

Synoptic CB: Porewater Nutrients

SEPTEMBER 2024 Samples

2025-07-18

Contents

0.1	Import Data & Clean	3
0.2	Assessing standard Curves	3
0.3	Dilution Corrections - ensure the latest dilution is kept	7
0.4	Performance Check	7
0.5	Analyze the Check Standards	9
0.6	Analyze Blanks	10
0.7	Analyze Duplicates	11
0.8	Spikes	12
0.9	Matrix Effects	13
0.10	Unit Converted Data Column Added (mg/L to uM)	13
0.11	Sample Flagging - Within range of standard curve	13
0.12	Pull out sample id information	13
0.13	Check to see if samples run match metadata & merge info	13
0.14	Visualize Data	14
0.15	Export Processed Data	16

```

##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 <- "07/10/2025"
sample_year <- "2025"
sample_month <- "SEPTEMBER"
user <- "Isabelle Van Benschoten"

#identify the files you want to read in
#read in as a list to accommodate ultiple runs in a month
NOx_files <- c("Raw Data/COMPASS_Synoptic_CB_202409_VNOx_1.csv",
              "Raw Data/COMPASS_Synoptic_CB_202409_VNOx_2.csv",
              "Raw Data/COMPASS_Synoptic_CB_202409_VNOx_3.csv")
NH3_P04_files <- c("Raw Data/COMPASS_Synoptic_CB_202409_NH3_P04_1.csv",
                    "Raw Data/COMPASS_Synoptic_CB_202409_NH3_P04_2.csv",
                    "Raw Data/COMPASS_Synoptic_CB_202409_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_202409.csv"

#record any notes about the run or anything other info here:
run_notes <- "Reduction efficiency check was only ran for some of the runs within this month."

#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 check was only ran for some of the runs within this month.

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

```

0.1 Import Data & Clean

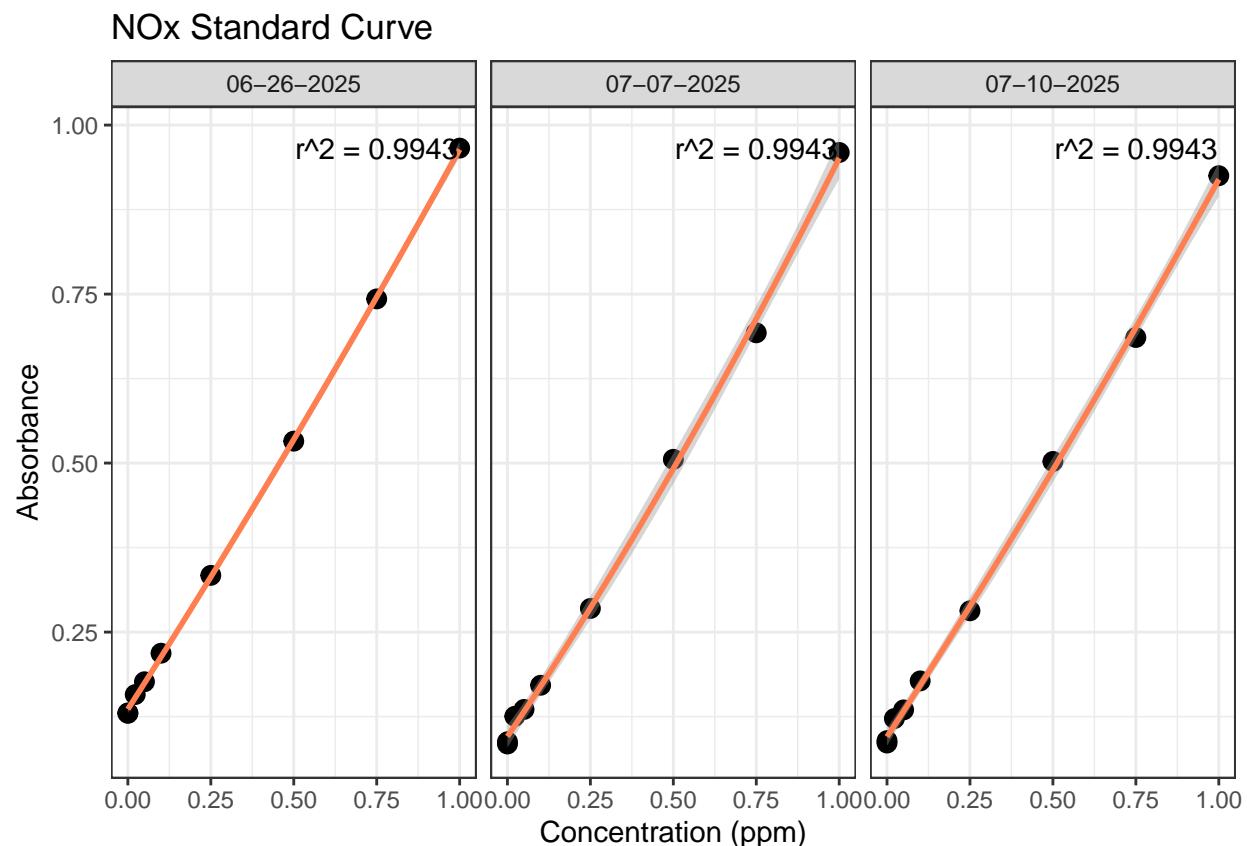
0.2 Assessing standard Curves

```
#Pull out standards data
```

```
## Assess Standard Curves
```

