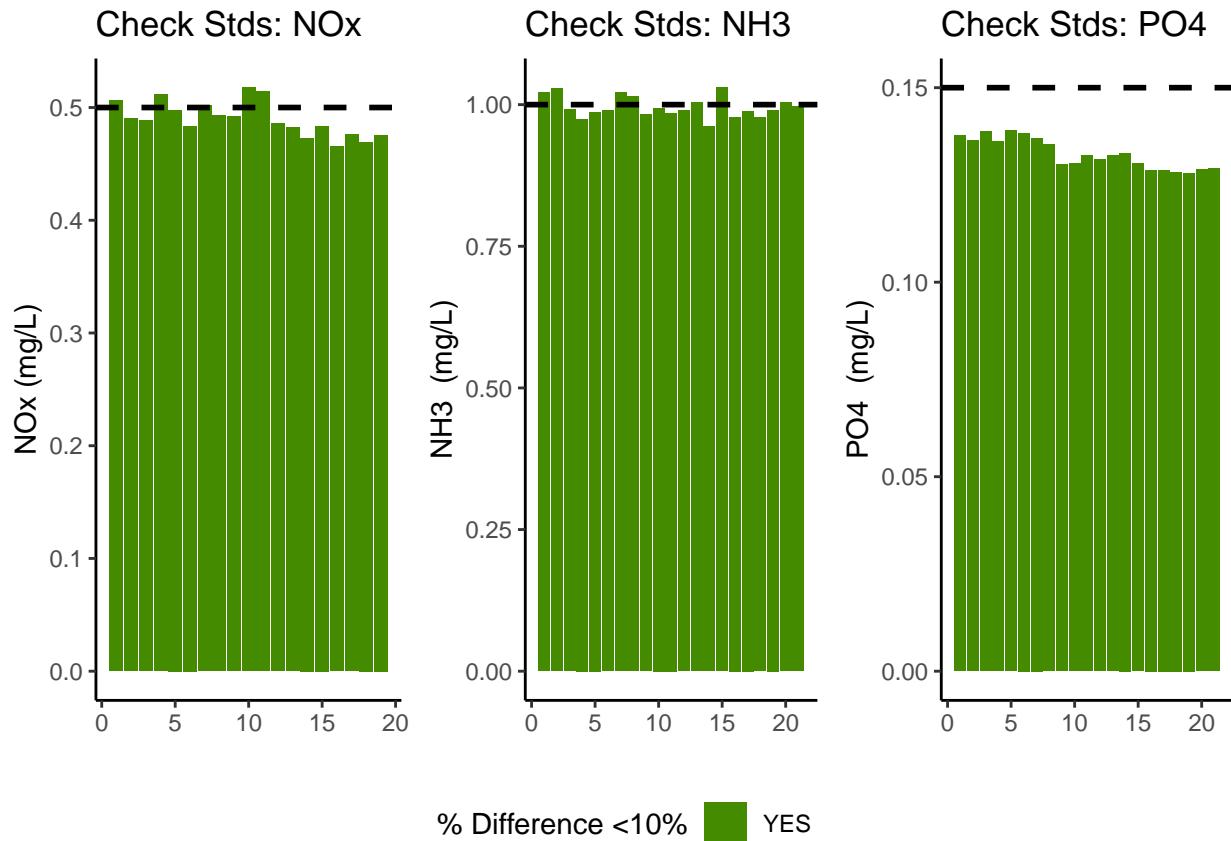
0.5 Analyze the Check Standards

```
## 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 Blank concentrations are lower than the lower 25% quartile of samples - PROCEED"

## [1] ">60% of NH3 Blank concentrations are lower than the lower 25% quartile of samples - PROCEED"

## [1] ">60% of PO4 Blank concentrations are lower than the lower 25% quartile of samples- PROCEED"
```

