

Synoptic CB: Porewater Nutrients

July 2023 Samples

2025-07-07

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```

##Run Information

cat("Run Information: Please Read
") #lets you know what section you're in

## Run Information: Please Read

#set the run date & user name
run_date <- "20240117"
sample_year <- 2023
sample_month <- 07
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_July2023_1.csv",
              "Raw Data/SEAL_COMPASS_Synoptic_NOx_July2023_2.csv",
              "Raw Data/SEAL_COMPASS_Synoptic_NOx_July2023_3.csv")
NH3_P04_files <- c("Raw Data/SEAL_COMPASS_Synoptic_NH3_P04_July2023_1.csv",
                    "Raw Data/SEAL_COMPASS_Synoptic_NH3_P04_July2023_2.csv",
                    "Raw Data/SEAL_COMPASS_Synoptic_NH3_P04_July2023_3.csv")

# Define the file path for QAQC log file - NO Need to change just check year
file_path <- "Raw Data/SEAL_COMPASS_Synoptic_QAACC_Log_2023.csv"
final_path <- "Processed Data/COMPASS_Synoptic_Nutrients_202307.xlsx"

#record any notes about the run or anything other info here:
run_notes <- "Run Notes: peChks for NOx and NH3 out of range, but all other
run metrics looked fine, so we are accepting the run with flags.
Blanks and Duplicates: Flags for NOx blanks out of range - because samples
have bdl concentrations, same problem for out of range duplicates"

#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)

## Run Notes: peChks for NOx and NH3 out of range, but all other
## run metrics looked fine, so we are accepting the run with flags.
## Blanks and Duplicates: Flags for NOx blanks out of range - because samples
## have bdl concentrations, same problem for out of range duplicates

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

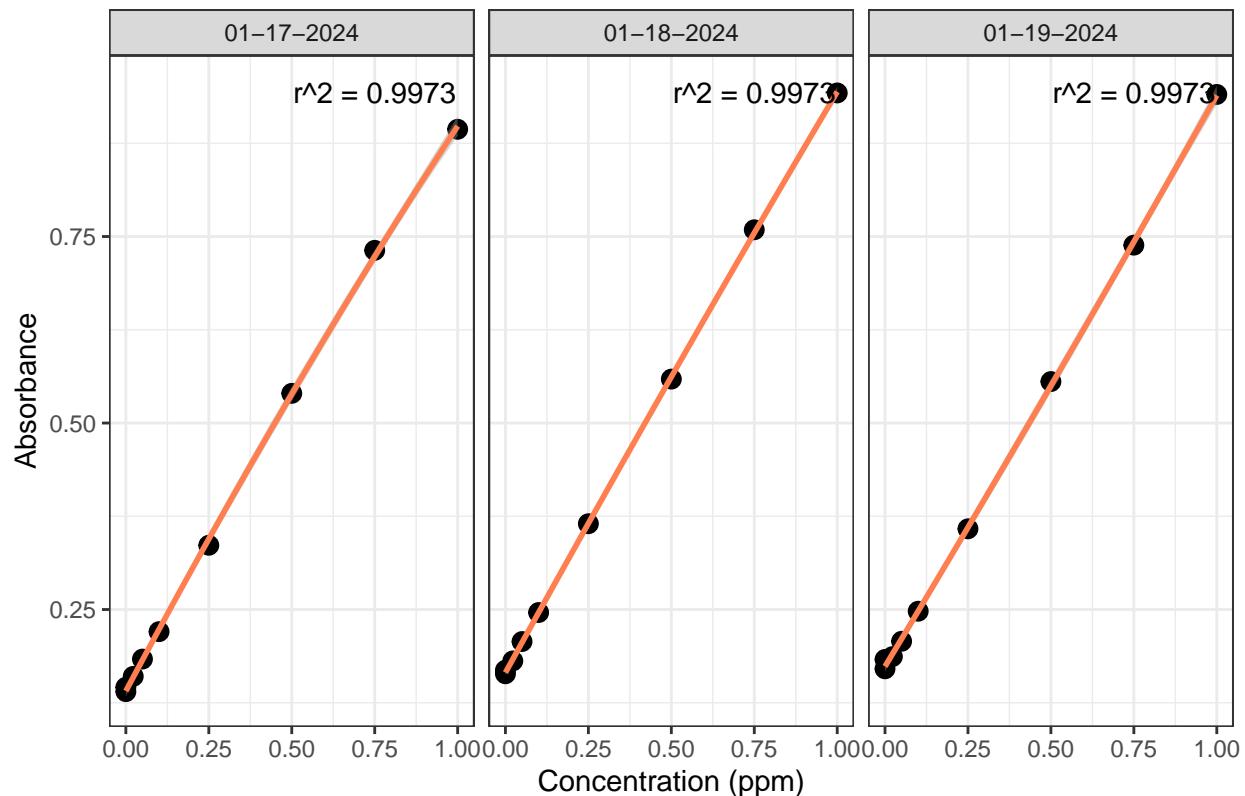
```

0.1 Import Data & Clean

0.2 Assessing standard Curves

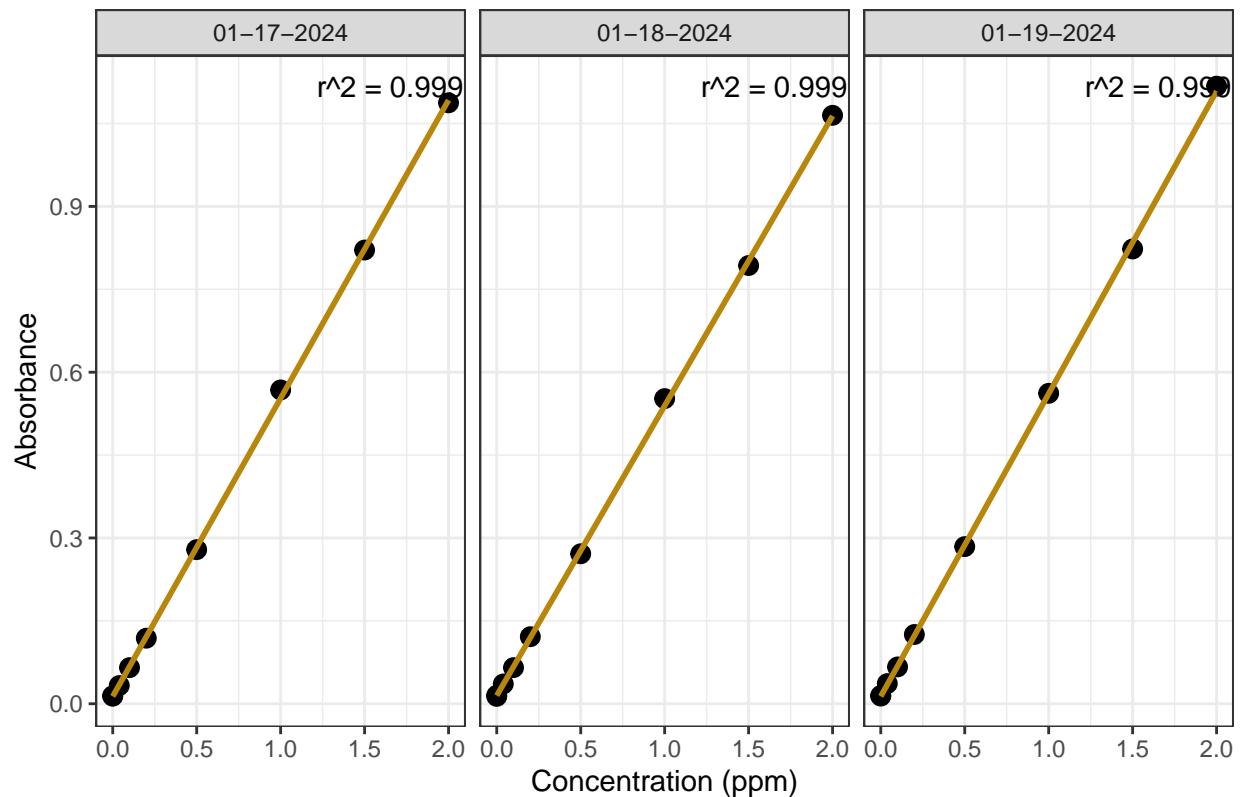
```
#Pull out standards data  
  
