

Synoptic CB: Porewater Nutrients

April 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 <- "20230604"
sample_year <- 2023
sample_month <- 04
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_April2023_1.csv",
              "Raw Data/SEAL_COMPASS_Synoptic_NOx_April2023_TEMPEST_May2023_2.csv")
NH3_P04_files <- c("Raw Data/SEAL_COMPASS_Synoptic_NH3_P04_April2023_1.csv",
                    "Raw Data/SEAL_COMPASS_Synoptic_NH3_P04_April2023_TEMPEST_May2023_2.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_202304.csv"

#record any notes about the run or anything other info here:
run_notes <- "NH3 3rd Party Check off, but all other run
parameters are fine so accepting this run.
NOx duplicates out of range due to low sample concentrations.
"

#samples to remove:
remove <- c("GCW_202304_TR_LysB_10cm_11", "GCW_202304_TR_LysB_20cm_13")
#these were put on the run twice and can be removed

#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)

## NH3 3rd Party Check off, but all other run
## parameters are fine so accepting this run.
## NOx duplicates out of range due to low sample concentrations.
## 

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

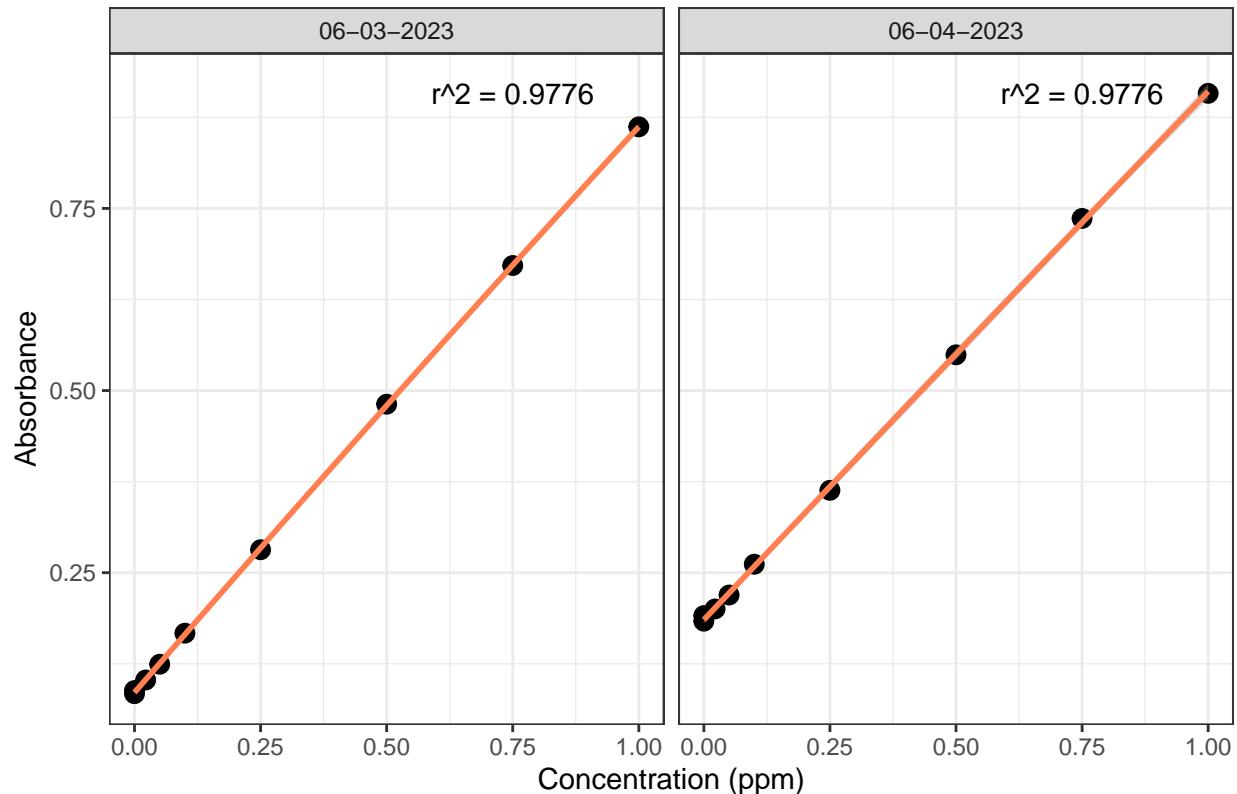
```

0.1 Import Data & Clean

0.2 Assessing standard Curves

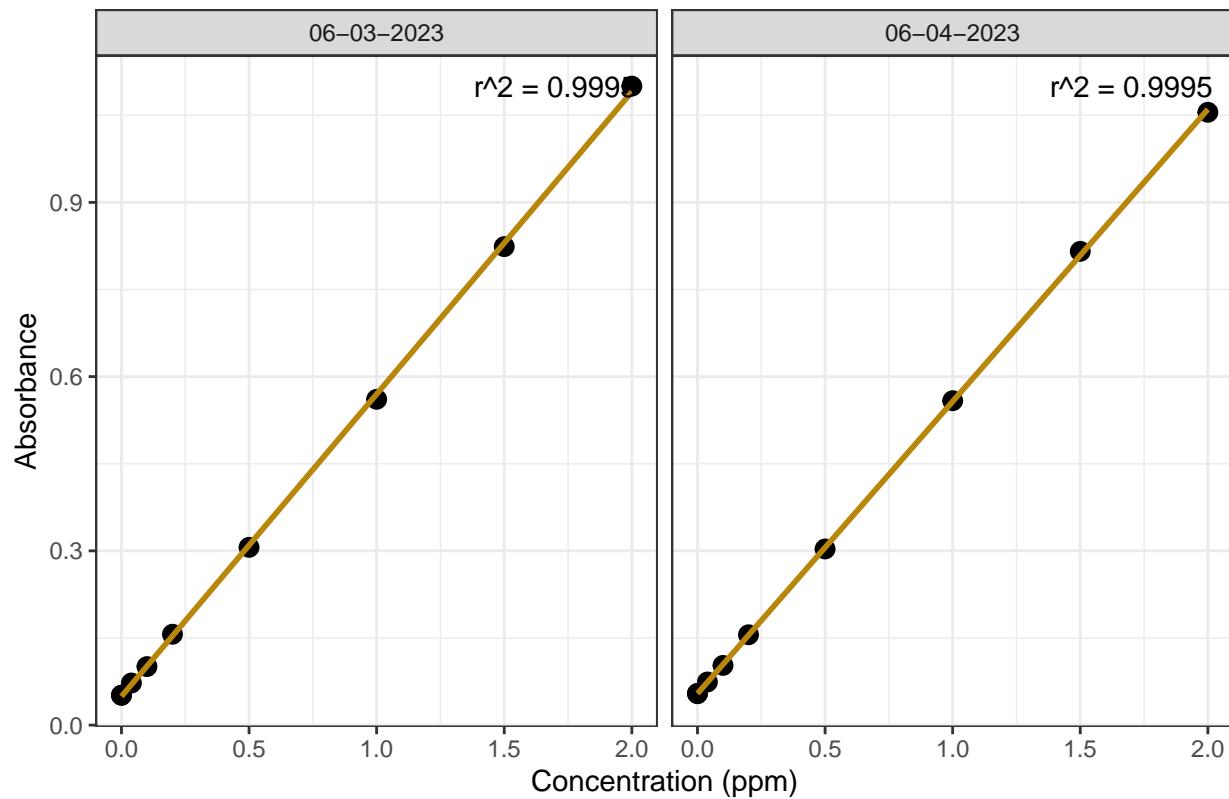
```
#Pull out standards data  
  
