

Synoptic CB: Porewater Nutrients

July 2024 Samples

2025-10-31

Contents

0.1	Import Data & Clean	3
0.2	Assessing standard Curves	3
0.3	Dilution Corrections - ensure the latest dilution is kept	6
0.4	Performance Check	6
0.5	Analyze the Check Standards	8
0.6	Analyze Blanks	9
0.7	Analyze Duplicates	10
0.8	Spikes	11
0.9	Matrix Effects	12
0.10	Unit Converted Data Column Added (mg/L to uM)	12
0.11	Sample Flagging - Within range of standard curve	12
0.12	Pull out sample id information	12
0.13	Check to see if samples run match metadata & merge info	12
0.14	Visualize Data	13
0.15	Export Processed Data	15

```

##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 <- "6/2/2025"
sample_year <- "2024"
sample_month <- "JULY"
user <- "Isabelle Van Benschoten"

#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_202407_VNOx_1.csv",
              "Raw Data/COMPASS_Synoptic_CB_202407_VNOx_2.csv",
              "Raw Data/COMPASS_Synoptic_CB_202407_VNOx_3.csv")
NH3_P04_files <- c("Raw Data/COMPASS_Synoptic_CB_202407_NH3_P04_1.csv",
                   "Raw Data/COMPASS_Synoptic_CB_202407_NH3_P04_2.csv",
                   "Raw Data/COMPASS_Synoptic_CB_202407_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_202407.csv"

#record any notes about the run or anything other info here:
run_notes <- "Reduction Efficiency was not ran for all of the runs included within this month.
               One NH3 check standard had high CV.
               One P04 blank had high CV.
               Over 60% of P04 Duplicates have a CV less than 10%."

#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)

## Reduction Efficiency was not ran for all of the runs included within this month.
##               One NH3 check standard had high CV.
##               One P04 blank had high CV.
##               Over 60% of P04 Duplicates have a CV less than 10%.

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

