

Synoptic CB: Porewater Nutrients

October 2023 Samples

2025-07-08

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```

##Run Information

cat("Run Information: Input by I. Van Benschoten") #lets you know what section you're in

## Run Information: Input by I. Van Benschoten

#set the run date & user name
run_date <- "01/27/24"
sample_year <- 2023
sample_month <- "October"
user <- "Stephanie Wilson"

#identify the files you want to read in
#read in as a list to accommodate multiple runs in a month
NOx_files <- c("Raw Data/SEAL_COMPASS_Synoptic_NOx_Oct2023_1.csv",
              "Raw Data/SEAL_COMPASS_Synoptic_NOx_Oct2023_2.csv",
              "Raw Data/SEAL_COMPASS_Synoptic_NOx_Oct2023_3.csv")
NH3_P04_files <- c("Raw Data/SEAL_COMPASS_Synoptic_NH3_P04_Oct2023_1.csv",
                   "Raw Data/SEAL_COMPASS_Synoptic_NH3_P04_Oct2023_2.csv",
                   "Raw Data/SEAL_COMPASS_Synoptic_NH3_P04_Oct2023_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_202310.csv"

#record any notes about the run or anything other info here:
run_notes <- "This run has limited spike checks for NH3 and P04.
peCheck for NH3 is out of range, all other run metrics are fine,
so accepting this run."

#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)

## This run has limited spike checks for NH3 and P04.
## peCheck for NH3 is out of range, all other run metrics are fine,
## so accepting this run.

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

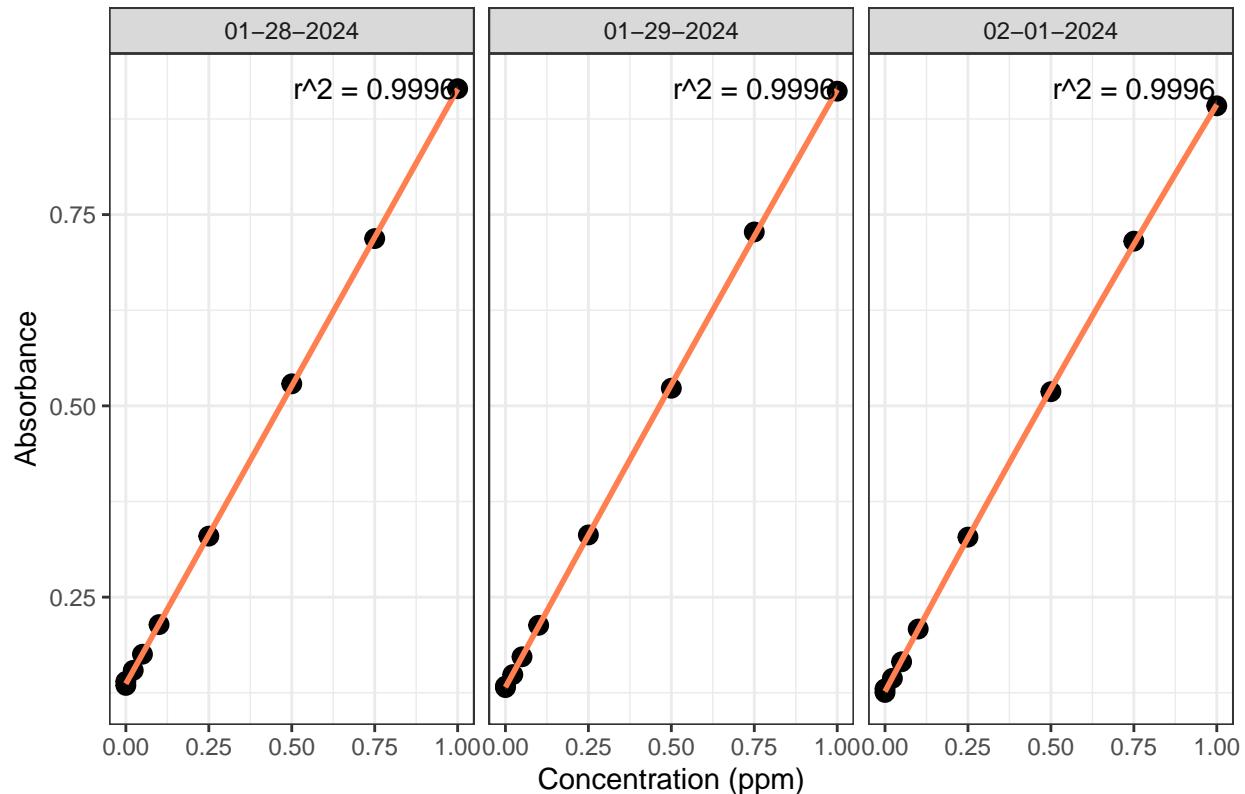
```

0.1 Import Data & Clean

0.2 Assessing standard Curves

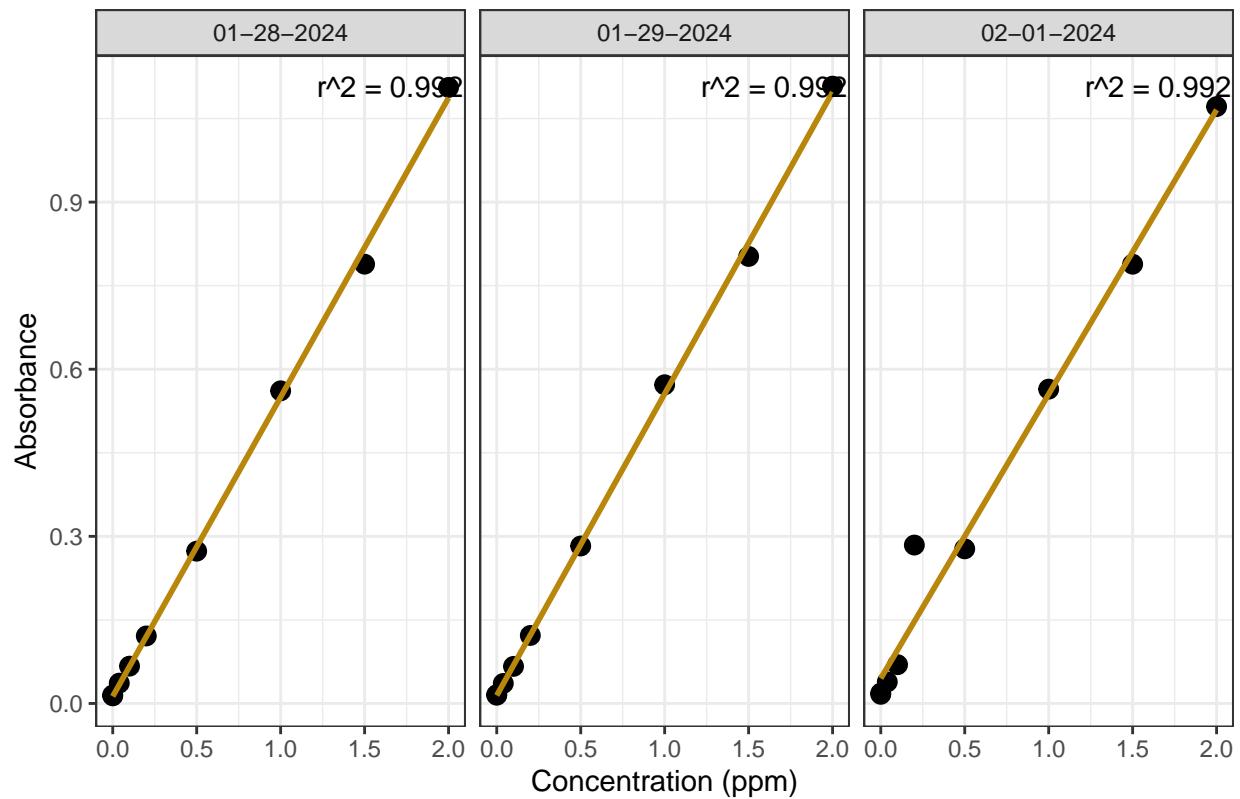
```
#Pull out standards data  
  