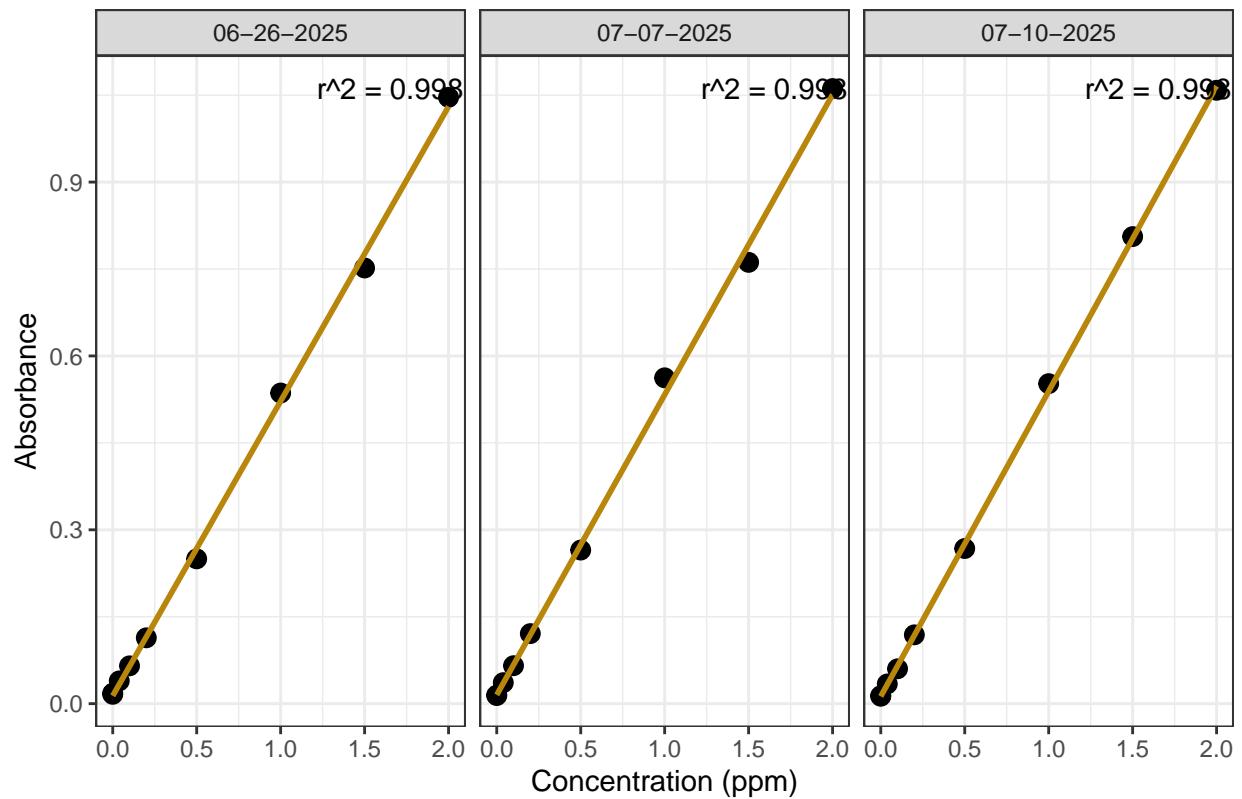
```
#Plot standards data
```

```
## Assess Standard Curves
```



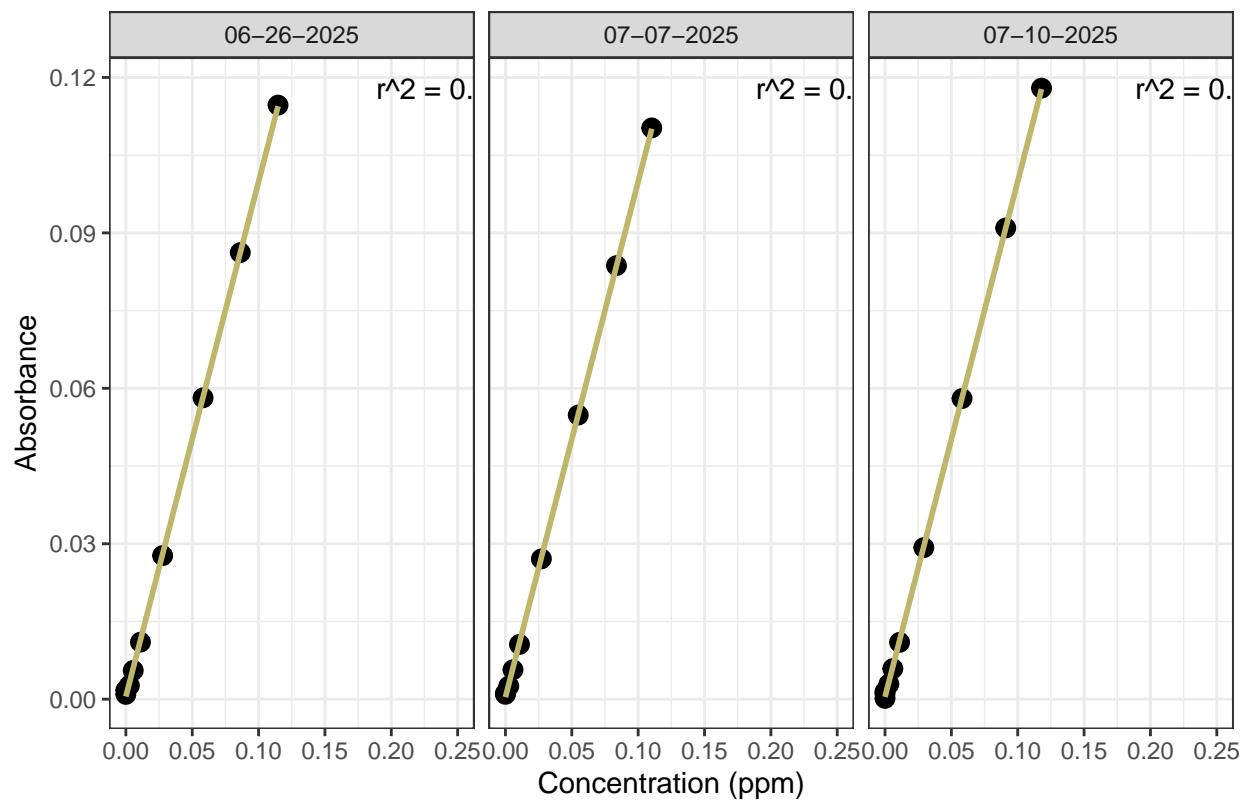
```
## `geom_smooth()` using formula = 'y ~ x'
```