```

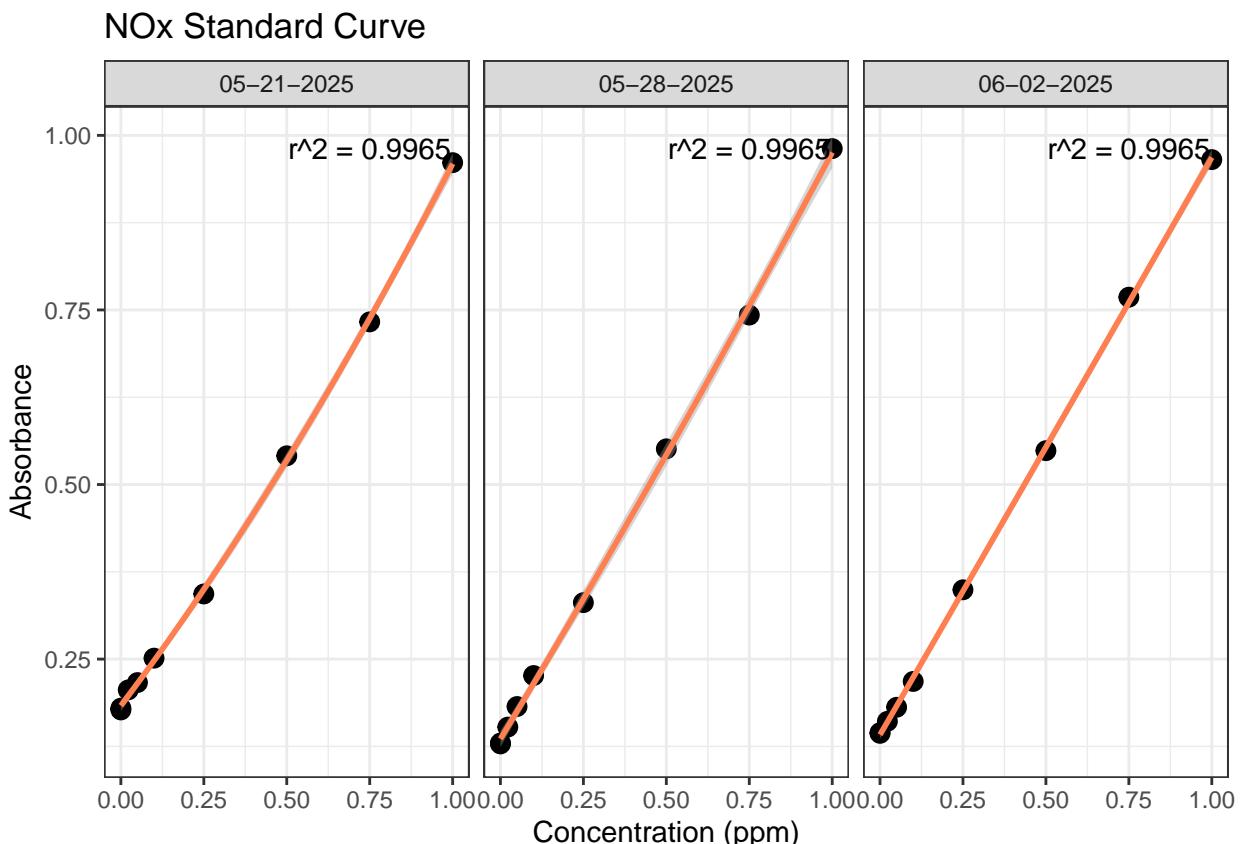
0.1 Import Data & Clean

0.2 Assessing standard Curves

```
## Assess Standard Curves
```

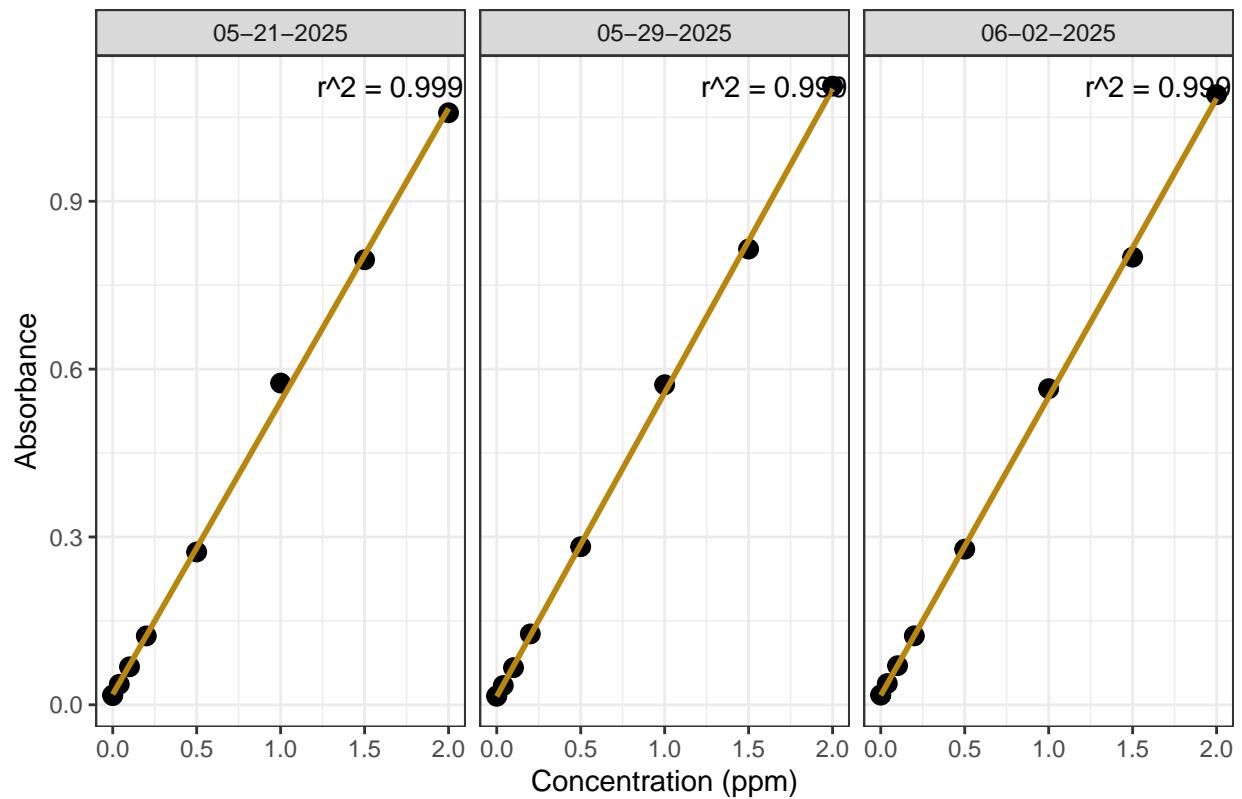
