

Synoptic CB: Porewater Nutrients

November 2024 Samples

2025-10-31

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```

##Run Information

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

## Run Information: NAME

#set the run date & user name
run_date <- "8/7/2025"
sample_year <- "2024"
sample_month <- "NOVEMBER"
user <- "Isabelle Van Benschoten"

##Data entered incorrectly
Old_ID_1 <- "SWH_202411_SWAMP_LycC_45cm"
New_ID_1 <- "SWH_202411_SWAMP_LysC_45cm"

#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/COMPASS_Synoptic_CB_202411_VNOx_1.csv",
               "Raw Data/COMPASS_Synoptic_CB_202411_VNOx_2.csv",
               "Raw Data/COMPASS_Synoptic_CB_202411_VNOx_3.csv")
NH3_P04_files <- c("Raw Data/COMPASS_Synoptic_CB_202411_NH3_P04_1.csv",
                    "Raw Data/COMPASS_Synoptic_CB_202411_NH3_P04_2.csv",
                    "Raw Data/COMPASS_Synoptic_CB_202411_NH3_P04_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_2024.csv"
final_path <- "Processed Data/COMPASS_Synoptic_Nutrients_202411.csv"

#record any notes about the run or anything other info here:
run_notes <- "One P04 check standard came back very high, all others were within range.
                A few duplicates were out of range but still within CV.
                SWH_202411_SWAMP_LycC_45cm, SWH_202411_TR_LysC_10cm,
                MSM_202411_TR_LysC_10cm, MSM_202411_TR_LysC_45cm were missing from metadata. "

#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_2024.csv"

cat(run_notes)

## One P04 check standard came back very high, all others were within range.
## A few duplicates were out of range but still within CV.
## SWH_202411_SWAMP_LycC_45cm, SWH_202411_TR_LysC_10cm,
## MSM_202411_TR_LysC_10cm, MSM_202411_TR_LysC_45cm were missing from metadata.

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

```

0.1 Import Data & Clean

```
##Fix data entered incorrectly
```

```
#####Fix Sample IDs#####
df_all$Sample_Name <- str_replace(df_all$Sample_Name, Old_ID_1, New_ID_1)
```

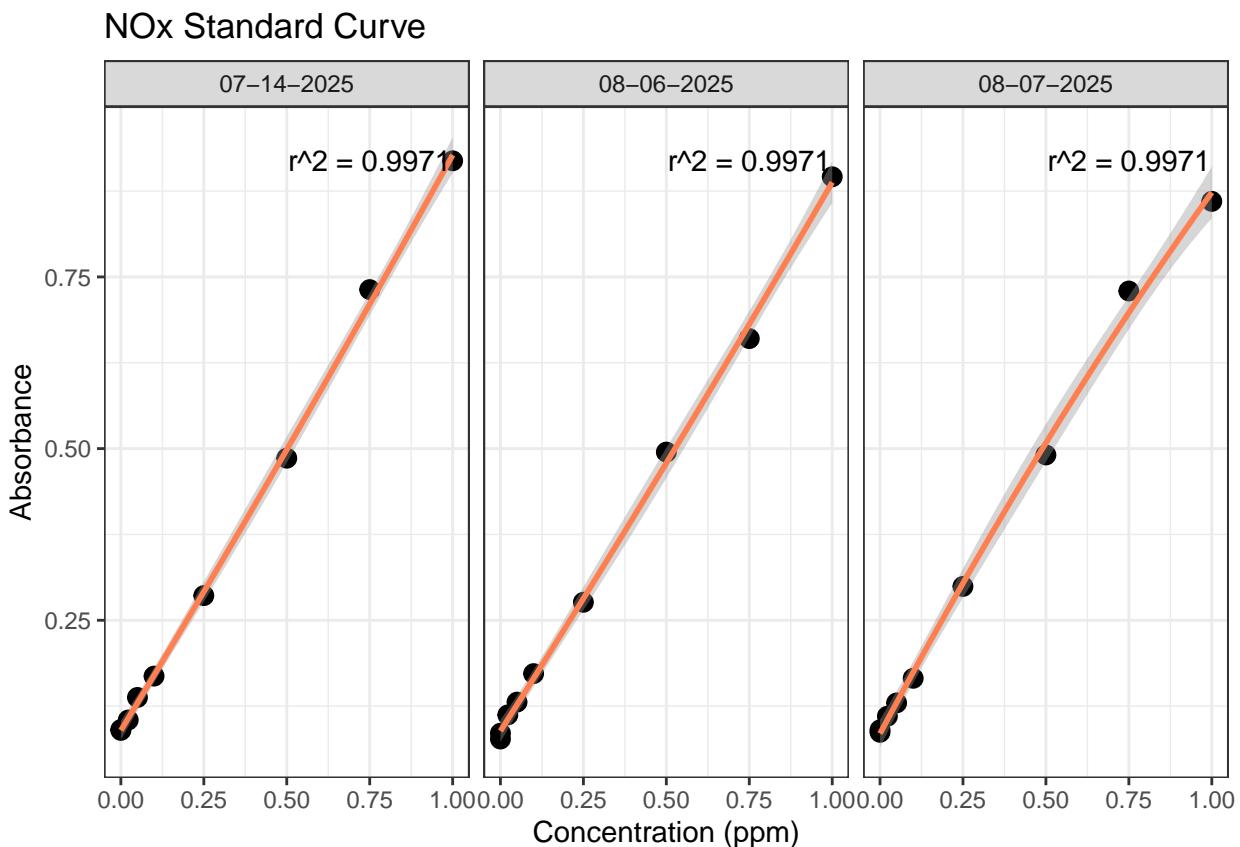
0.2 Assessing standard Curves