## Assess Standard Curves  
  
#Plot standards data  
  
## Assess Standard Curves
```

NOx Standard Curve



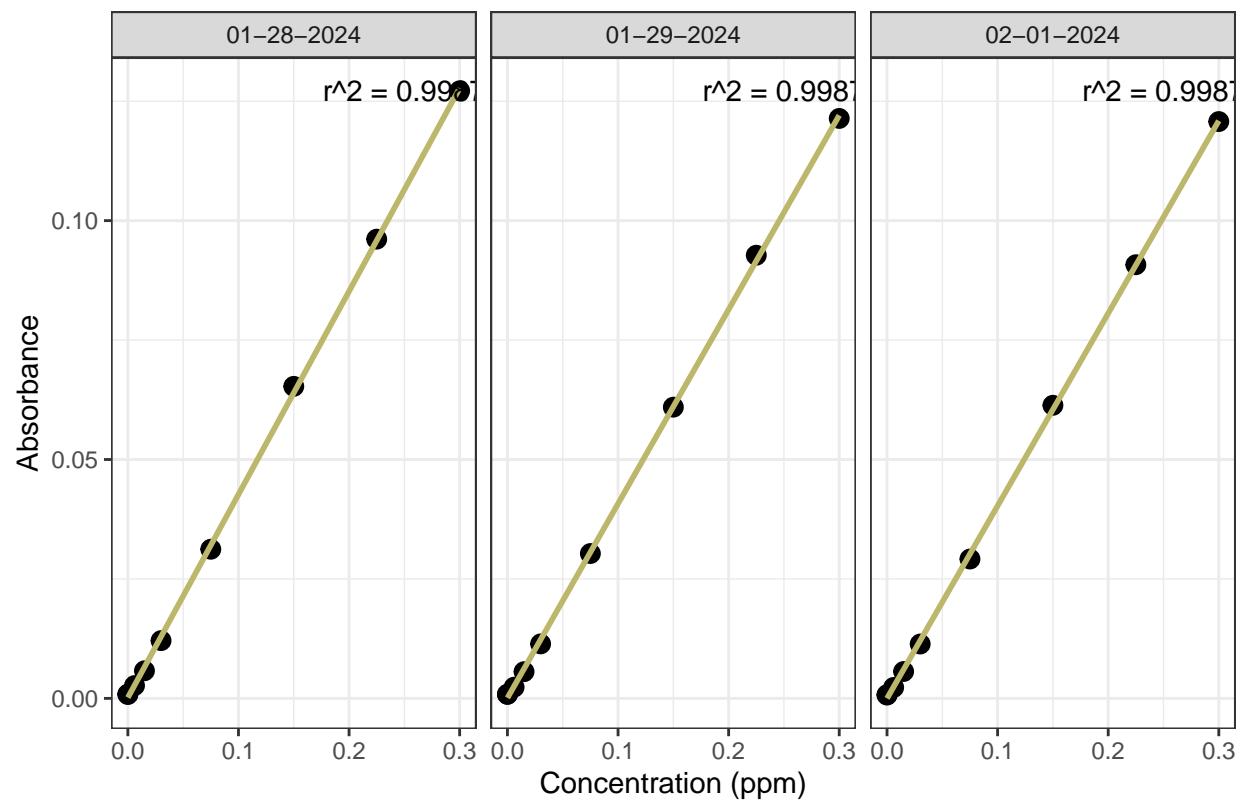
```
## `geom_smooth()` using formula = 'y ~ x'
```

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."
```