```
#Plot standards data
```

```
## Assess Standard Curves
```



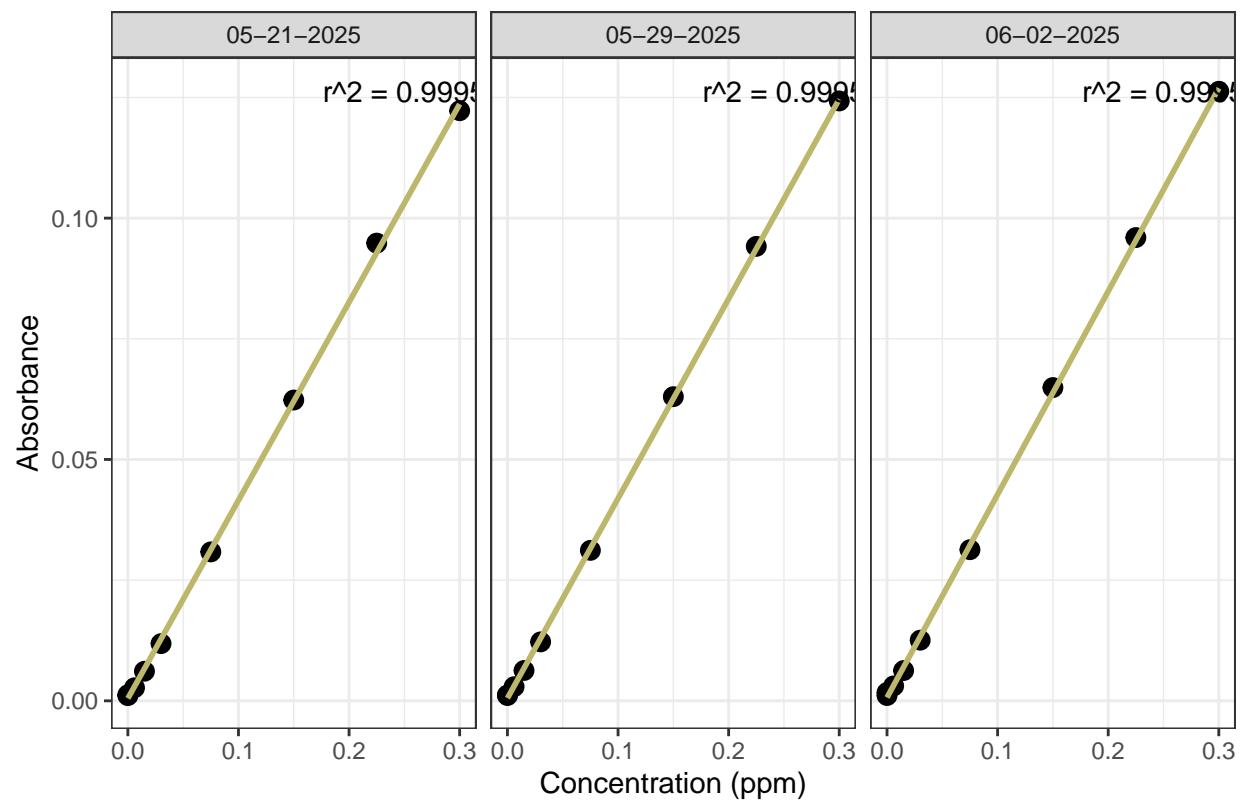
```
## `geom_smooth()` using formula = 'y ~ x'
```

