Synoptic CB: Porewater Nutrients

November 2024 Samples

2025-10-31

Contents

##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 <- "8/7/2025"
  sample_year <- "2024"
  sample_month <- "NOVEMBER"
  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_202411_VNOx_1.csv",
                 "Raw Data/COMPASS_Synoptic_CB_202411_VNOx_2.csv",
                 "Raw Data/COMPASS_Synoptic_CB_202411_VNOx_3.csv")
  NH3_PO4_files <- c("Raw Data/COMPASS_Synoptic_CB_202411_NH3_PO4_1.csv",
                     "Raw Data/COMPASS_Synoptic_CB_202411_NH3_PO4_2.csv",
                     "Raw Data/COMPASS_Synoptic_CB_202411_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_202411.csv"

#record any notes about the run or anything other info here:
  run_notes <- "One PO4 check standard came back very high, all others were within range.
                A few duplicates were out of range but still within CV.
                SWH_202411_SWAMP_LycC_45cm, SWH_202411_TR_LysC_10cm,
                MSM_202411_TR_LysC_10cm, MSM_202411_TR_LysC_45cm were missing from metadata. "

#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)
```

```
## One PO4 check standard came back very high, all others were within range.
##                 A few duplicates were out of range but still within CV.
##                 SWH_202411_SWAMP_LycC_45cm, SWH_202411_TR_LysC_10cm,
##                 MSM_202411_TR_LysC_10cm, MSM_202411_TR_LysC_45cm were missing from metadata.
```

##Setup

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

0.1 Import Data & Clean

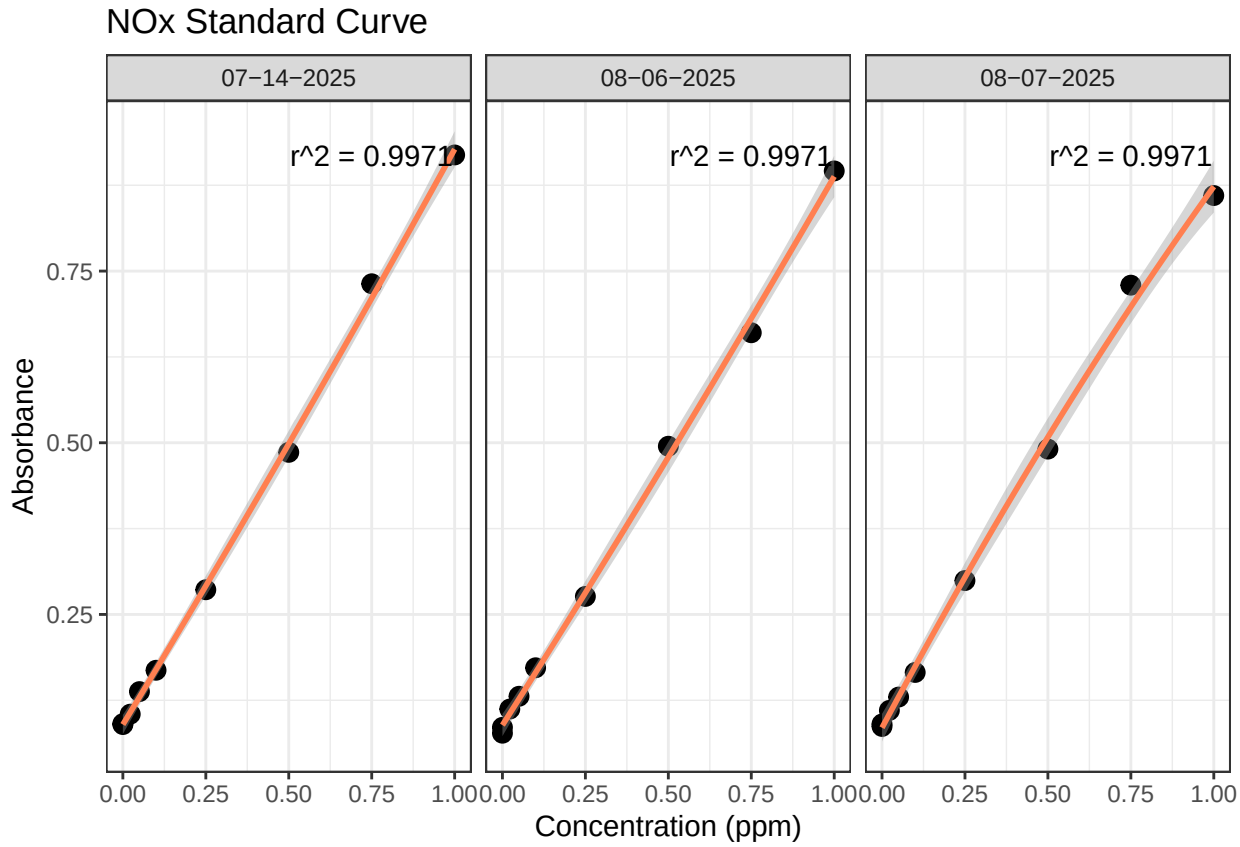
0.2 Assessing standard Curves

#Pull out standards data

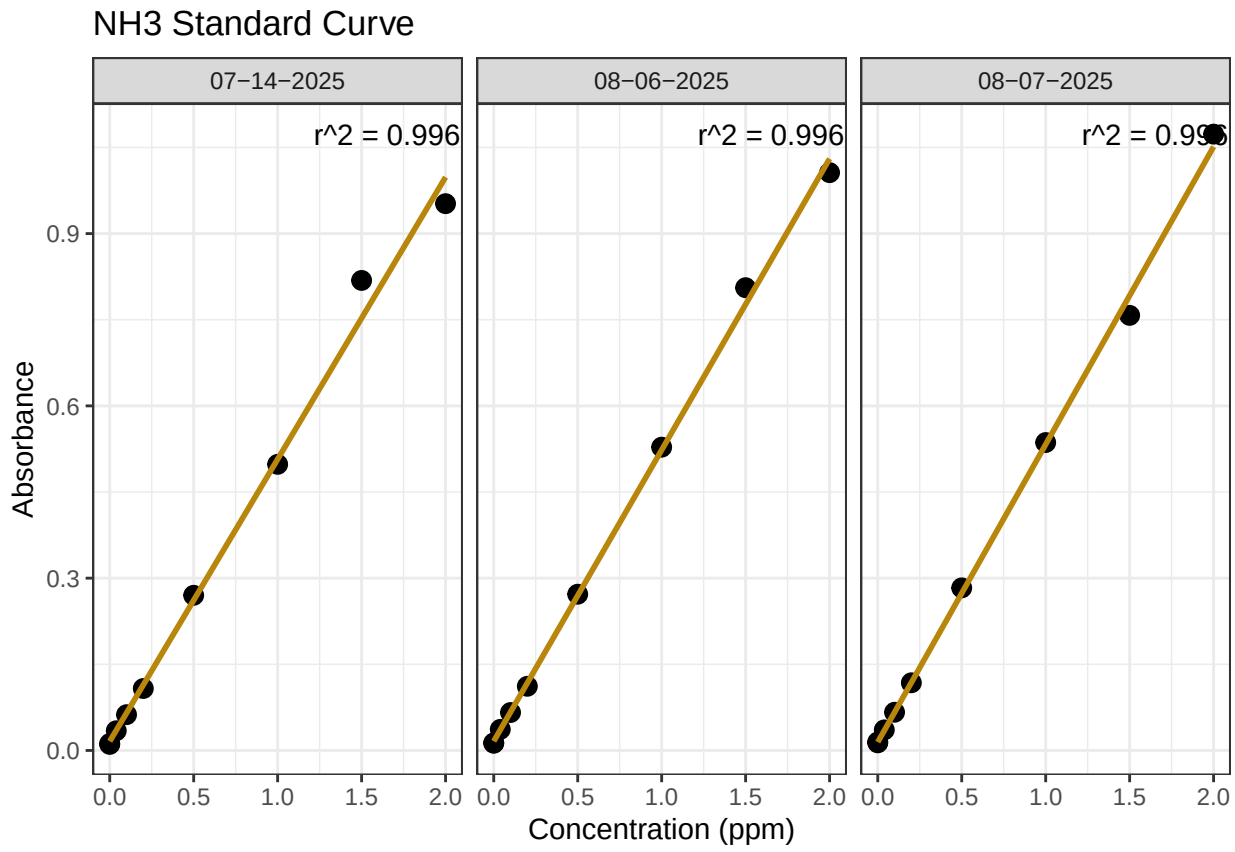
```
## Assess Standard Curves
```

#Plot standards data

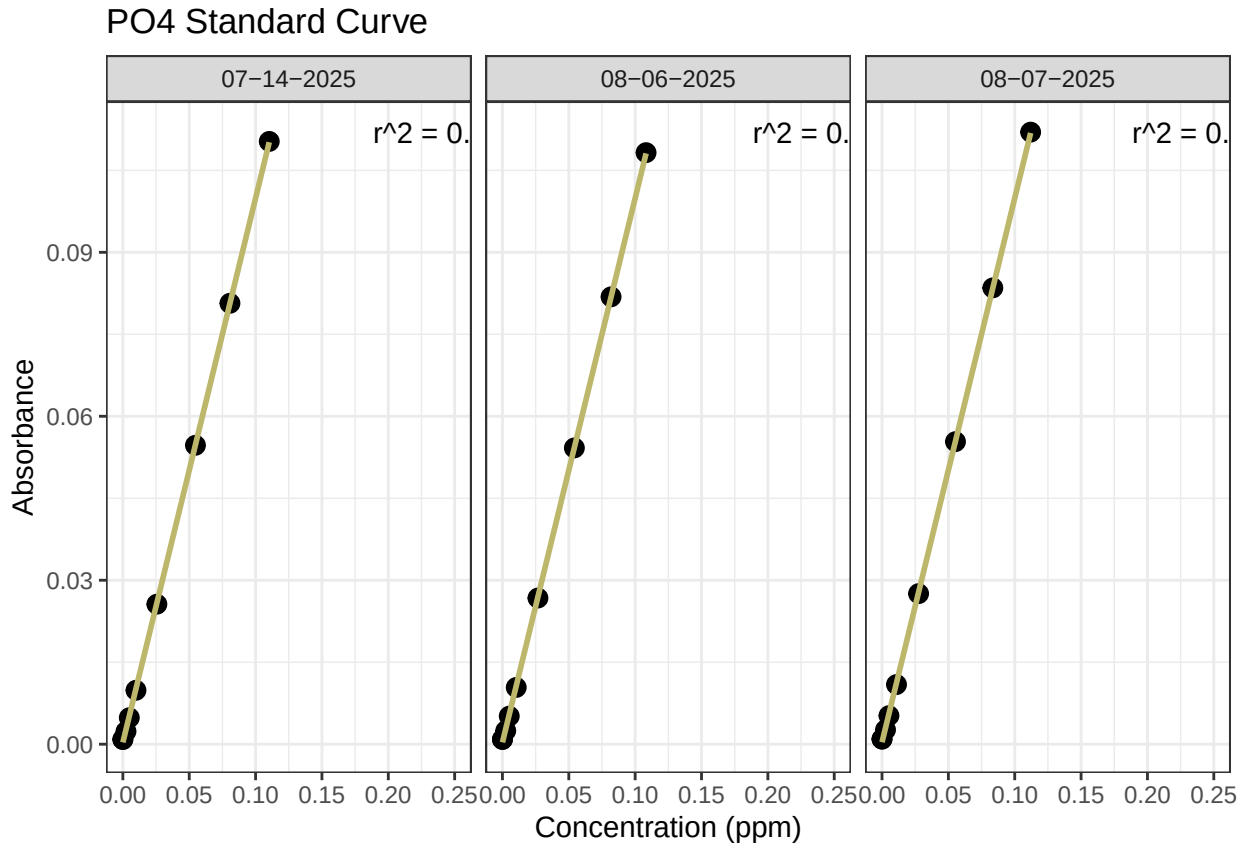
```
## Assess Standard Curves
```