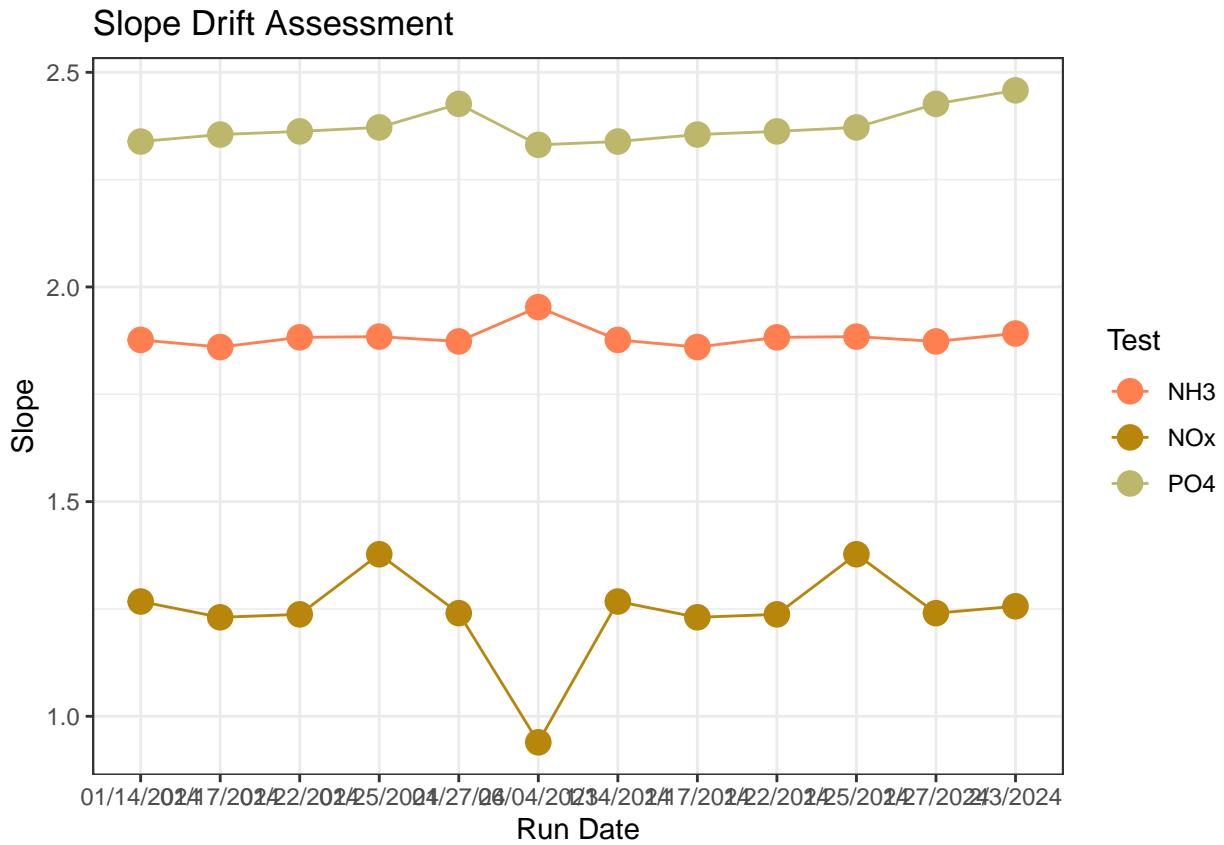


Table 1: Average Slope by Analyte

Test	avg_slope
NH3	1.883
NOx	1.242
PO4	2.375

0.3 Dilution Corrections - ensure the latest dilution is kept

```
## Dilution Corrections

## Duplicated samples: GCW_202310_TR_LysB_20cm, GCW_202310_WC_LysA_45cm, MSM_202310_TR_LysA_20cm, MSM_202310_WC_LysB_45cm

## 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 = 0.7126627
```

```
## Expected = 0.706
```

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

```
## Run mean = 1.482162
```

```
## Expected = 0.948
```

