Synoptic CB: Porewater Nutrients

July 2023 Samples

2025-07-08

Contents

##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 <- "01/17/2024"
  sample_year <- 2023
  sample_month <- 07
  user <- "Stephanie Wilson"

#identify the files you want to read in
  #read in as a list to accommadate ultiple runs in a month
  NOx_files <- c("Raw Data/SEAL_COMPASS_Synoptic_NOx_July2023_1.csv",
                 "Raw Data/SEAL_COMPASS_Synoptic_NOx_July2023_2.csv",
                 "Raw Data/SEAL_COMPASS_Synoptic_NOx_July2023_3.csv")
  NH3_PO4_files <- c("Raw Data/SEAL_COMPASS_Synoptic_NH3_PO4_July2023_1.csv",
                     "Raw Data/SEAL_COMPASS_Synoptic_NH3_PO4_July2023_2.csv",
                     "Raw Data/SEAL_COMPASS_Synoptic_NH3_PO4_July2023_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_202307.xlsx"

#record any notes about the run or anything other info here:
  run_notes <- "Run Notes: peChks for NOx and NH3 out of range, but all other
  run metrics looked fine, so we are accepting the 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)
```

```
## Run Notes: peChks for NOx and NH3 out of range, but all other
##   run metrics looked fine, so we are accepting the run.
```

##Setup

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

0.1 Import Data & Clean

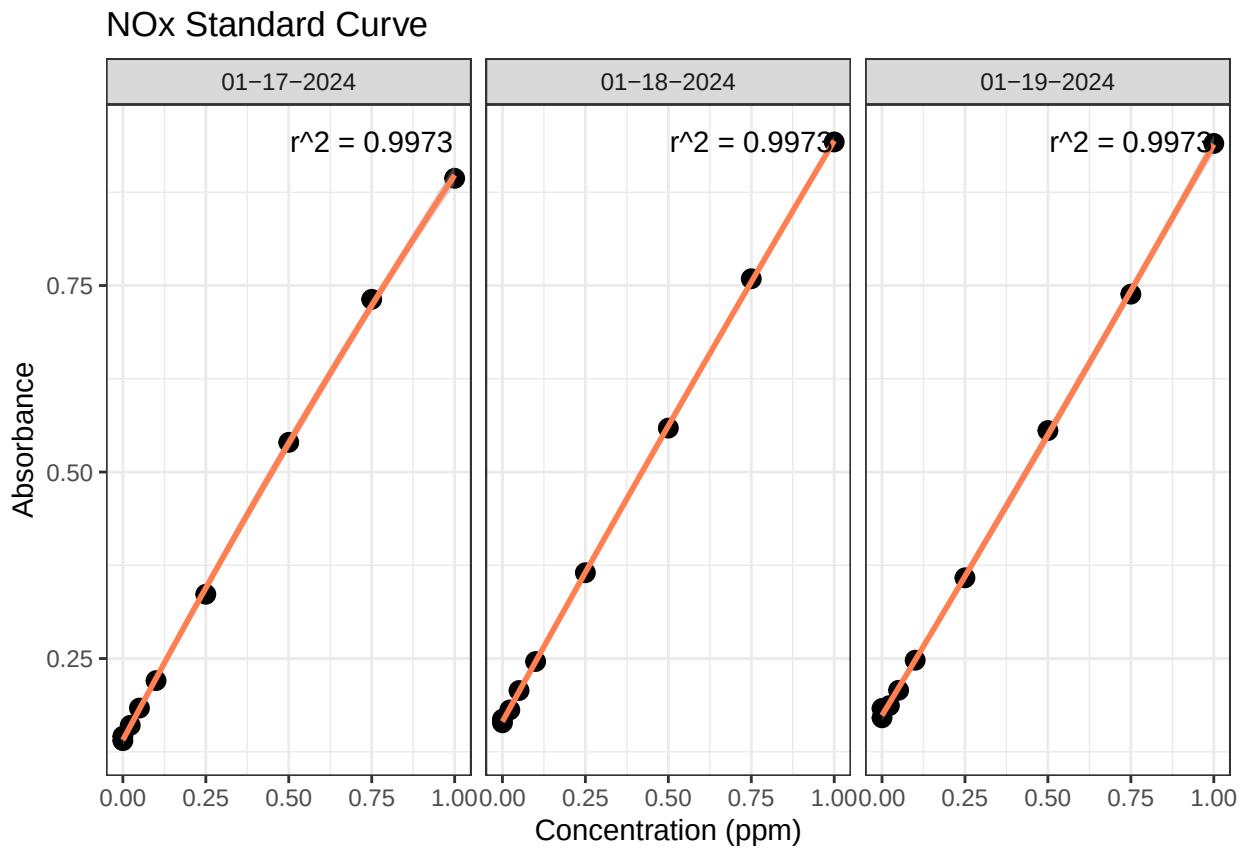
0.2 Assessing standard Curves

#Pull out standards data

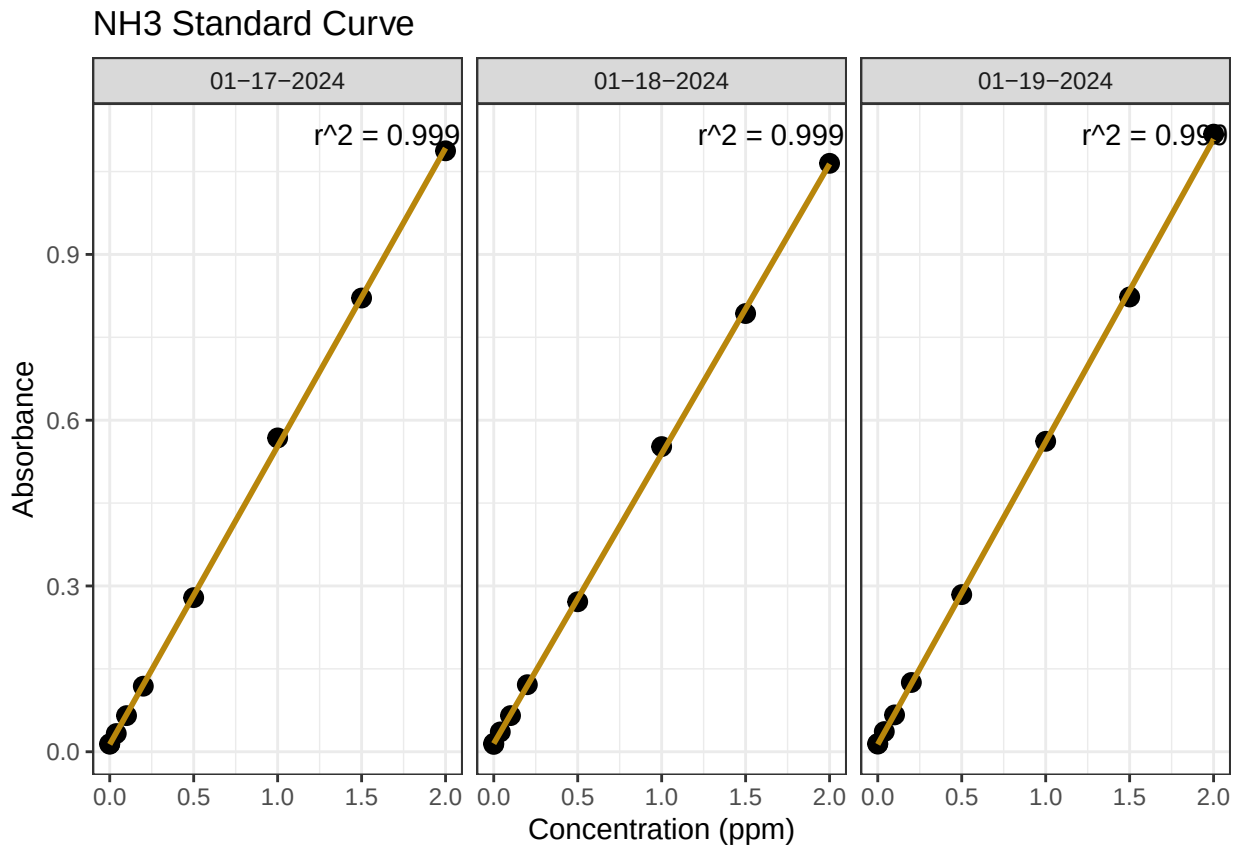
```
## Assess Standard Curves
```

#Plot standards data

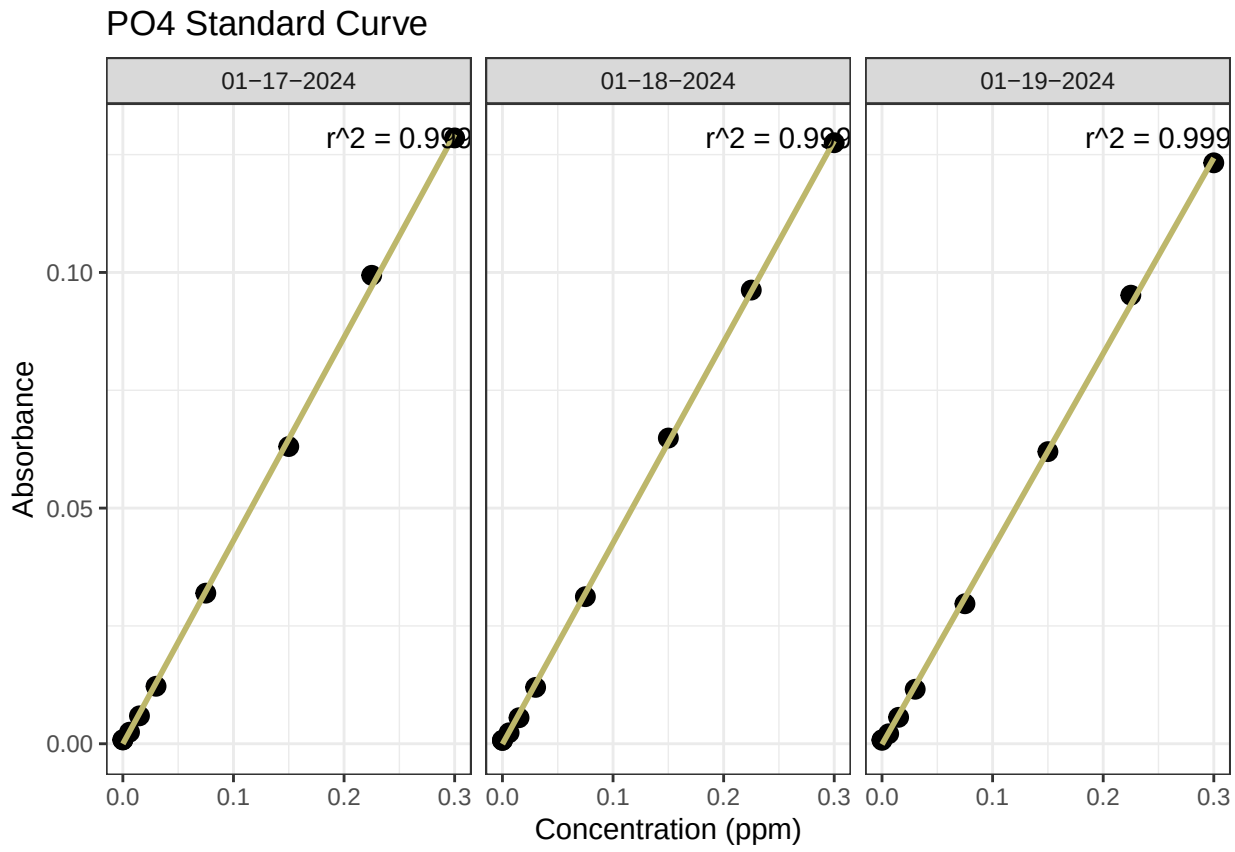
```
## Assess Standard Curves
```




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




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