```
#Pull out standards data
```

```
## Assess Standard Curves
```

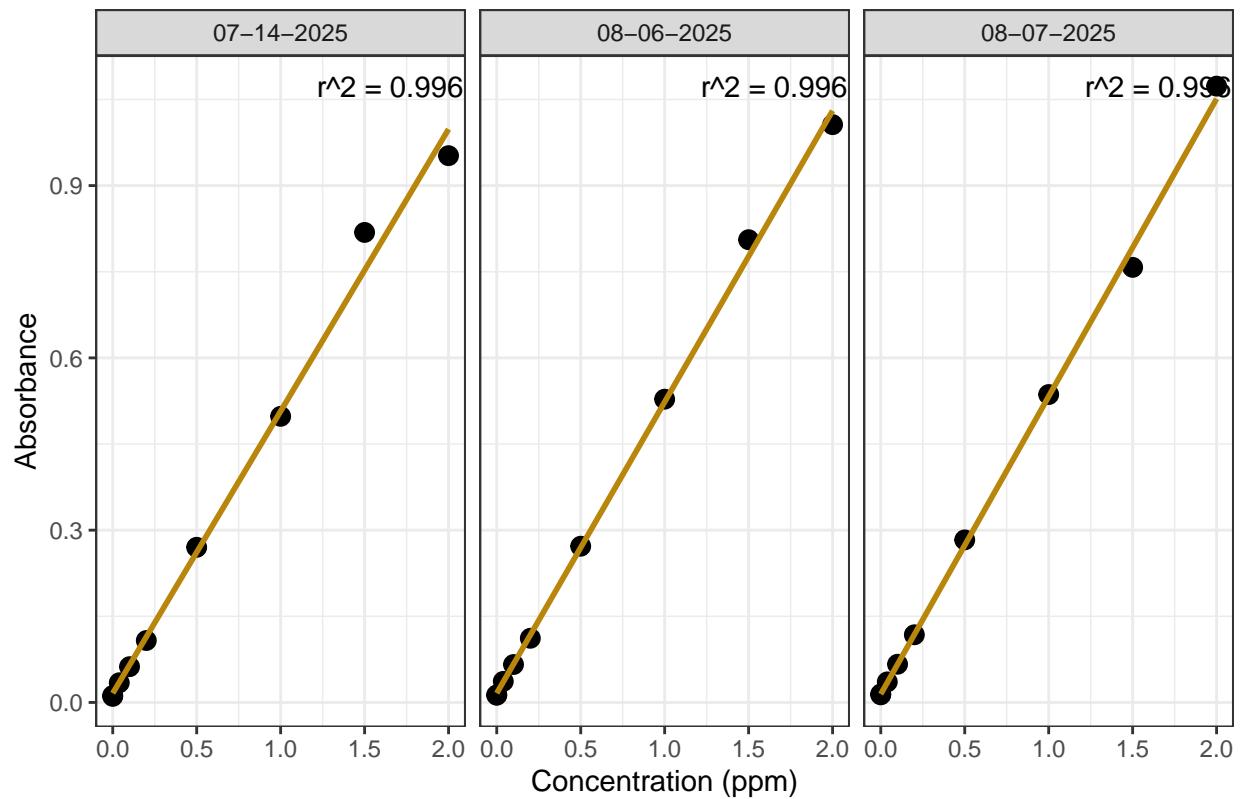
```
#Plot standards data
```