## Assess Standard Curves  
  
#Plot standards data  
  
## Assess Standard Curves
```

NOx Standard Curve



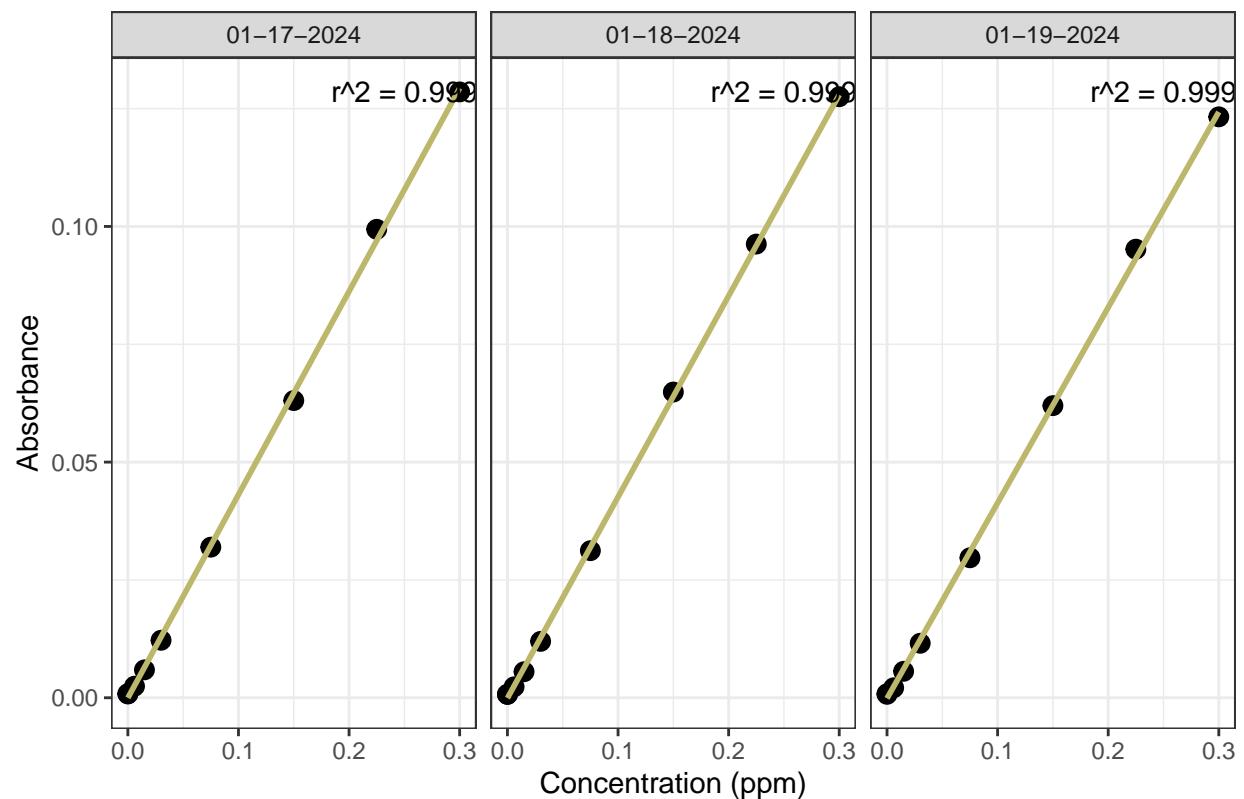
```
## `geom_smooth()` using formula = 'y ~ x'
```

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

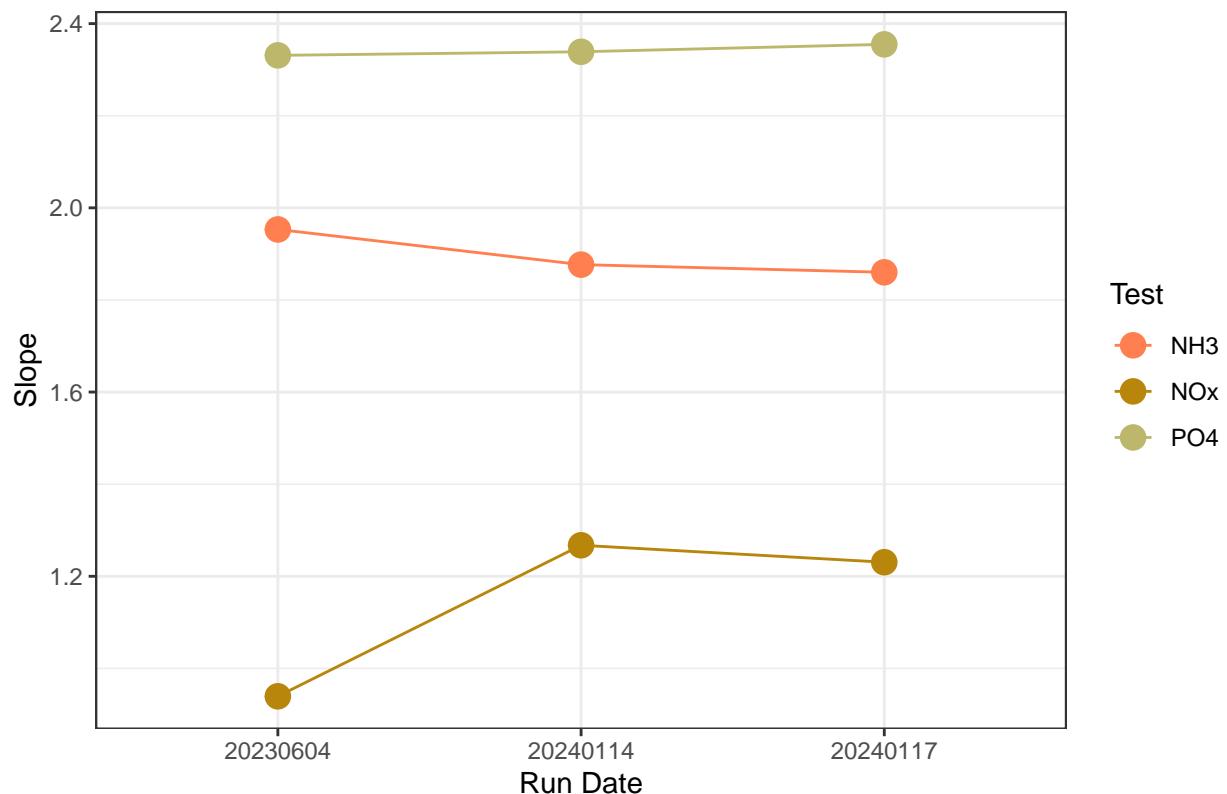


Table 1: Average Slope by Analyte

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_202307_UP_LysC_20cm, MSM_202307_TR_LysA_20cm, MSM_202307_TR_LysB_10cm, MSM_202307_TR_LysC_10cm

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

0.4 Performance Check

```
## [1] "NOx pe Check has a % Difference >20% - REASSESS"
```

```
## Run mean = 2.511515
```

Expected = 0.706

[1] "NH3 pe Check has a % Difference >20% - REASSESS"