```
## `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."
```

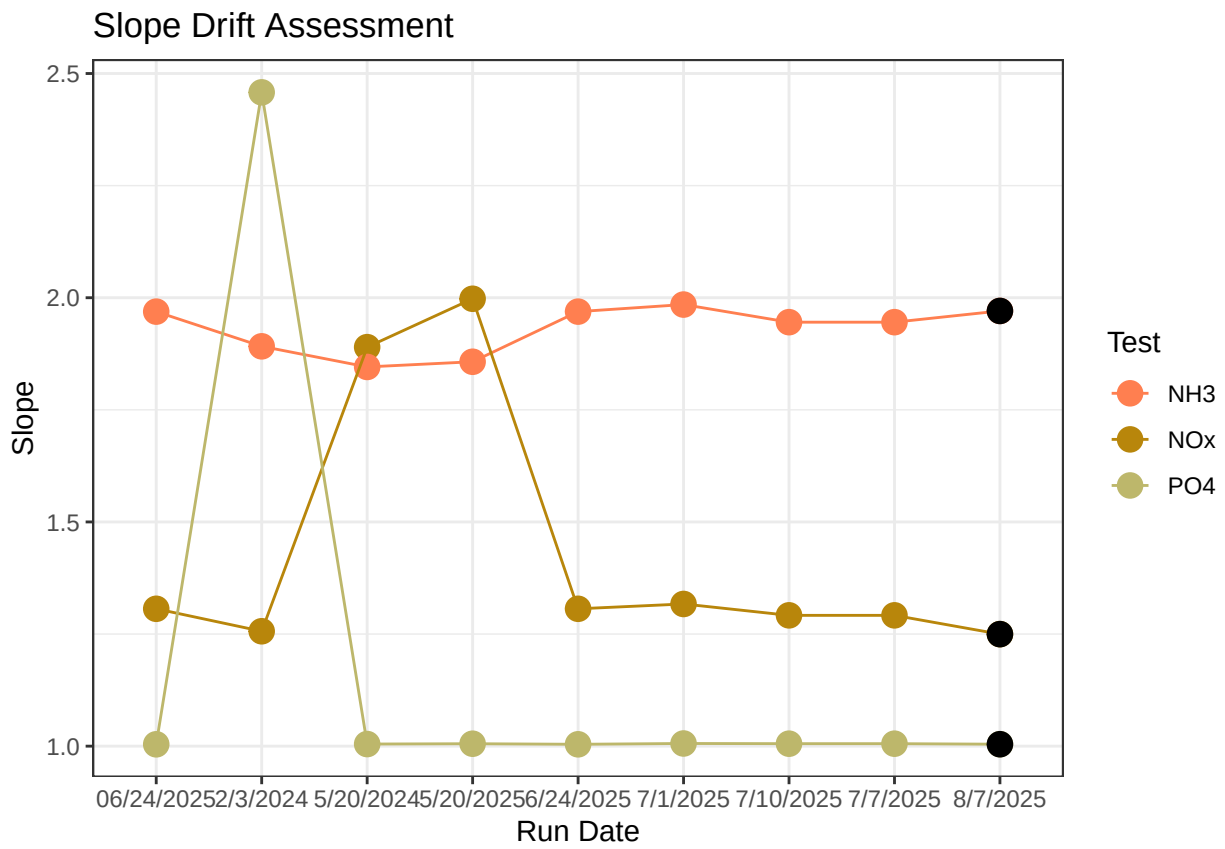


Table 1: Average Slope by Analyte

Test	avg_slope
NH3	1.931
NOx	1.434
PO4	1.166

0.3 Dilution Corrections - ensure the latest dilution is kept

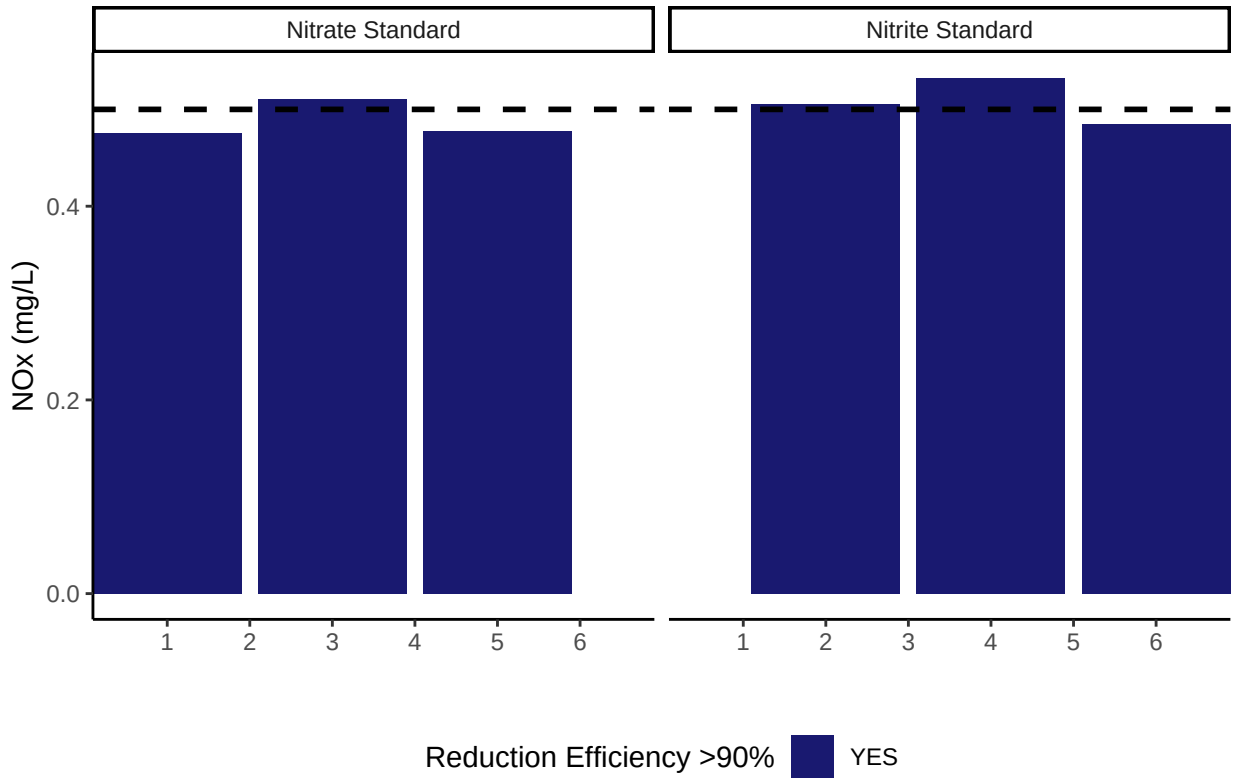
```
## Dilution Corrections