## Assess Standard Curves  
  
#Plot standards data  
  
## Assess Standard Curves
```

NOx Standard Curve



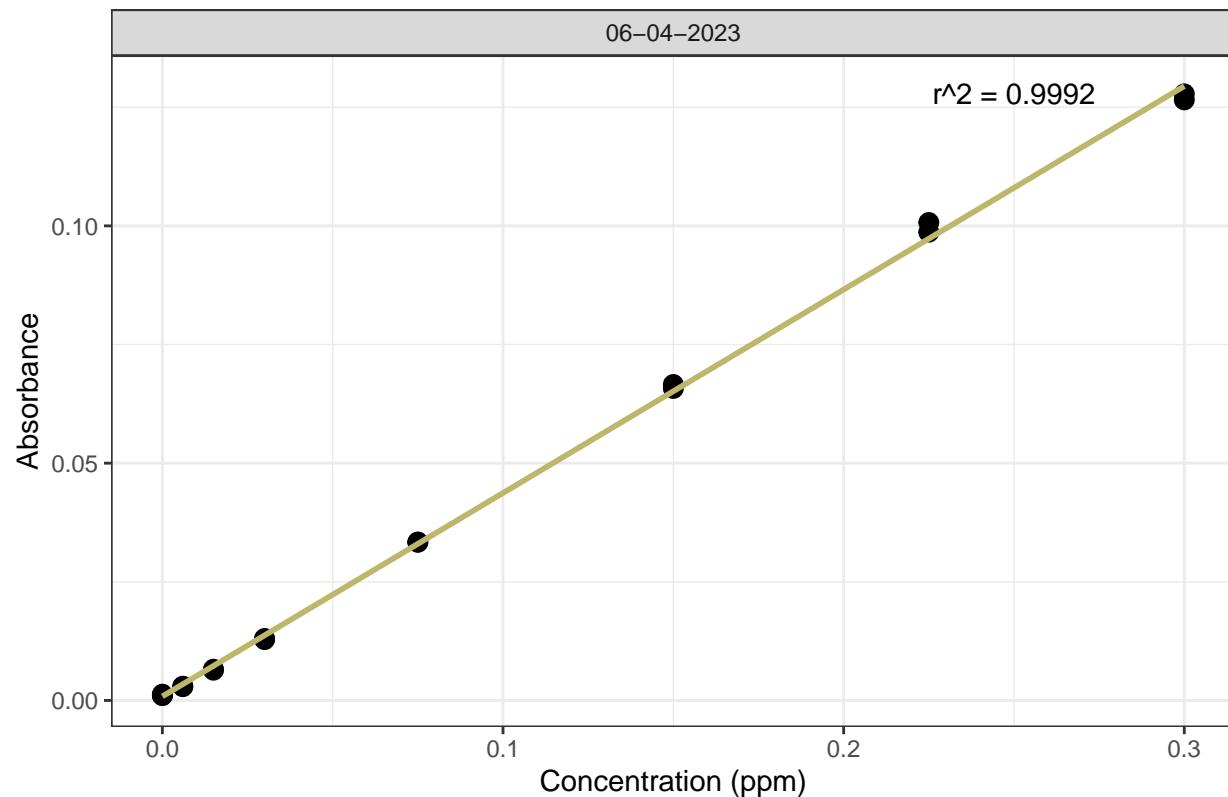
```
## `geom_smooth()` using formula = 'y ~ x'
```

NH3 Standard Curve



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

PO4 Standard Curve