```
## Run mean = 0.820844
```

Expected = 0.948

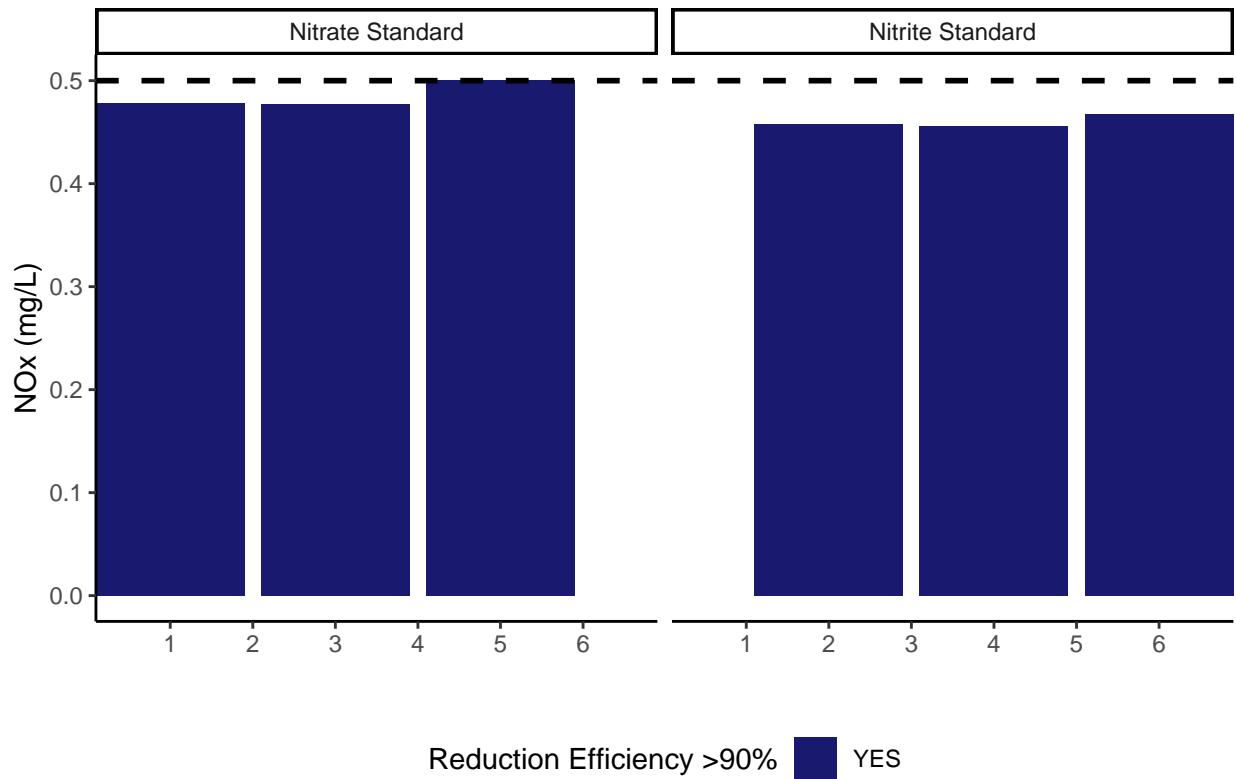
```
## [1] "P04 pe Check has a % Difference <20% - PROCEED"
```

```
## Run mean = 0.878815
```

```
## Expected = 0.818
```

```
#Check NOx Reduction Efficiency
```

```
## Assess Reduction Efficiency
```



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

```
## [1] 94.57947
```

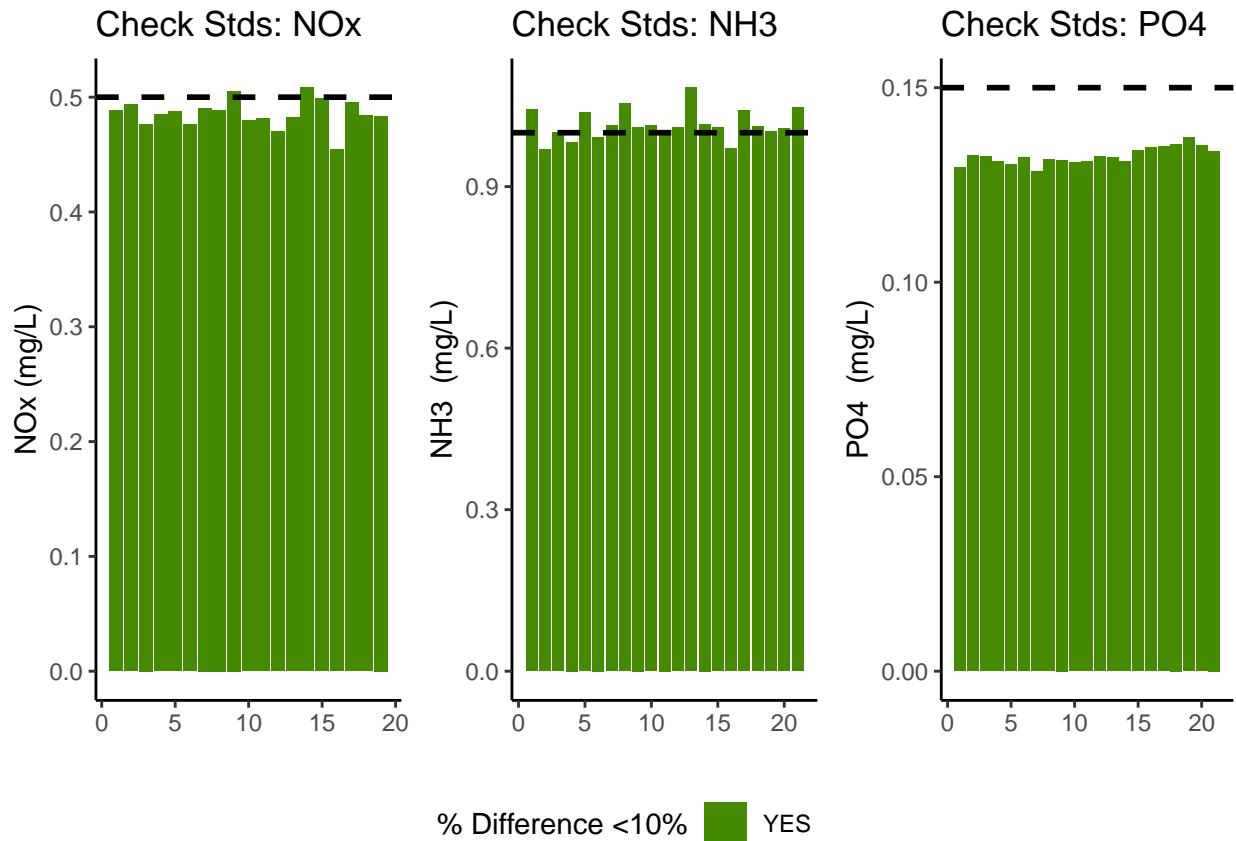
0.5 Analyze the Check Standards