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."
```

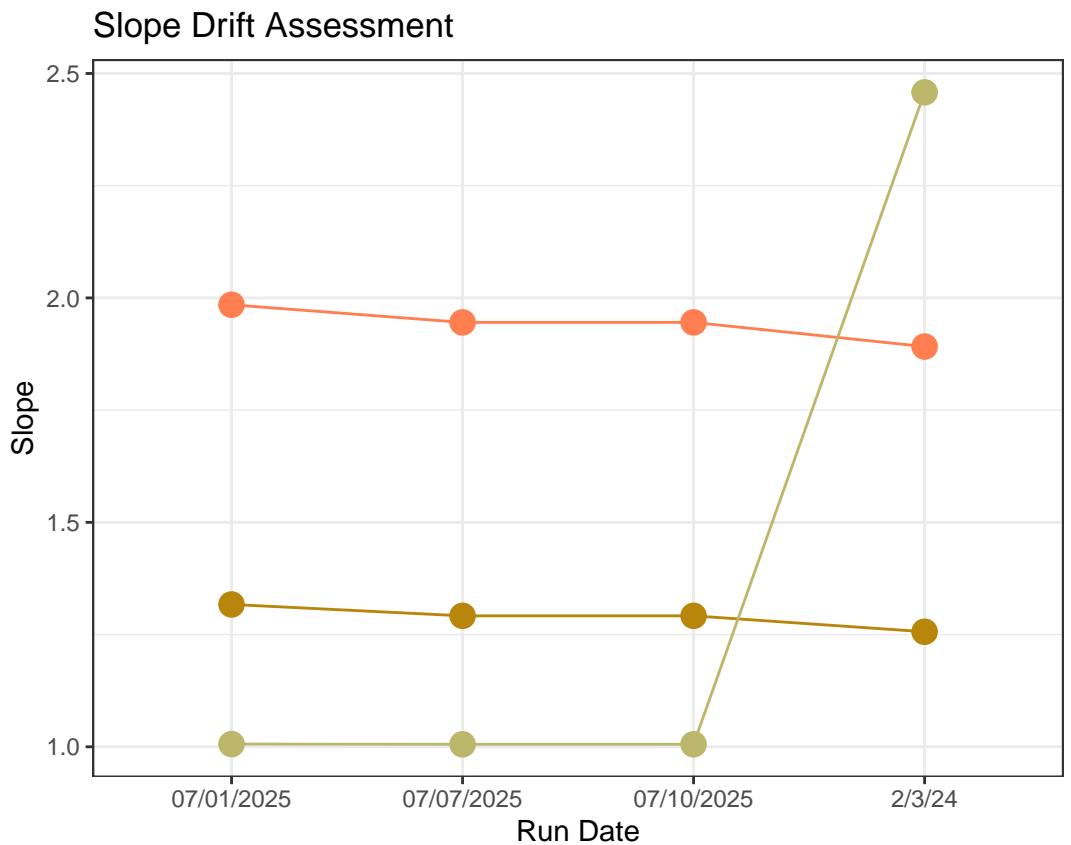


Table 1: Average Slope by Analyte

Test	avg_slope
NH3	1.942
NOx	1.289
PO4	1.369

0.3 Dilution Corrections - ensure the latest dilution is kept

0.4 Performance Check

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

## Run mean = 1.649319

## Expected = 1.51

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

## Run mean = 1.143141

## Expected = 1.034

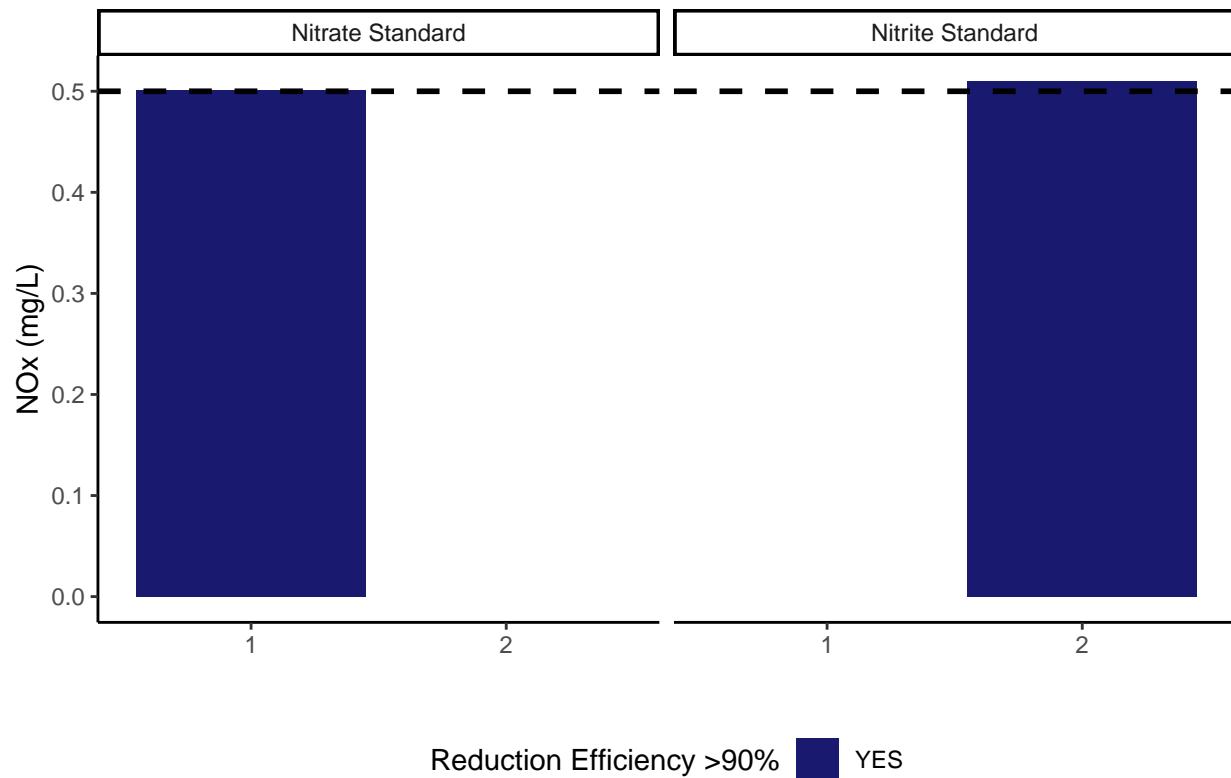
## [1] "PO4 pe Check has a % Difference <25% - PROCEED"

## Run mean = 0.946821

## Expected = 0.824

##Check NOx Reduction Efficiency

## Assess Reduction Efficiency
```