```
## [1] "NOx Curve r2 is below cutoff! - REASSESS"  
## [1] "NH3 Curve r2 GOOD - PROCEED"  
## [1] "PO4 Curve r2 GOOD - PROCEED"  
## [1] "QAQC log file exists and has been read into the code."  
## `geom_line()`: Each group consists of only one observation.  
## i Do you need to adjust the group aesthetic?
```

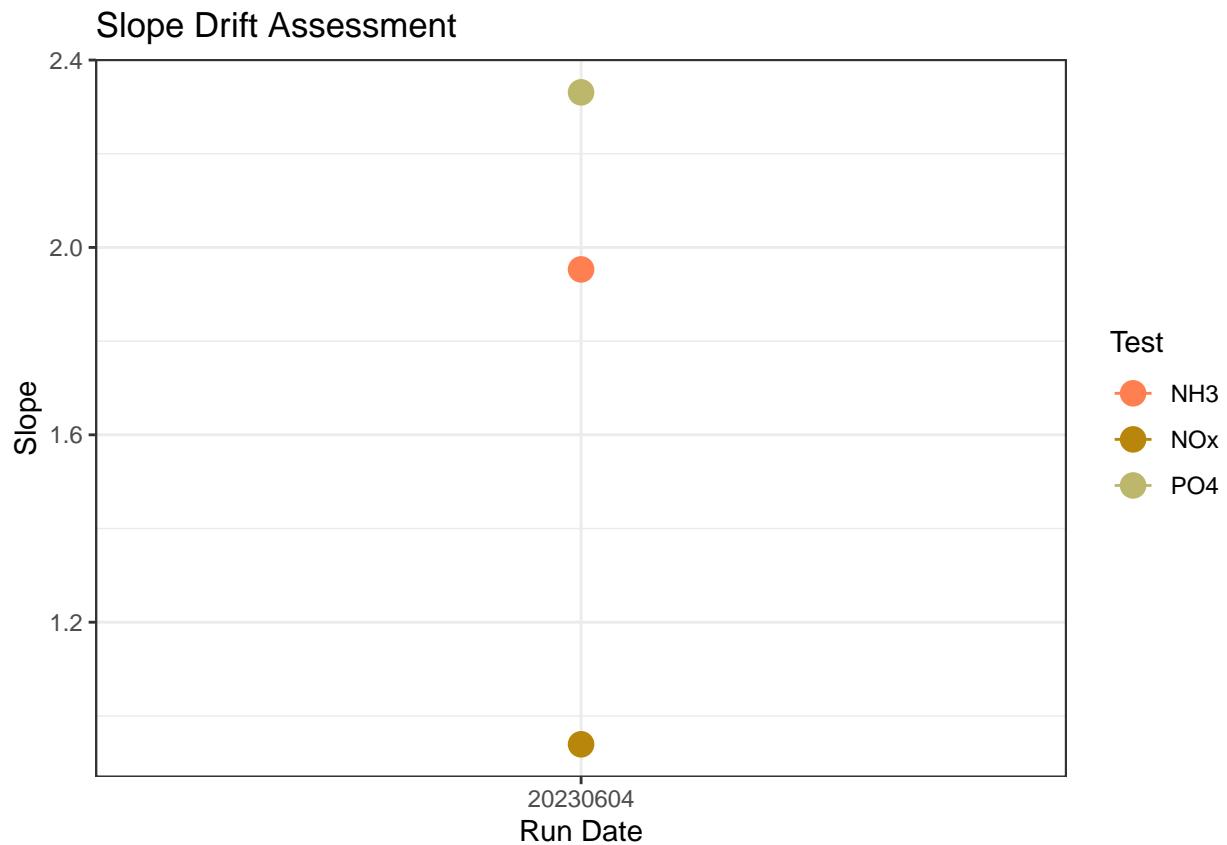


Table 1: Average Slope by Analyte

Test	avg_slope
NH3	1.953
NOx	0.939
PO4	2.331

0.3 Dilution Corrections - ensure the latest dilution is kept

```
## Dilution Corrections

## Duplicated samples: TEMPEST_20230513_CON_C6, MSM_202304_WC_LysC_45cm

## Duplicated samples with NO dilution present (possible input error): TEMPEST_20230513_CON_C6
```

0.4 Performance Check