## Duplicated samples: GCW_202411_WC_LysB_10cm, MSM_202411_TR_LysA_20cm, MSM_202411_TR_LysB_20cm, MSM_2

##
##  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 = 1.57518

## Expected  = 1.51

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

## Run mean = 1.209981

## Expected  = 1.034

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

## Run mean = 0.8969137

## Expected  = 0.824
```

##Check NOx Reduction Efficiency

```
## Assess Reduction Efficiency
```




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

```
## [1] 99.48873
```

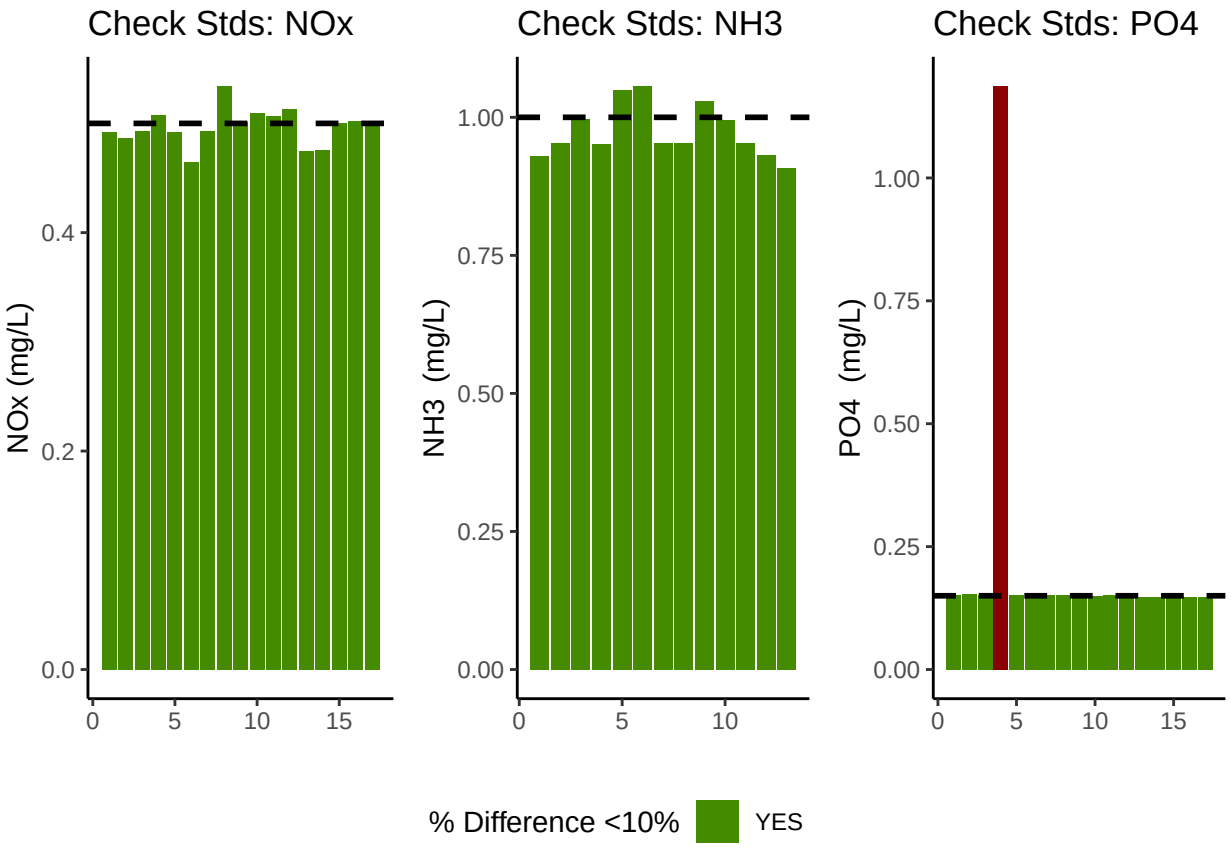
0.5 Analyze the Check Standards

