Synoptic CB: Porewater Nutrients

July 2024 Samples

2025-10-31

Contents

Run Information

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

```
## Run Information: NAME
```

```r
#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_PO4_files <- c("Raw Data/COMPASS_Synoptic_CB_202407_NH3_PO4_1.csv",
                     "Raw Data/COMPASS_Synoptic_CB_202407_NH3_PO4_2.csv",
                     "Raw Data/COMPASS_Synoptic_CB_202407_NH3_PO4_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 PO4 blank had high CV.
                Over 60% of PO4 Duplicates have a CV less than 10%.
                Some sample IDs are missing from metadata:
                SWH_202407_UP_LysC_10cm, SWH_202407_WC_LysA_45cm"

#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 PO4 blank had high CV.
##               Over 60% of PO4 Duplicates have a CV less than 10%.
##               Some sample IDs are missing from metadata:
##               SWH_202407_UP_LysC_10cm, SWH_202407_WC_LysA_45cm
```

Setup

Read in metadata and create similar sample IDs for matching to samples
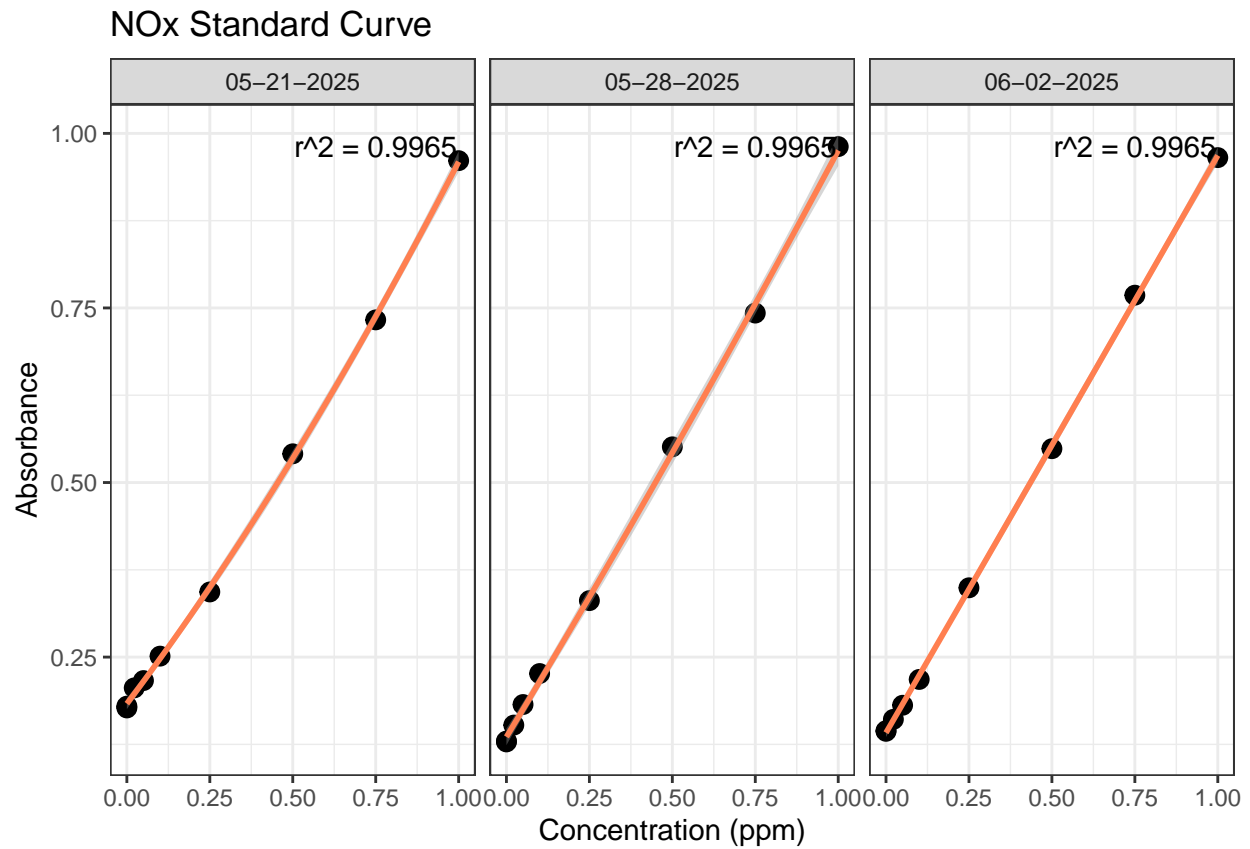
0.1 Import Data & Clean