```
## [1] NA

## Run mean = NaN

## Expected = 0.706

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

## Run mean = 1.257933

## Expected = 0.948

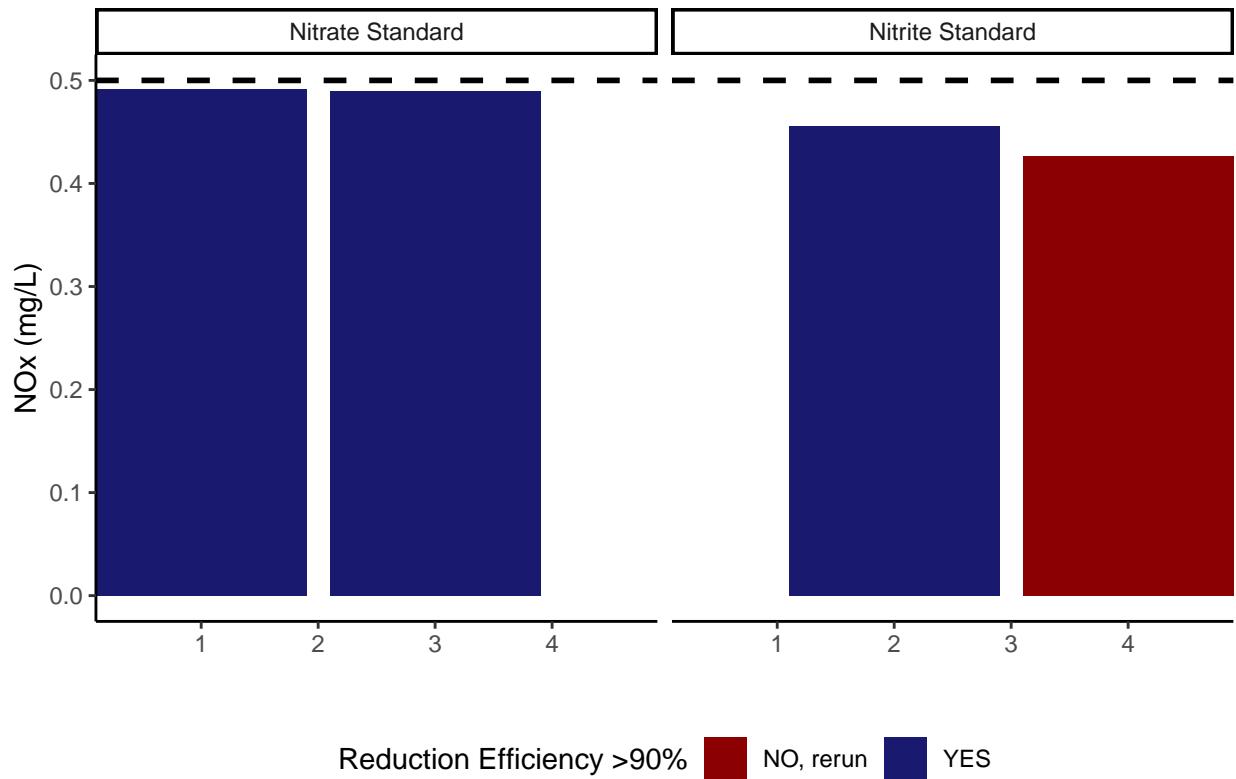
## [1] "PO4 pe Check has a % Difference <20% - PROCEED"

## Run mean = 0.873426

## Expected = 0.818
```

```
#Check NOx Reduction Efficiency
```

```
## Assess Reduction Efficiency
```



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

```
## [1] 93.1661
```

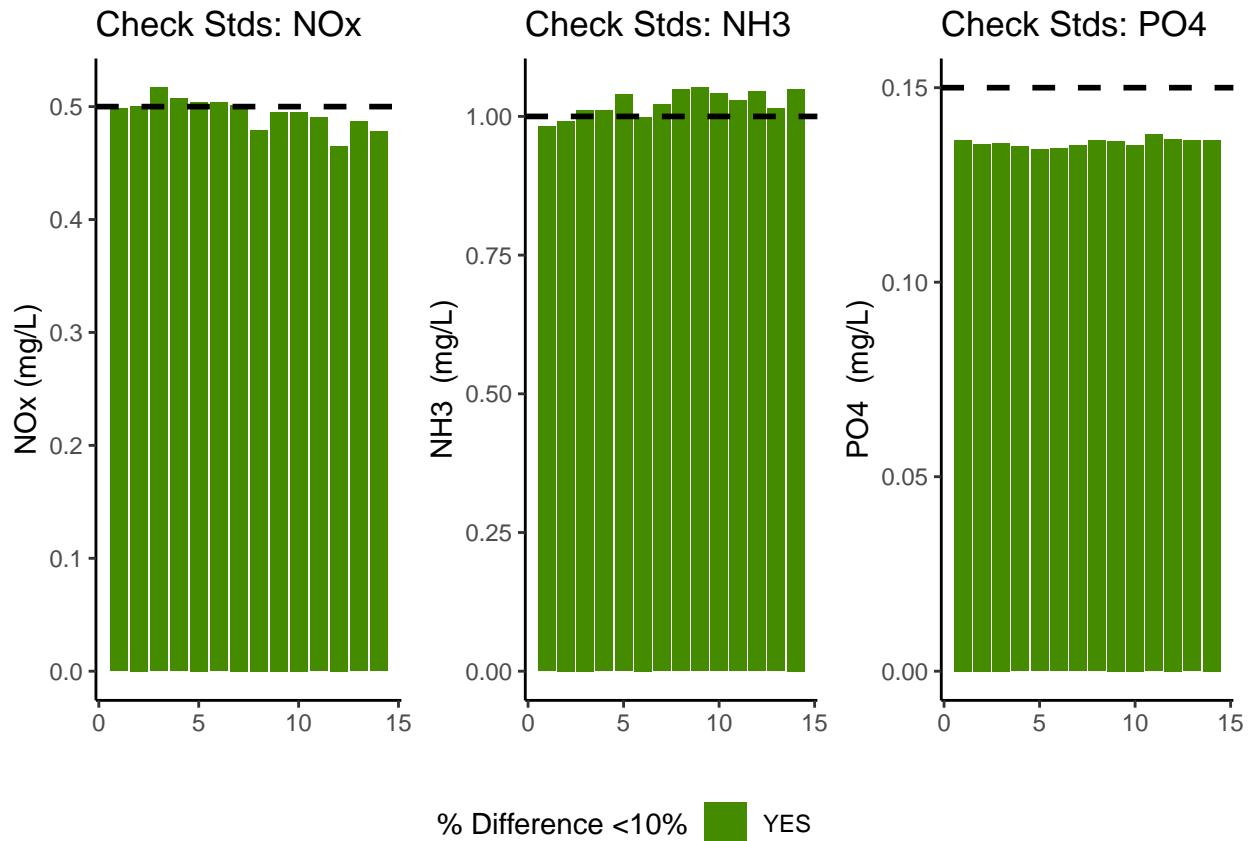
0.5 Analyze the Check Standards