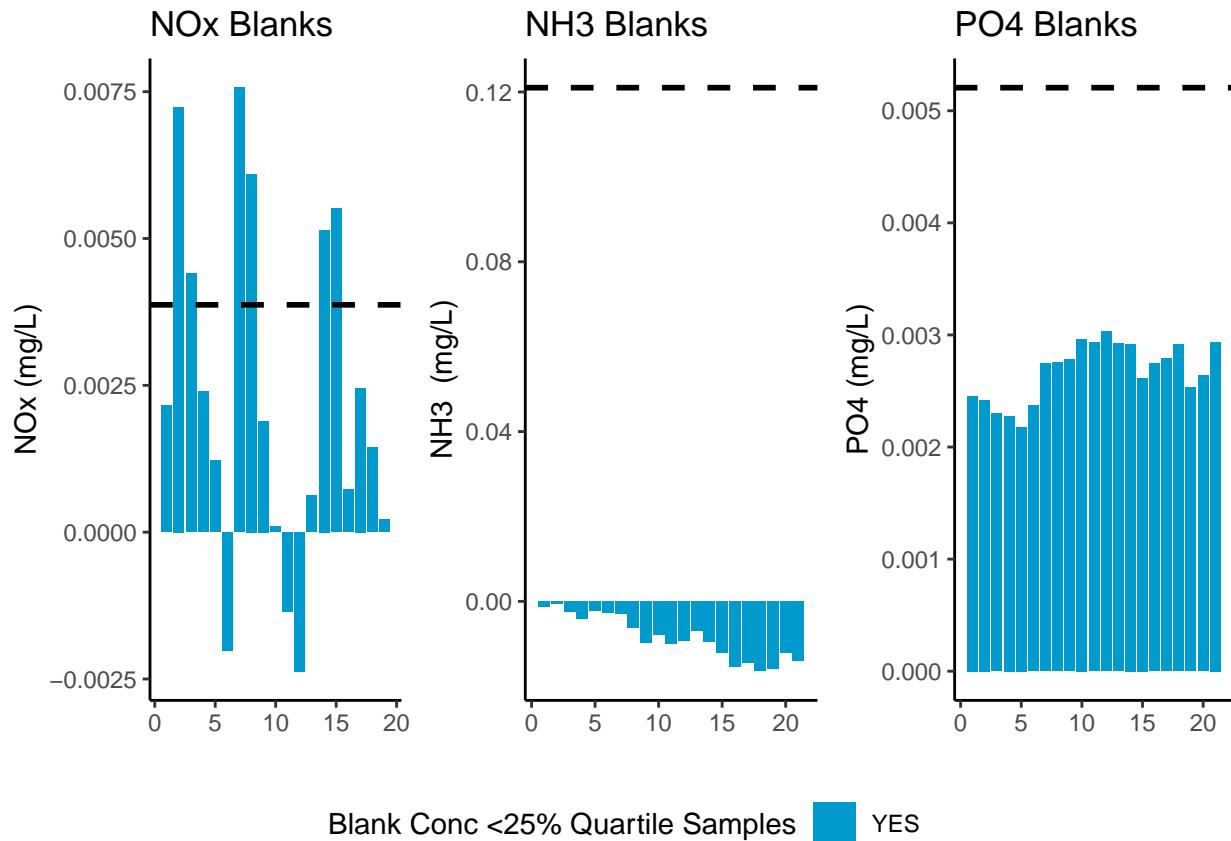


Table 2: Mean Concentration of Blanks

Test	Blank_Mean_Conc
NOx	0.0023
NH3	-0.0084
PO4	0.0027

0.7 Analyze Duplicates