```
## Assess Standard Curves
```



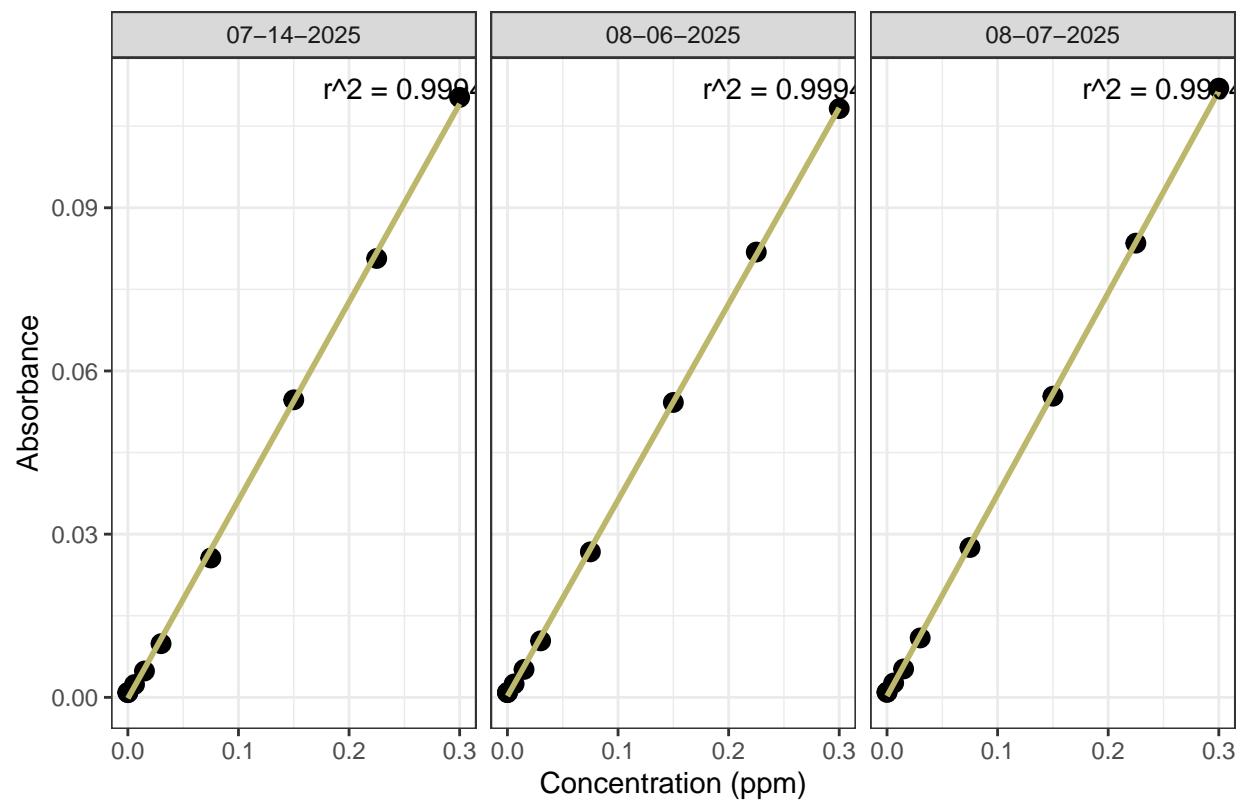
```
## `geom_smooth()` using formula = 'y ~ x'
```

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

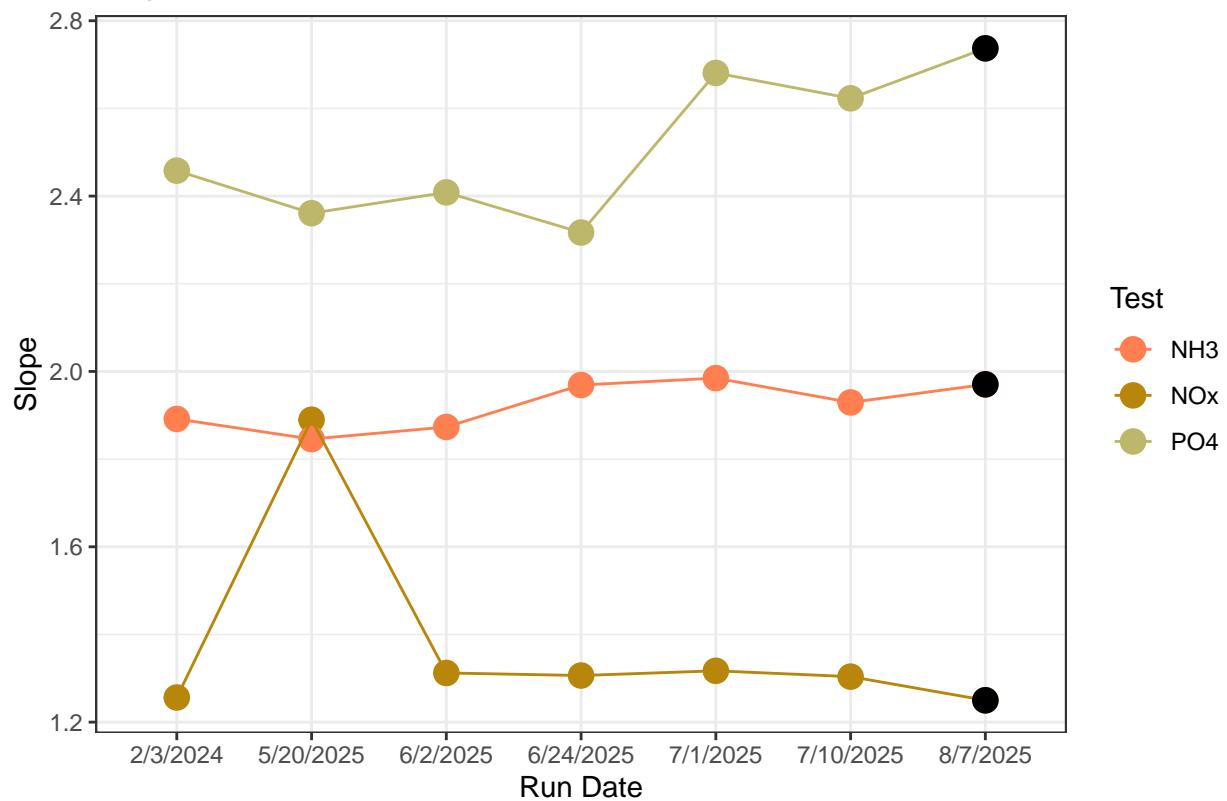


Table 1: Average Slope by Analyte

Test	avg_slope
NH3	1.923
NOx	1.376
PO4	2.512

0.3 Dilution Corrections - ensure the latest dilution is kept

```
## Dilution Corrections

## Duplicated samples: GCW_202411_WC_LysB_10cm, MSM_202411_TR_LysA_20cm, MSM_202411_TR_LysB_20cm, MSM_202411_TR_LysB_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 = 1.57518