```
## 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"
```

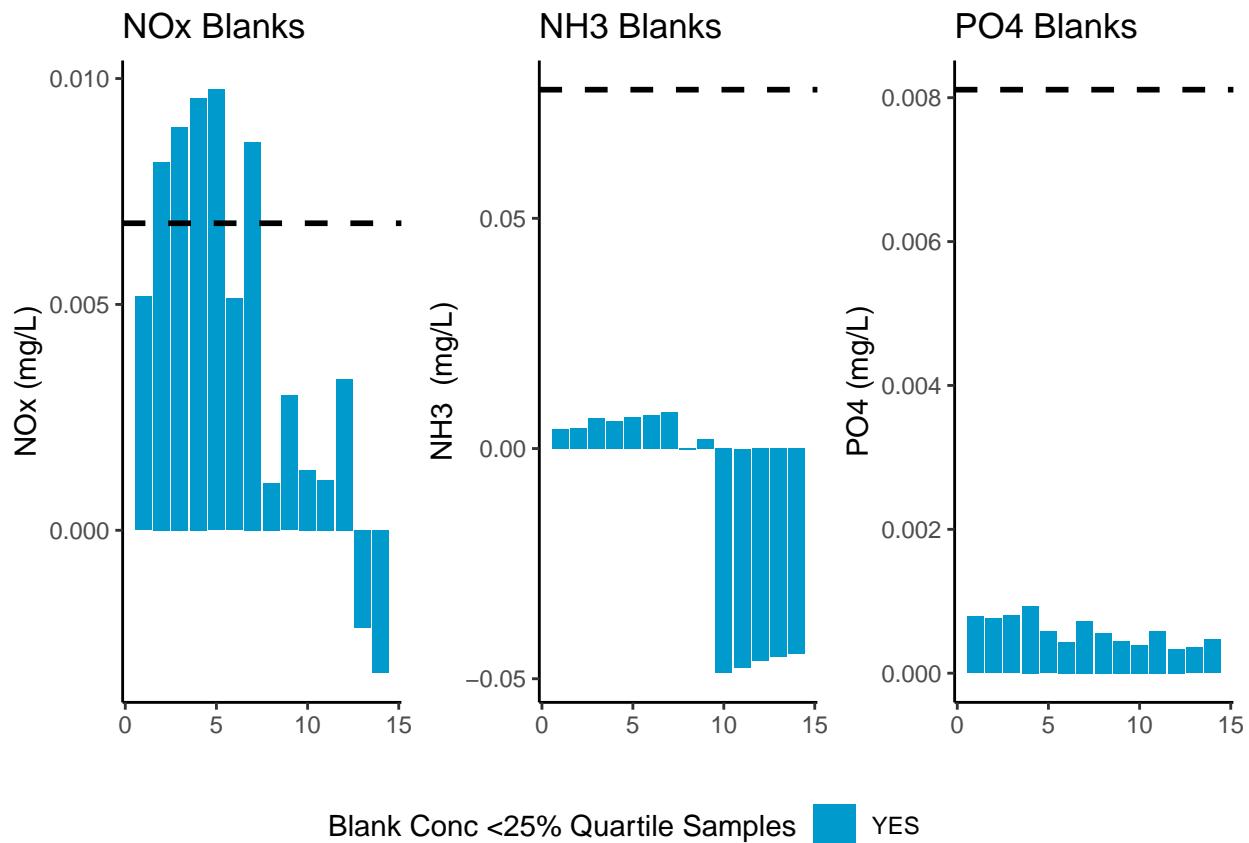


Table 2: Mean Concentration of Blanks

Test	Blank_Mean_Conc
NOx	0.0043
NH3	-0.0134
PO4	0.0006

0.7 Analyze Duplicates

```
## Analyze Duplicates

## Warning: Returning more (or less) than 1 row per `summarise()`' group was deprecated in
## dplyr 1.1.0.
## i Please use `reframe()` instead.
## i When switching from `summarise()` to `reframe()`, remember that `reframe()`
##   always returns an ungrouped data frame and adjust accordingly.
## Call `lifecycle::last_lifecycle_warnings()` to see where this warning was
## generated.

