Synoptic CB: Porewater Nutrients

May 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 <- "5/12/2025"
  sample_year <- "2024"
  sample_month <- "MAY"
  user <- "Isabelle Van Benschoten"

##Data entered incorrectly
Old_ID_1 <- "SWH_202405_SWAMP_LysA_10"
New_ID_1 <- "SWH_202405_SWAMP_LysA_10cm"

#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_202405_VNox_1.csv",
                 "Raw Data/COMPASS_Synoptic_CB_202405_VNox_2.csv",
                 "Raw Data/COMPASS_Synoptic_CB_202405_VNox_4.csv")
  NH3_PO4_files <- c("Raw Data/COMPASS_Synoptic_CB_202405_NH3_PO4_1.csv",
                     "Raw Data/COMPASS_Synoptic_CB_202405_NH3_PO4_2.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_202405.csv"

#record any notes about the run or anything other info here:
  run_notes <- "Some sample IDs are missing from metadata:
  MSM_202405_UP_LysA_10cm
  MSM_202405_UP_LysA_20cm
  MSM_202405_WC_LysC_20cm
  GWI_202405_TR_LysC_45cm.
  It looks like NH3 was only ran for GCW, MSM, and SWH.
  It looks like PO4 was only ran for GCW and MSM.
  Mean NOx Reduction Efficiency is less than 95% (94.18327%).
  Most of the NOx blanks are above the lower 25% quartile of samples.
  3 NOx dups and one NH3 dup have high CVs, but more than 60% have low CVs.
  2 NOx spikes have high CVs, but more than 60% have low CVs."

#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)
```

```
## Some sample IDs are missing from metadata:
##   MSM_202405_UP_LysA_10cm
##   MSM_202405_UP_LysA_20cm
##   MSM_202405_WC_LysC_20cm
##   GWI_202405_TR_LysC_45cm.
##   It looks like NH3 was only ran for GCW, MSM, and SWH.
```

```
##   It looks like PO4 was only ran for GCW and MSM.
##   Mean NOx Reduction Efficiency is less than 95% (94.18327%).
##   Most of the NOx blanks are above the lower 25% quartile of samples.
##   3 NOx dups and one NH3 dup have high CVs, but more than 60% have low CVs.
##   2 NOx spikes have high CVs, but more than 60% have low CVs.
```

##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$Sample_Name[df_all$Sample_Name == Old_ID_1] <- New_ID_1
```