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."
```

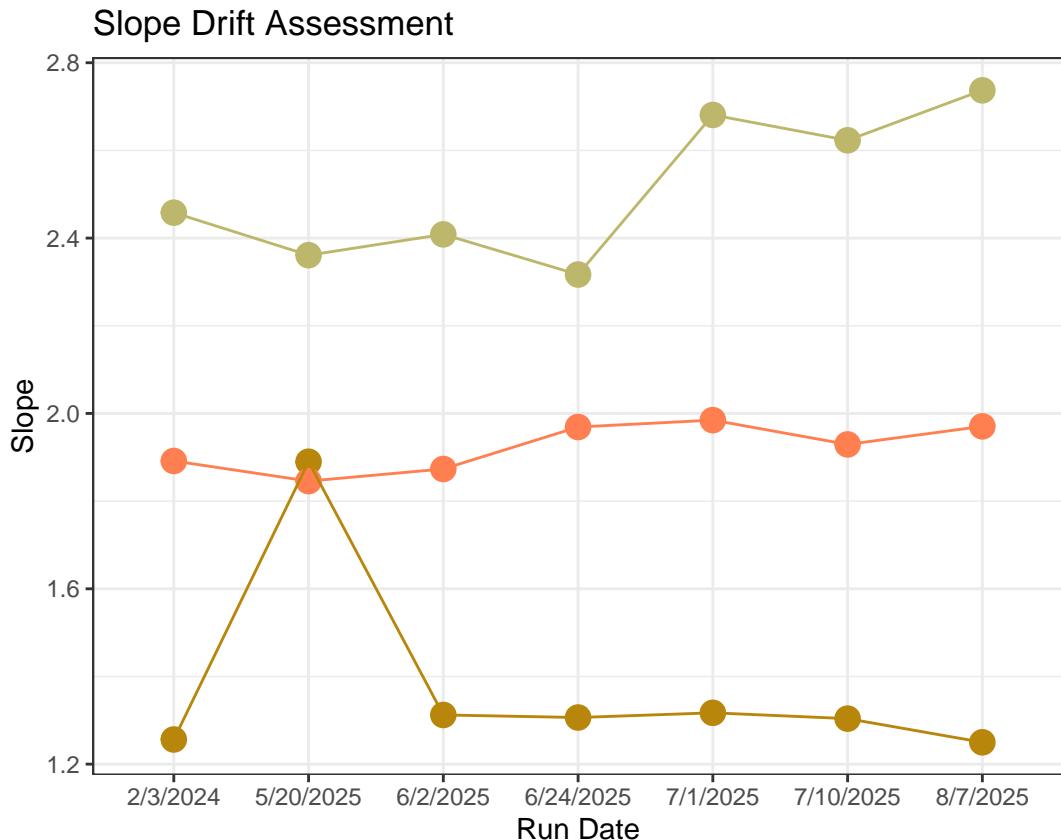


Table 1: Average Slope by Analyte

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: pe_Chk_NOx, GCW_202407_WC_LysA_45cm, GCW_202407_TR_LysB_45cm, GCW_202407_WC_LysC

## 
## 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 = 1.656071

## Expected = 1.51
```

```

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

## Run mean = 1.284822

## Expected = 1.034

## [1] "P04 pe Check has a % Difference <25% - PROCEED"

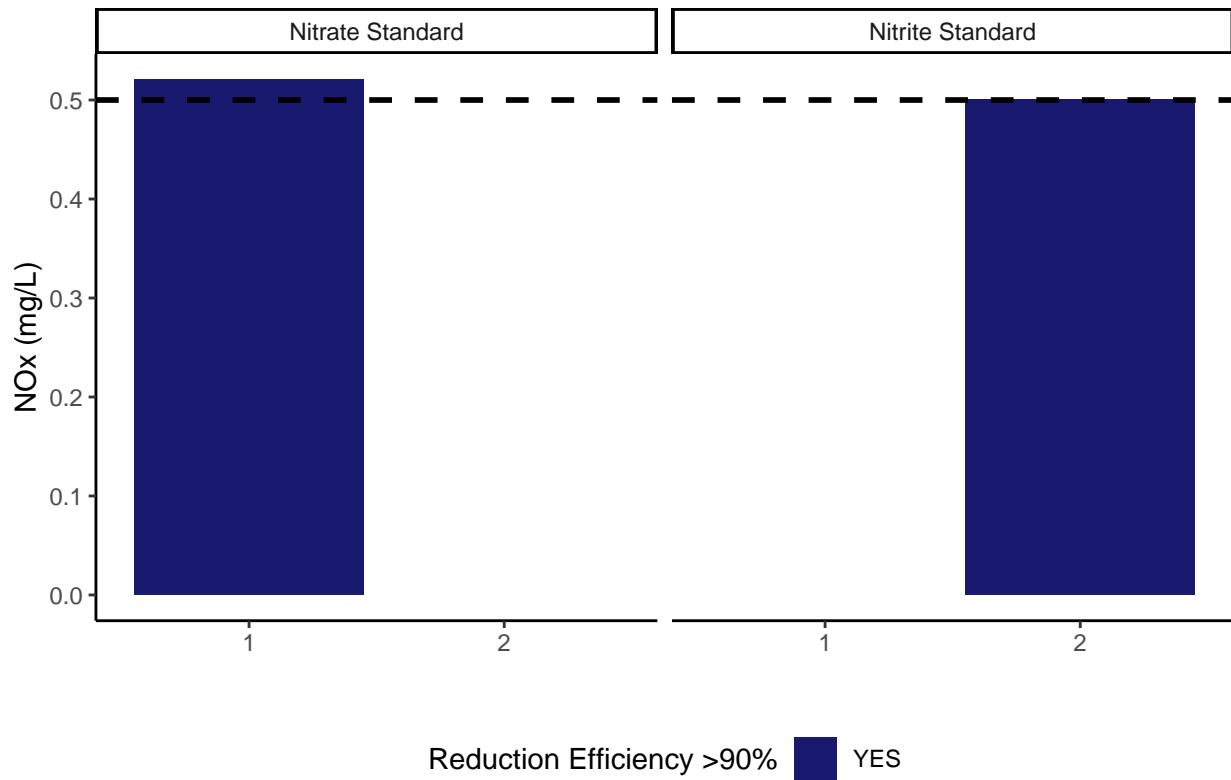
## Run mean = 0.885617

## Expected = 0.824

##Check NOx Reduction Efficiency

## Assess Reduction Efficiency