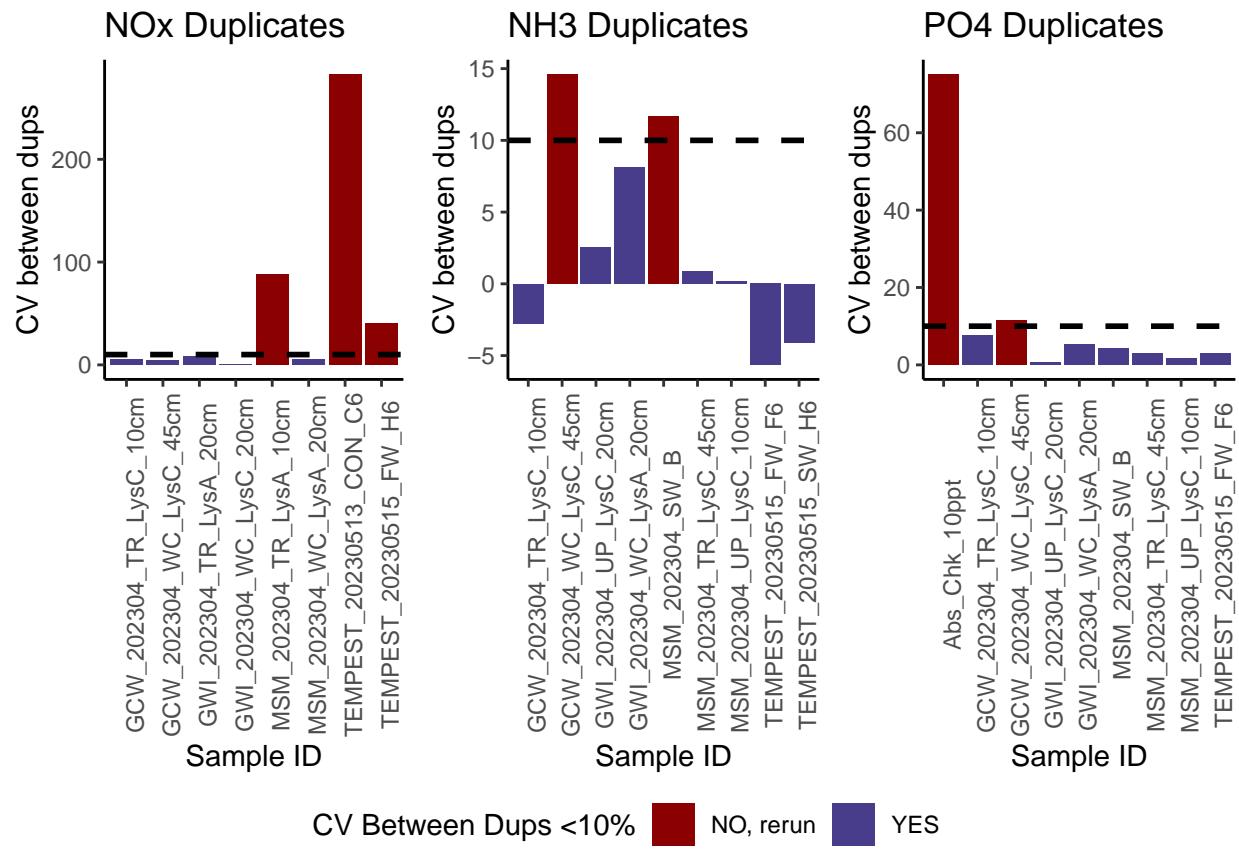
## Warning: Returning more (or less) than 1 row per `summarise()`' group was deprecated in
## dplyr 1.1.0.
## i Please use `reframe()` instead.
## i When switching from `summarise()` to `reframe()`, remember that `reframe()`
##   always returns an ungrouped data frame and adjust accordingly.
## Call `lifecycle::last_lifecycle_warnings()` to see where this warning was
## generated.