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

```
## [1] 101.1063
```

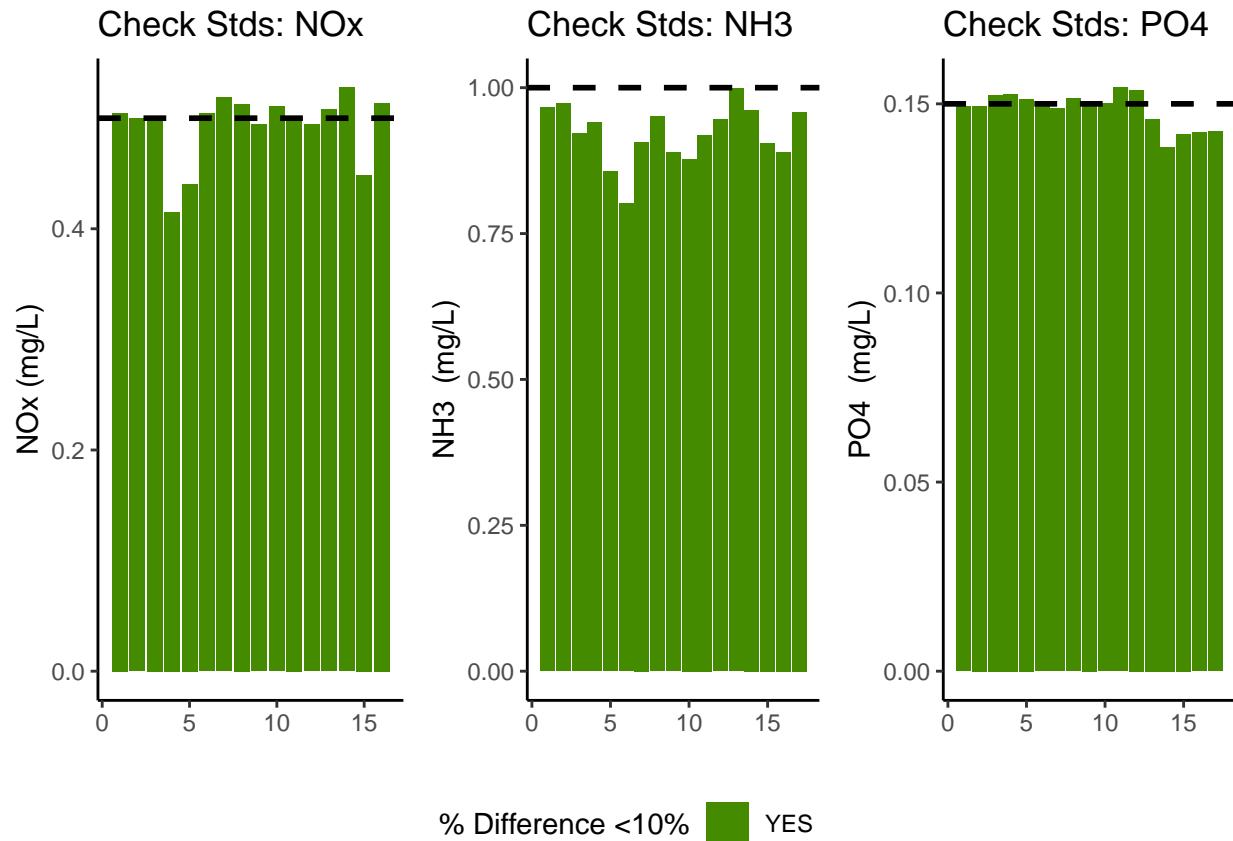
0.5 Analyze the Check Standards

```
## 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"
```