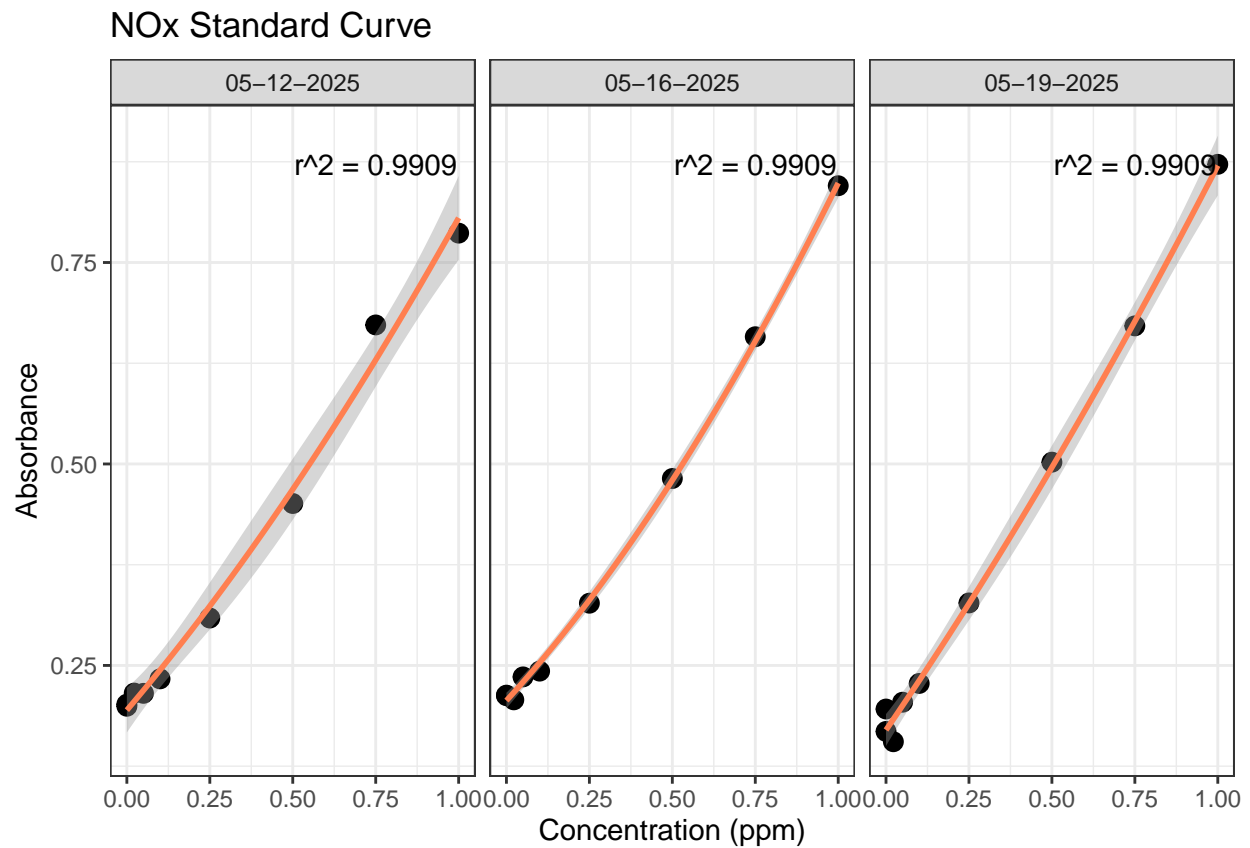## 0.2 Assessing standard Curves

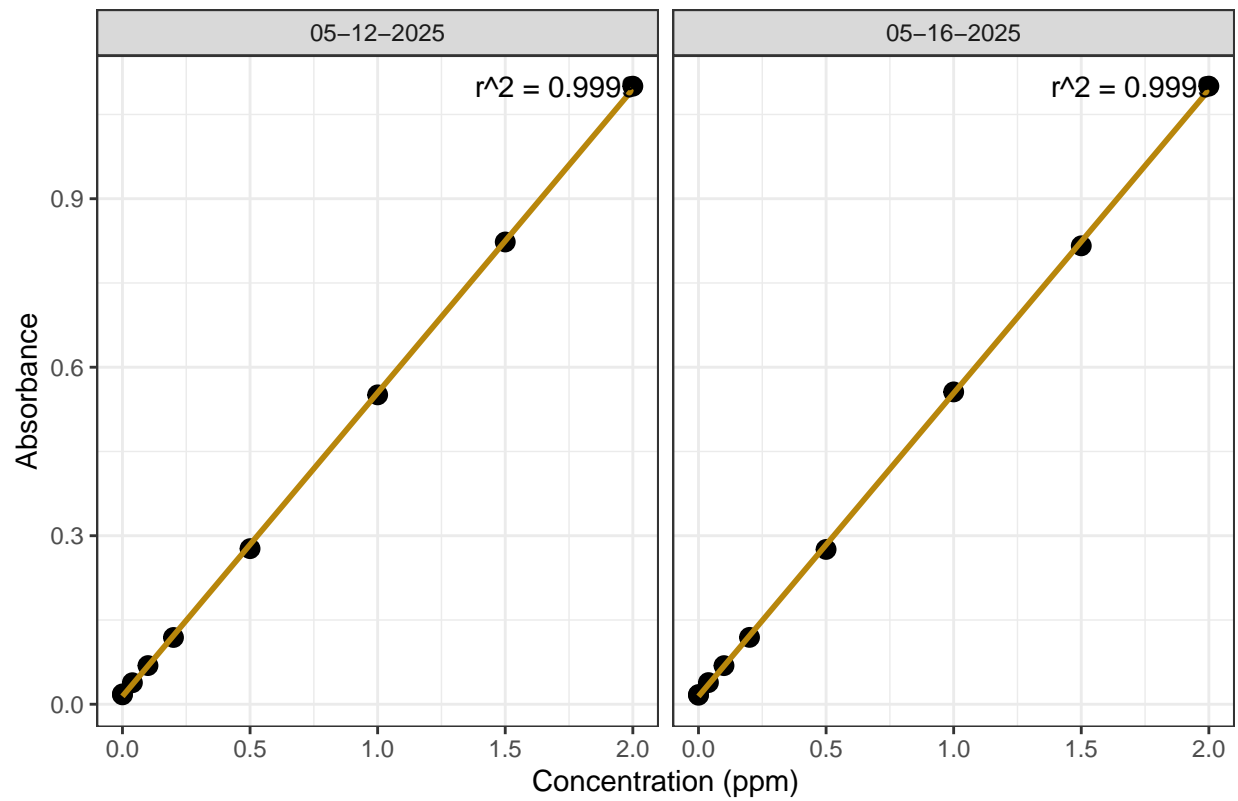#Pull out standards data

Assess Standard Curves

0.3 Plot standards data