## [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.
```

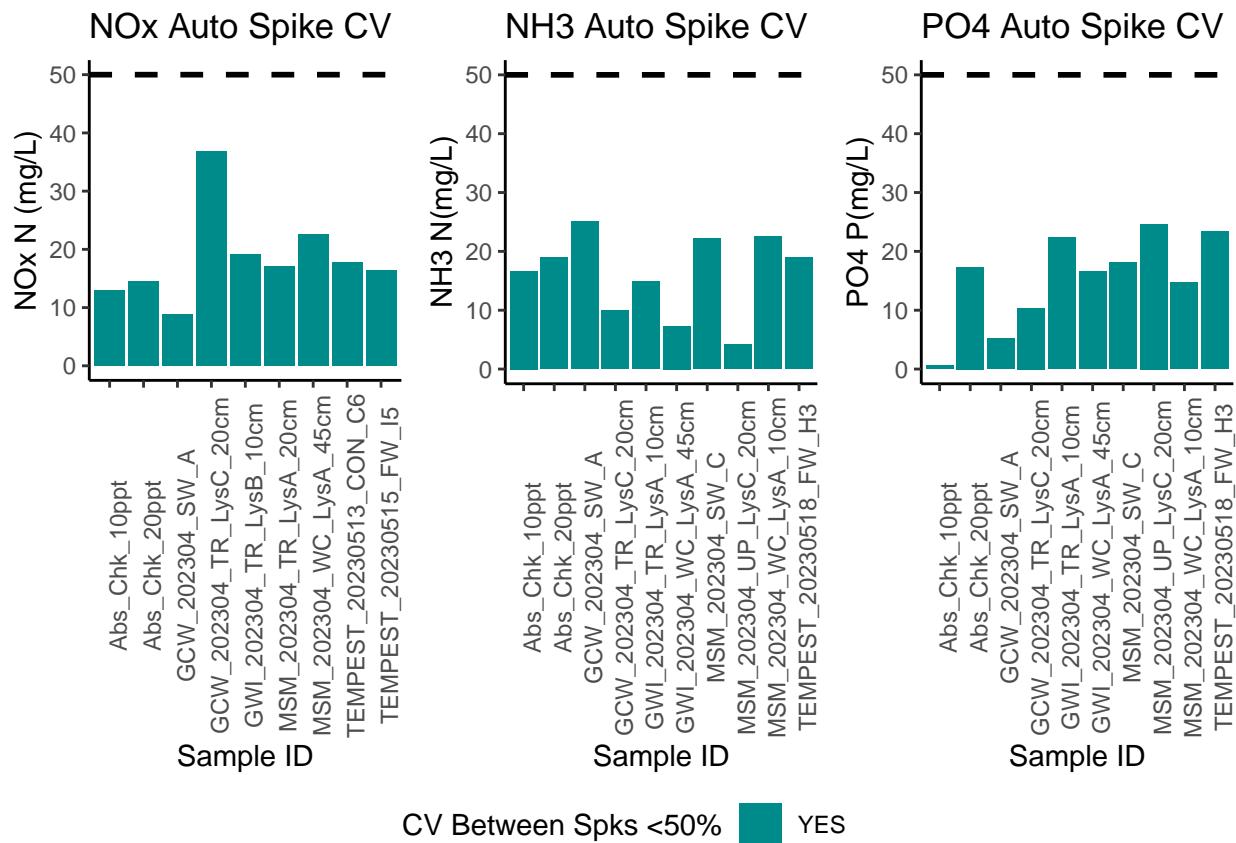


0.8 Spikes

```
## [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 27 rows [21, 22, 23, 46,  
## 47, 48, 72, 73, 74, 95, 96, 97, 141, 142, 143, 167, 168, 169, 193, 194, ...].
```

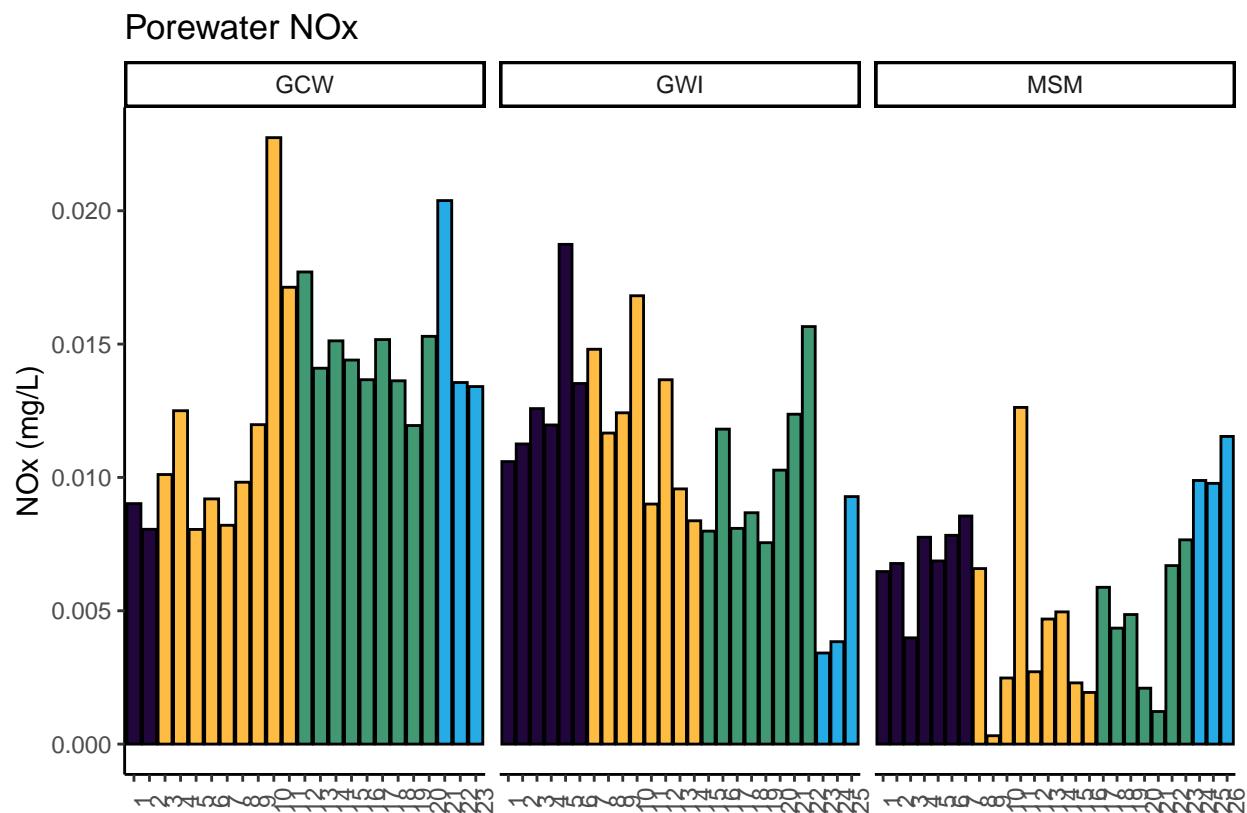
0.13 Pulling Rhizon Samples

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

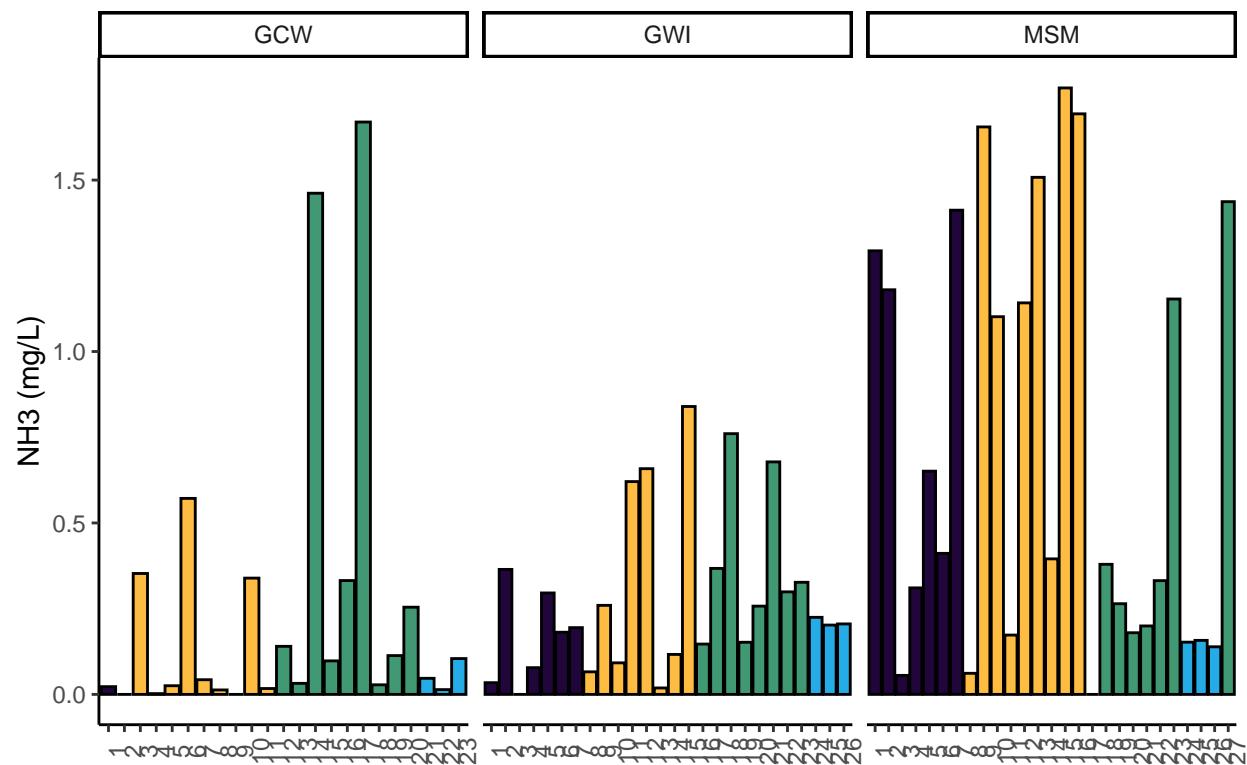
```
## Check Sample IDs with Metadata  
  