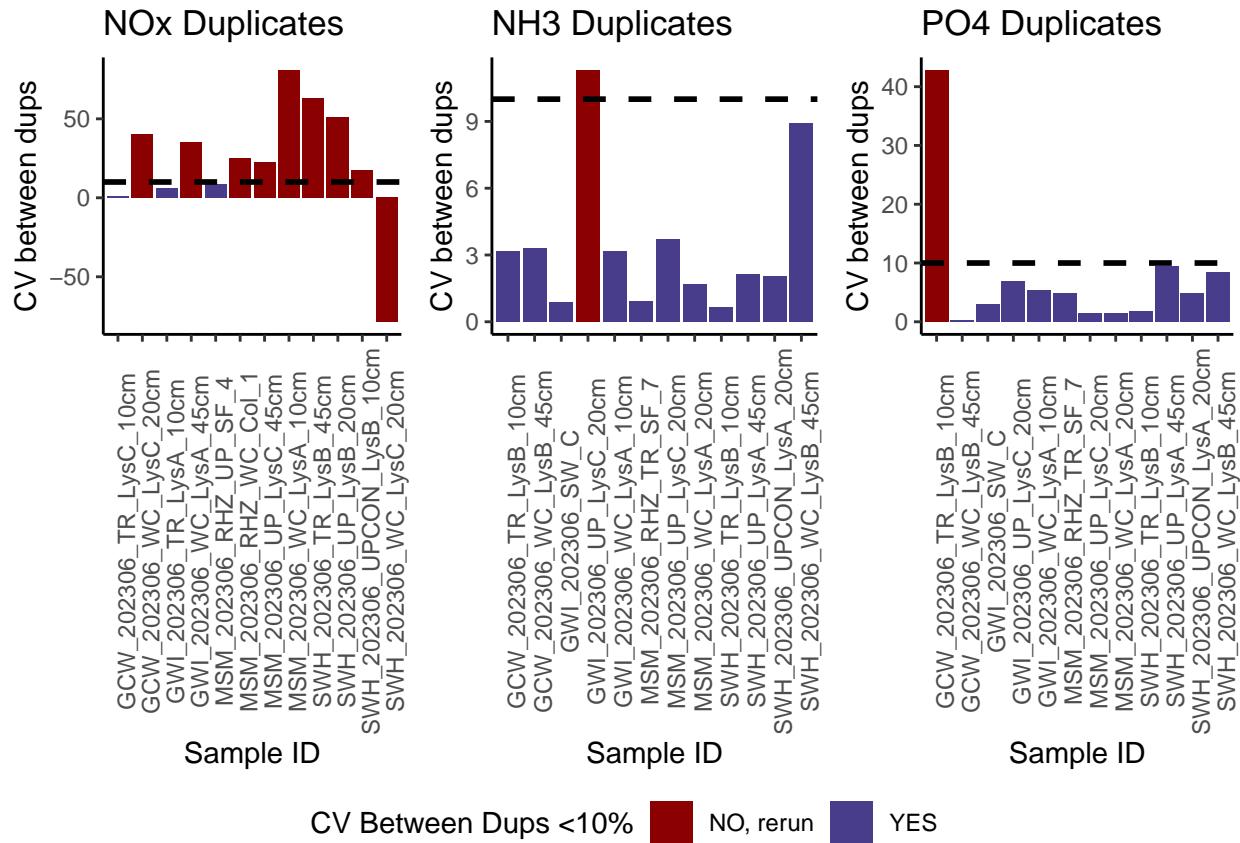
```
## Analyze Duplicates

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

## [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.
```