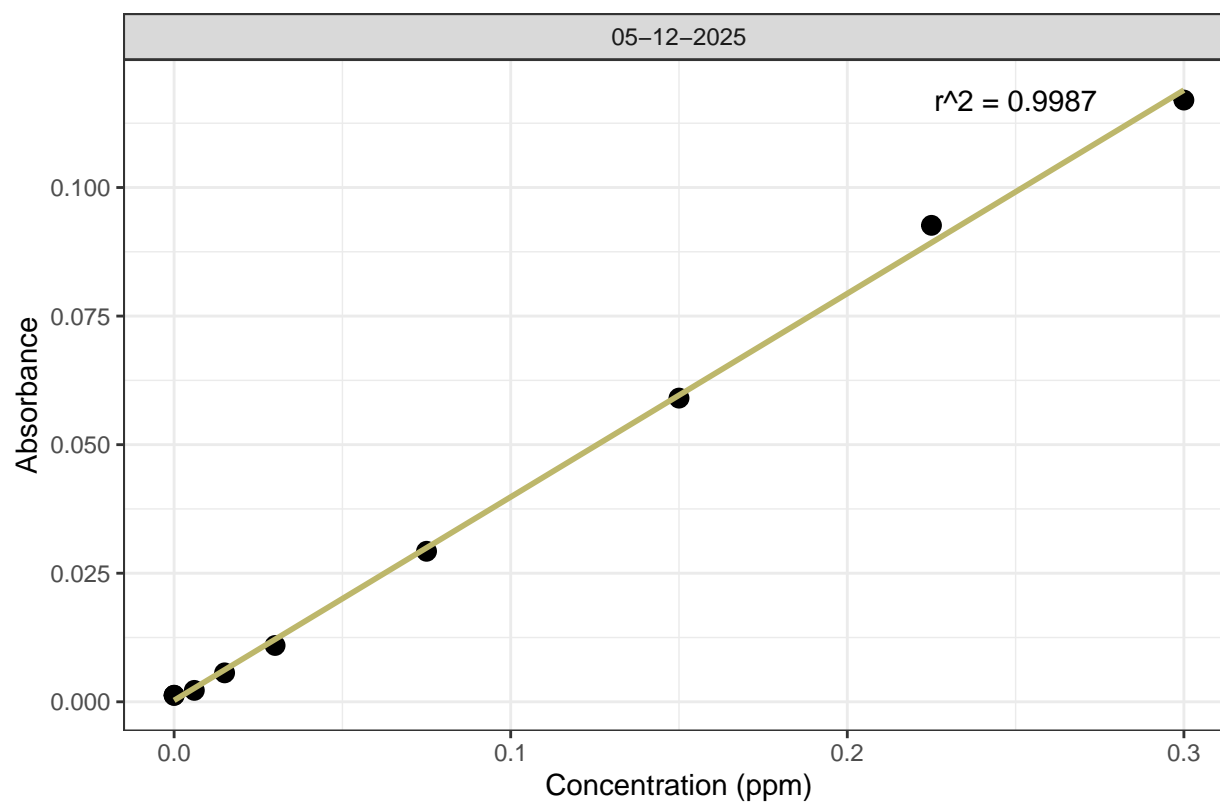
Assess Standard Curves

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
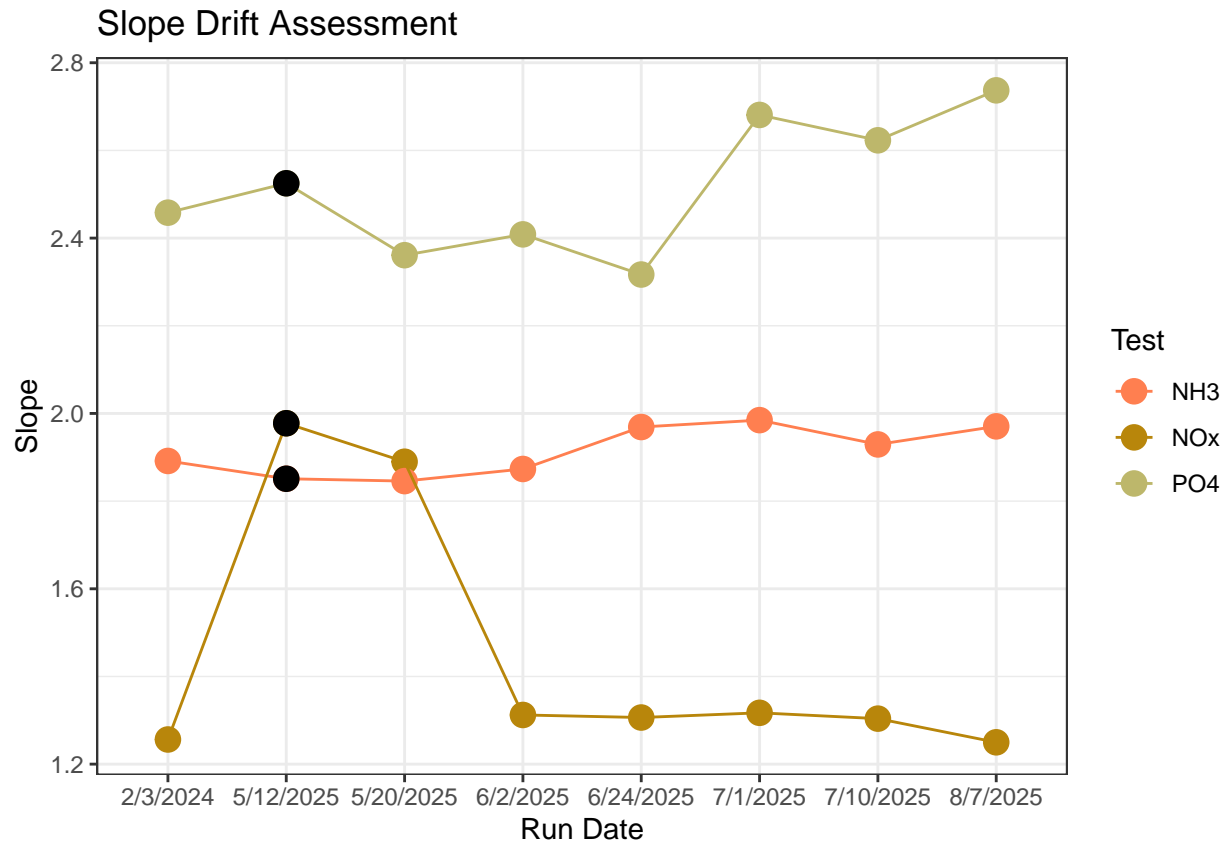
Table 1: Average Slope by Analyte