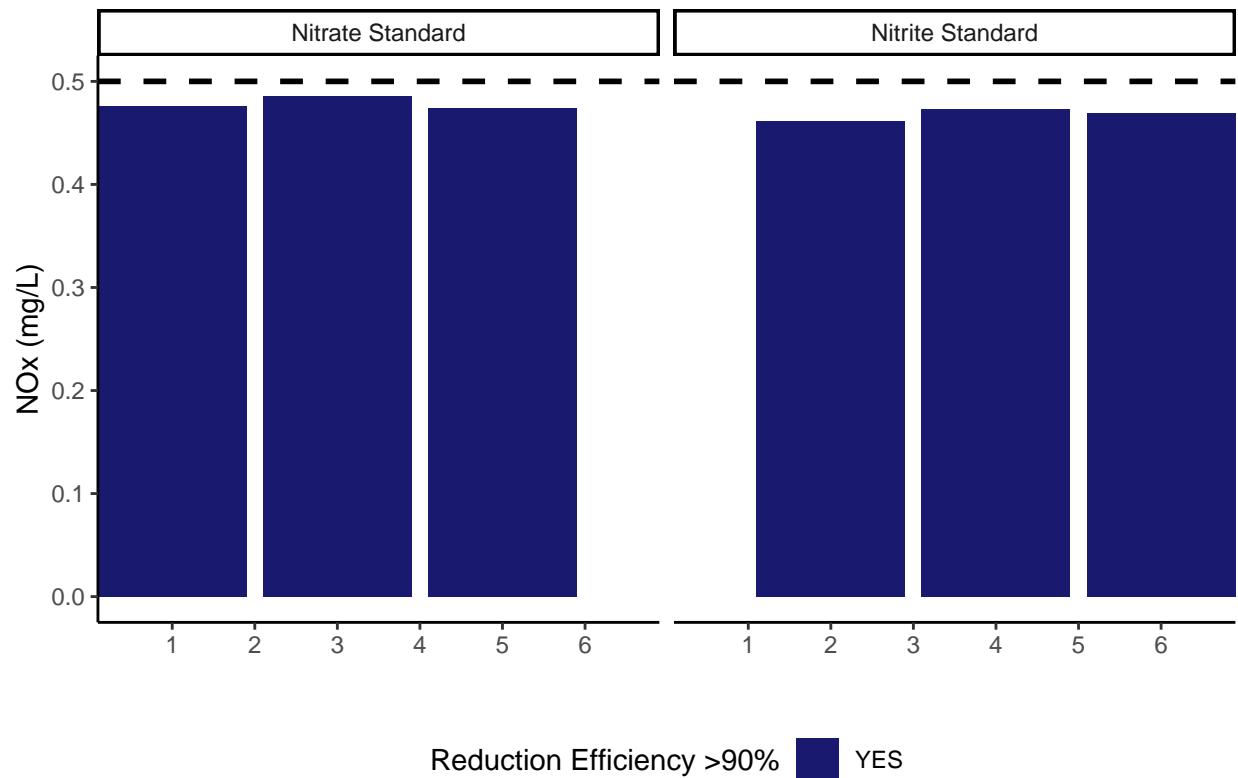
```
## [1] "PO4 pe Check has a % Difference <25% - PROCEED"
```

```
## Run mean = 0.9255853
```

```
## Expected = 0.818
```

```
#Check NOx Reduction Efficiency
```

```
## Assess Reduction Efficiency
```



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

```
## [1] 94.6084
```

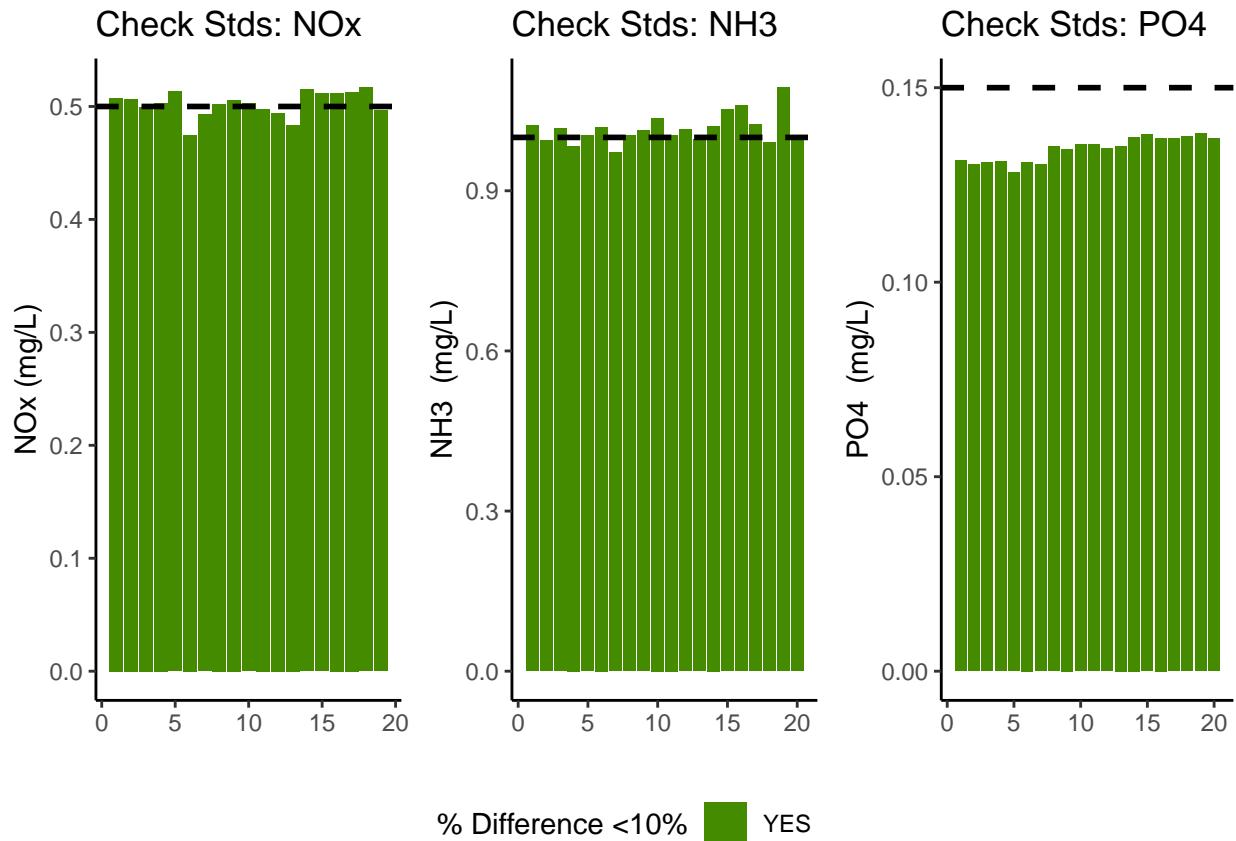
0.5 Analyze the Check Standards

```
## 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"
```