0.2 Assessing standard Curves

Assess Standard Curves
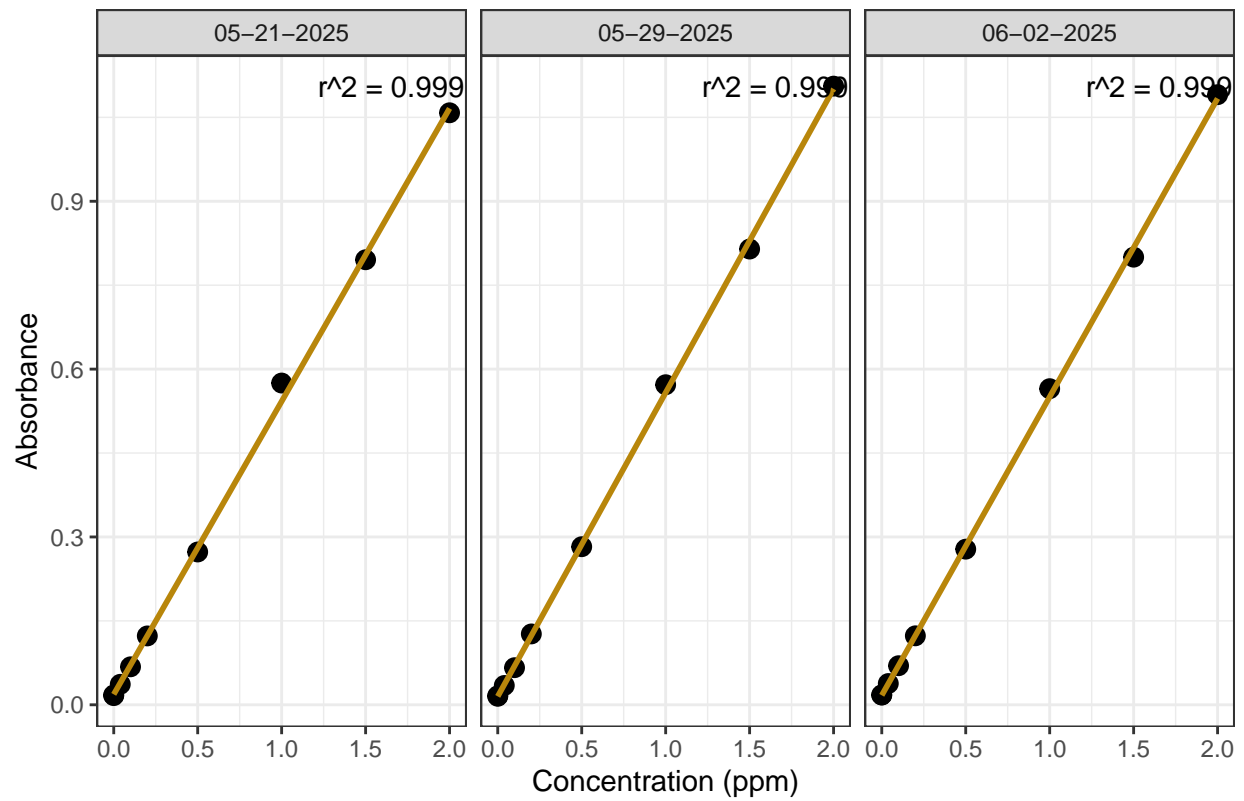
#Plot standards data