```



```

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

## [1] 102.1556

```

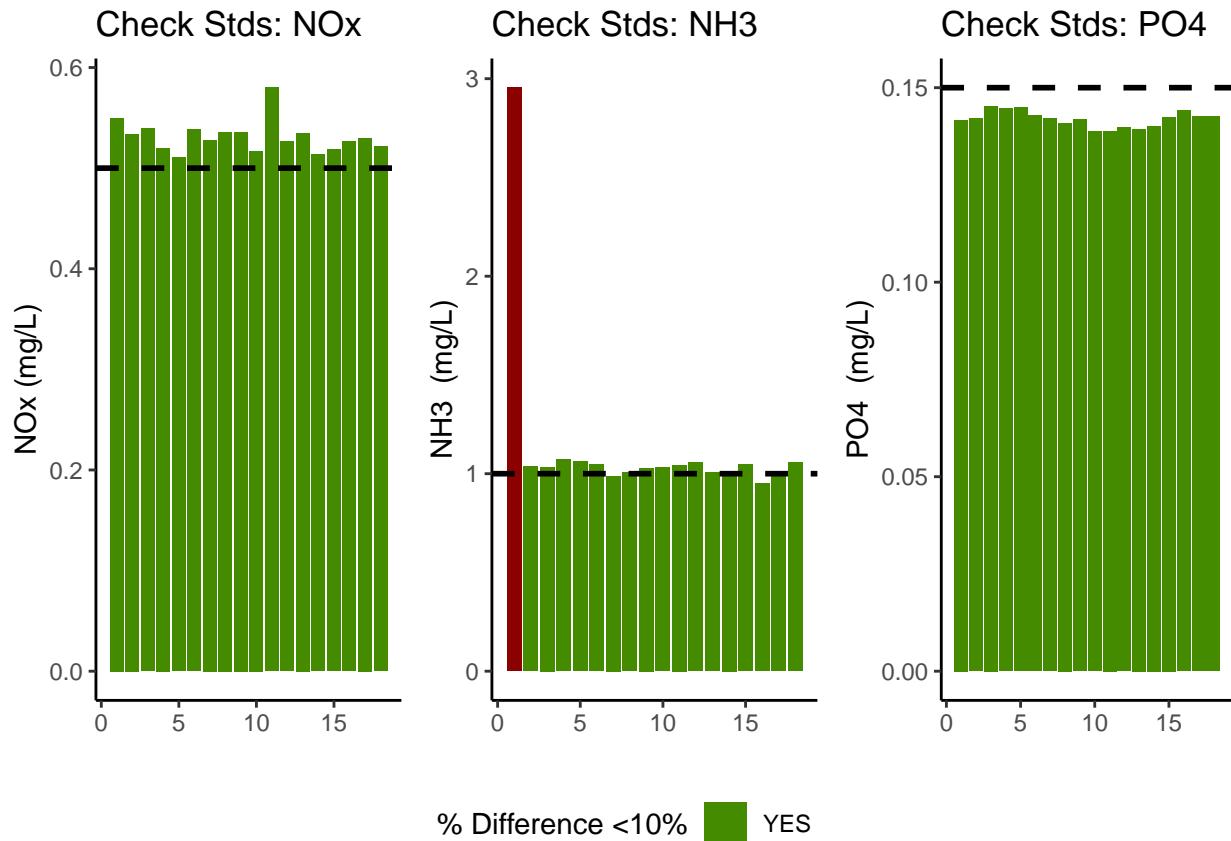
0.5 Analyze the Check Standards

```
## Analyze Check Standards

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

## [1] "NH3 CHECK STANDARD RSD TOO HIGH - REASSESS"

## [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"
```