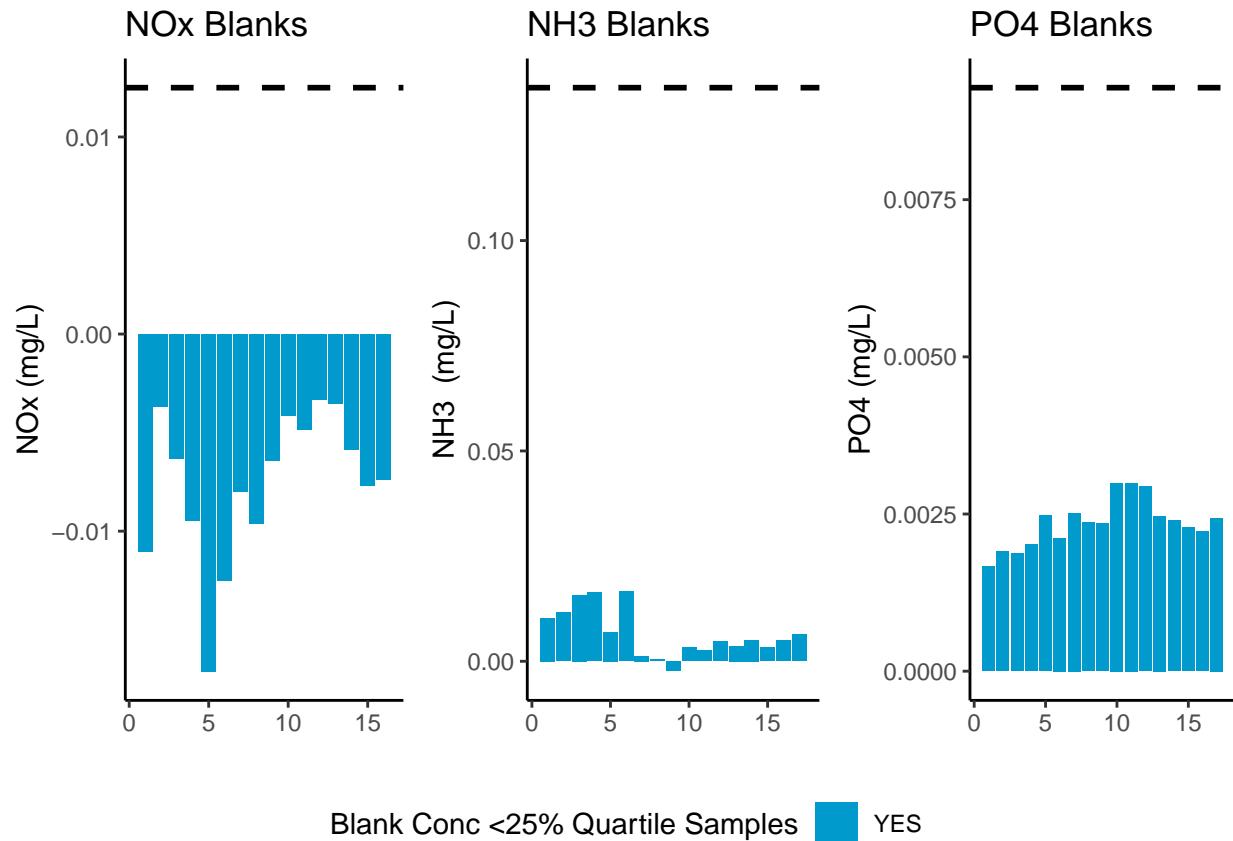


Table 2: Mean Concentration of Blanks

Test	Blank_Mean_Conc
NOx	-0.0076
NH3	0.0065
PO4	0.0024

0.7 Analyze Duplicates

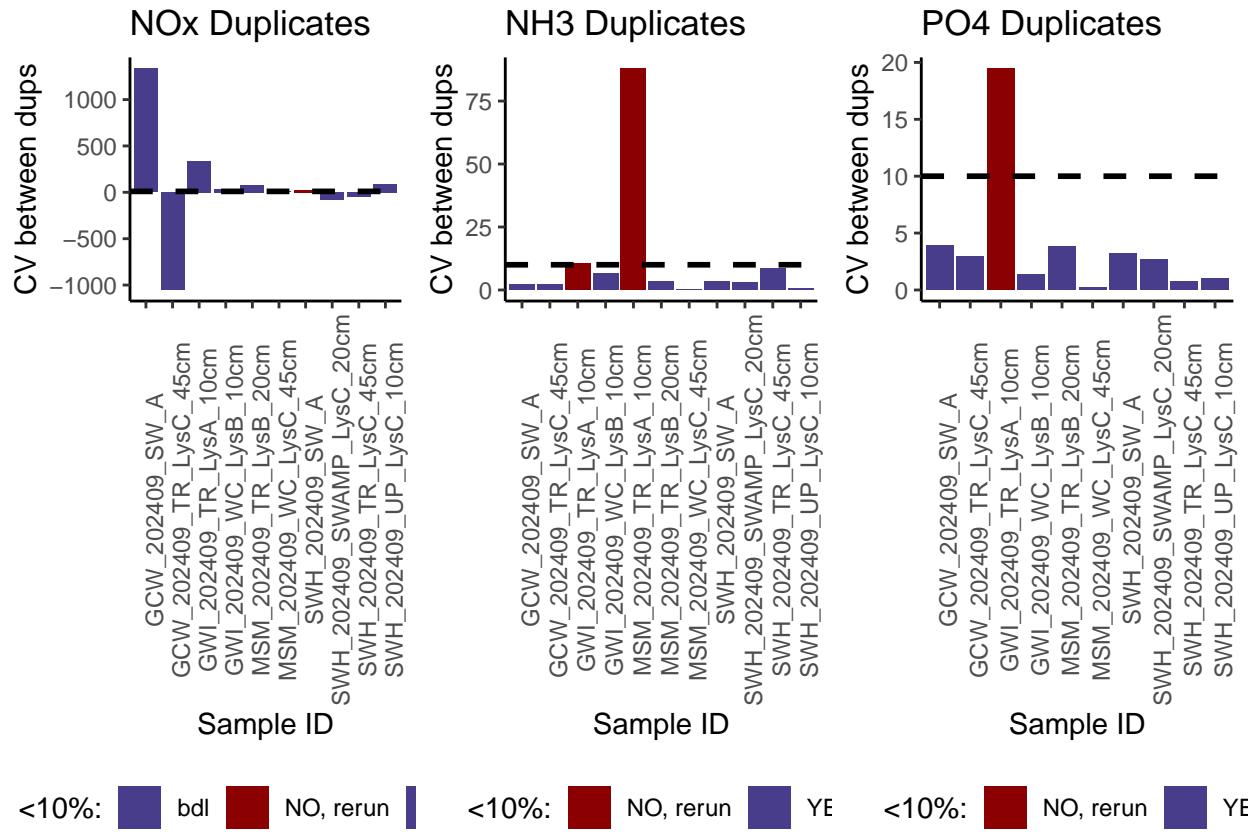
```
## Analyze Duplicates

## [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.
```