## All sample IDs are present in metadata.  
  
## Warning: Expected 5 pieces. Missing pieces filled with 'NA' in 27 rows [21, 22, 23, 46,  
## 47, 48, 72, 73, 74, 95, 96, 97, 141, 142, 143, 167, 168, 169, 193, 194, ...].
```

0.15 Visualize Data

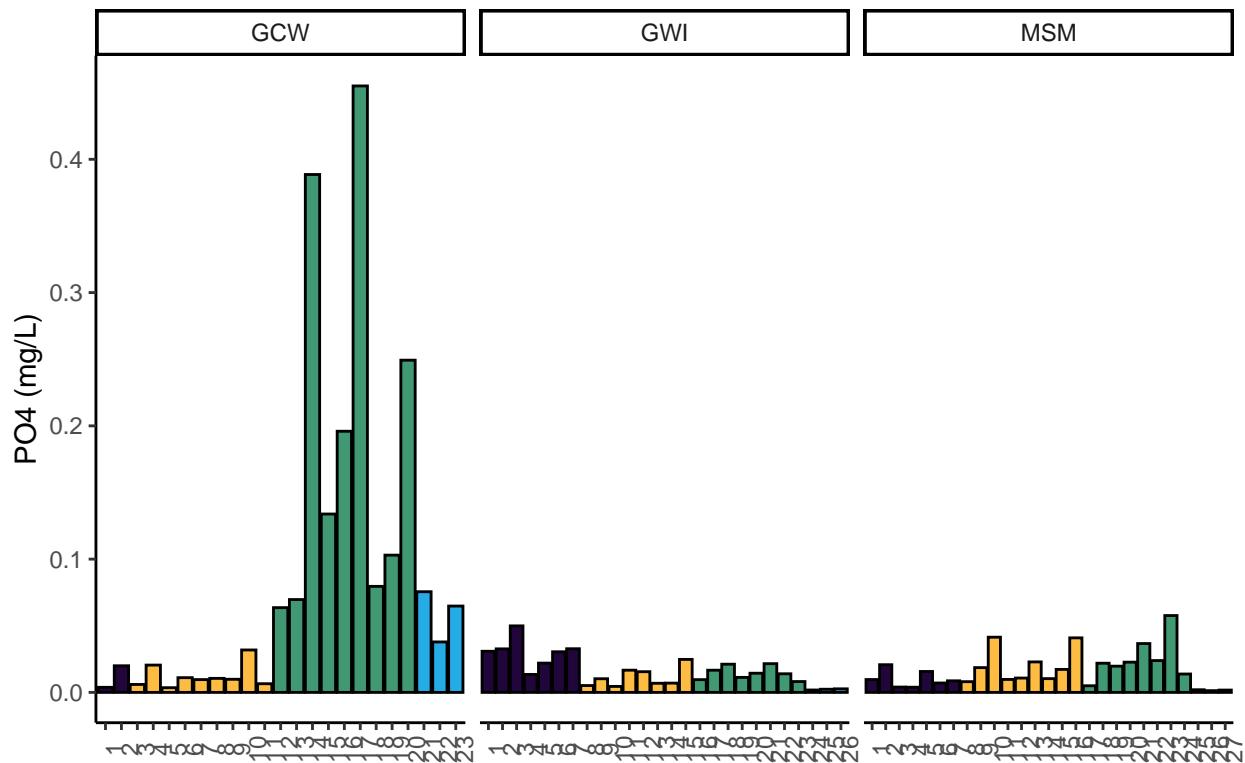
```
## Visualize Data
```



Porewater NH3



Porewater PO4



0.16 Export Processed Data

#end