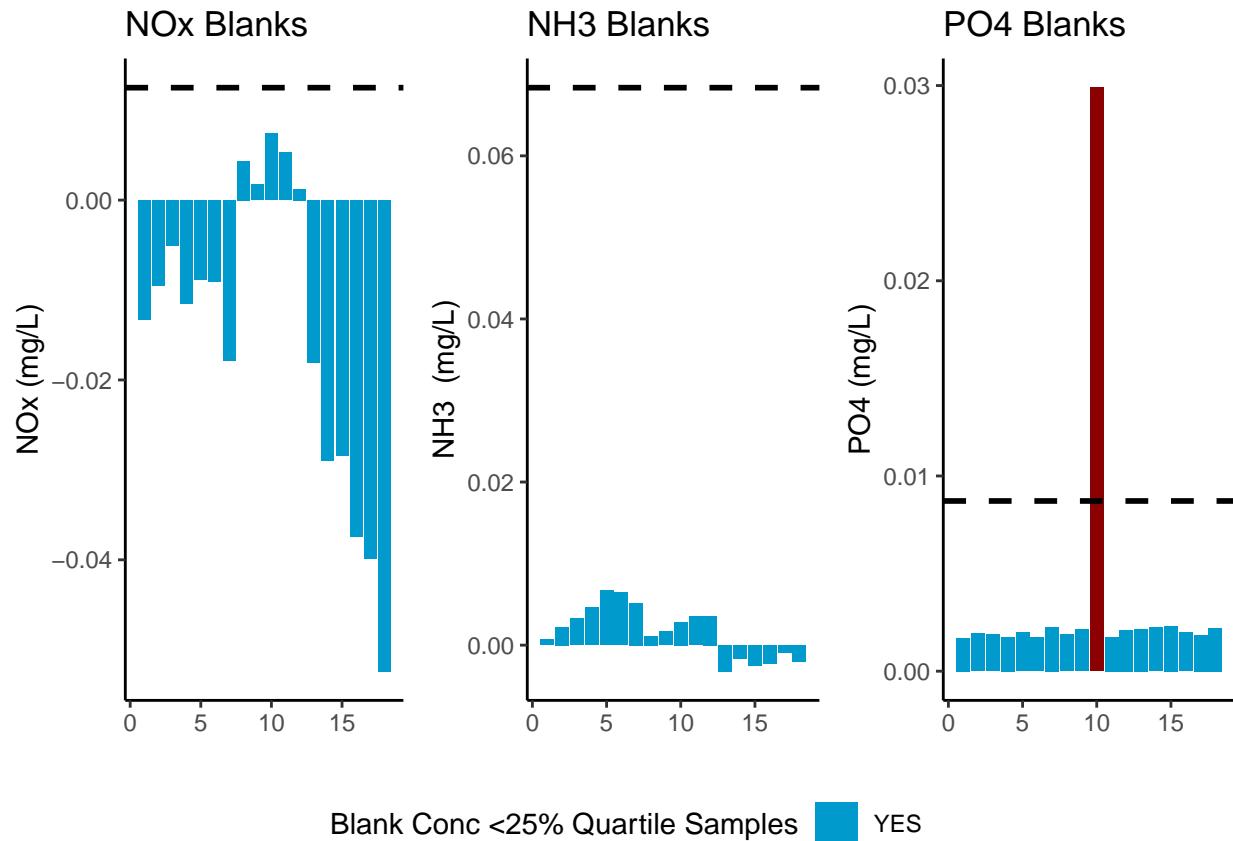


Table 2: Mean Concentration of Blanks

Test	Blank_Mean_Conc
NOx	-0.0145
NH3	0.0016
PO4	0.0035

0.7 Analyze Duplicates

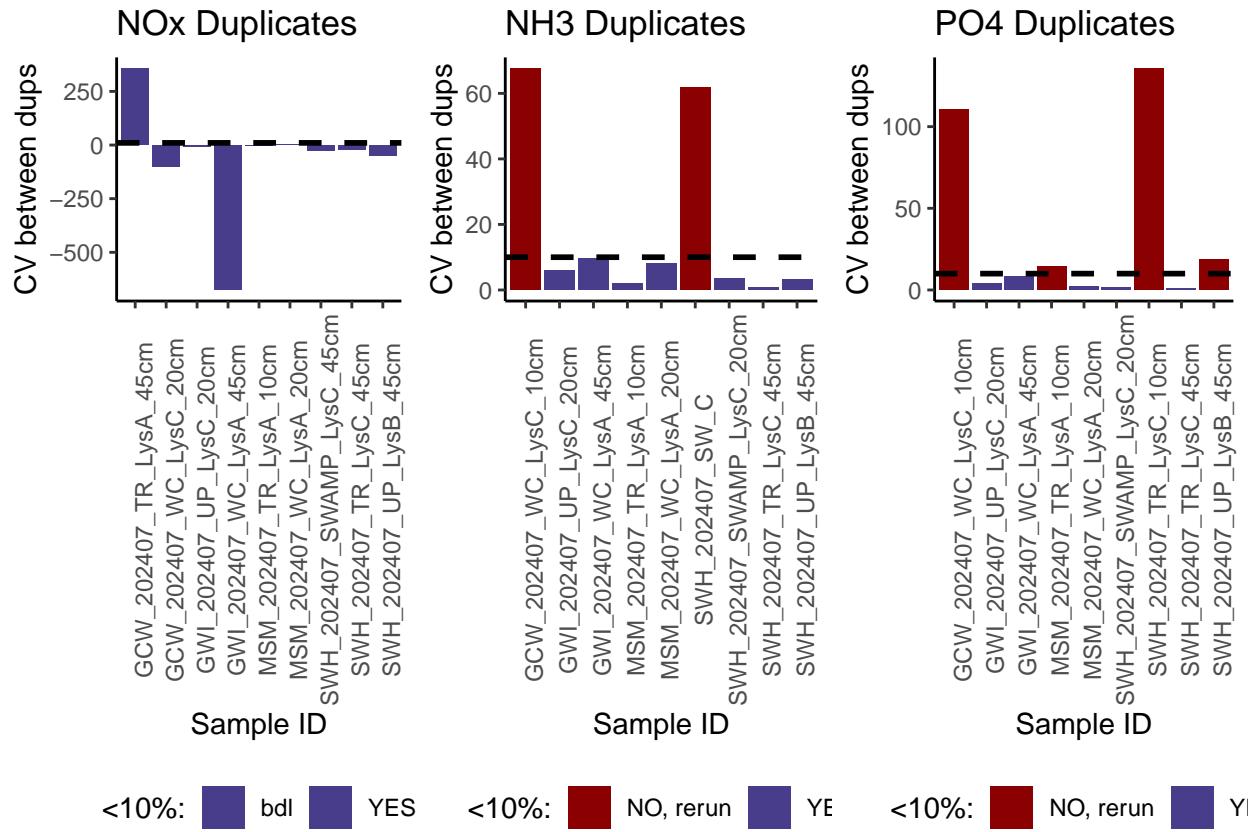
```
## Analyze Duplicates

## [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% - 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.
```