```
## Analyze Check Standards
```

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

```
## [1] "NH3 Check Standard RSD within Range - PROCEED"
```

```
## [1] "PO4 CHECK STANDARD RSD TOO HIGH - REASSESS"
```




```
## [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"
```

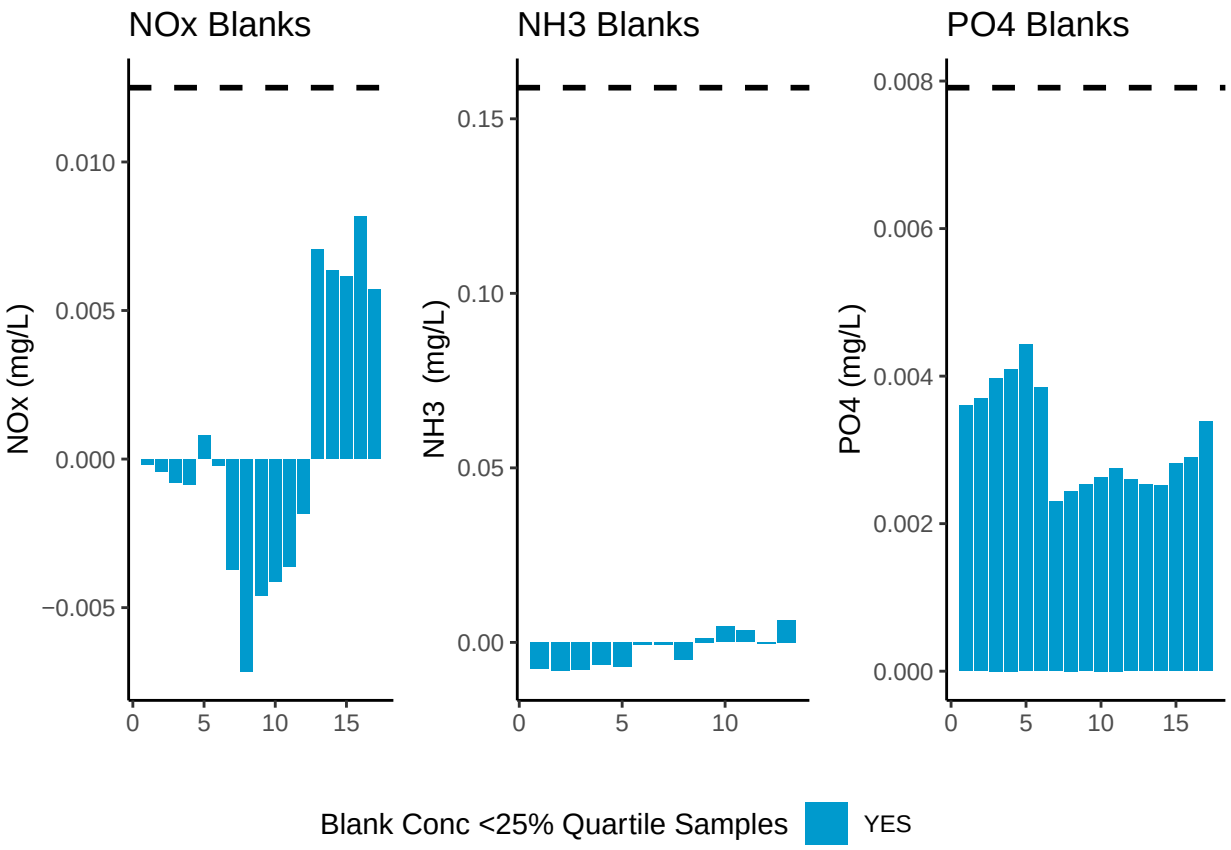


Table 2: Mean Concentration of Blanks

Test	Blank_Mean_Conc
NOx	0.0004
NH3	-0.0022
PO4	0.0031

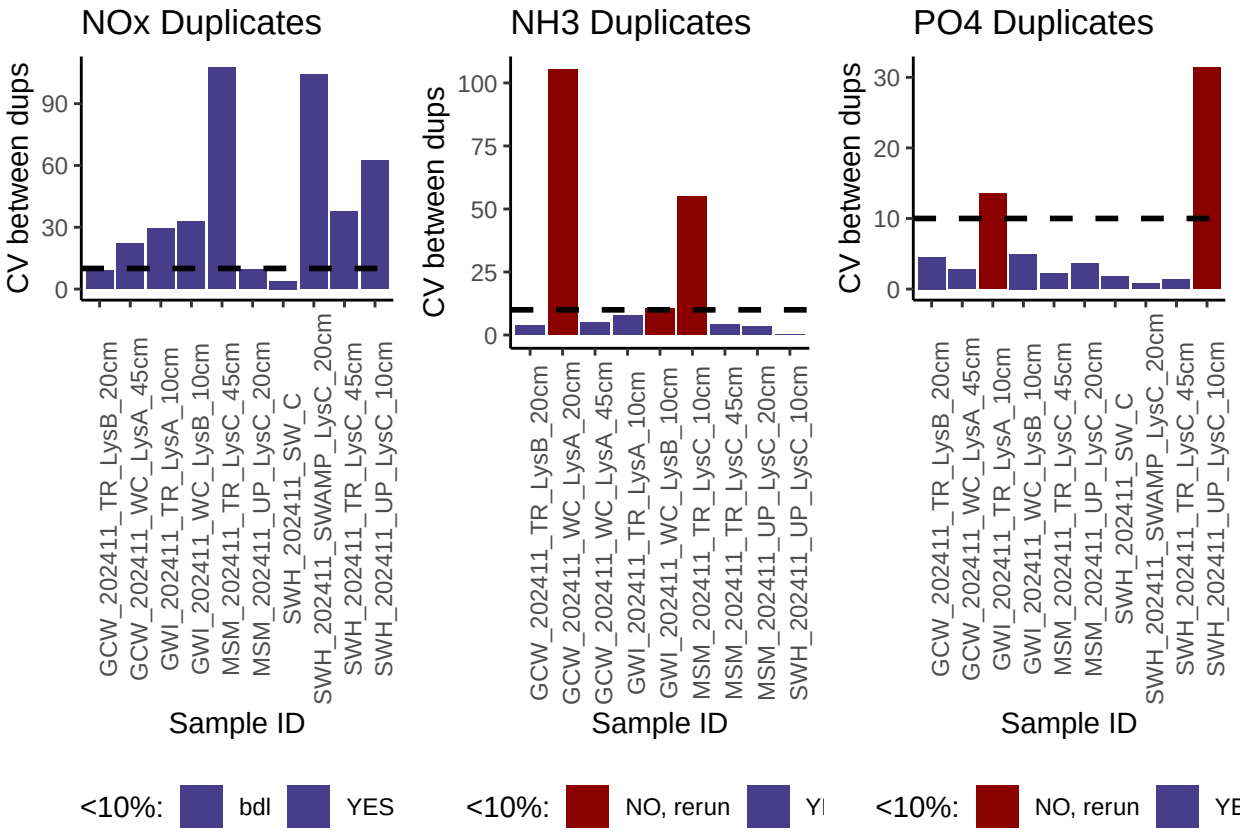
0.7 Analyze Duplicates