Test	avg_slope
NH3	1.914
NOx	1.452
PO4	2.514

0.4 Dilution Corrections - ensure the latest dilution is kept

```
## Dilution Corrections

## Duplicated samples: MSM_TR_202405_LysA_20cm, MSM_TR_202405_LysB_45cm, MSM_TR_202405_LysC_45cm, GCW_W(

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

0.5 Performance Check

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

## Run mean = 1.575157

## Expected  = 1.51

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

## Run mean = 1.037336

## Expected  = 1.034

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

## Run mean = 0.94957

## Expected  = 0.824
```
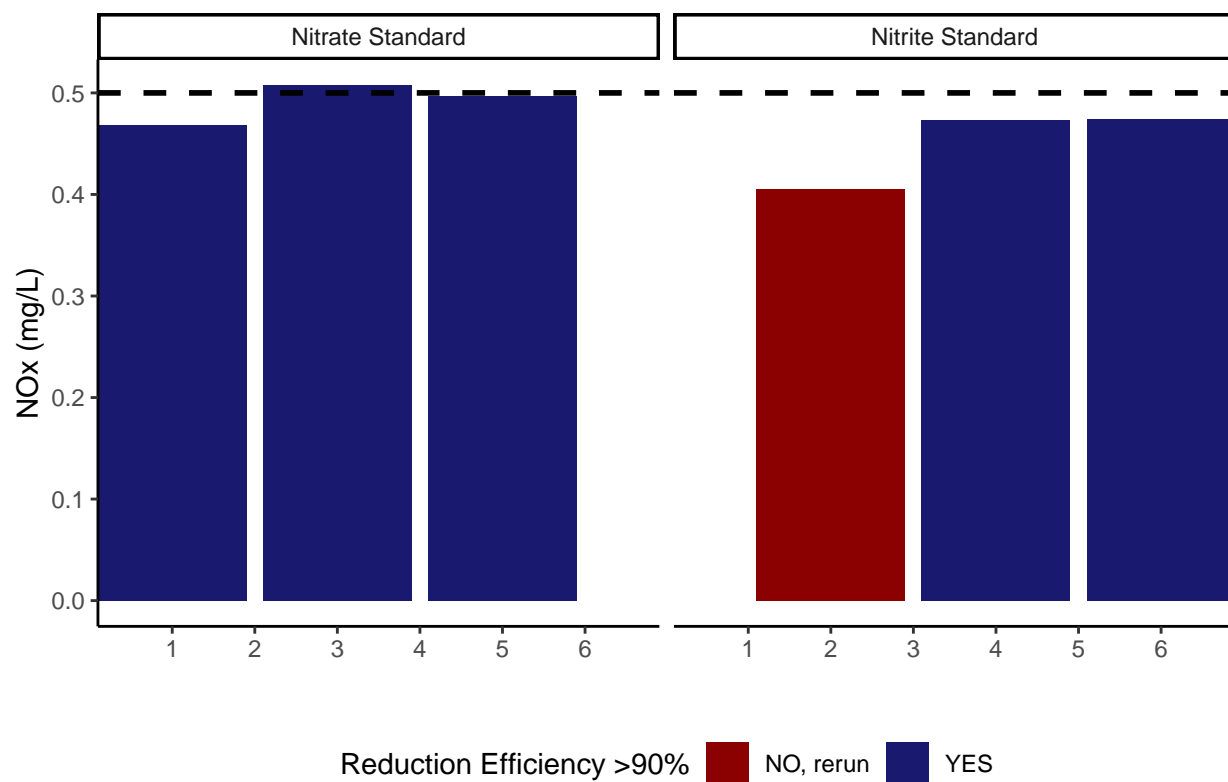
##Check NOx Reduction Efficiency

```
## Assess Reduction Efficiency
```

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

## [1] 94.18327
```
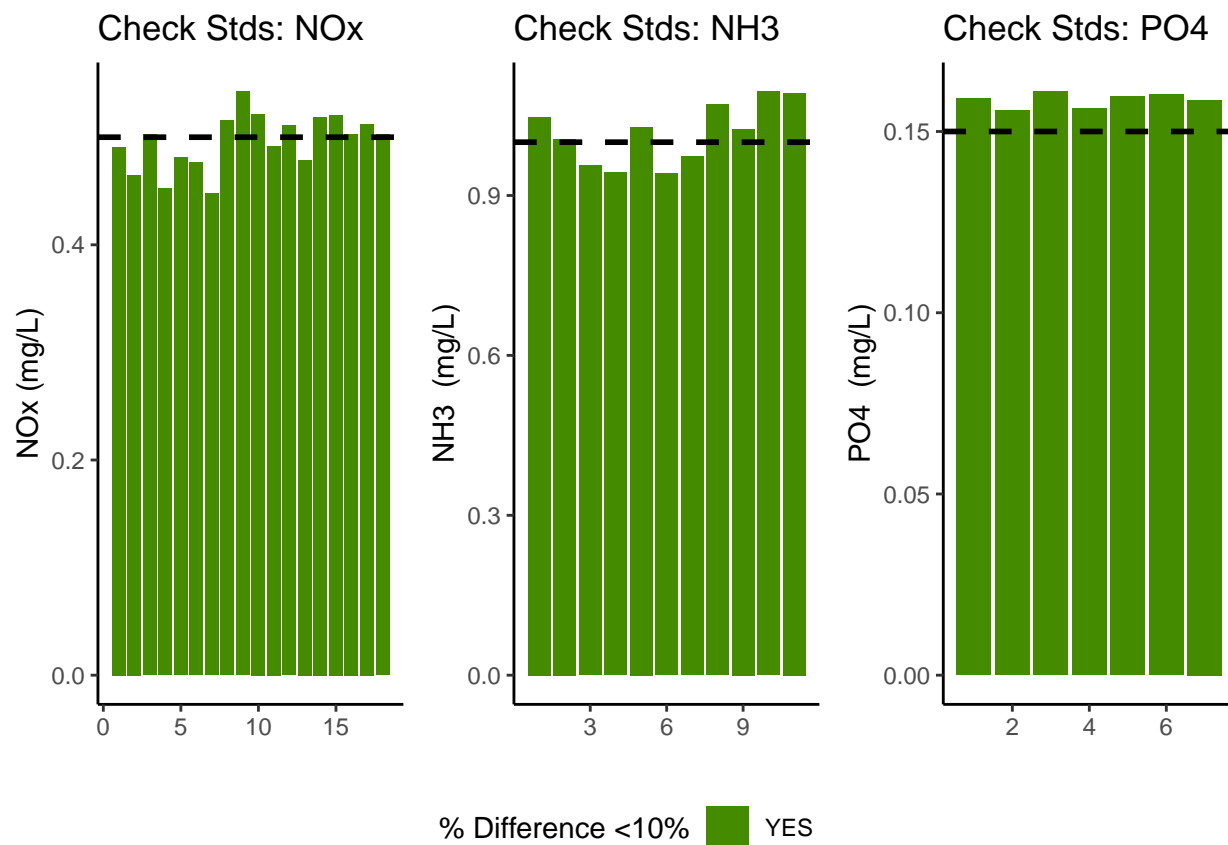
0.6 Analyze the Check Standards

```
## 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"
```

0.7 Analyze Blanks