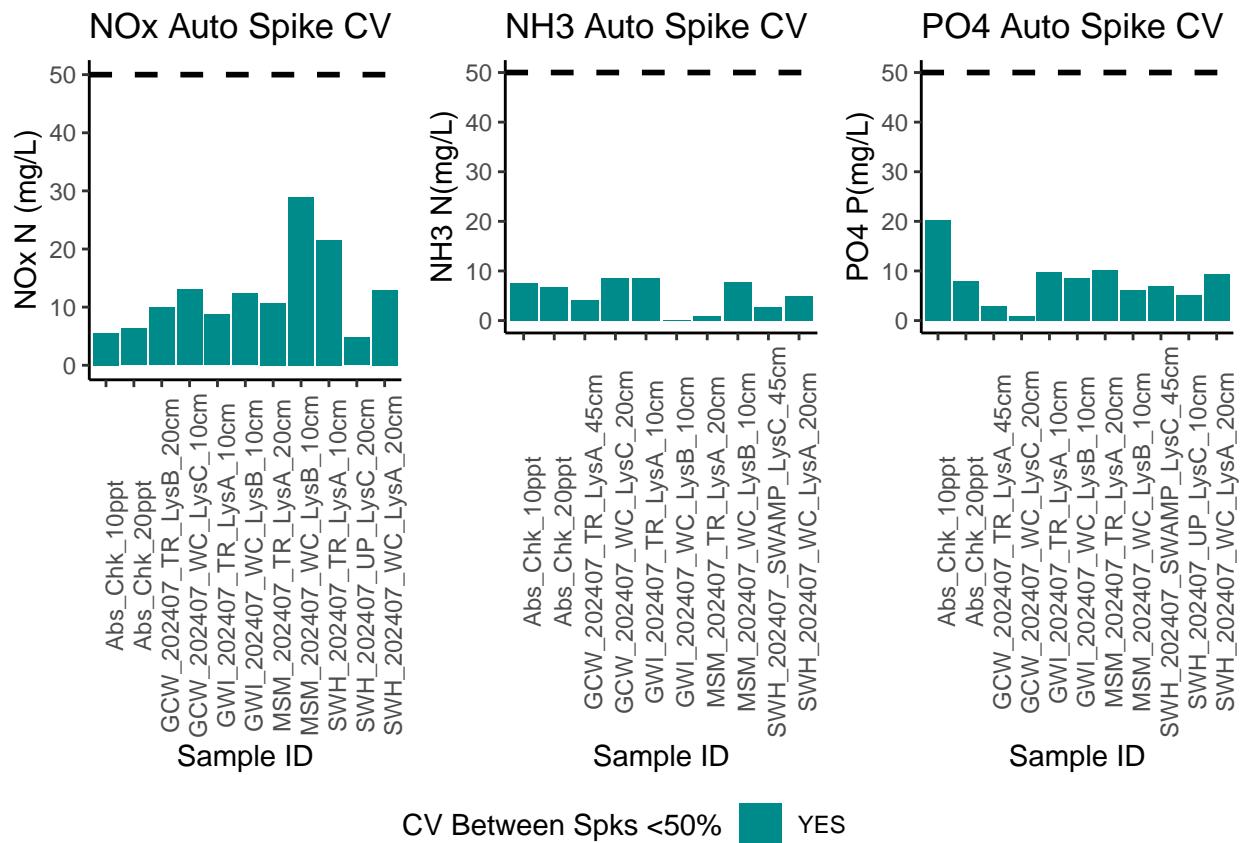


0.8 Spikes

```
## [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
```

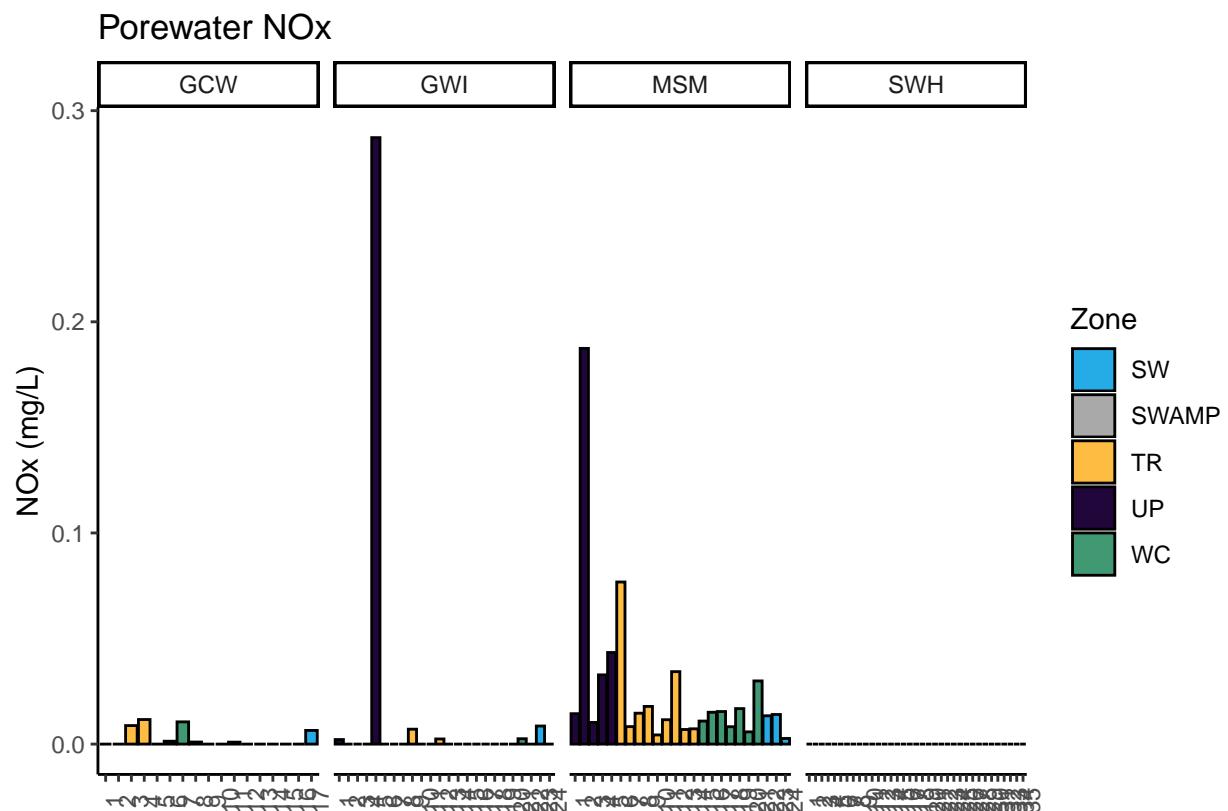
```
## Warning: Expected 5 pieces. Missing pieces filled with 'NA' in 36 rows [22, 23, 24, 39,  
## 40, 41, 63, 64, 65, 98, 99, 100, 121, 122, 123, 136, 137, 138, 159, 160, ...].
```