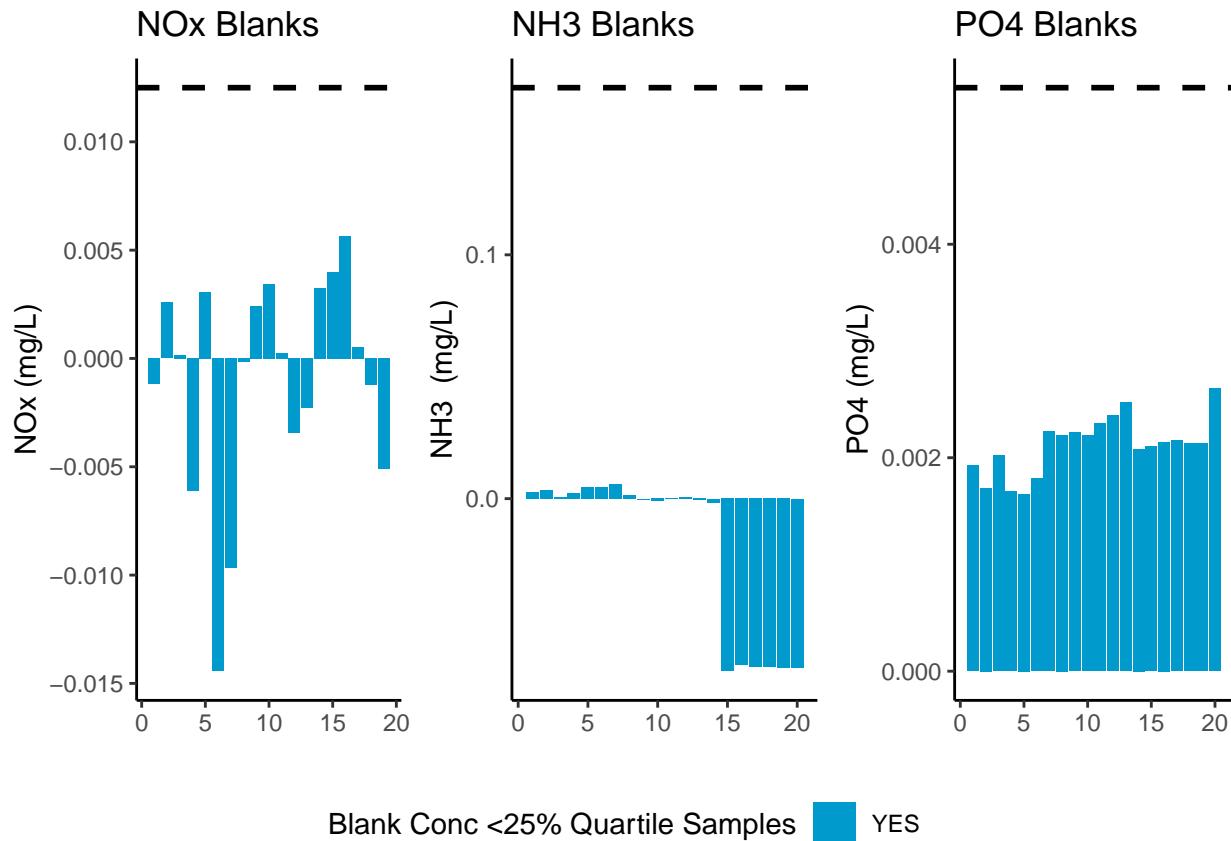


Table 2: Mean Concentration of Blanks

Test	Blank_Mean_Conc
NOx	-0.0010
NH3	-0.0196
PO4	0.0021

0.7 Analyze Duplicates

```

## Analyze Duplicates

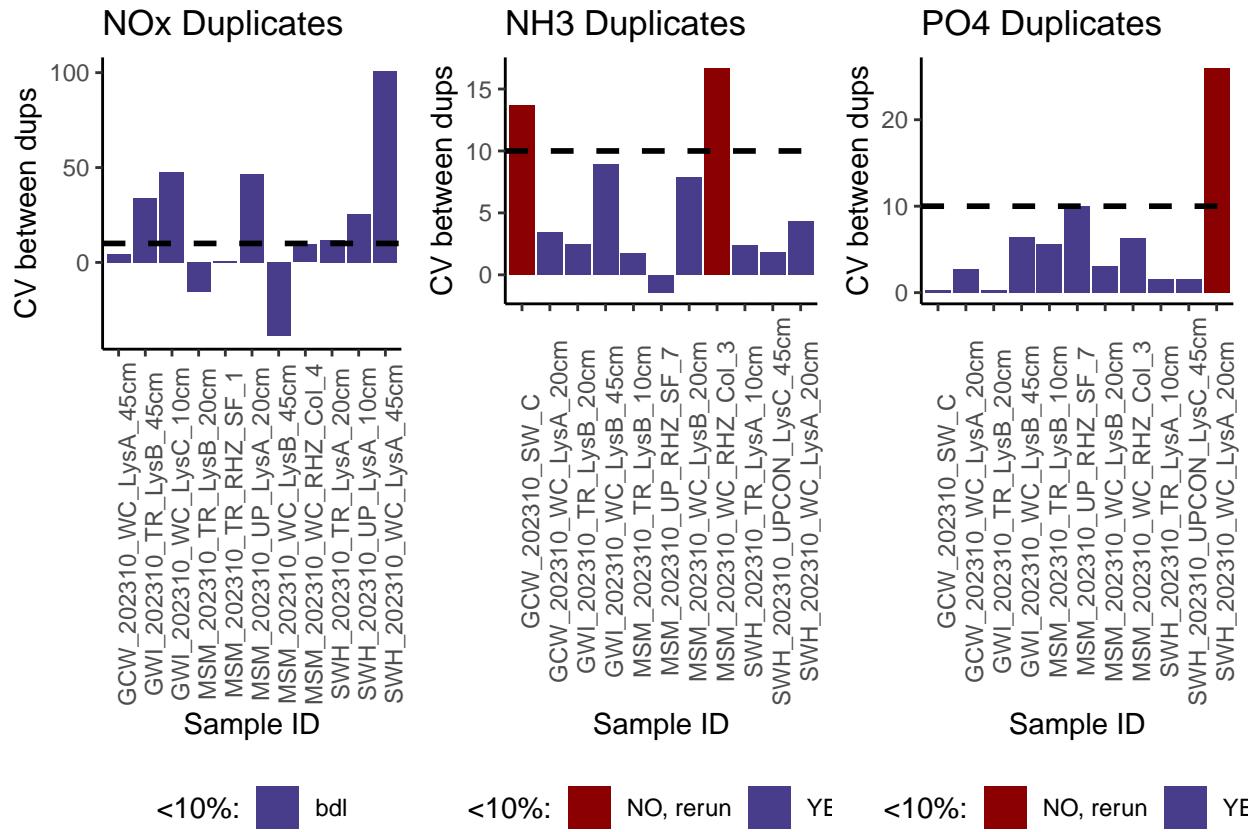
## [1] ">60% of NOx Duplicates have a CV <10% - PROCEED"

## [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.

```