```
## Assess Blanks

## [1] "<60% of NOx Blanks are below the lower 25% quartile of samples or 1/2 the detection limit - REAS

## [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"
```
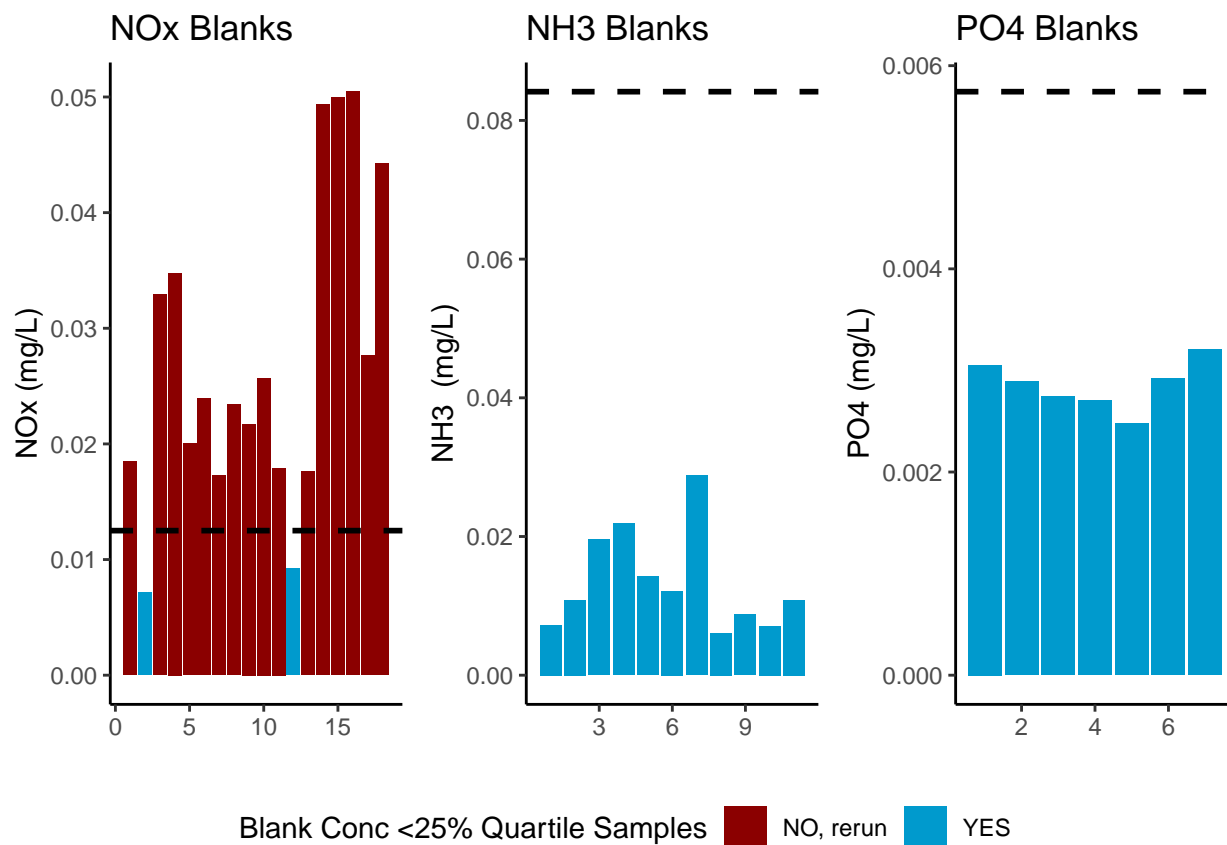

Table 2: Mean Concentration of Blanks

Test	Blank_Mean_Conc
NOx	0.0273
NH3	0.0134
PO4	0.0029

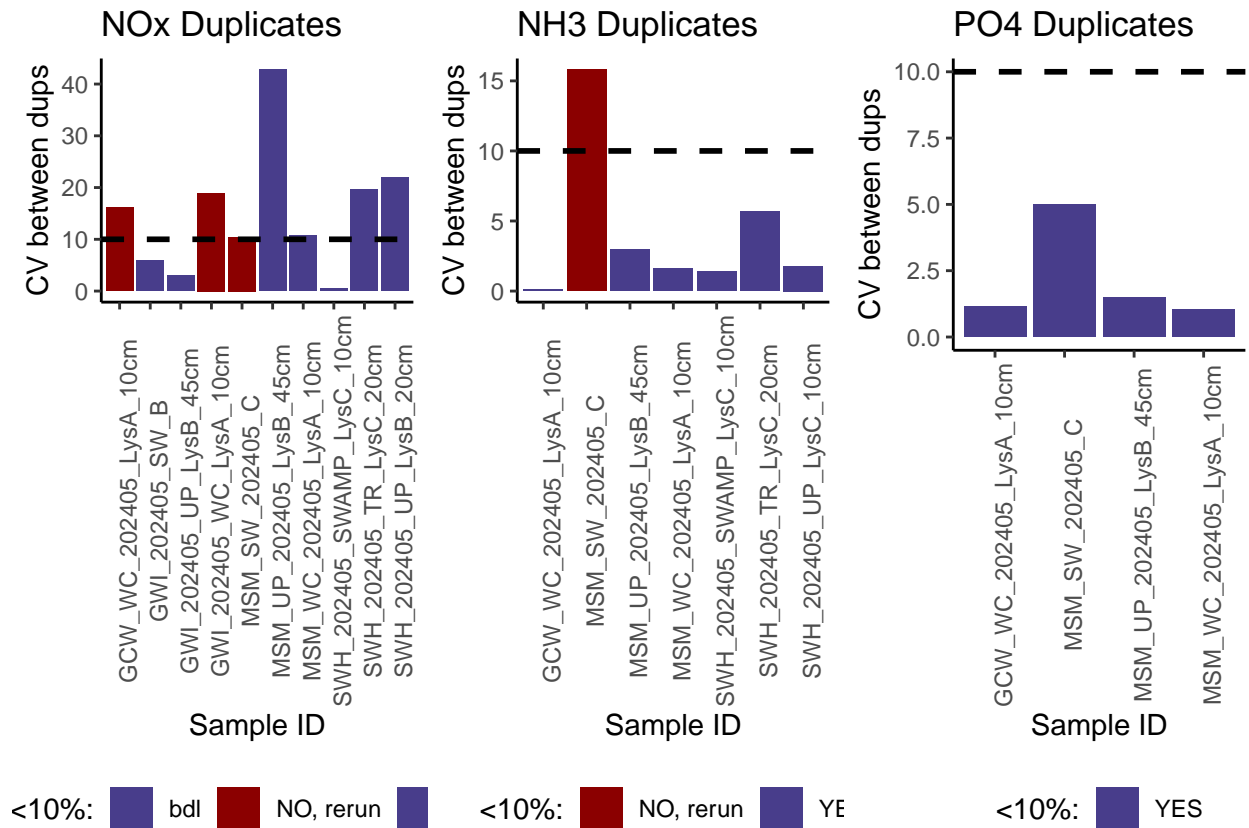## 0.8 Analyze Duplicates