## Expected = 1.51

## [1] "NH3 pe Check has a % Difference <25% - PROCEED"

## Run mean = 1.209981

## Expected = 1.034

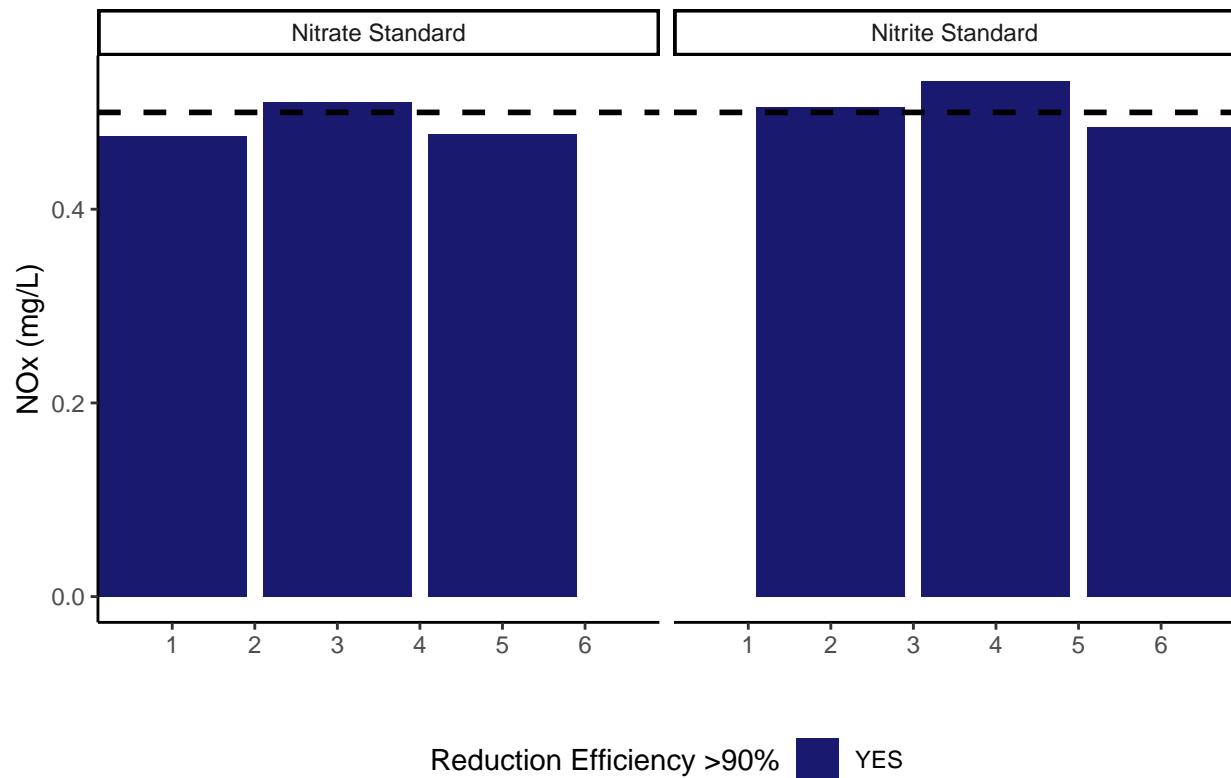
## [1] "PO4 pe Check has a % Difference <25% - PROCEED"

## Run mean = 0.8969137

## Expected = 0.824

##Check NOx Reduction Efficiency

## Assess Reduction Efficiency
```



```
## [1] "Mean NOx Reduction Efficiency >95% - PROCEED"
```

```
## [1] 99.48873
```

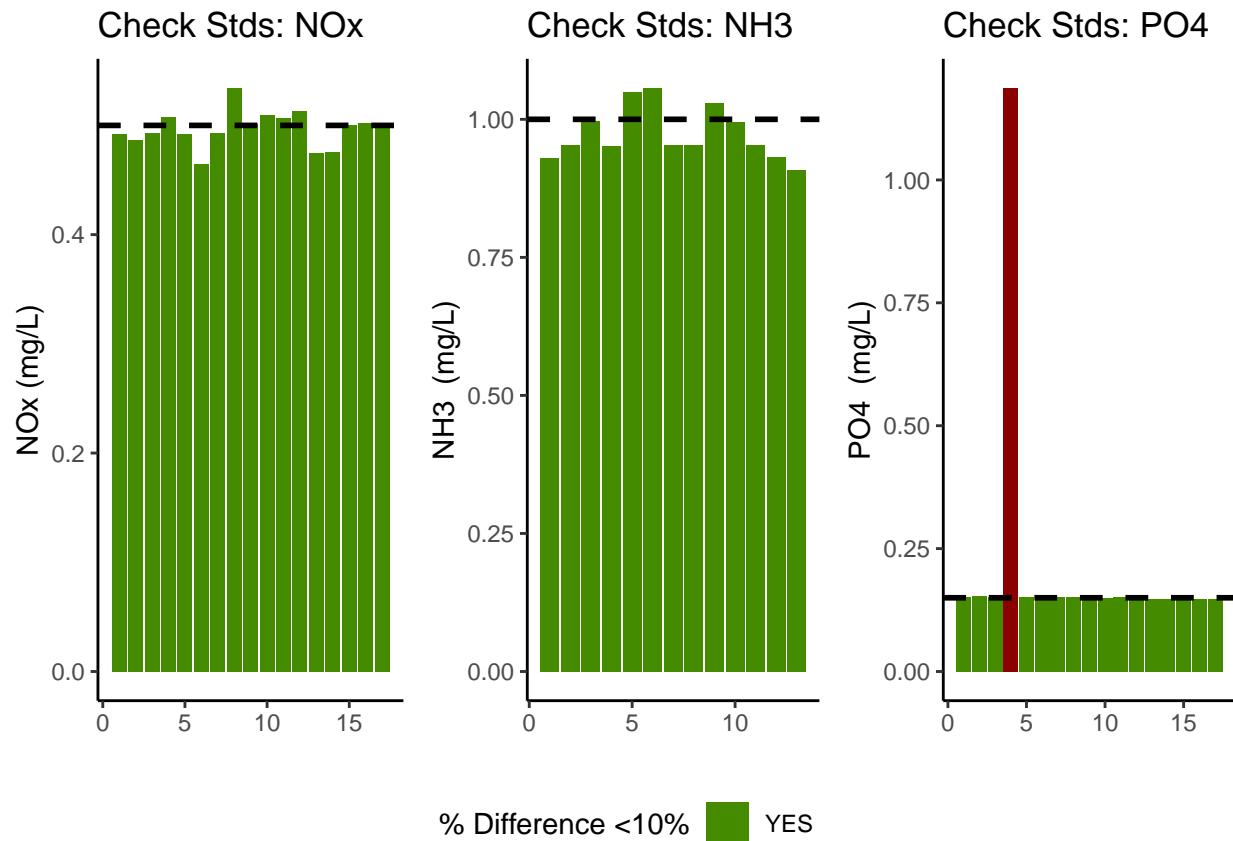
0.5 Analyze the Check Standards