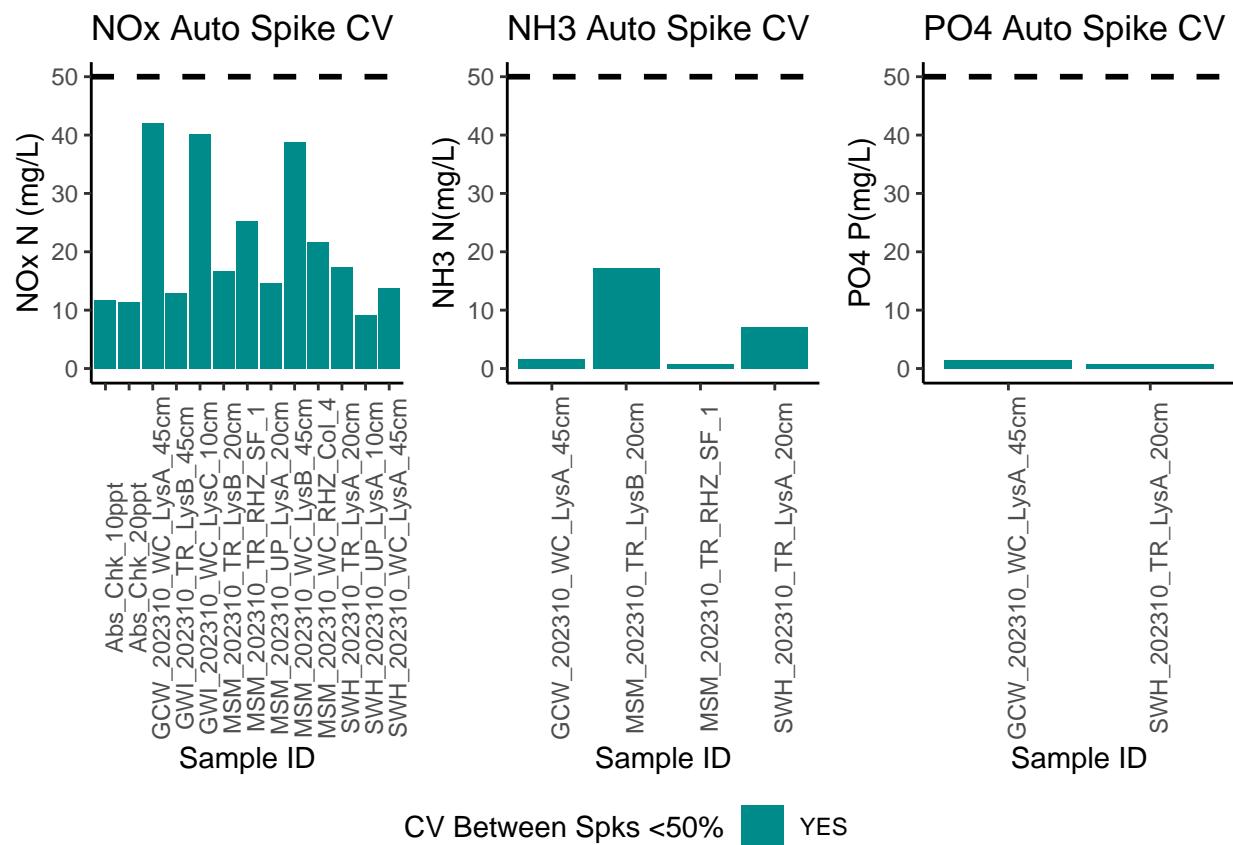


0.8 Spikes

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

```
## [1] ">60% of NH3 Spikes have a CV <50% - PROCEED"
```

```
## [1] ">60% of PO4 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 [17, 18, 19, 44,  
## 45, 46, 83, 84, 85, 107, 108, 109, 124, 125, 126, 146, 147, 148, 163, 164,  
## ...].
```