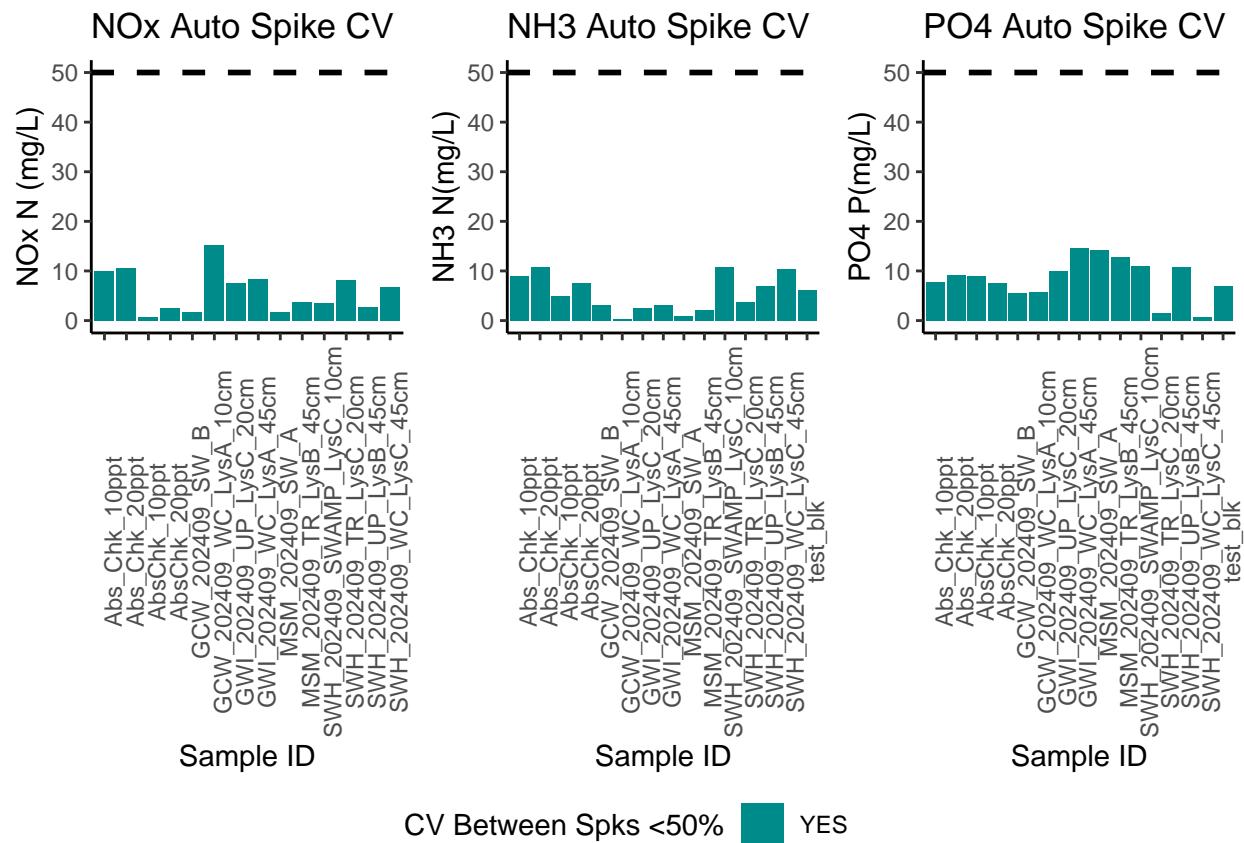


0.8 Spikes

```
## [1] ">60% of 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

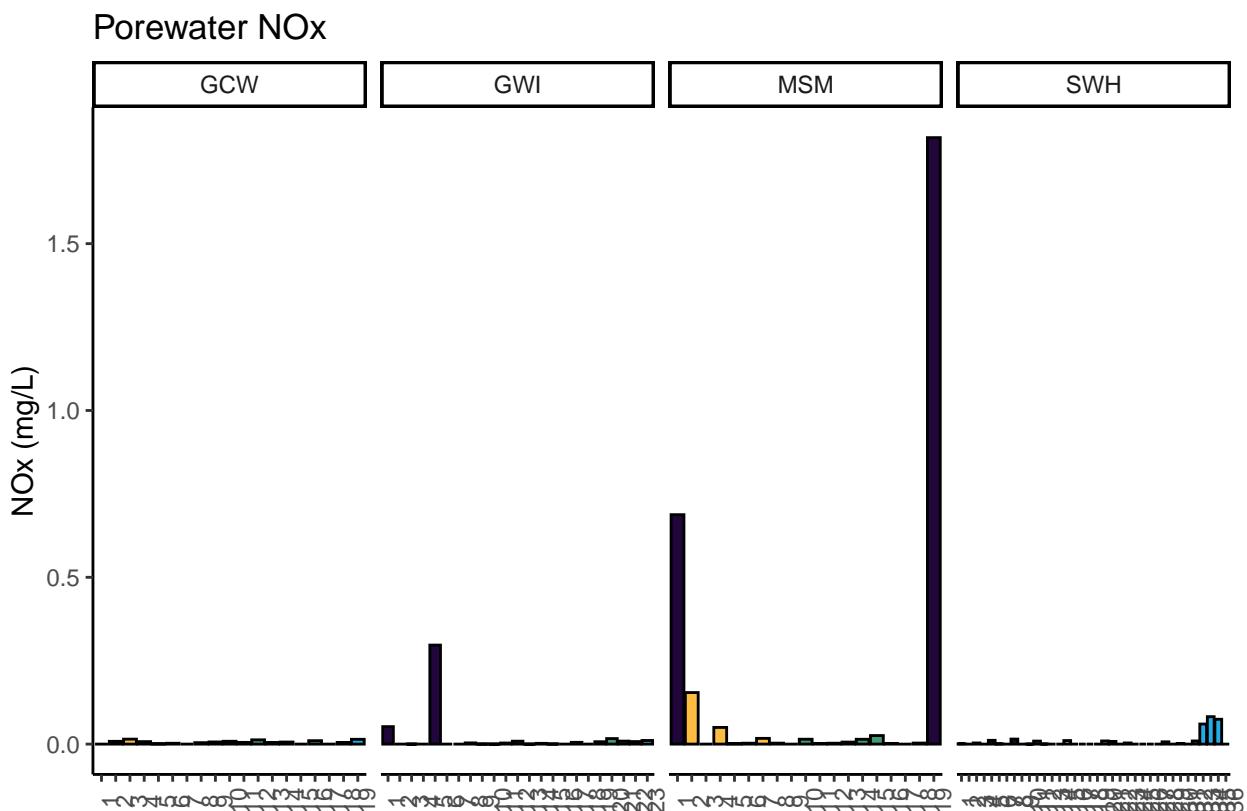
```
## Sample Processing  
  
## Warning: Expected 5 pieces. Missing pieces filled with 