```
## Analyze Check Standards

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

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

## [1] "PO4 CHECK STANDARD RSD TOO HIGH - REASSESS"
```



```
## [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"
```

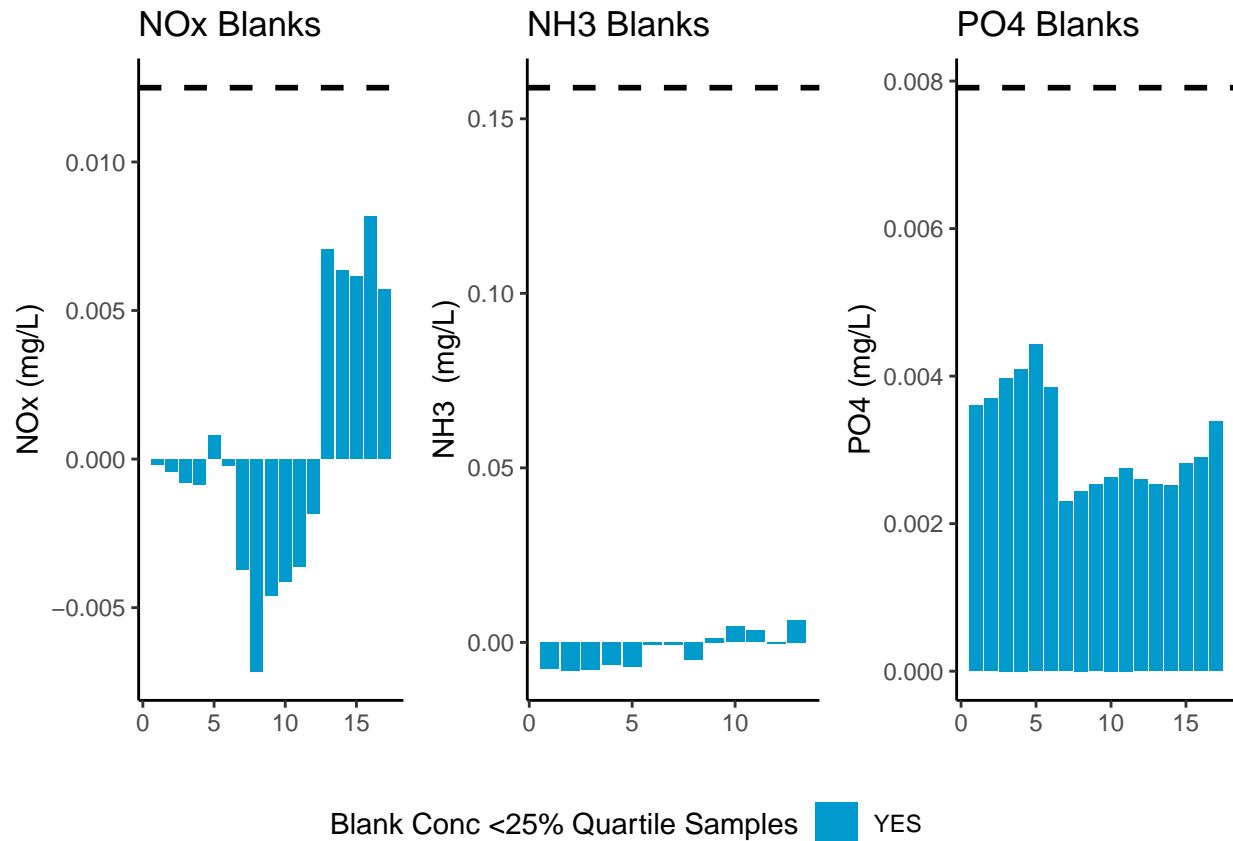


Table 2: Mean Concentration of Blanks

Test	Blank_Mean_Conc
NOx	0.0004
NH3	-0.0022
PO4	0.0031

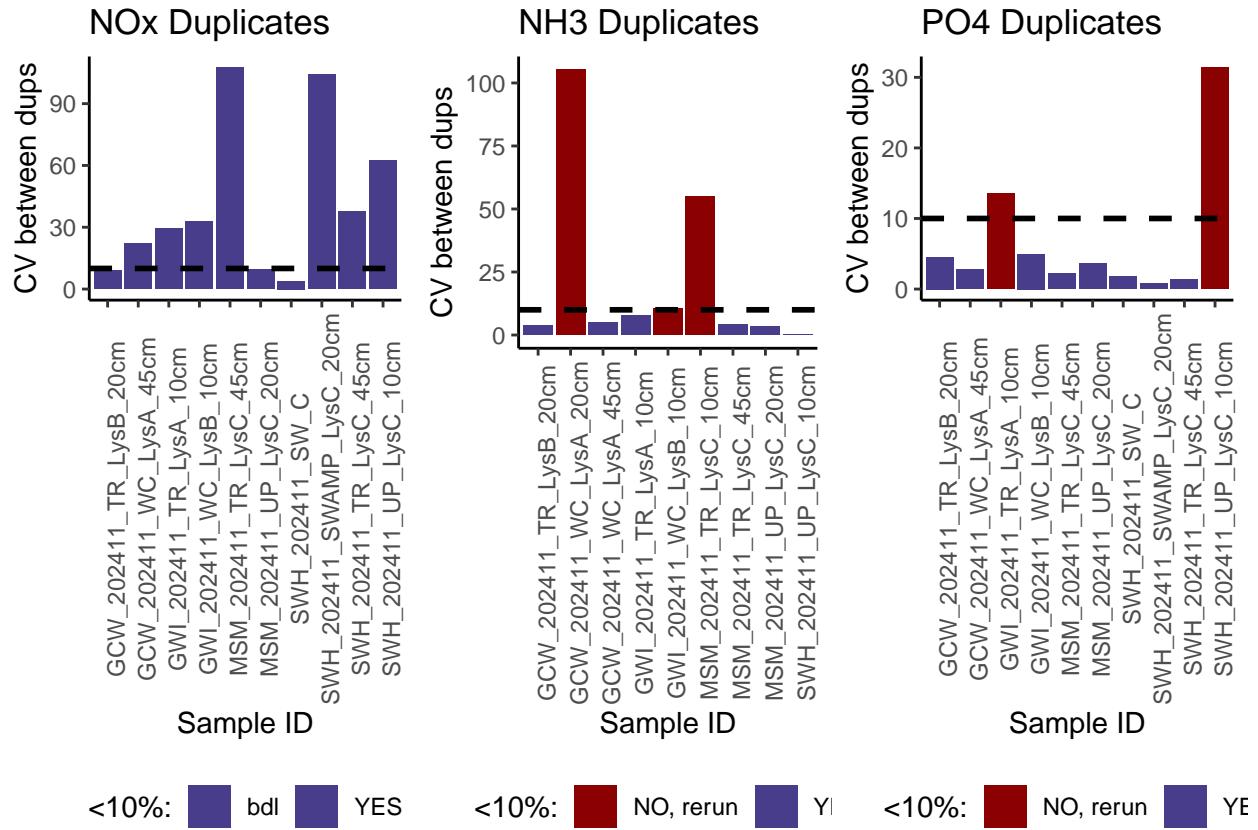
0.7 Analyze Duplicates