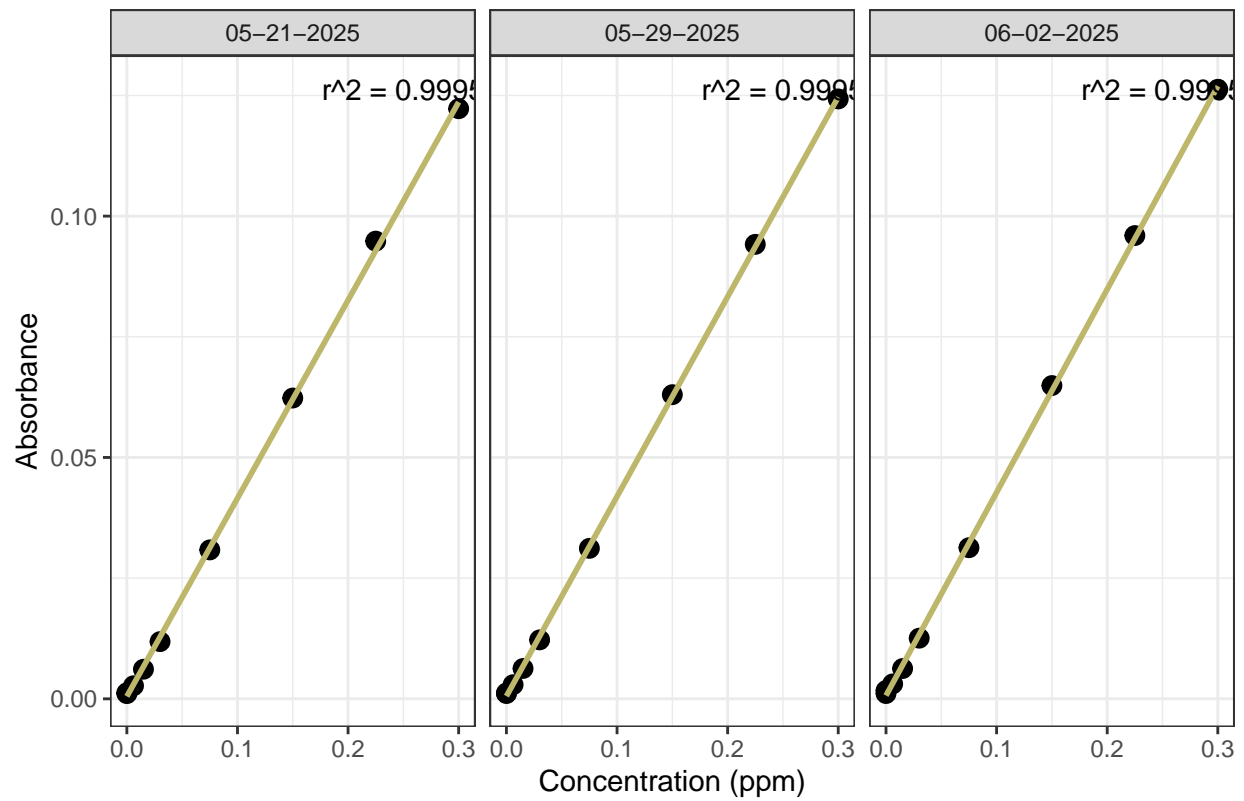## Assess Standard Curves

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 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
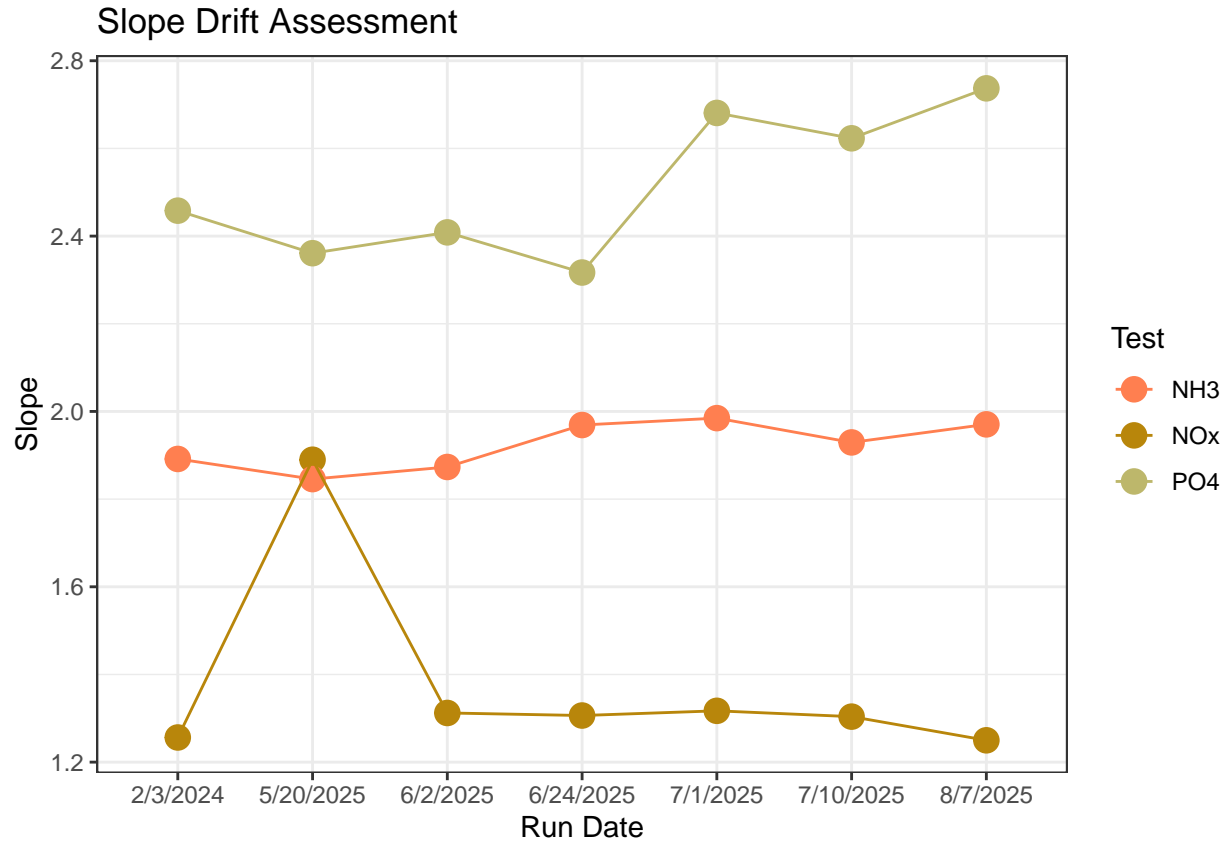