```
## [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."
```

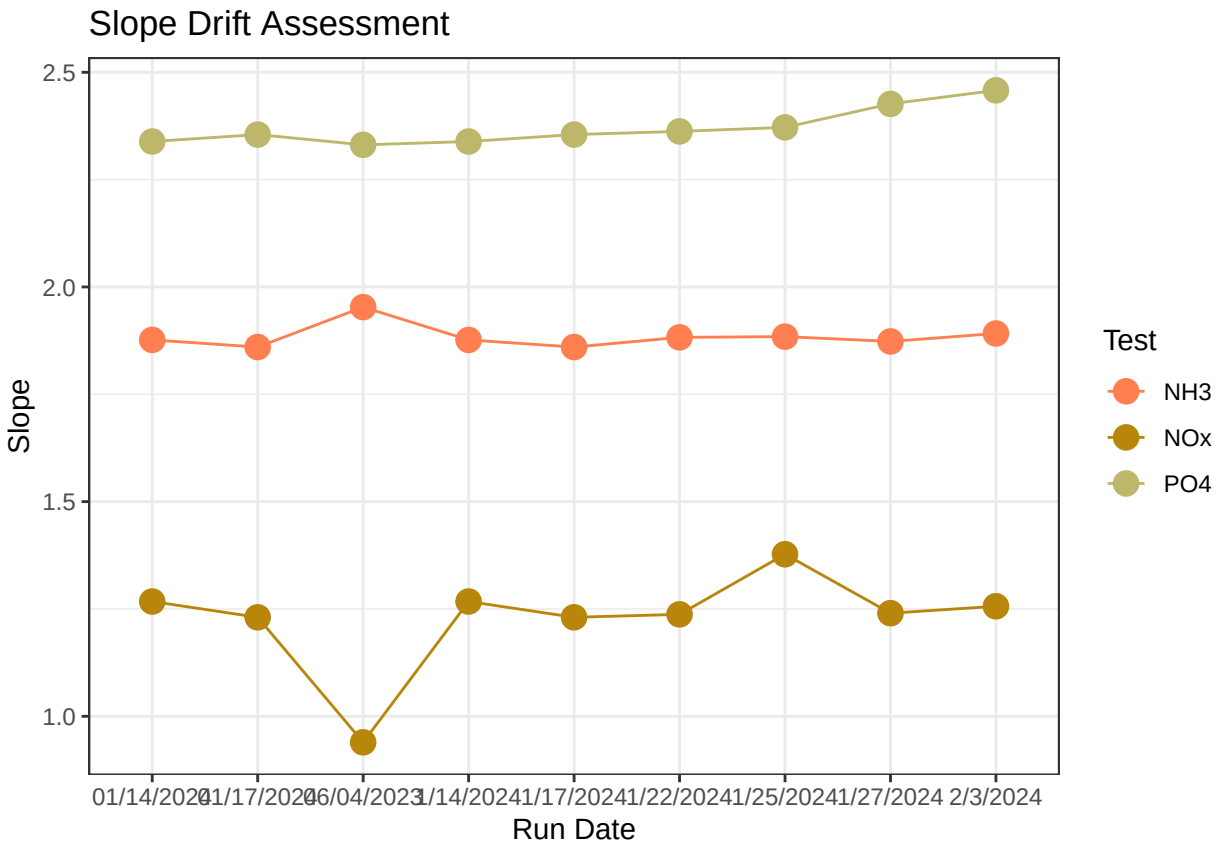


Table 1: Average Slope by Analyte

Test	avg_slope
NH3	1.884
NOx	1.227
PO4	2.371

0.3 Dilution Corrections - ensure the latest dilution is kept

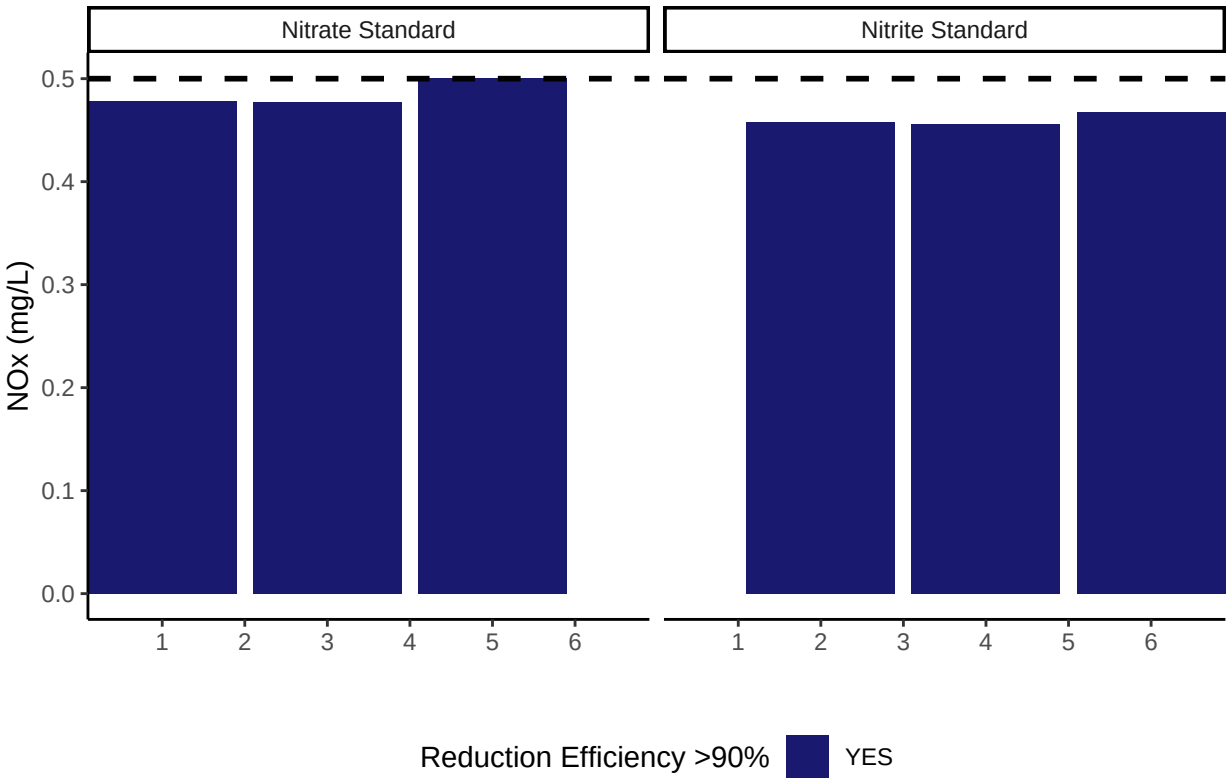
```
## Dilution Corrections