```
## 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"
```



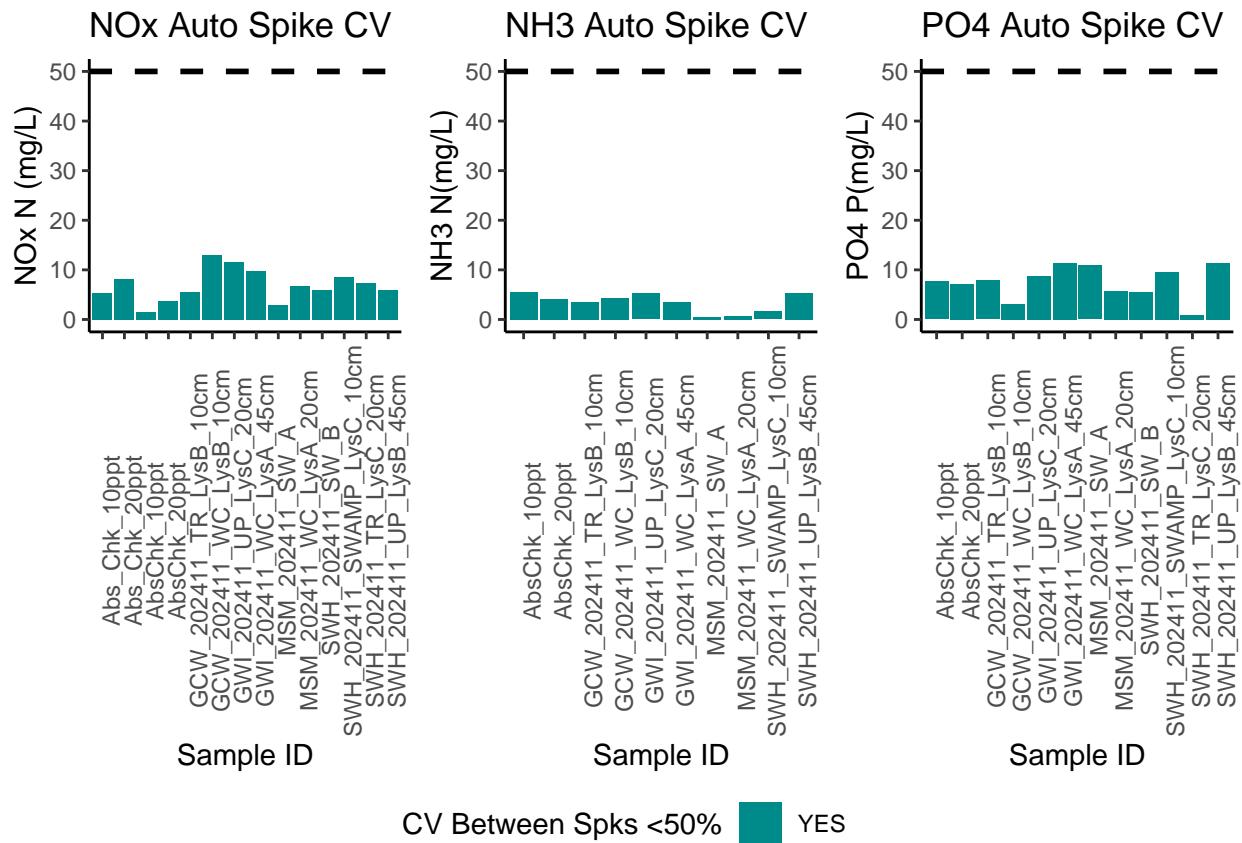
0.8 Spikes