```
## 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"
```



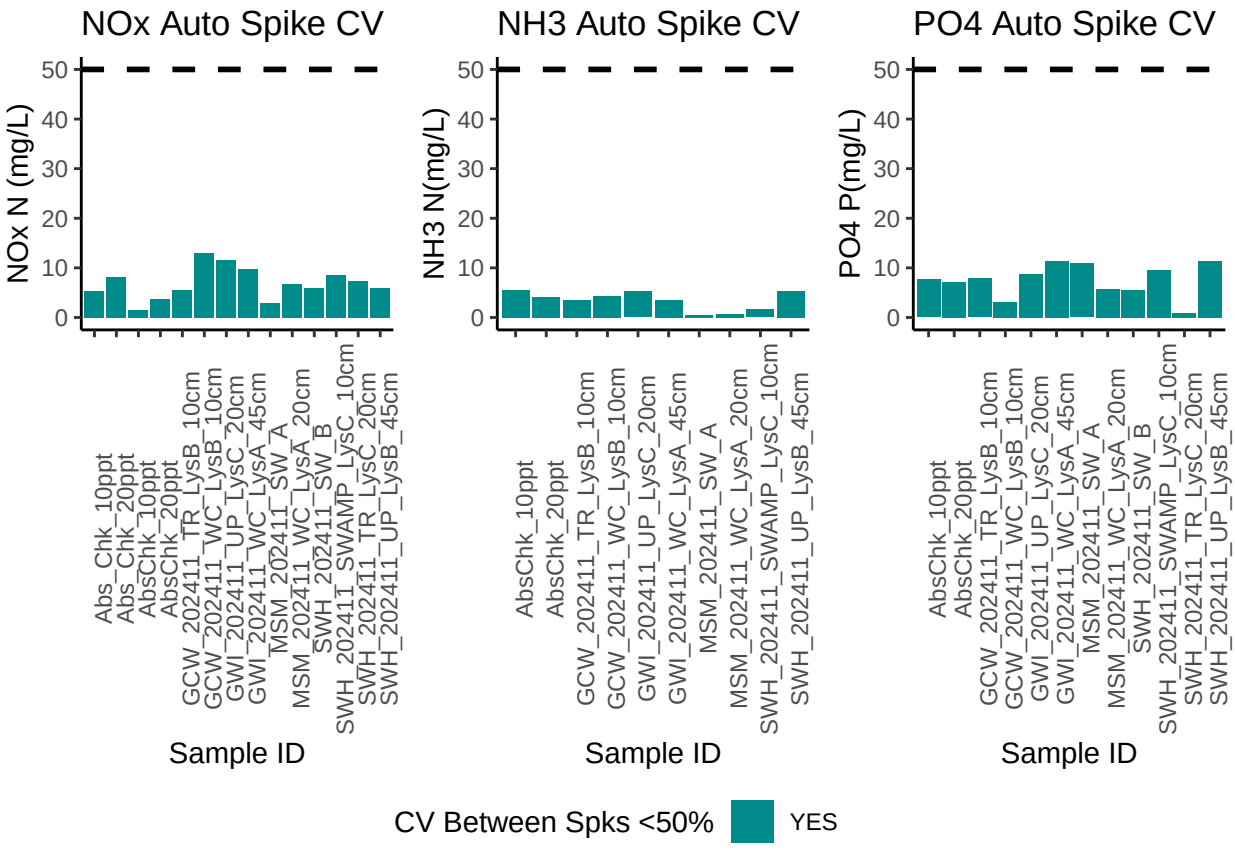
0.8 Spikes