## Duplicated samples: MSM_202307_UP_LysC_20cm, MSM_202307_TR_LysA_20cm, MSM_202307_TR_LysB_10cm, MSM_2

## All duplicated samples have valid dilutions. No naming issues detected.
```

0.4 Performance Check

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

## Run mean = 2.511515

## Expected  = 0.706

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

## Run mean = 0.820844

## Expected  = 0.948

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

## Run mean = 0.878815

## Expected  = 0.818
```

#Check NOx Reduction Efficiency

```
## Assess Reduction Efficiency
```




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

```
## [1] 94.57947
```

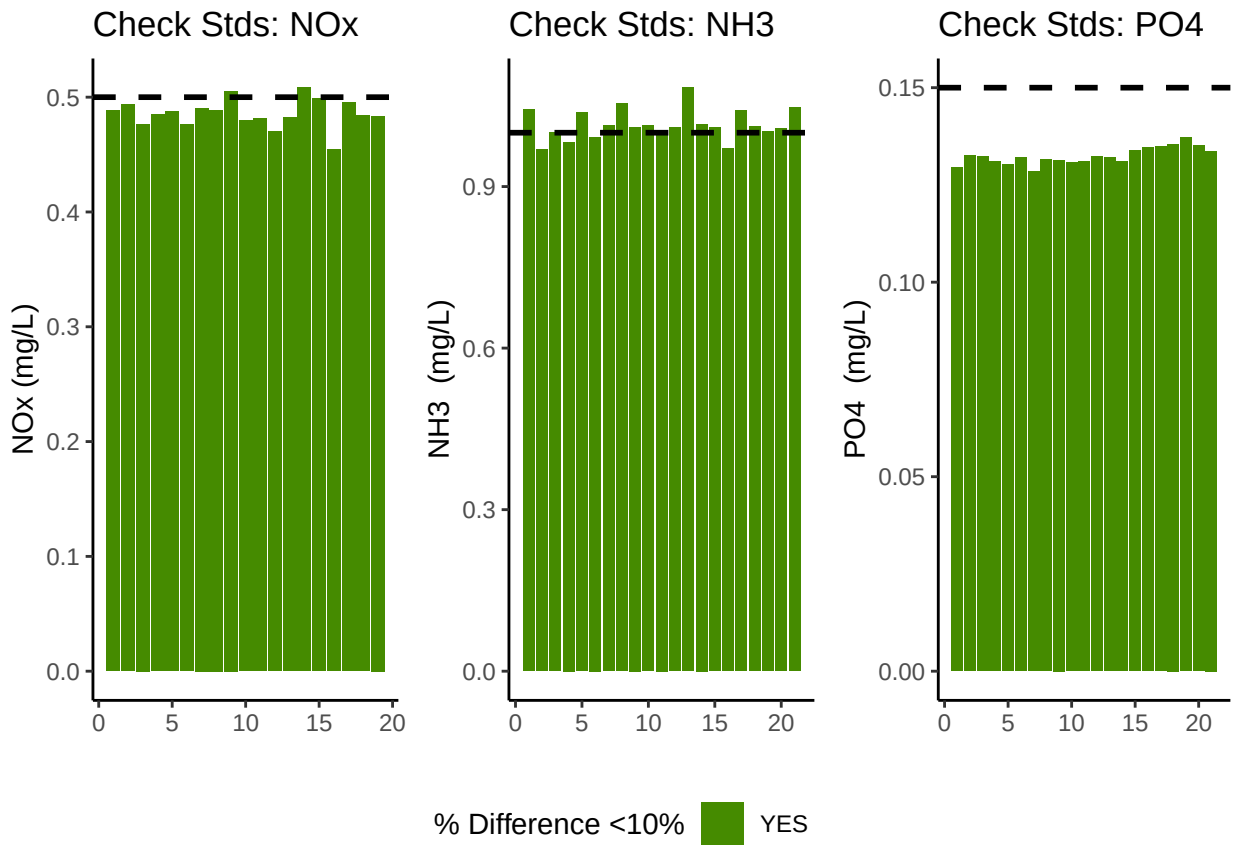
0.5 Analyze the Check Standards

```
## 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"
```