```
## 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"
```

0.9 Spikes

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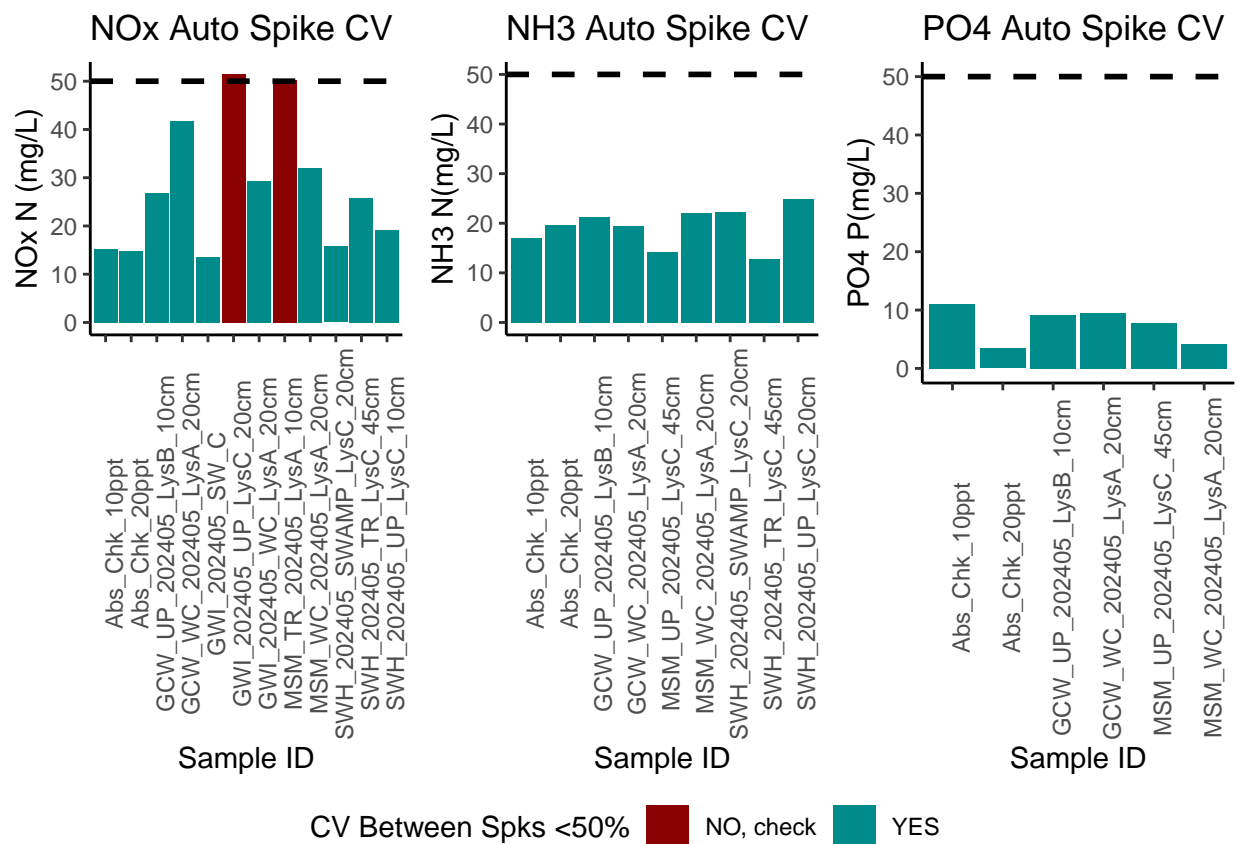
```
## [1] ">60% of Spikes have a CV <50% - PROCEED"
```