```
## 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 blaks are lower 25% quartile of samples - REASSESS"

## [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"
```

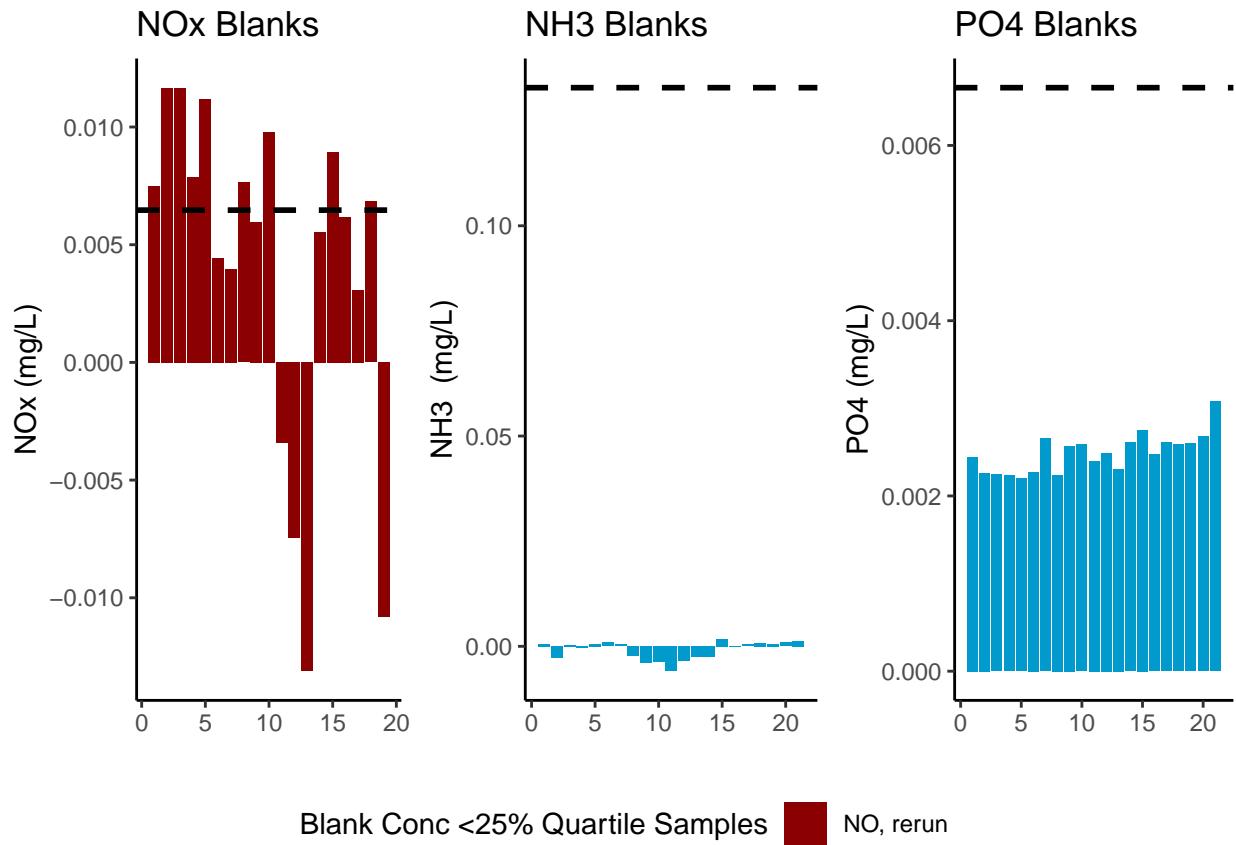