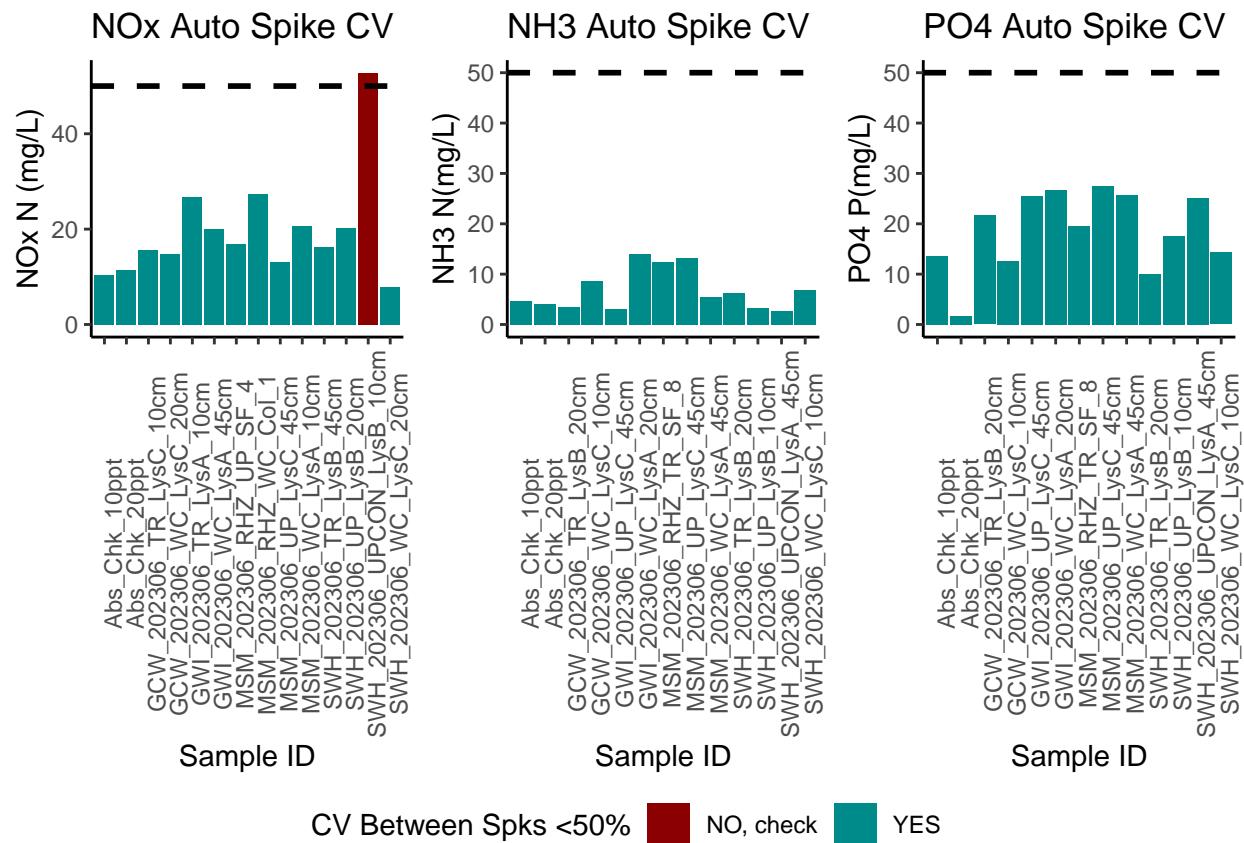


0.8 Spikes

```
## [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,  
## ...].
```

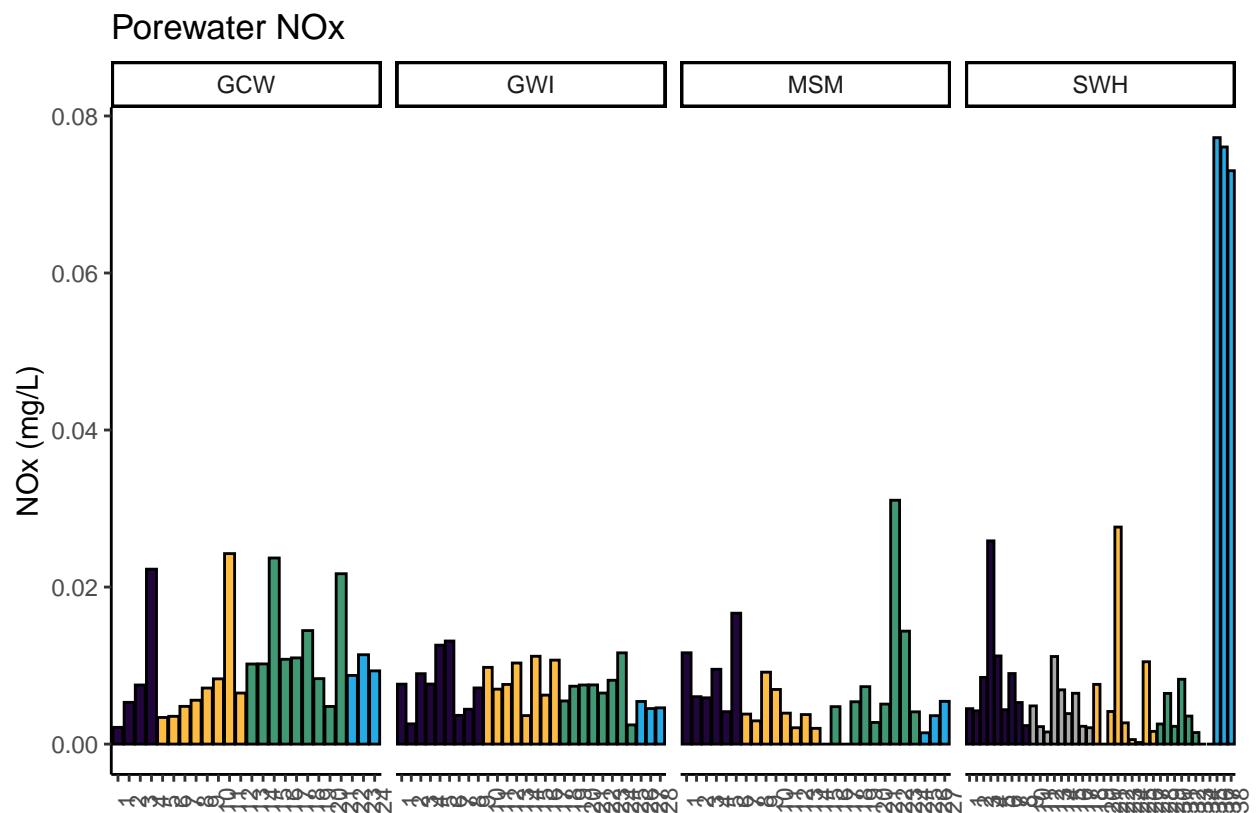
0.13 Pulling Out Rhizon Samples

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

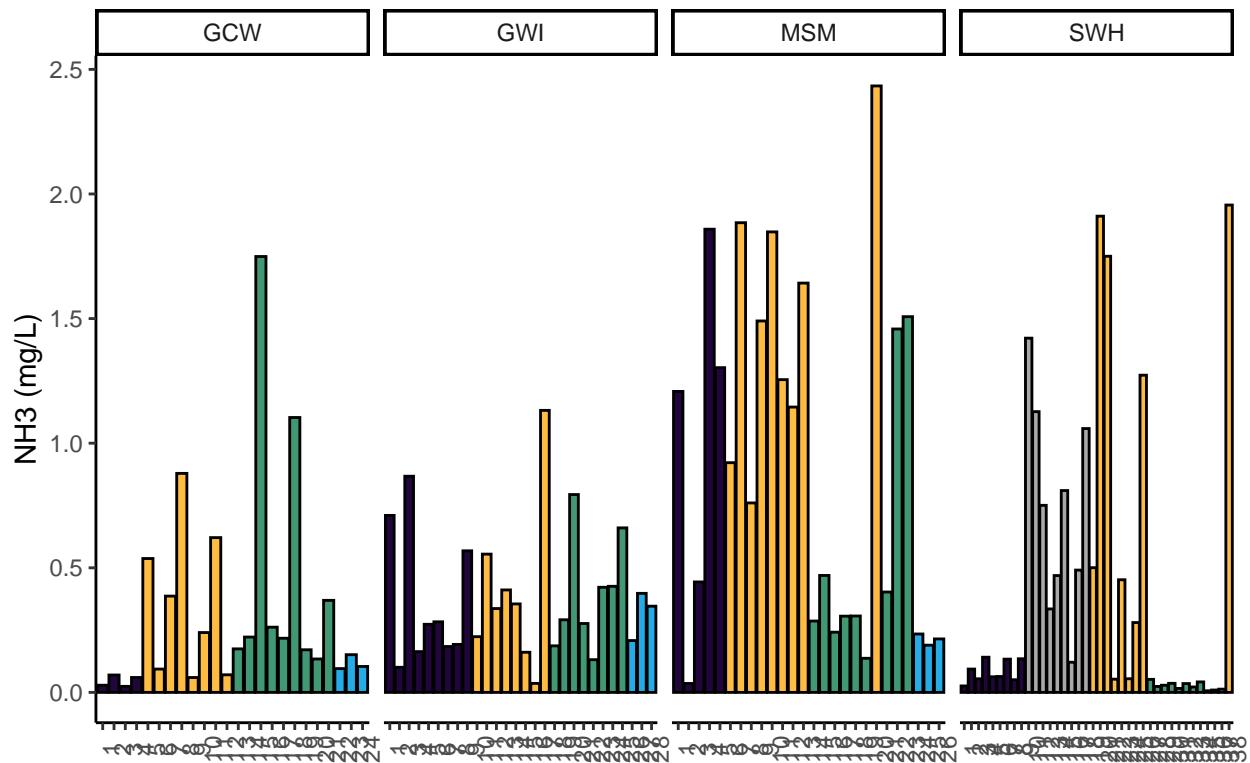
```
## Check Sample IDs with Metadata  
  
## All sample IDs are present in metadata.  
  
## Warning: Expected 5 pieces. Missing pieces filled with 'NA' in 36 rows [22, 23, 24, 49,  
## 50, 51, 87, 88, 89, 115, 116, 117, 139, 140, 141, 181, 182, 183, 209, 210,  
## ...].
```