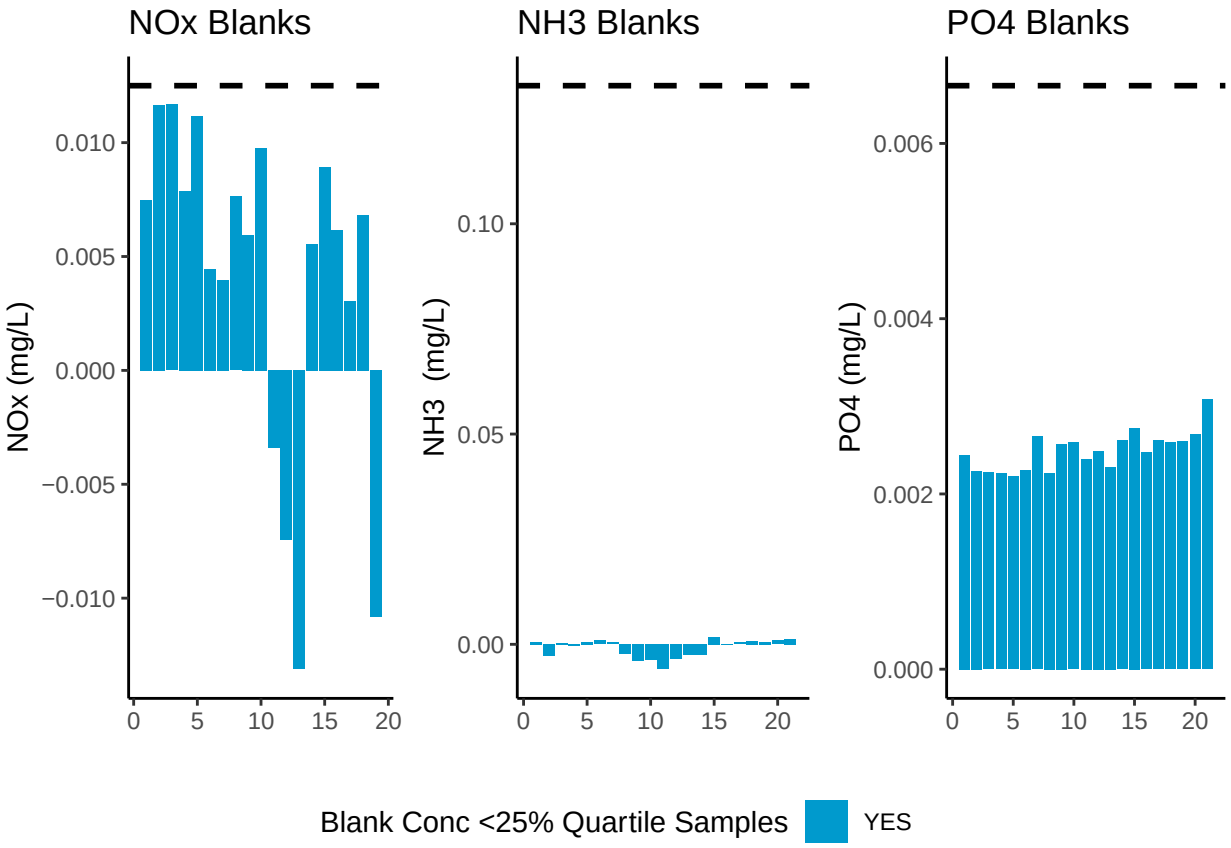
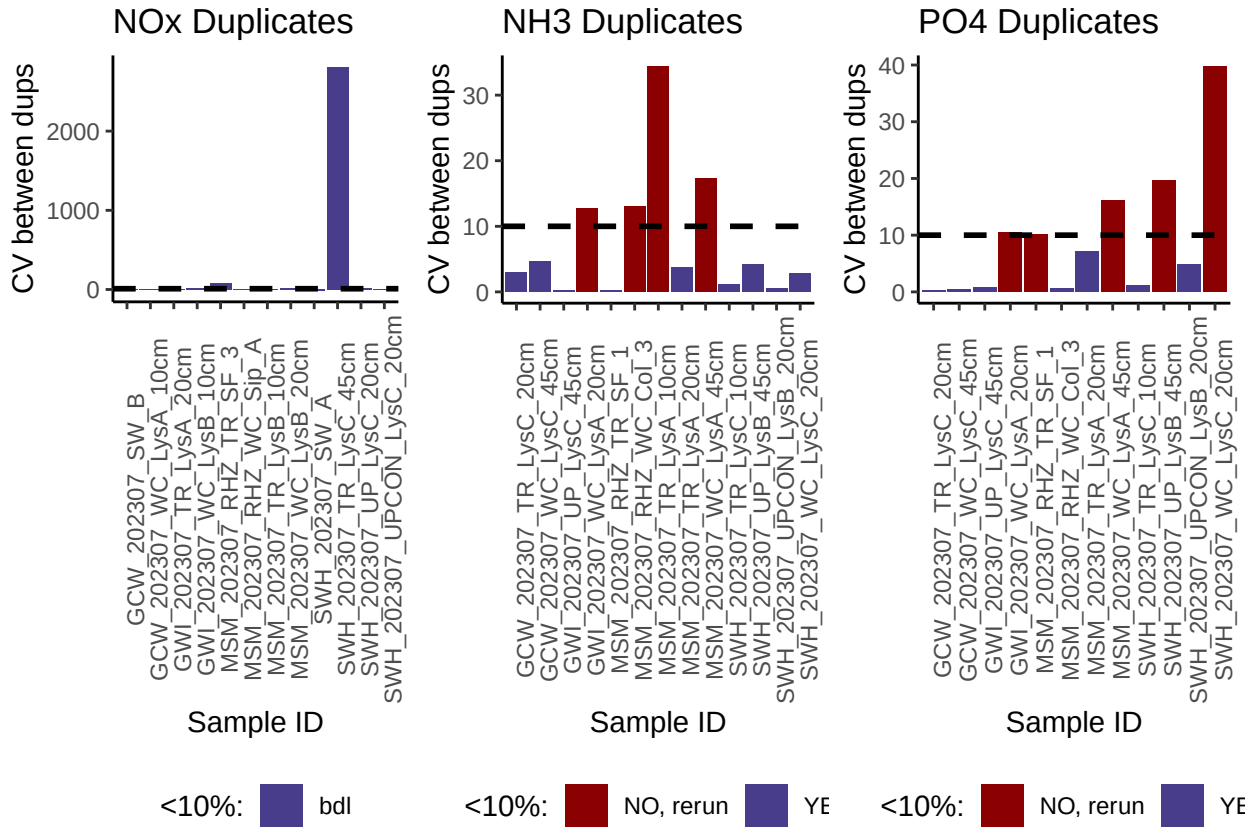