Table 1: Average Slope by Analyte

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: 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
```

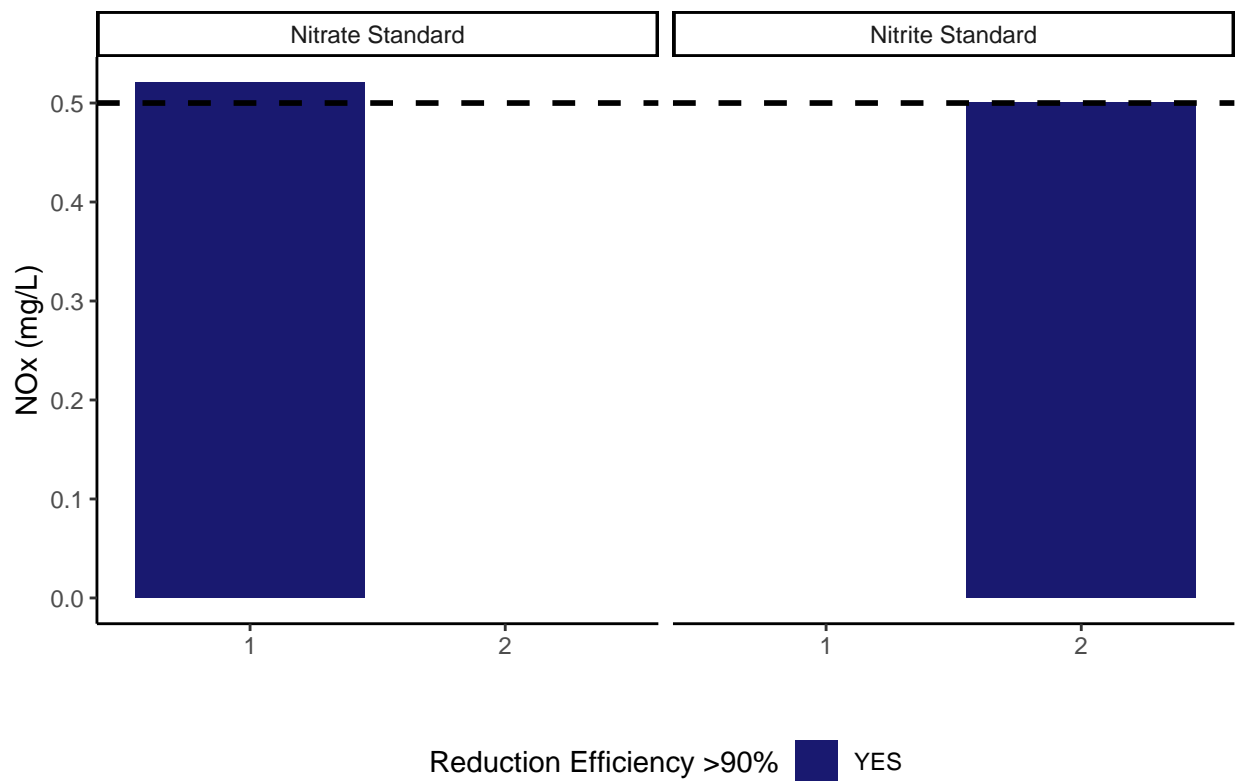## [1] "NH3 pe Check has a % Difference <25% - PROCEED"

Run mean = 1.284822

Expected = 1.034

[1] "PO4 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

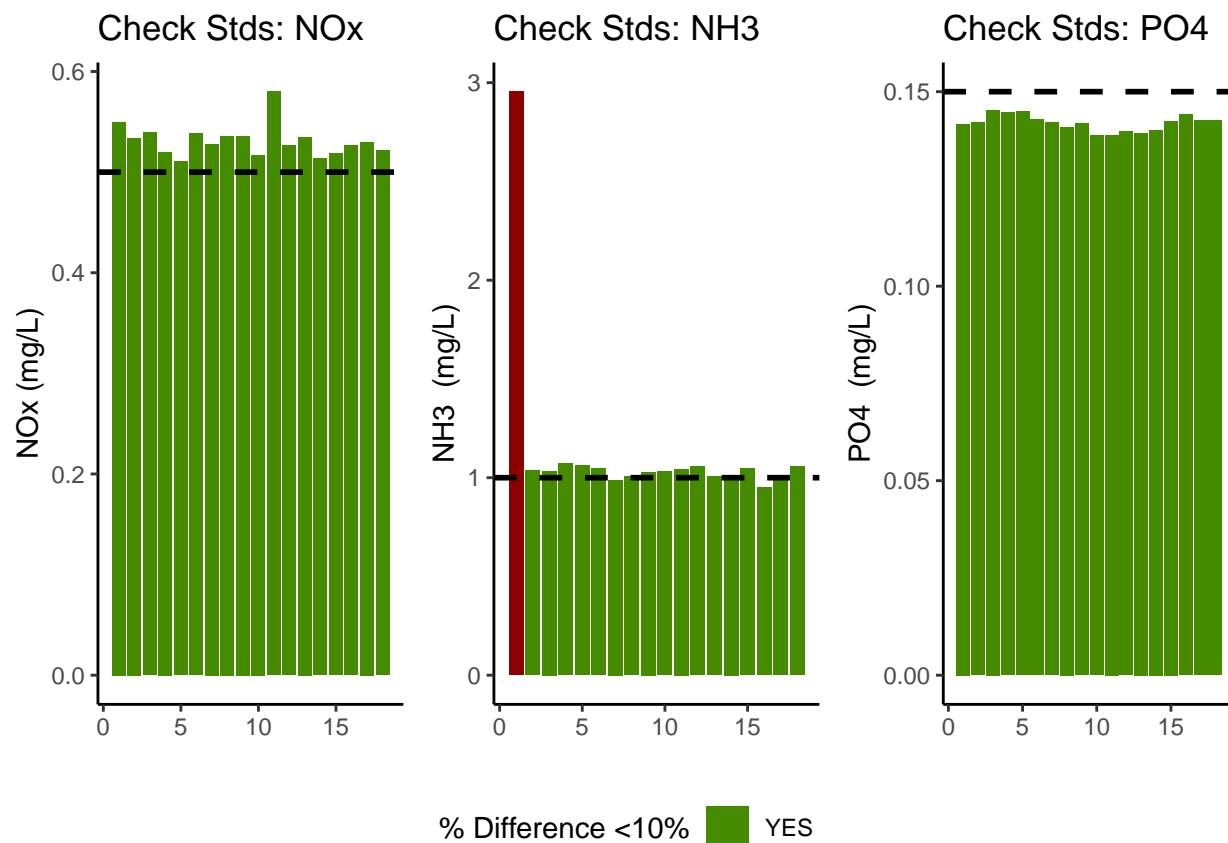## 0.5 Analyze the Check Standards