```
## [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"

## 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.
```



0.9 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

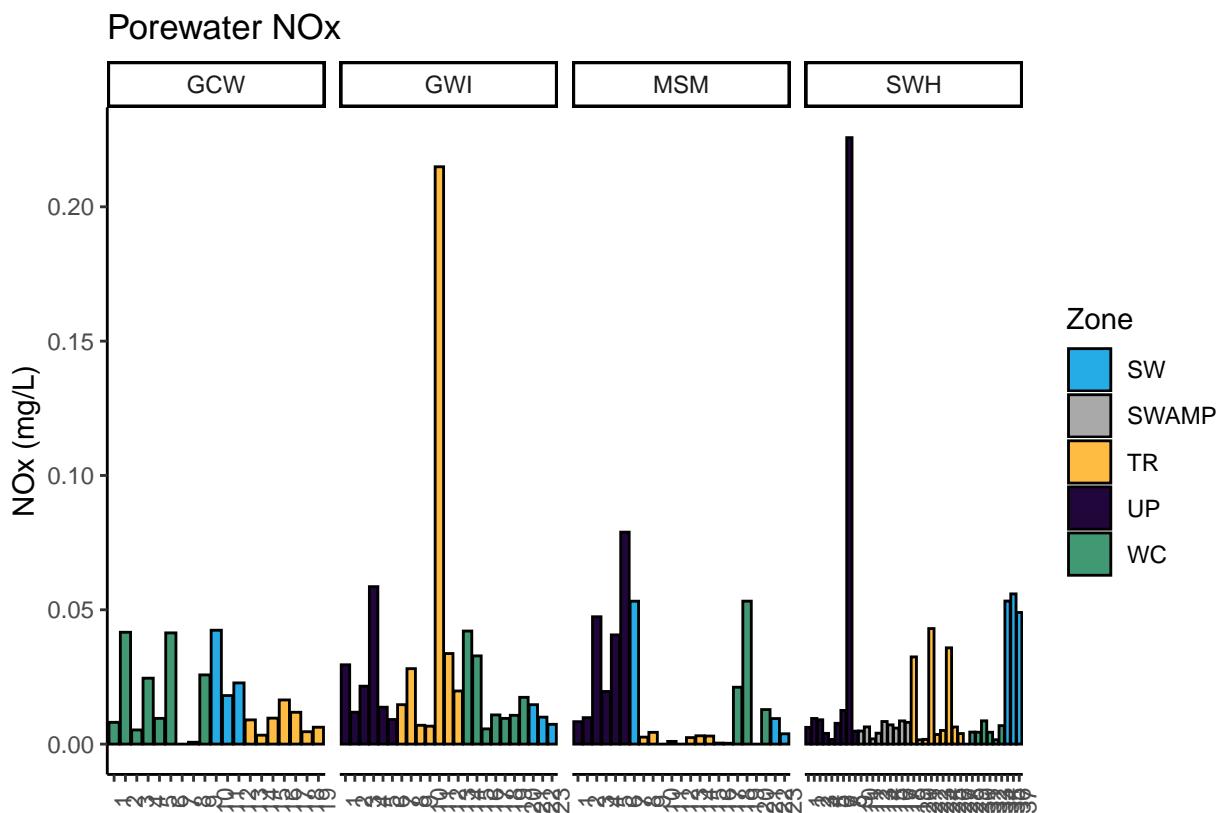
```
## Sample Processing
```

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

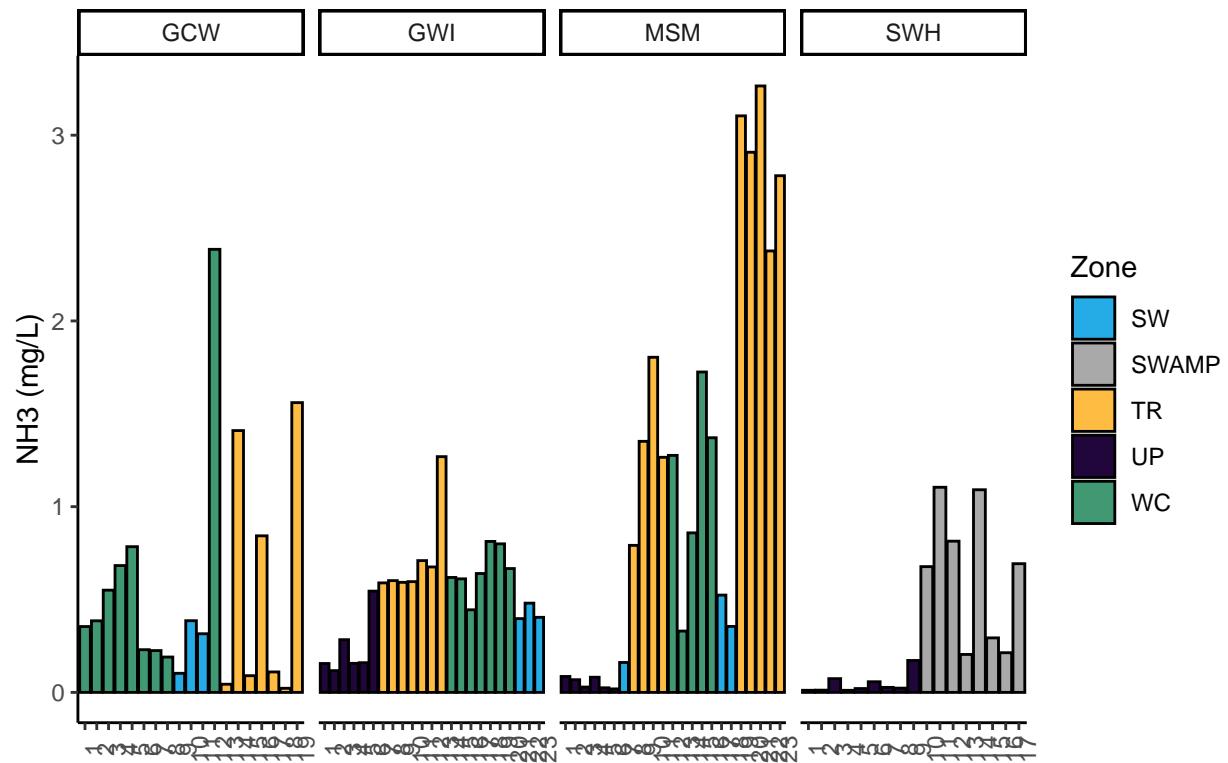
```
## Check Sample IDs with Metadata  
  