Table 2: Mean Concentration of Blanks

Test	Blank_Mean_Conc
NOx	0.0041
NH3	-0.0009
PO4	0.0025

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.
```

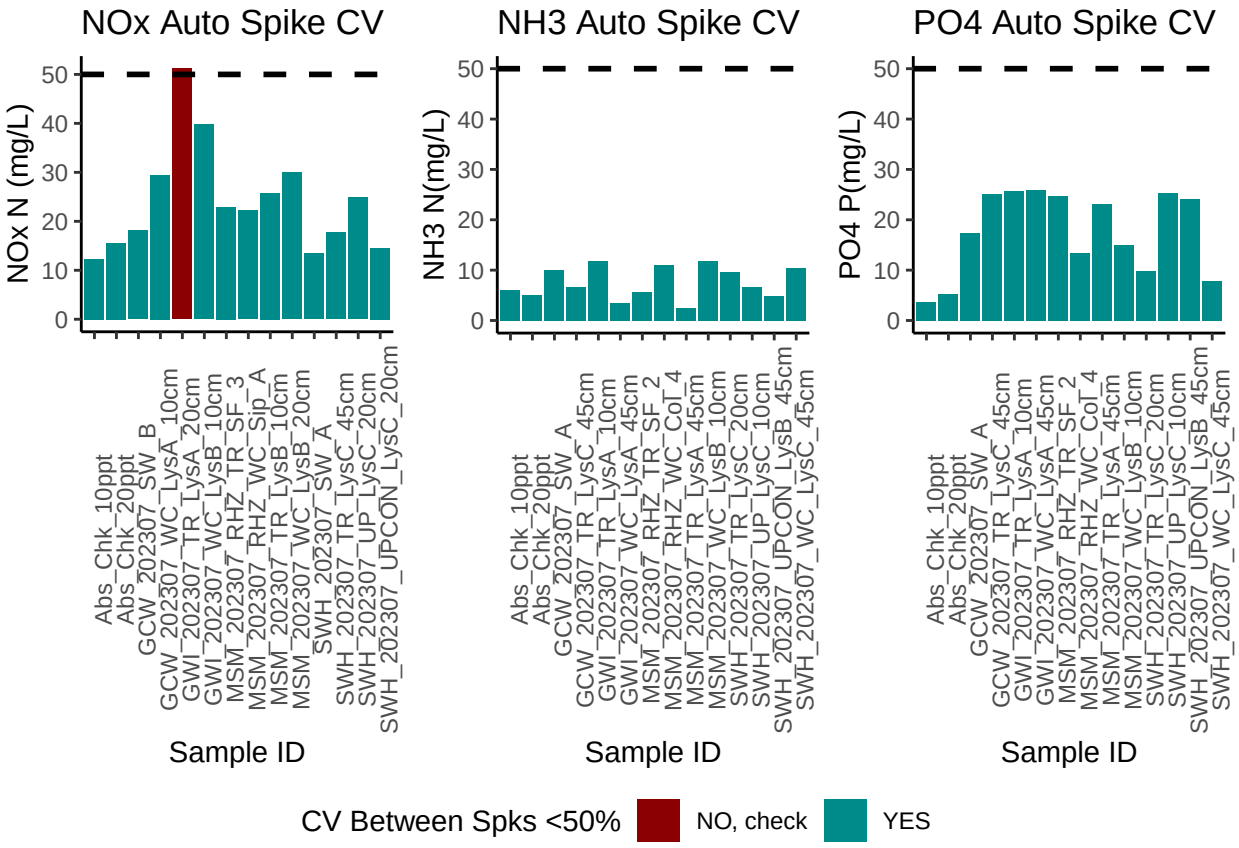


0.8 Spikes