```
## [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"
```

```
## 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.
```



0.9 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
```

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

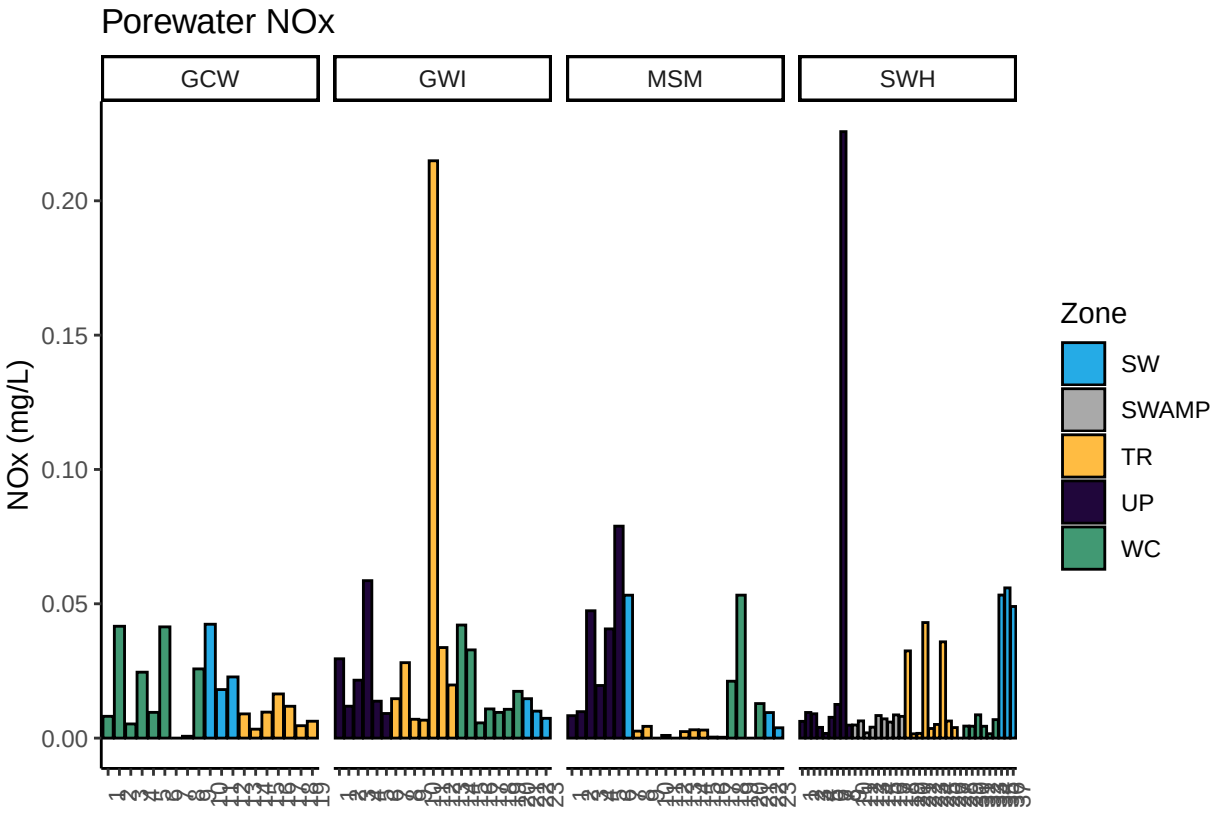
```
## Check Sample IDs with Metadata
```