Table 2: Mean Concentration of Blanks

Test	Blank_Mean_Conc
NOx	0.0041
NH3	-0.0009
PO4	0.0025

0.7 Analyze Duplicates

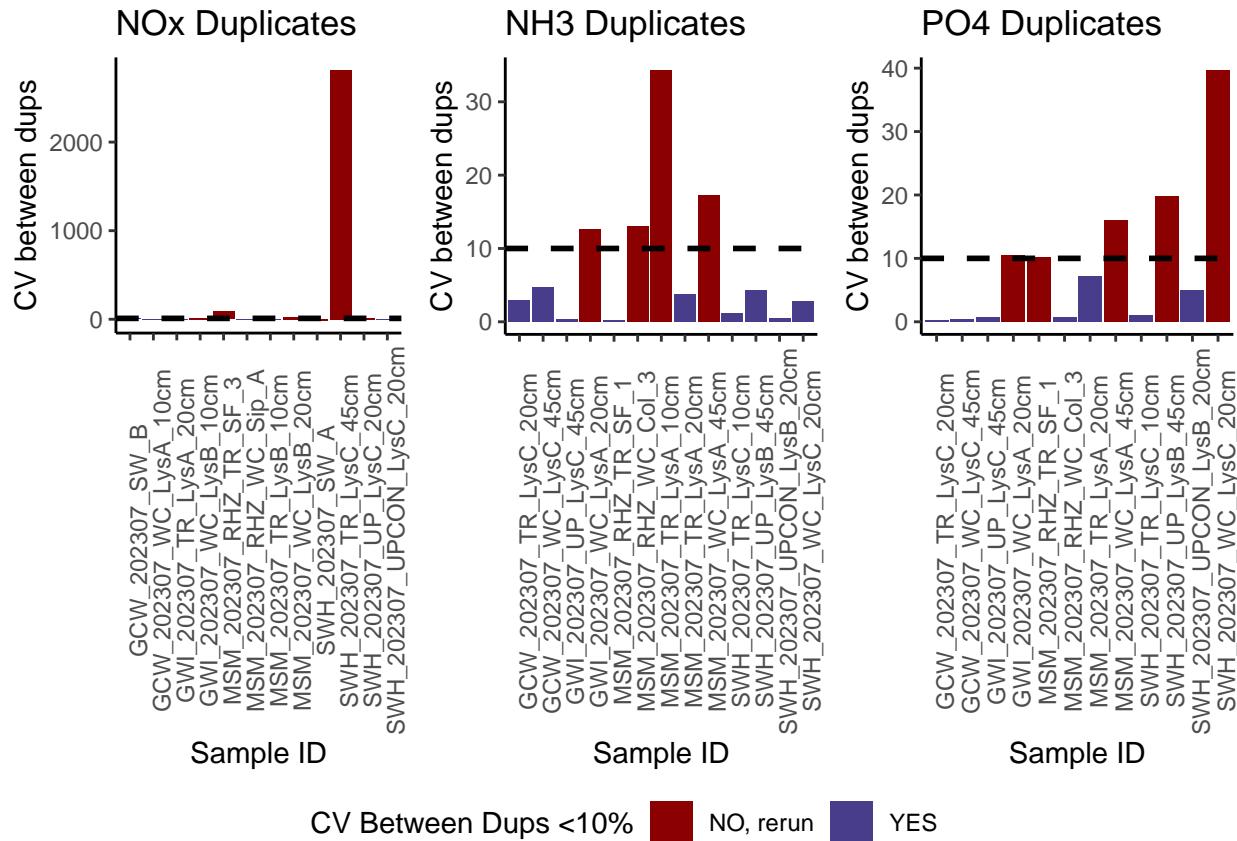
```
## Analyze Duplicates