```
## 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"
```
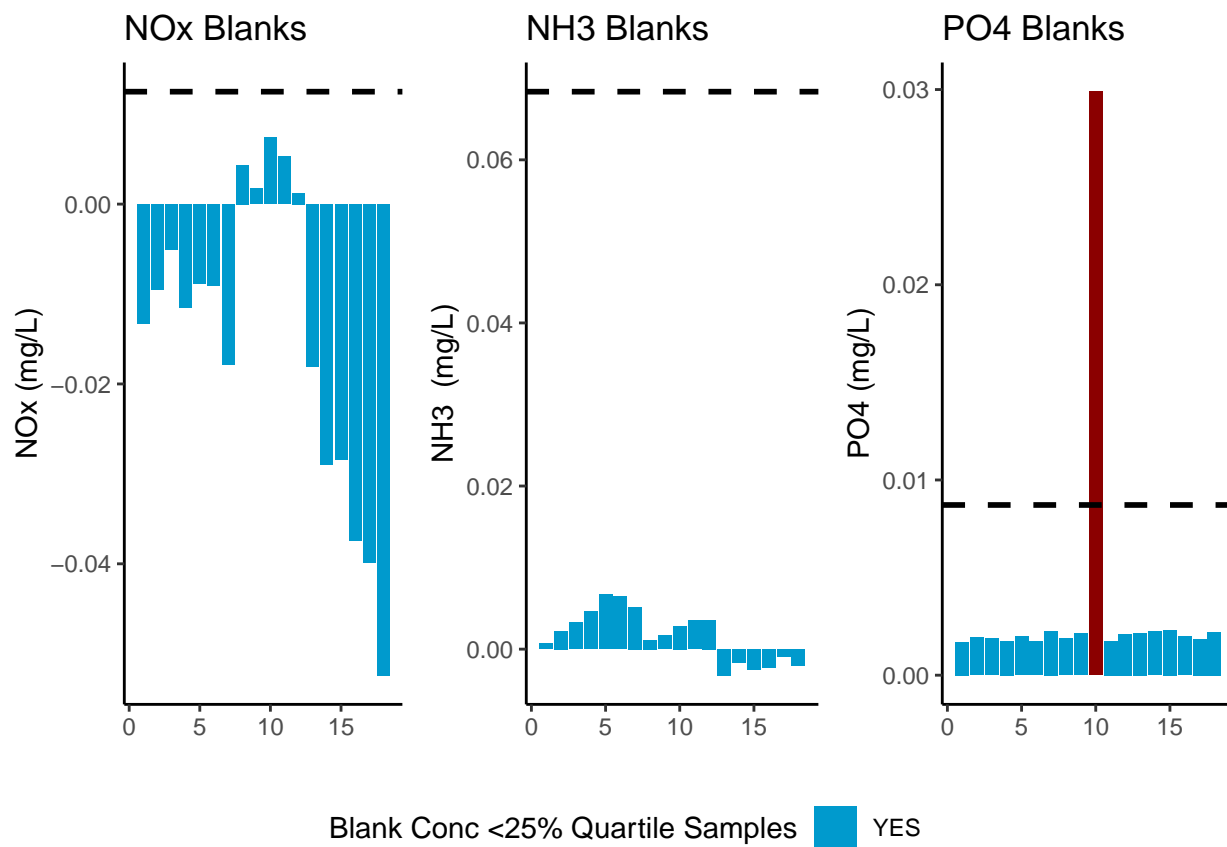

Table 2: Mean Concentration of Blanks

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.
```