0.13 Pulling Rhizon Samples

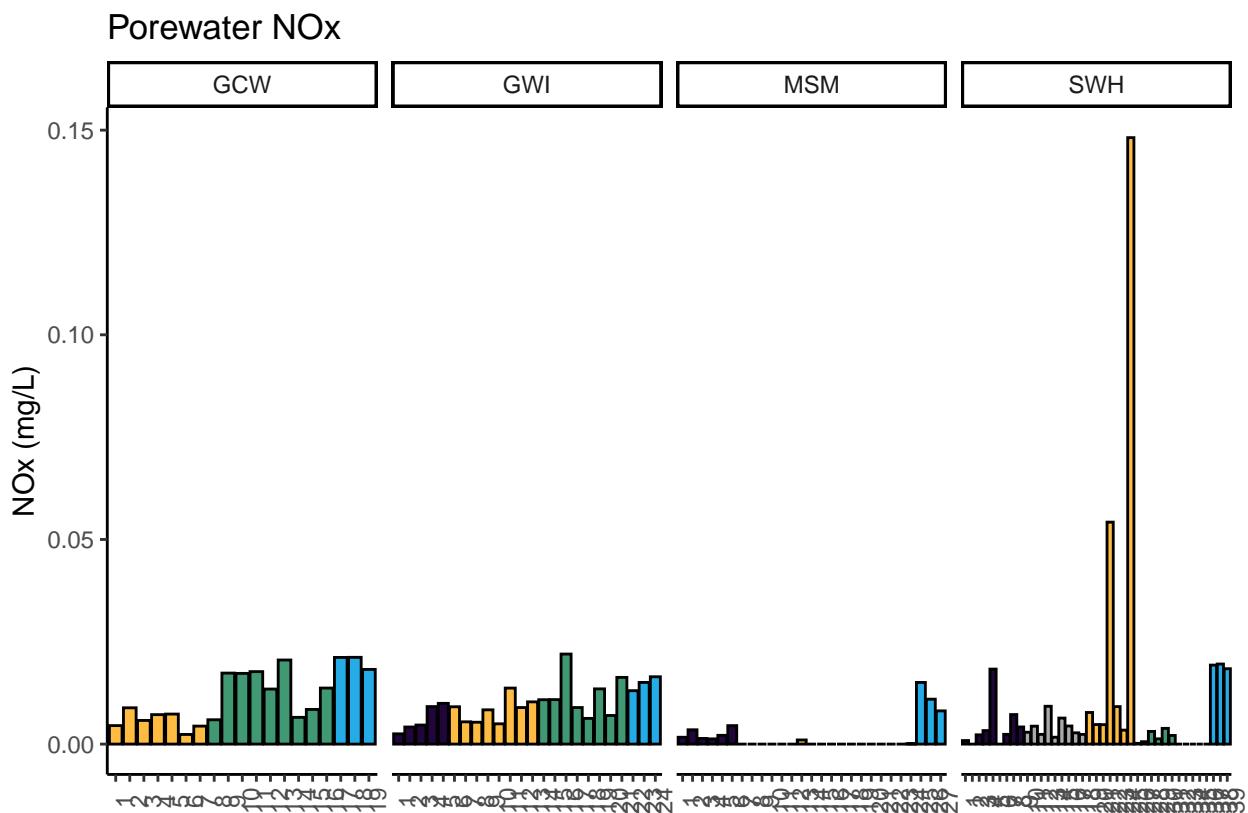
0.14 Check to see if samples run match metadata & merge info

```
## Check Sample IDs with Metadata  
  
## All sample IDs are present in metadata.
```