## [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% - REASSESS"

## 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.
```

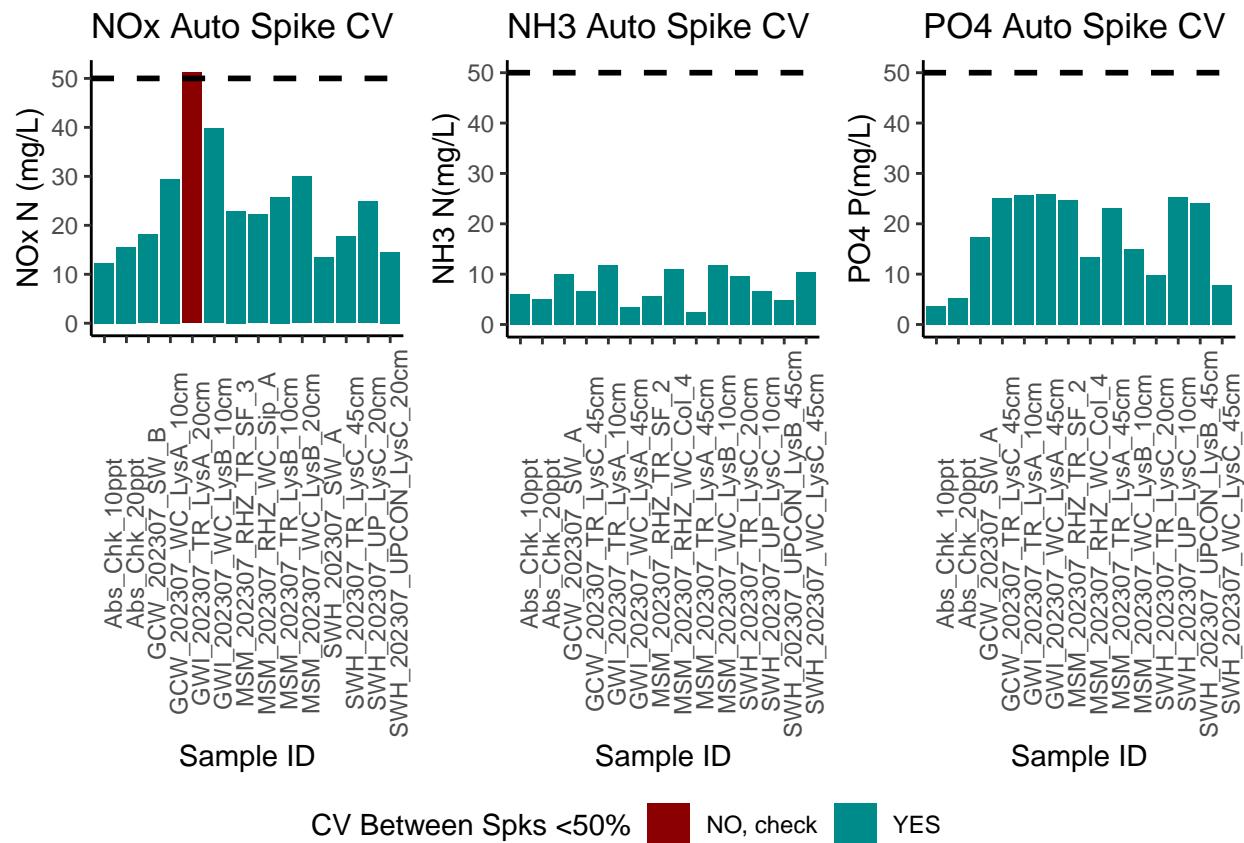


0.8 Spikes

```
## [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 [19, 20, 21, 44,  
## 45, 46, 83, 84, 85, 110, 111, 112, 131, 132, 133, 167, 168, 169, 199, 200,  
## ...].
```

0.13 Pulling Rhizon Samples

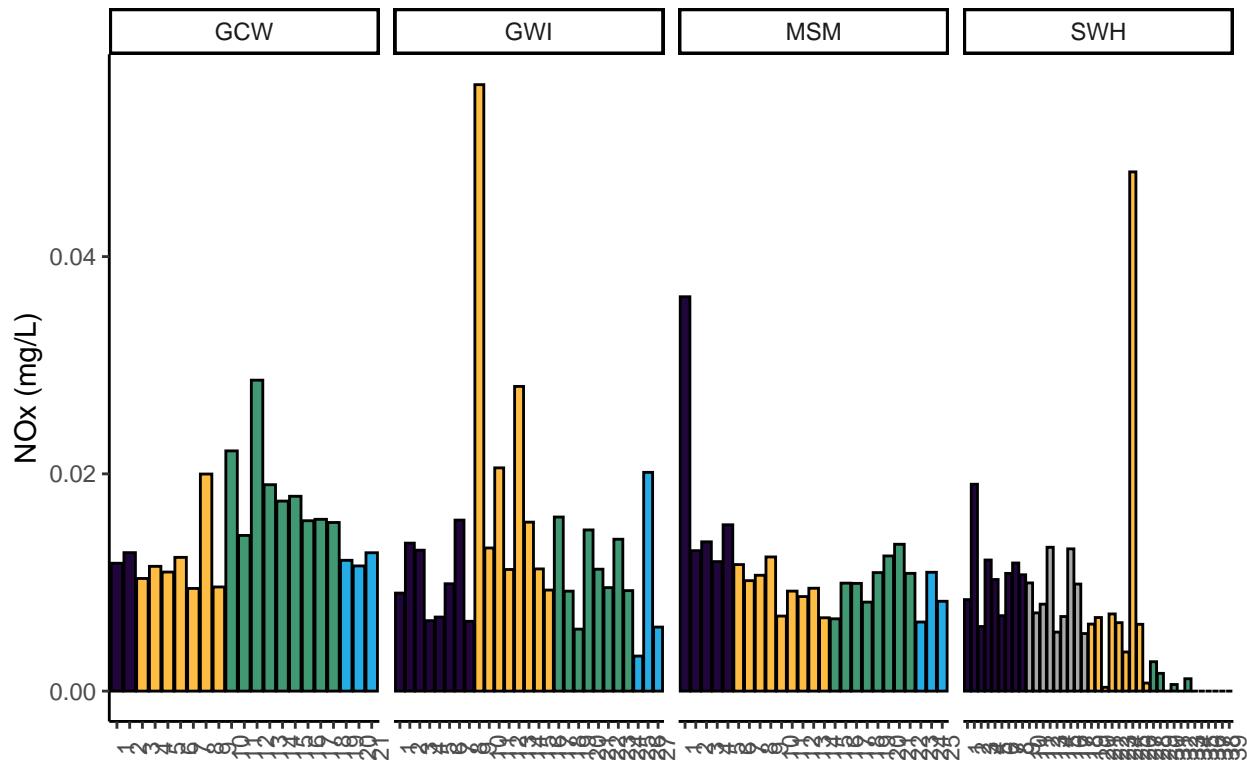
0.14 Check to see if samples run match metadata & merge info