```
## [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 [19, 20, 21, 44,
## 45, 46, 83, 84, 85, 110, 111, 112, 131, 132, 133, 167, 168, 169, 199, 200,
## ...].
```

0.13 Pulling Rhizon Samples

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

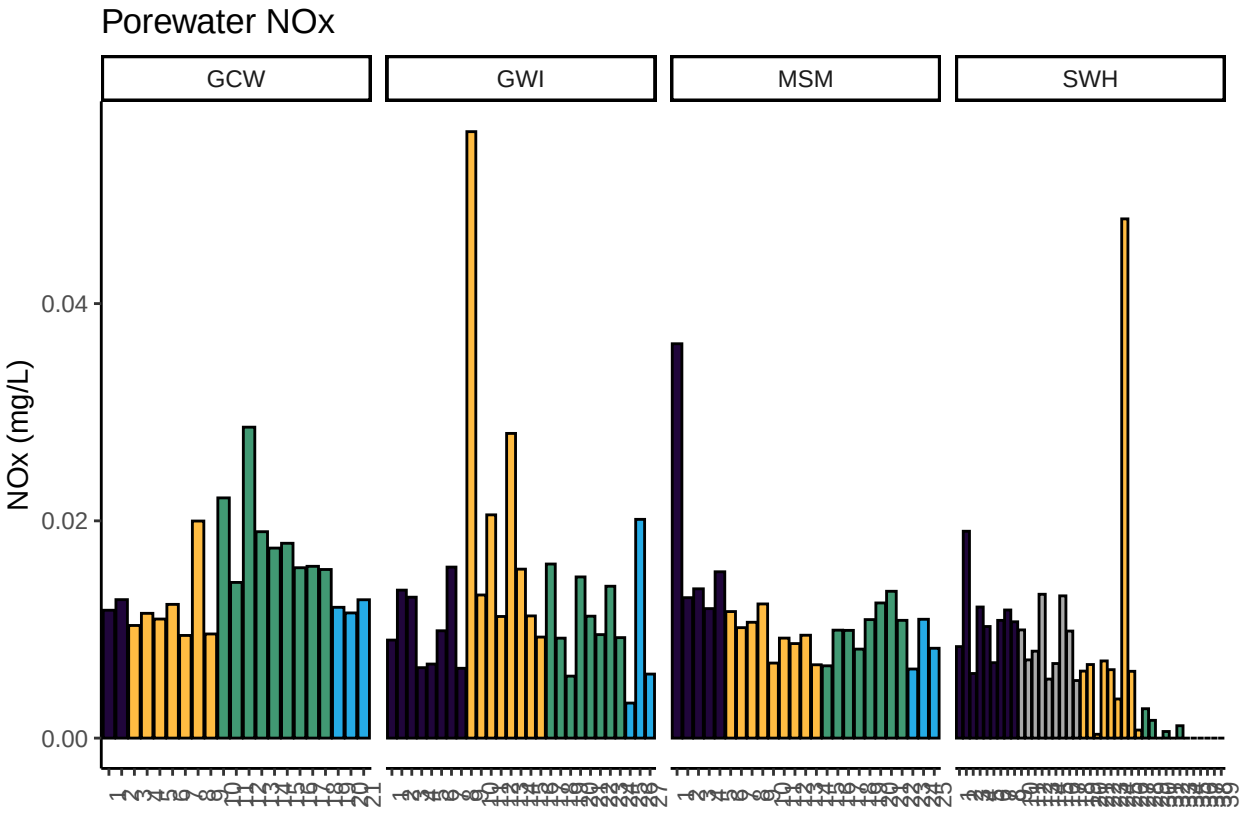
```
## Check Sample IDs with Metadata
```

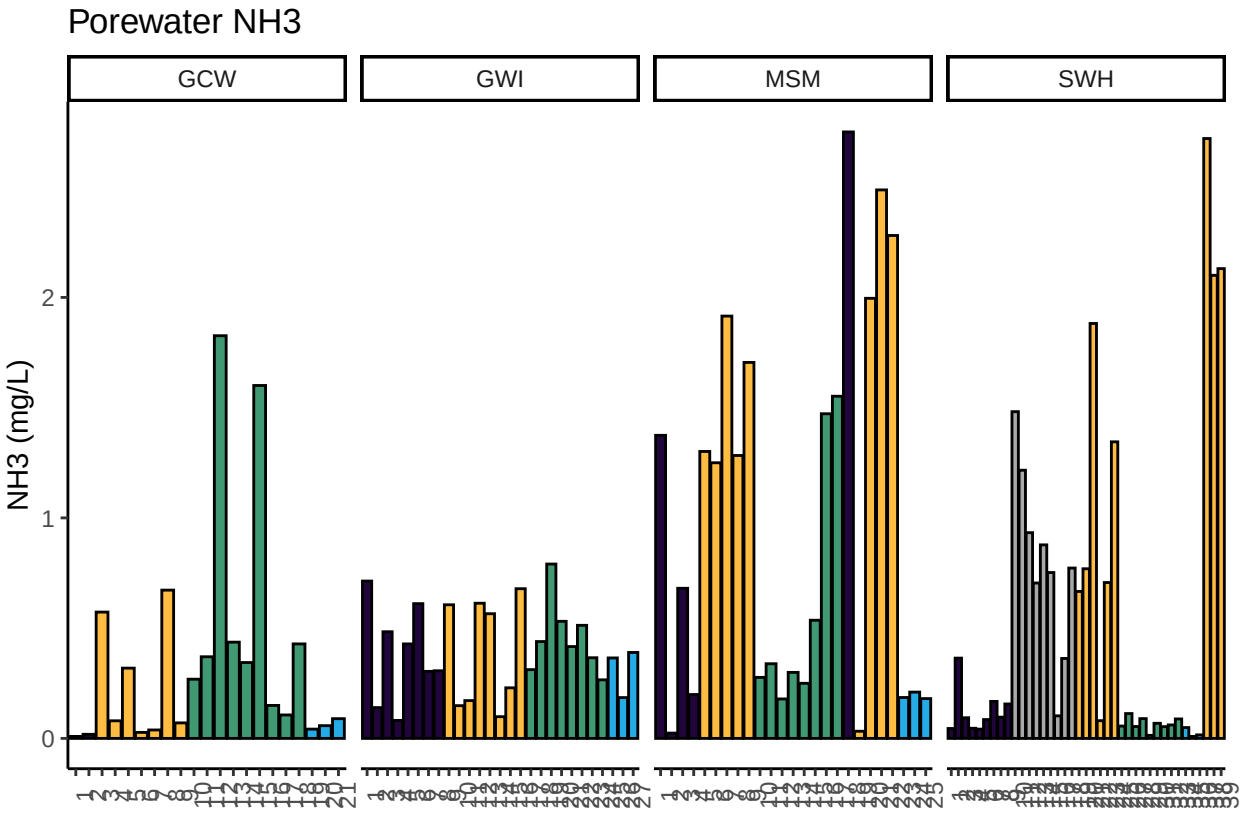
```