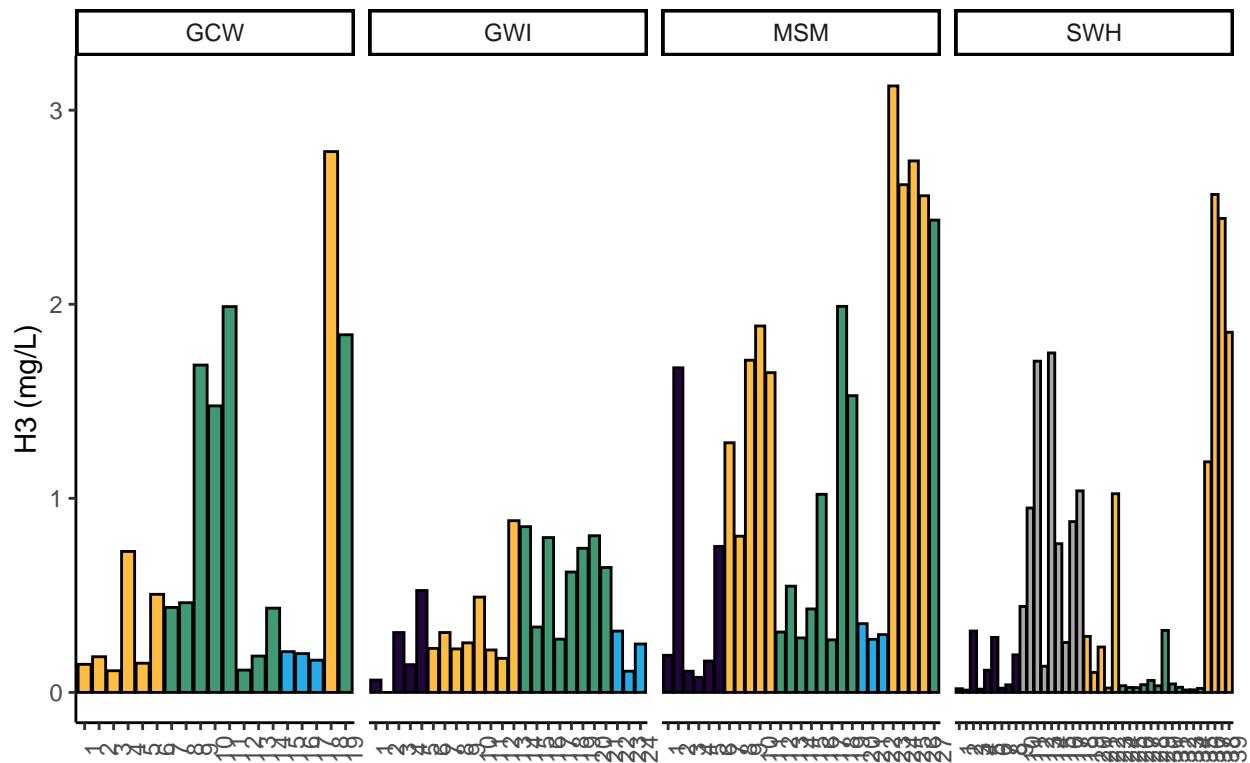
```
## Warning: Expected 5 pieces. Missing pieces filled with 'NA' in 36 rows [17, 18, 19, 44,  
## 45, 46, 83, 84, 85, 107, 108, 109, 124, 125, 126, 146, 147, 148, 163, 164,  
## ...].
```

0.15 Visualize Data

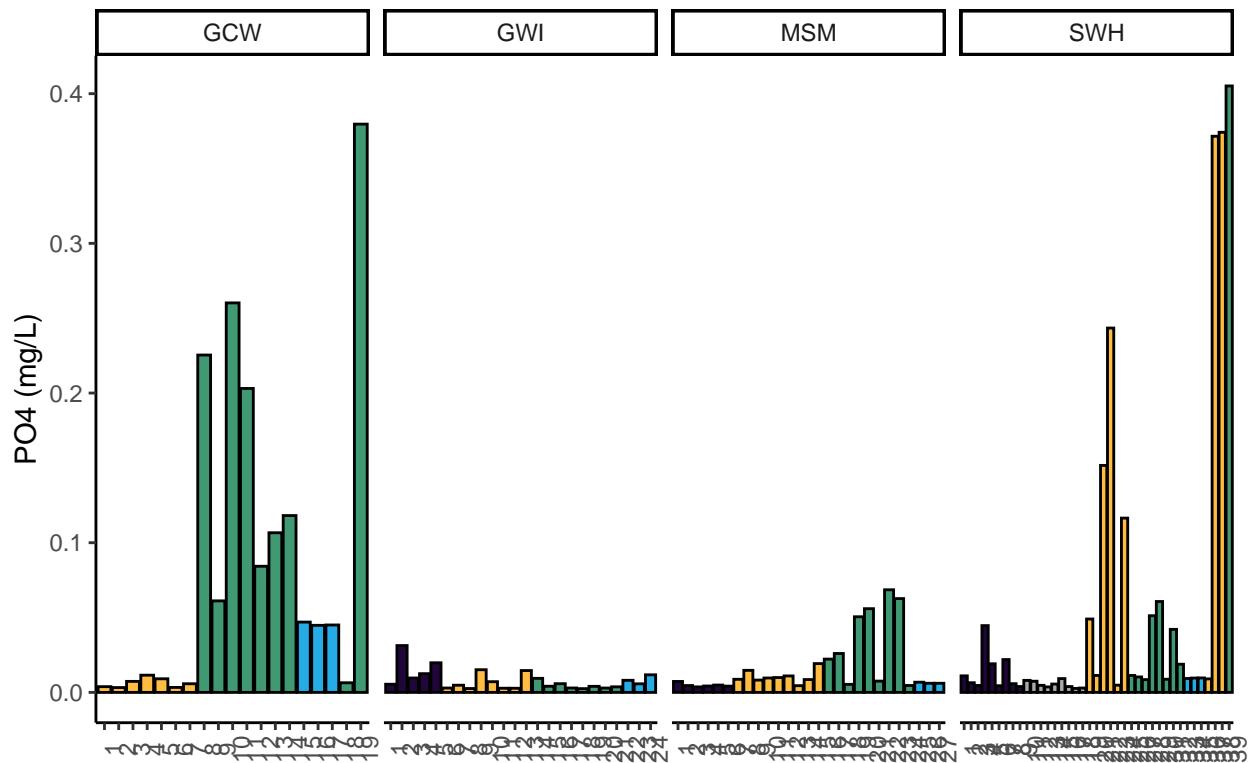
```
## Visualize Data
```



Porewater NH₃



Porewater PO4



0.16 Export Processed Data

#end