'NA' in 36 rows [33, 34, 35, 52,  
## 53, 54, 71, 72, 73, 95, 96, 97, 124, 125, 126, 159, 160, 161, 186, 187, ...].
```

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

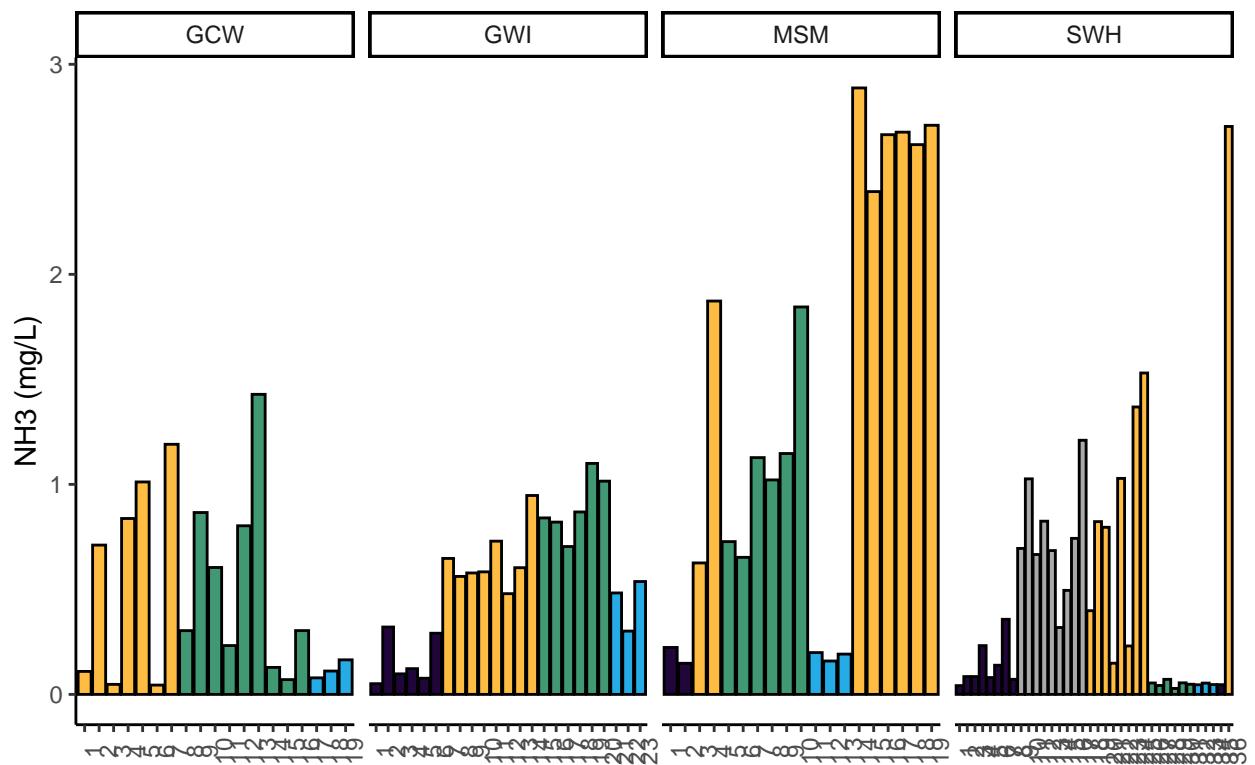
```
## Check Sample IDs with Metadata  
  