0.15 Visualize Data

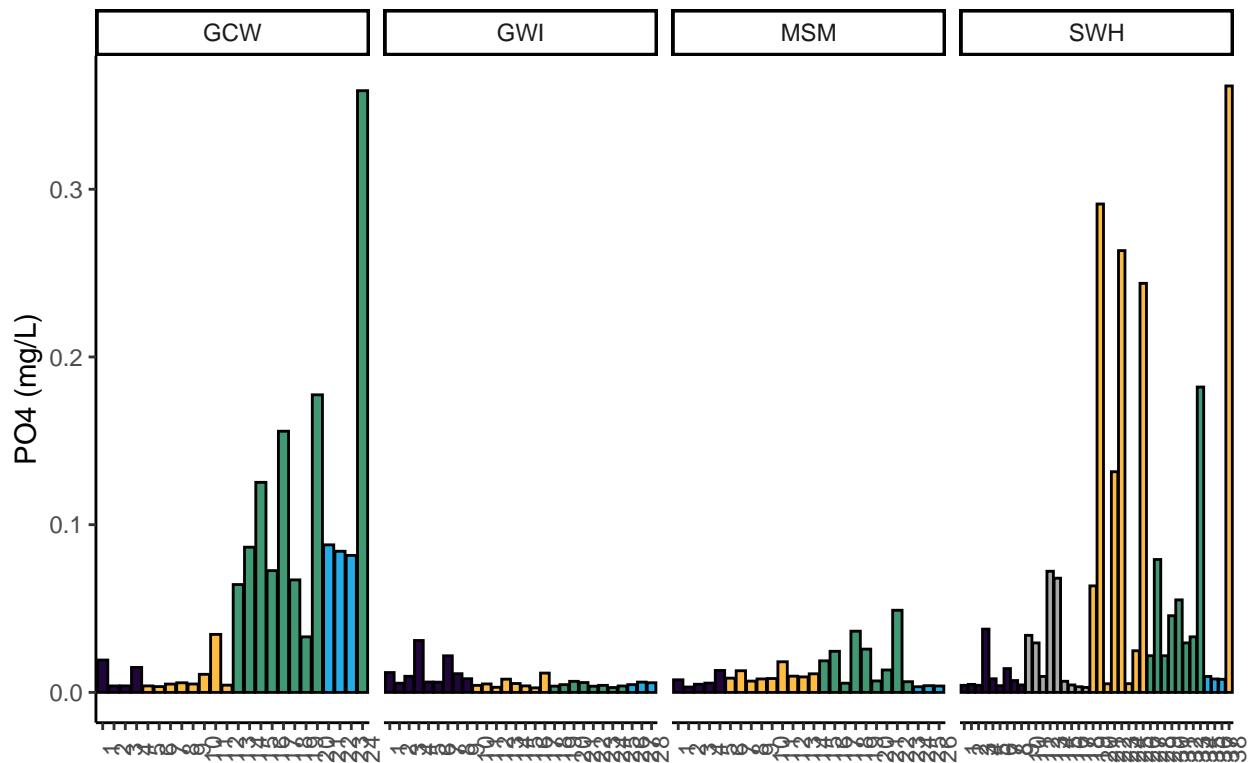
```
## Visualize Data
```



Porewater NH₃



Porewater PO4



0.16 Export Processed Data

```
#end
```