```
## Check Sample IDs with Metadata  
  
## All sample IDs are present in metadata.  
  
## Warning: Expected 5 pieces. Missing pieces filled with 'NA' in 36 rows [19, 20, 21, 44,  
## 45, 46, 83, 84, 85, 110, 111, 112, 131, 132, 133, 167, 168, 169, 199, 200,  
## ...].
```

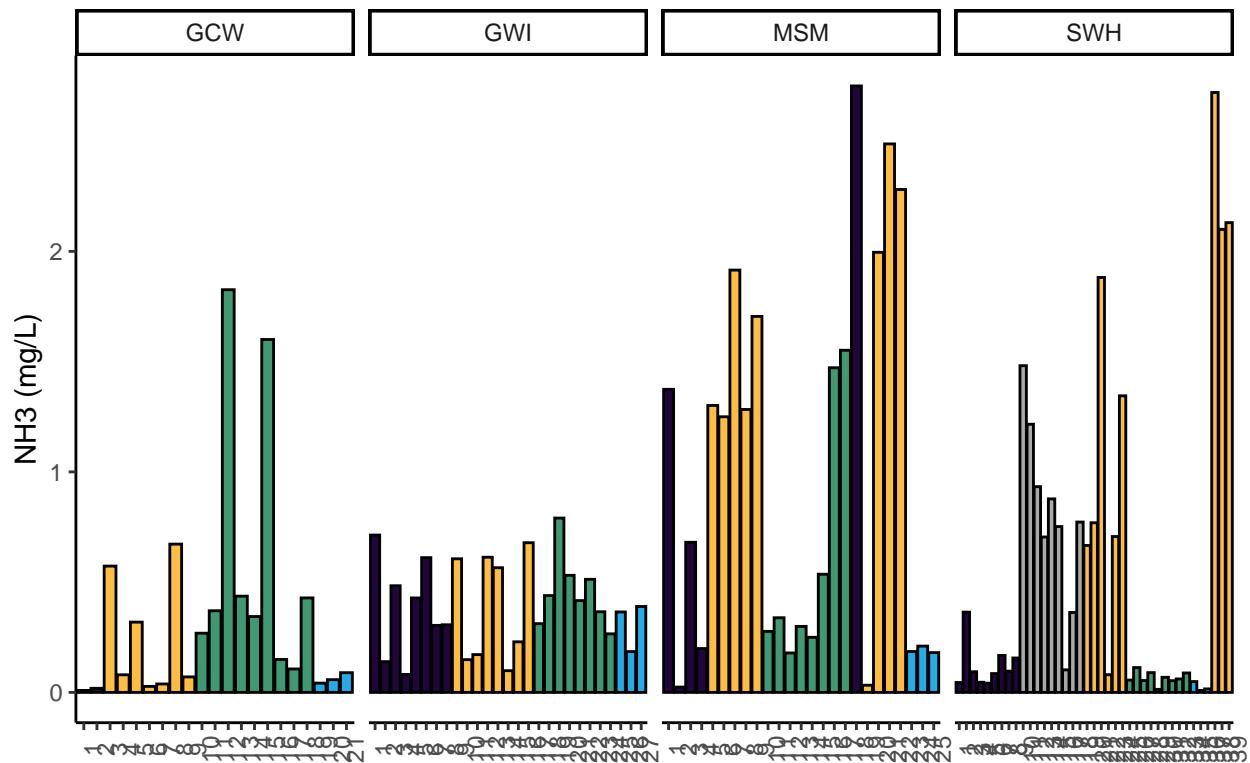
0.15 Visualize Data

```
## Visualize Data
```

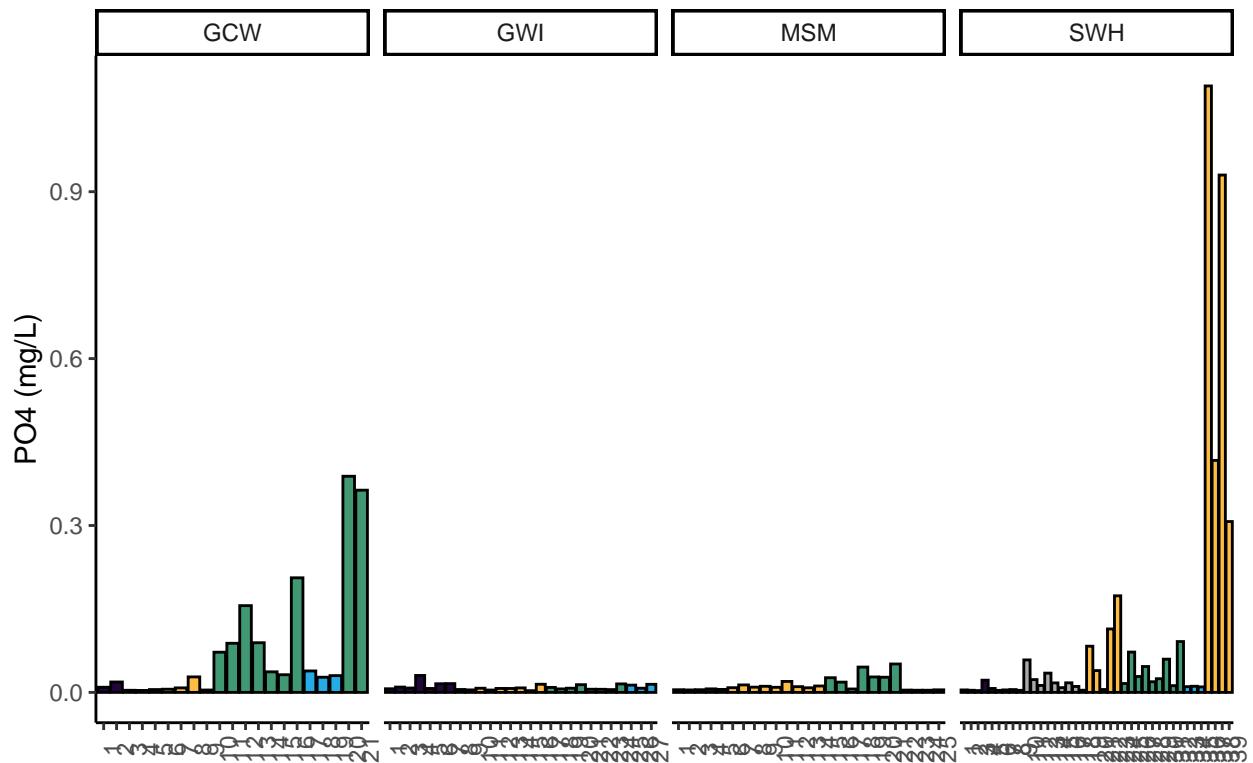
Porewater NOx



Porewater NH₃



Porewater PO4



0.16 Export Processed Data

```
#end
```