## All sample IDs are present in metadata.
```

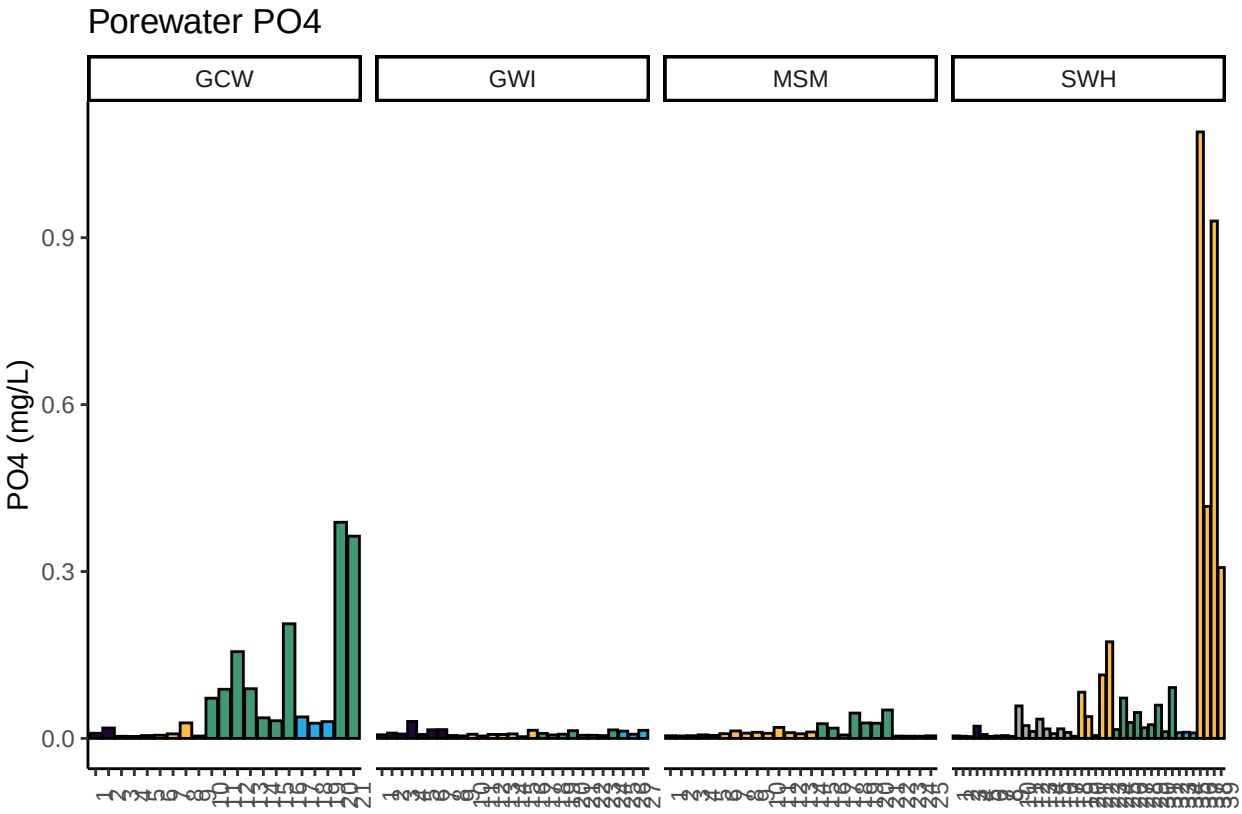
```
## Warning: Expected 5 pieces. Missing pieces filled with `NA` in 36 rows [19, 20, 21, 44,
## 45, 46, 83, 84, 85, 110, 111, 112, 131, 132, 133, 167, 168, 169, 199, 200,
## ...].
```

0.15 Visualize Data

```
## Visualize Data
```




Porewater NH3
GCW
GWI
MSM
SWH
NH3 (mg/L)
0
1
2



0.16 Export Processed Data

#end