## Some sample IDs are missing from metadata.  
  
## [1] "SWH_202409_SWAMP_LycC_45cm" "MSM_202409_UP_LysA_45cm"  
  
## Warning: Expected 5 pieces. Missing pieces filled with 'NA' in 36 rows [33, 34, 35, 52,  
## 53, 54, 71, 72, 73, 95, 96, 97, 124, 125, 126, 159, 160, 161, 186, 187, ...].
```

0.14 Visualize Data

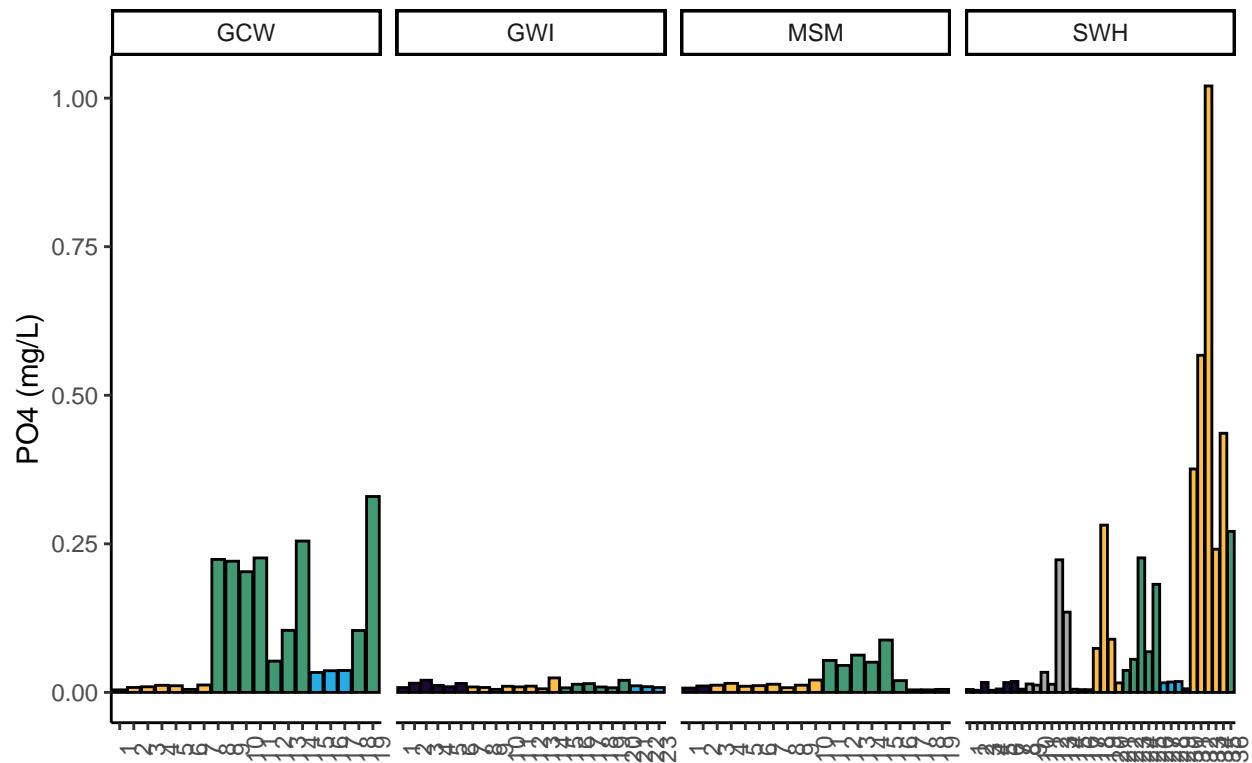
```
## Visualize Data
```



Porewater NH₃



Porewater PO4



0.15 Export Processed Data

```
#end
```