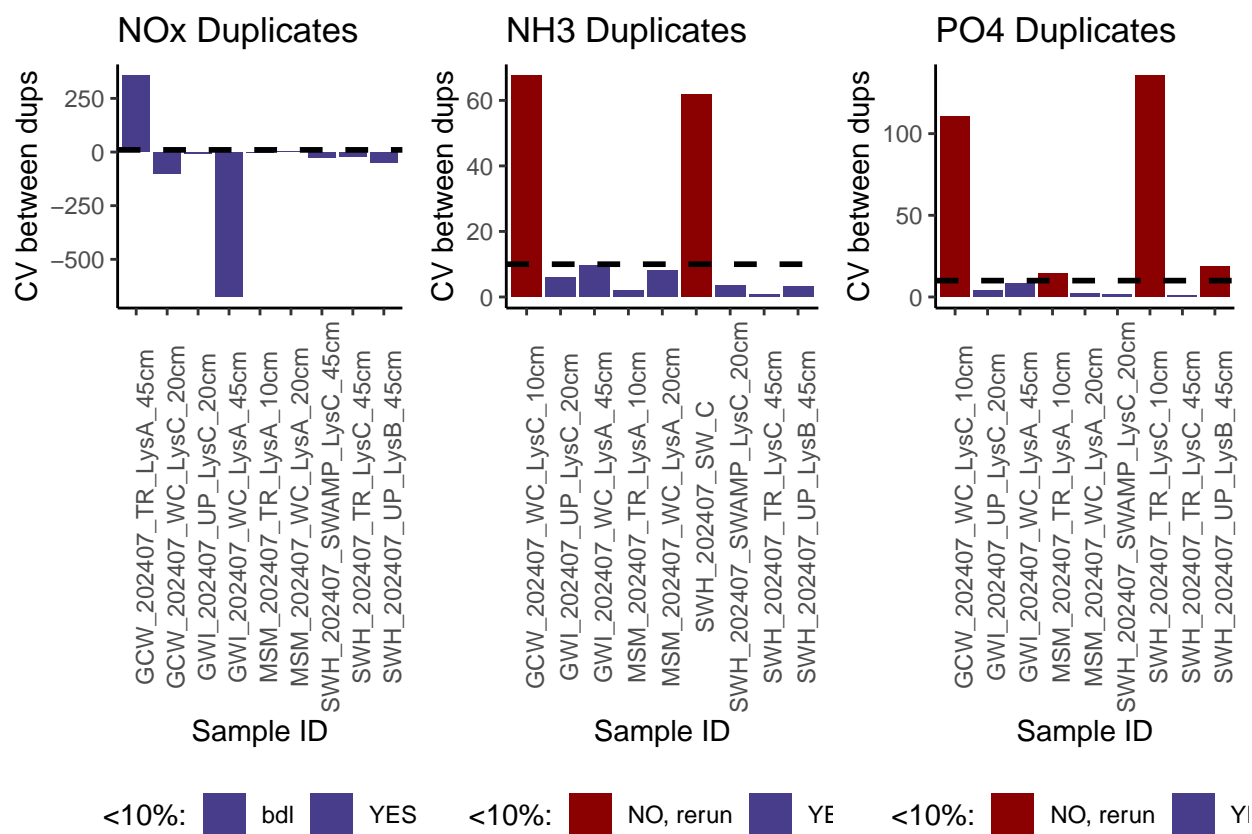
0.8   Spikes

```
## [1] ">60% of Spikes have a CV <50% - PROCEED"
```
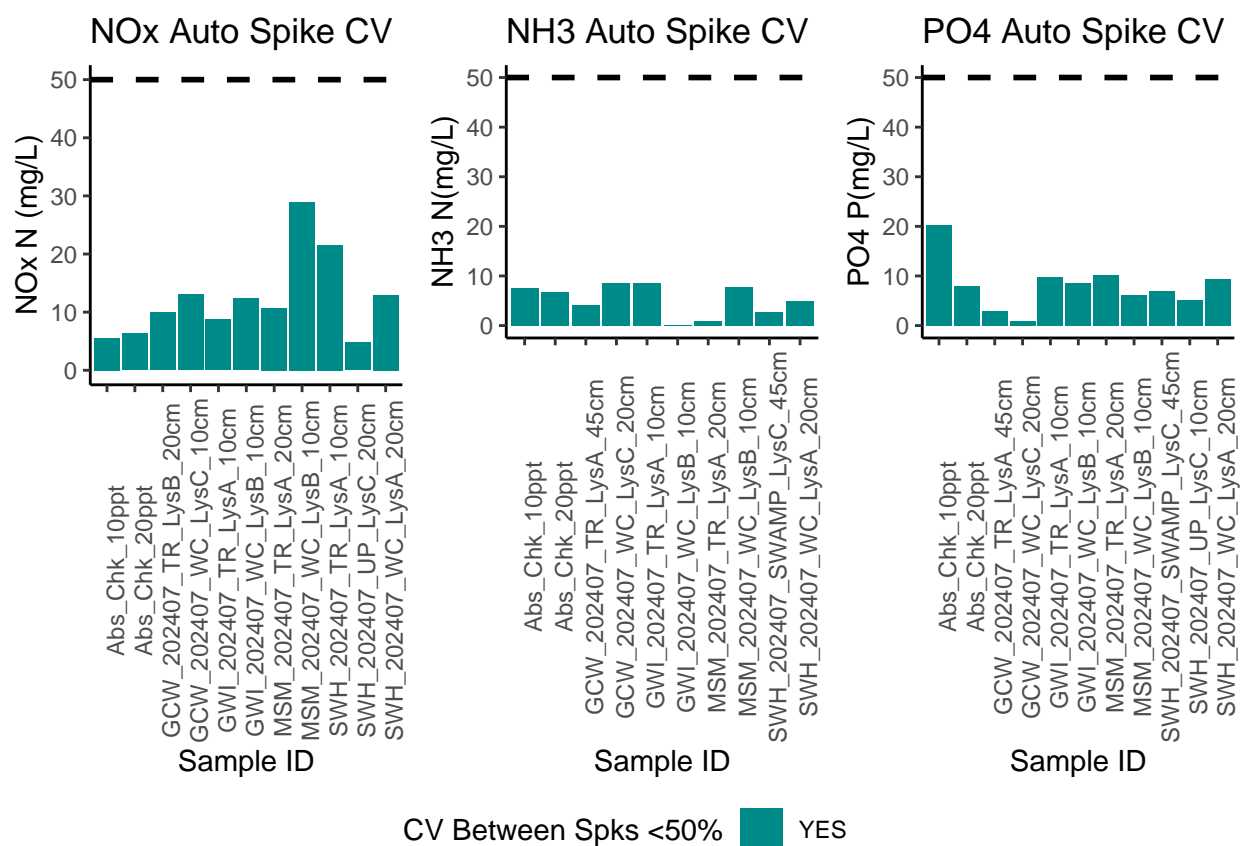
```
## [1] ">60% of Spikes have a CV <50% - PROCEED"
```