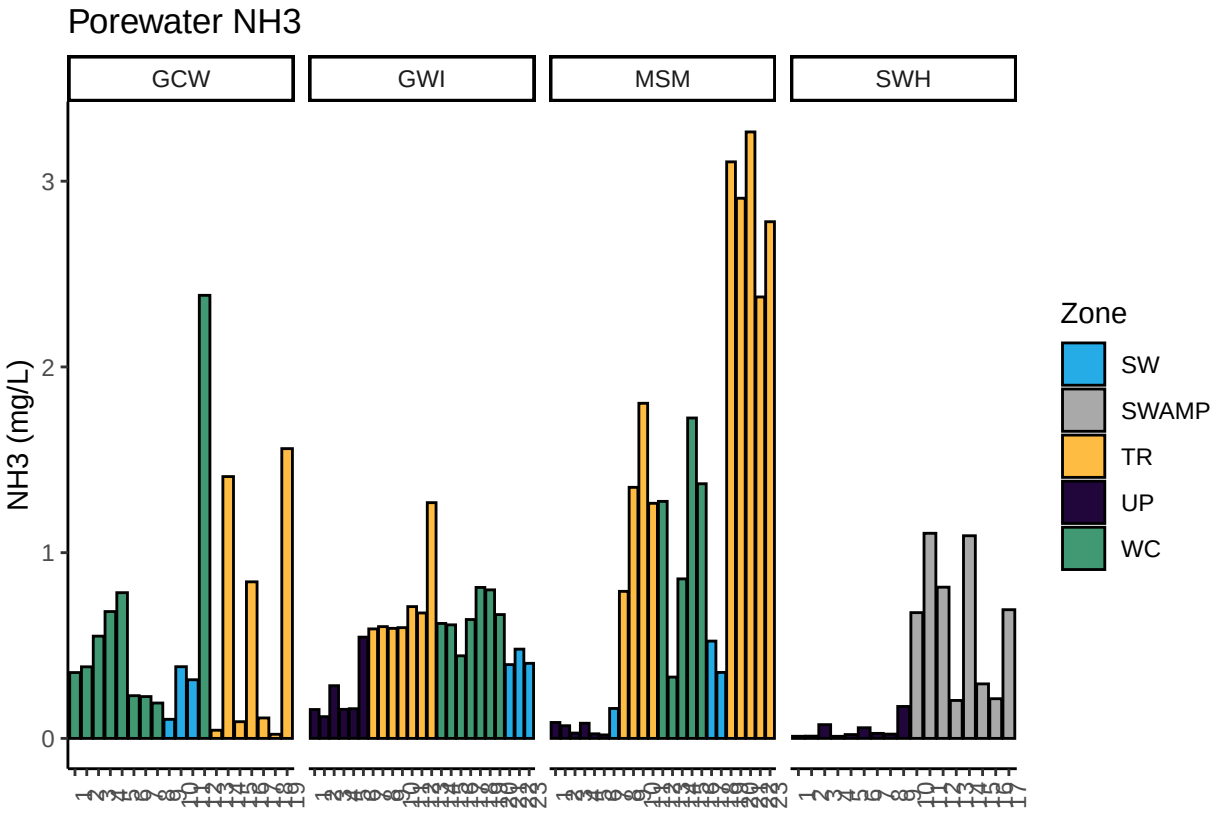
```
## Some sample IDs are missing from metadata.
```

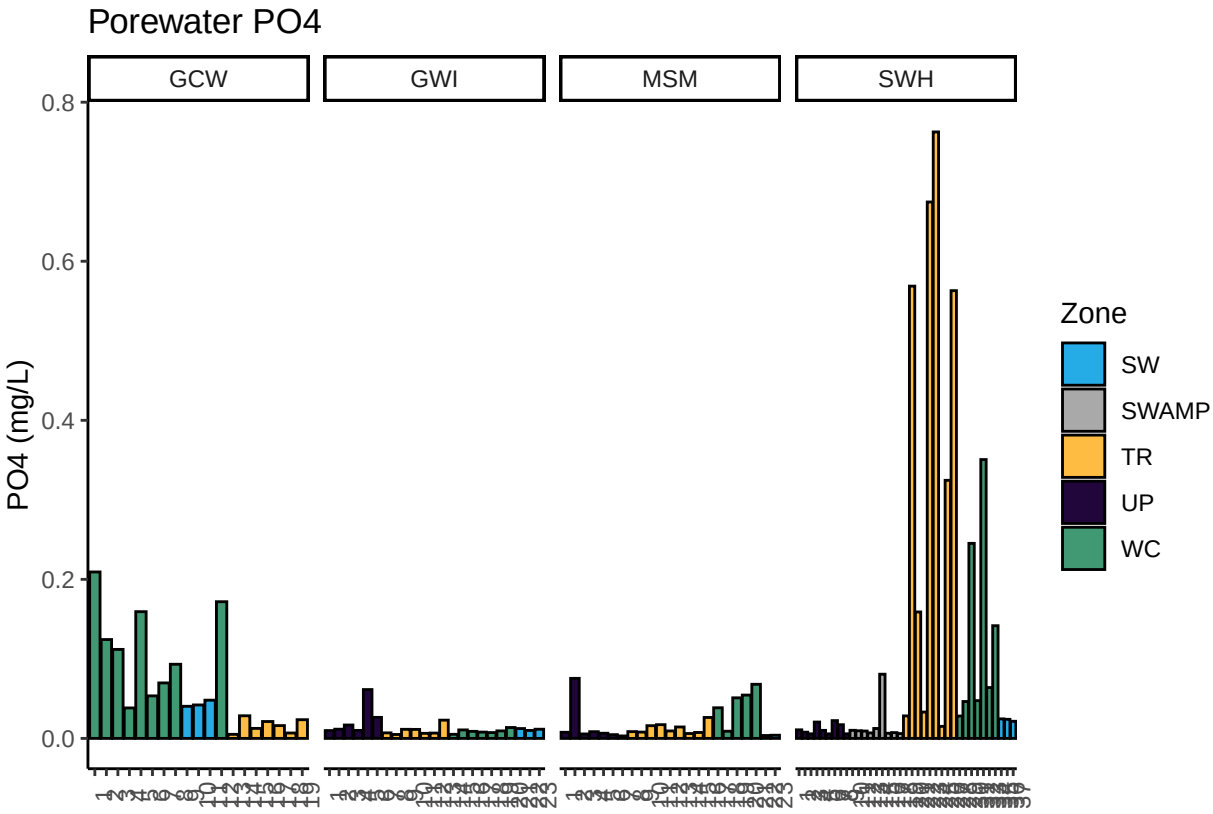
```
## [1] "SWH_202411_SWAMP_LycC_45cm" "SWH_202411_TR_LysC_10cm"
## [3] "MSM_202411_TR_LysC_10cm"    "MSM_202411_TR_LysC_45cm"
```

0.14 Visualize Data

```
## Visualize Data
```




Porewater NH3
GCW
GWI
MSM
SWH
NH3 (mg/L)
0
1
2
3
Zone
SW
SWAMP
TR
UP
WC



0.15 Export Processed Data

#end