## All sample IDs are present in metadata.
```

0.14 Visualize Data

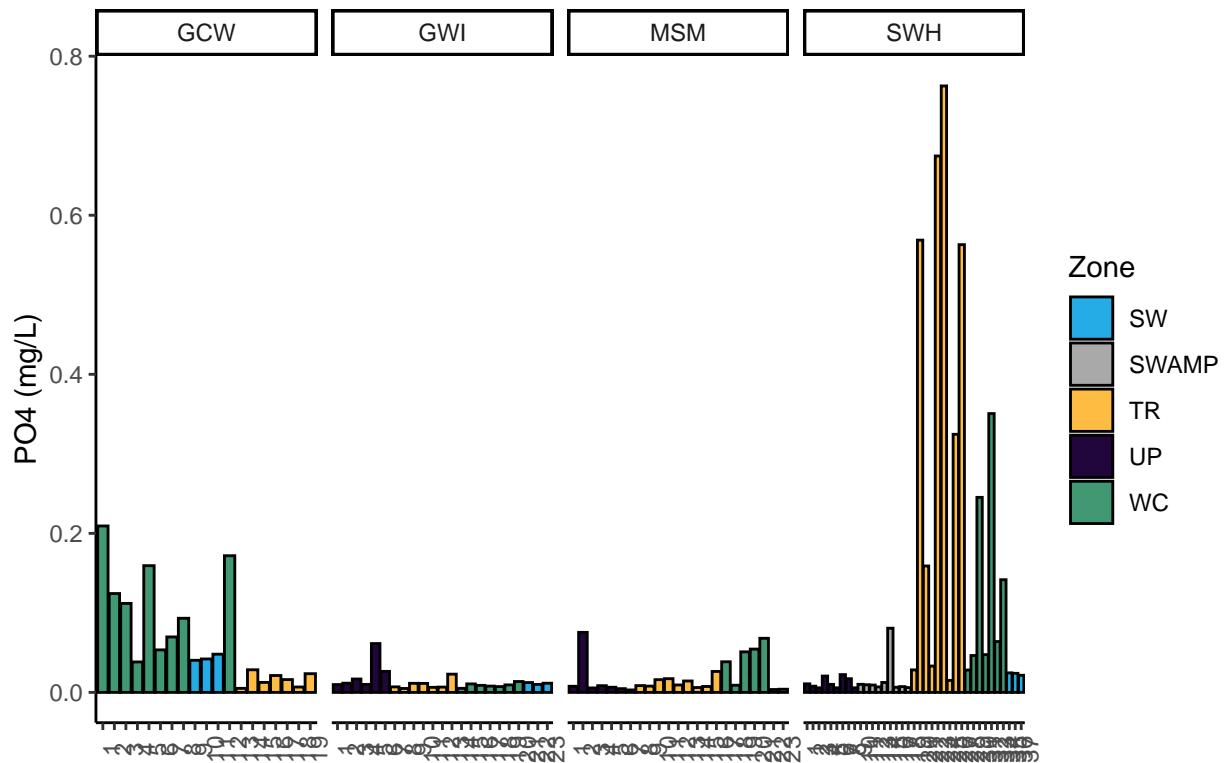
```
## Visualize Data
```



Porewater NH₃



Porewater PO4



0.15 Export Processed Data

```
#end
```