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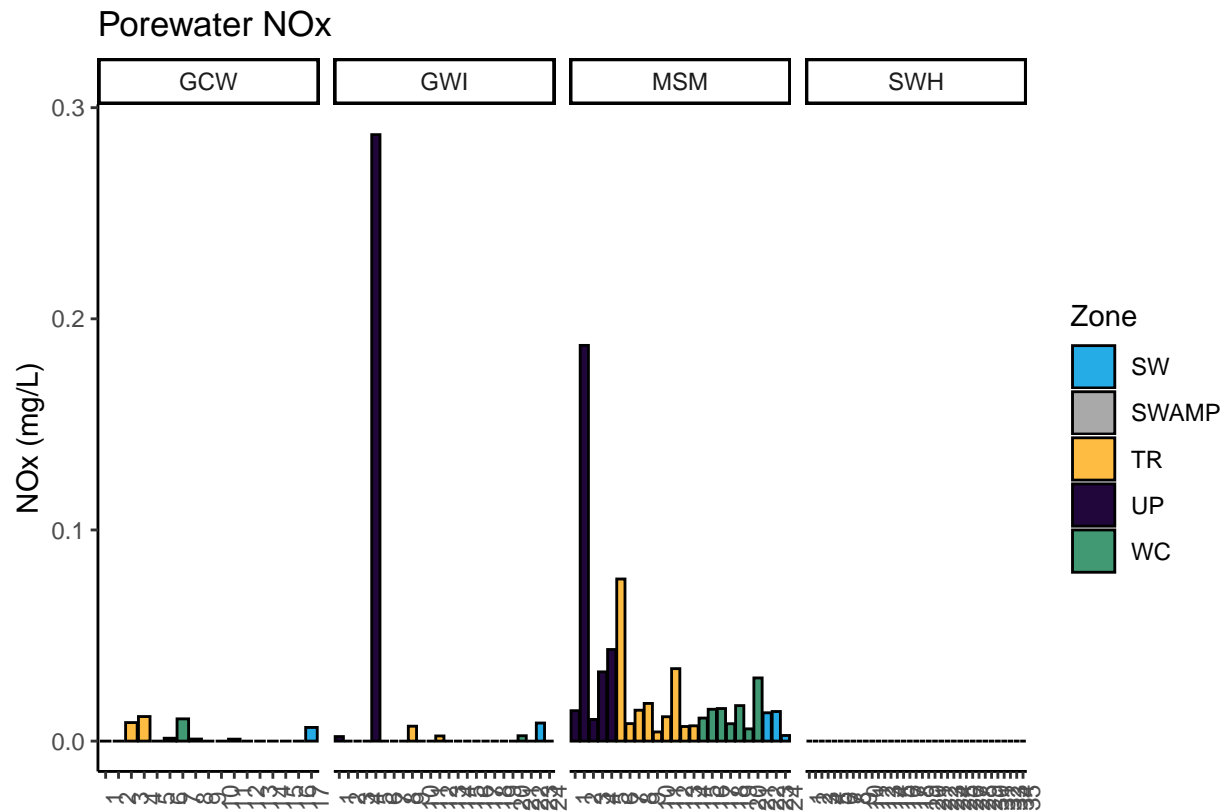
```
## Check Sample IDs with Metadata
```

```
## Some sample IDs are missing from metadata.
```
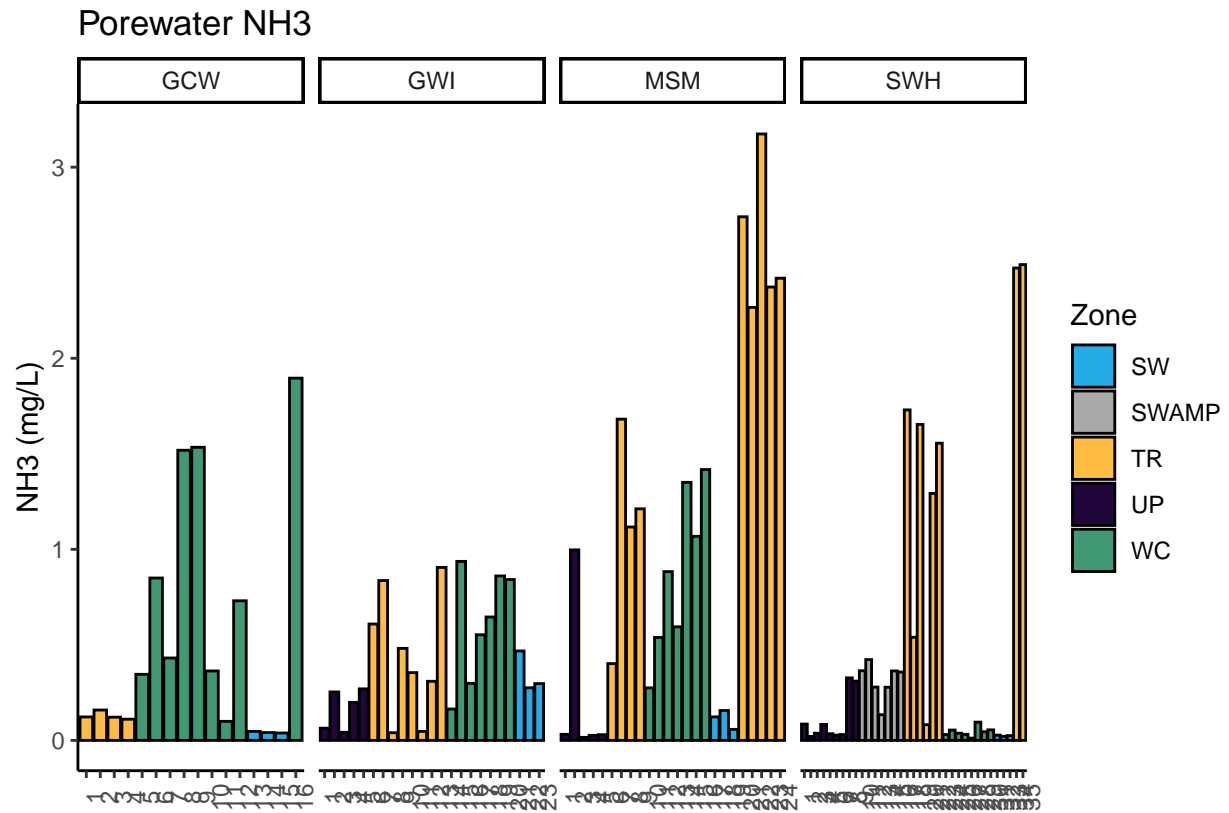
```
## [1] "SWH_202407_UP_LysC_10cm" "SWH_202407_WC_LysA_45cm"
```
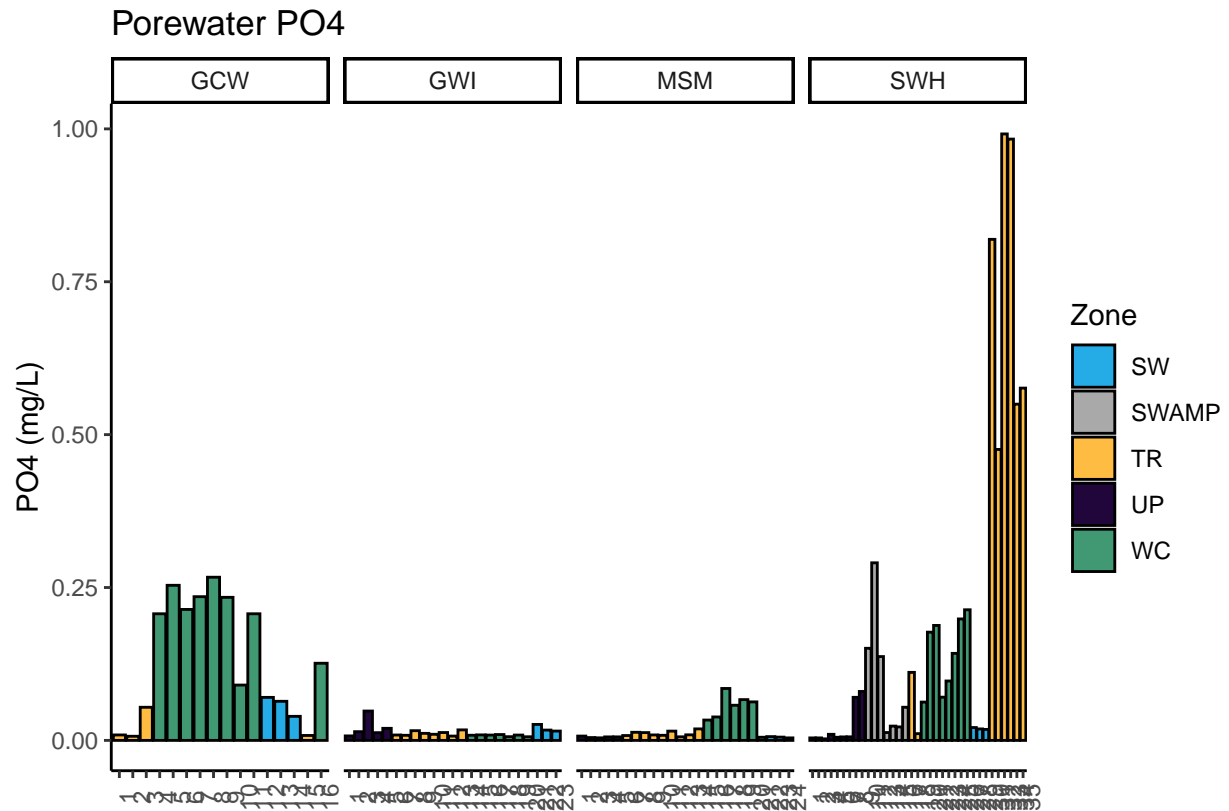
```
## Warning: Expected 5 pieces. Missing pieces filled with 'NA' in 36 rows [22, 23, 24, 39,
## 40, 41, 63, 64, 65, 98, 99, 100, 121, 122, 123, 136, 137, 138, 159, 160, ...].
```

0.14 Visualize Data

```
## Visualize Data
```


Porewater NOx

Porewater NH3

Porewater PO4

0.15   Export Processed Data

#end