```
## [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.
```

0.10 Matrix Effects

```
## [1] "NO NOx Matrix Effect, PROCEED"
```

```
## [1] "NO NH3 Matrix Effect, PROCEED"
```

```
## [1] "NO PO4 Matrix Effect, PROCEED"
```

0.11 Unit Converted Data Column Added (mg/L to uM)

0.12 Sample Flagging - Within range of standard curve

```
## Sample Flagging
```

0.13 Pull out sample id information

```
## Sample Processing
```

0.14 Check to see if samples run match metadata & merge info
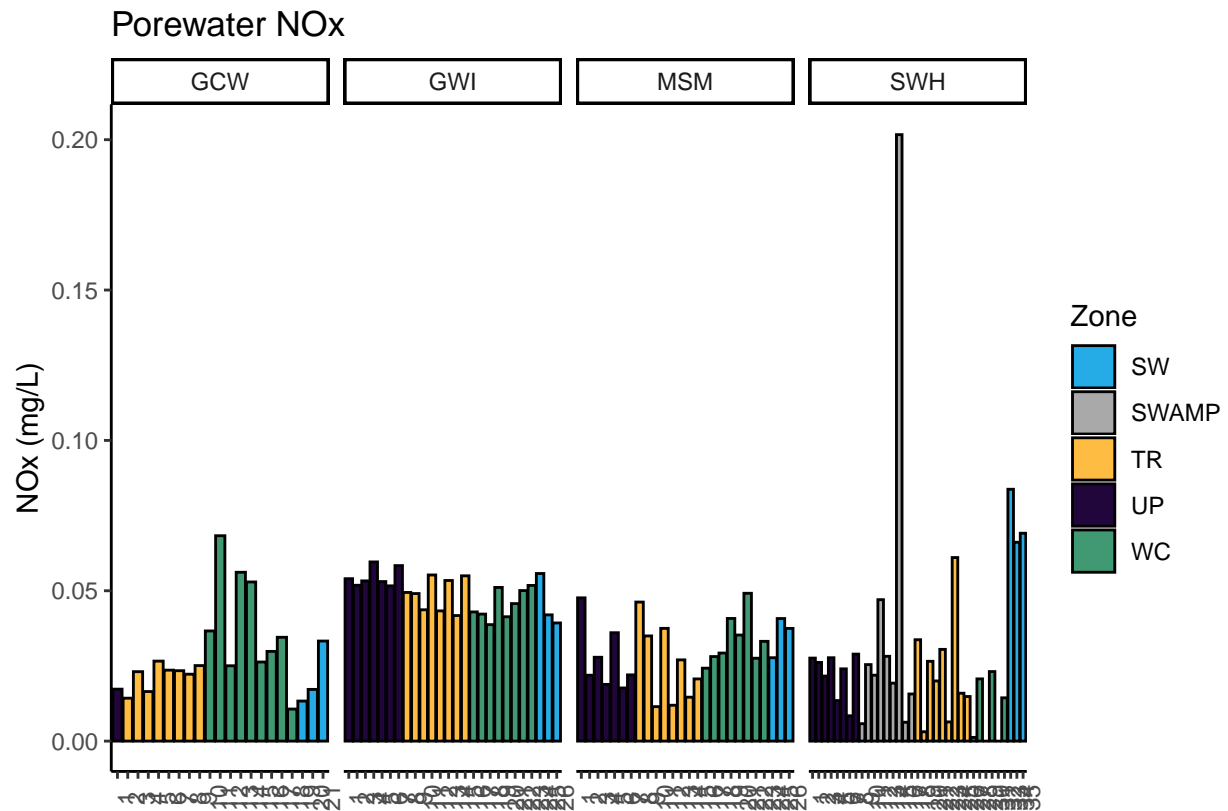
```
## Check Sample IDs with Metadata
```