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

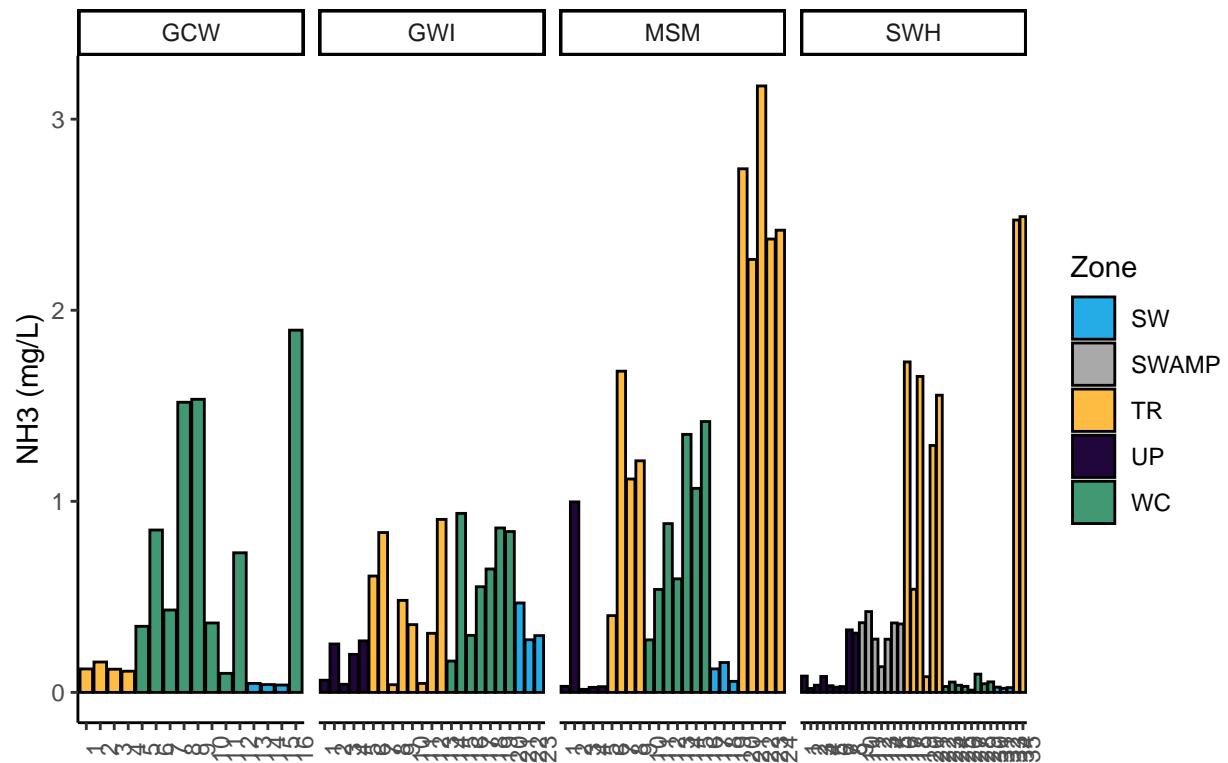
```
## Check Sample IDs with Metadata  
  
## All sample IDs are present in metadata.  
  
## Warning: Expected 5 pieces. Missing pieces filled with 'NA' in 36 rows [22, 23, 24, 39,  
## 40, 41, 63, 64, 65, 98, 99, 100, 121, 122, 123, 136, 137, 138, 159, 160, ...].
```

0.14 Visualize Data

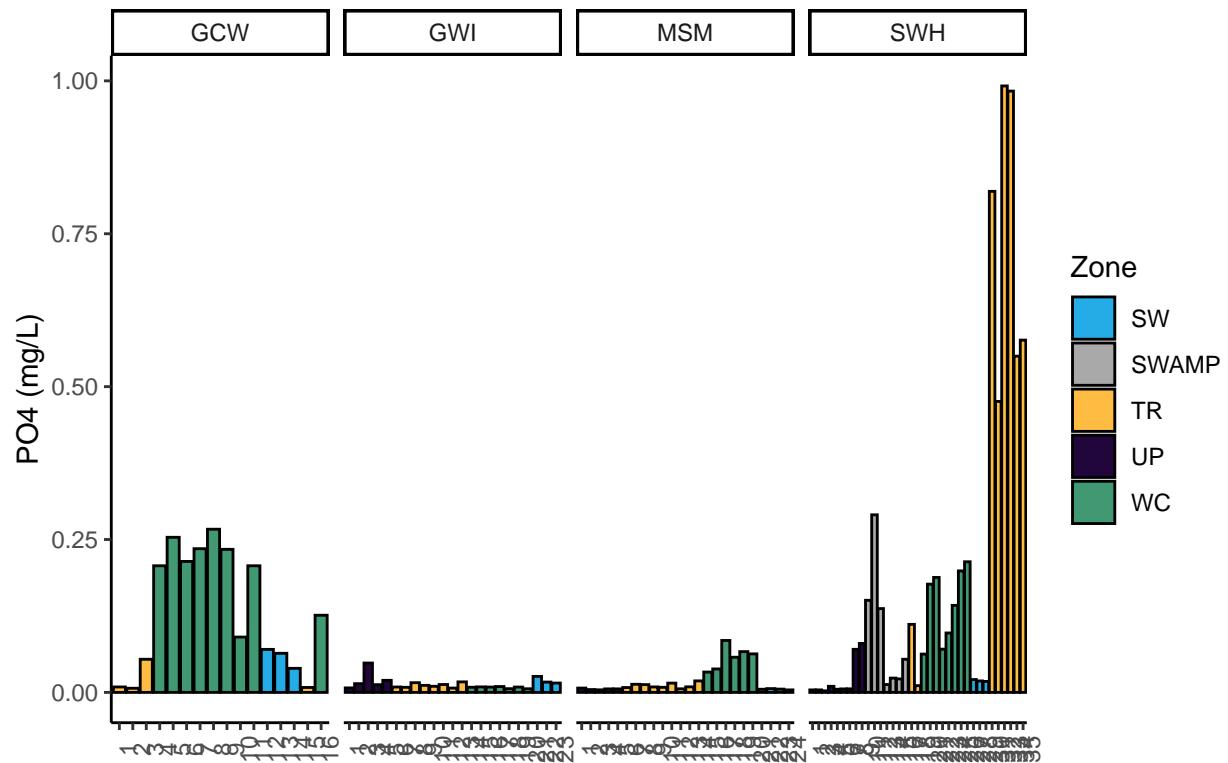
```
## Visualize Data
```



Porewater NH₃



Porewater PO4



0.15 Export Processed Data

```
#end
```