```
## Some sample IDs are missing from metadata.
```
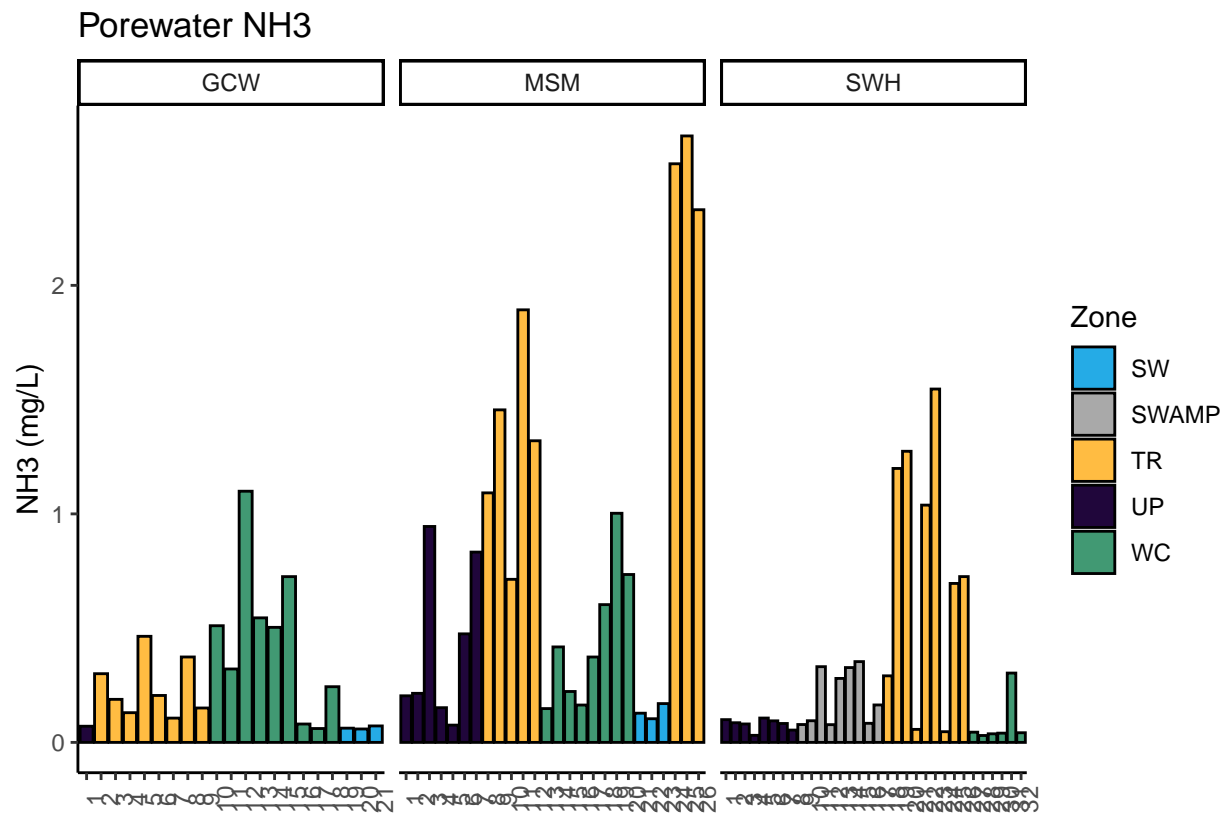
```
## [1] "MSM_202405_UP_LysA_10cm" "MSM_202405_UP_LysA_20cm"
## [3] "MSM_202405_WC_LysC_20cm" "GWI_202405_TR_LysC_45cm"
```
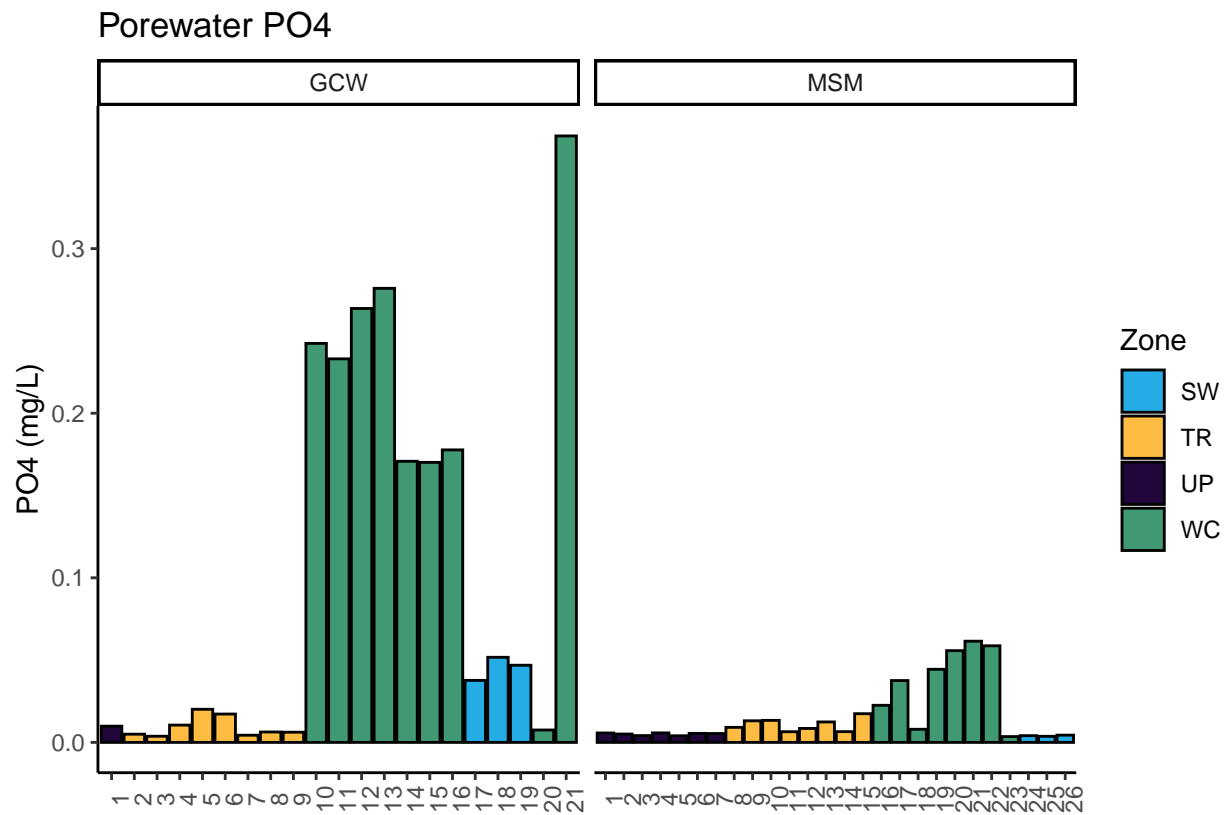
0.15 Visualize Data

```
## Visualize Data
```


Porewater NOx

Porewater NH3

Porewater PO4

0.16 Export Processed Data

#end