Synoptic CB: Porewater Nutrients

September 2023 Samples

2025-07-08

Contents

##Run Information

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

```
## Run Information: Input by User
```

```r
#set the run date & user name
  run_date <- "01/25/2024"
  sample_year <- 2023
  sample_month <- 09
  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_Sept2023_1.csv",
                 "Raw Data/SEAL_COMPASS_Synoptic_NOx_Sept2023_2.csv",
                 "Raw Data/SEAL_COMPASS_Synoptic_NOx_Sept2023_3.csv")
  NH3_PO4_files <- c("Raw Data/SEAL_COMPASS_Synoptic_NH3_PO4_Sept2023_1.csv",
                     "Raw Data/SEAL_COMPASS_Synoptic_NH3_PO4_Sept2023_2.csv",
                     "Raw Data/SEAL_COMPASS_Synoptic_NH3_PO4_Sept2023_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_202309.csv"

#record any notes about the run or anything other info here:
  run_notes <- "This run was stopped and restarted part way through due to
  insufficient water and/or reaction segments.
  There are fewer spikes for PO4 and NH3 in this run due to stop and rerun.
  NH3 peCheck is high, but other run metrics okay, so accepting this 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)
```

```
## This run was stopped and restarted part way through due to
##   insufficient water and/or reaction segments.
##   There are fewer spikes for PO4 and NH3 in this run due to stop and rerun.
##   NH3 peCheck is high, but other run metrics okay, so accepting this run.
```

##Setup

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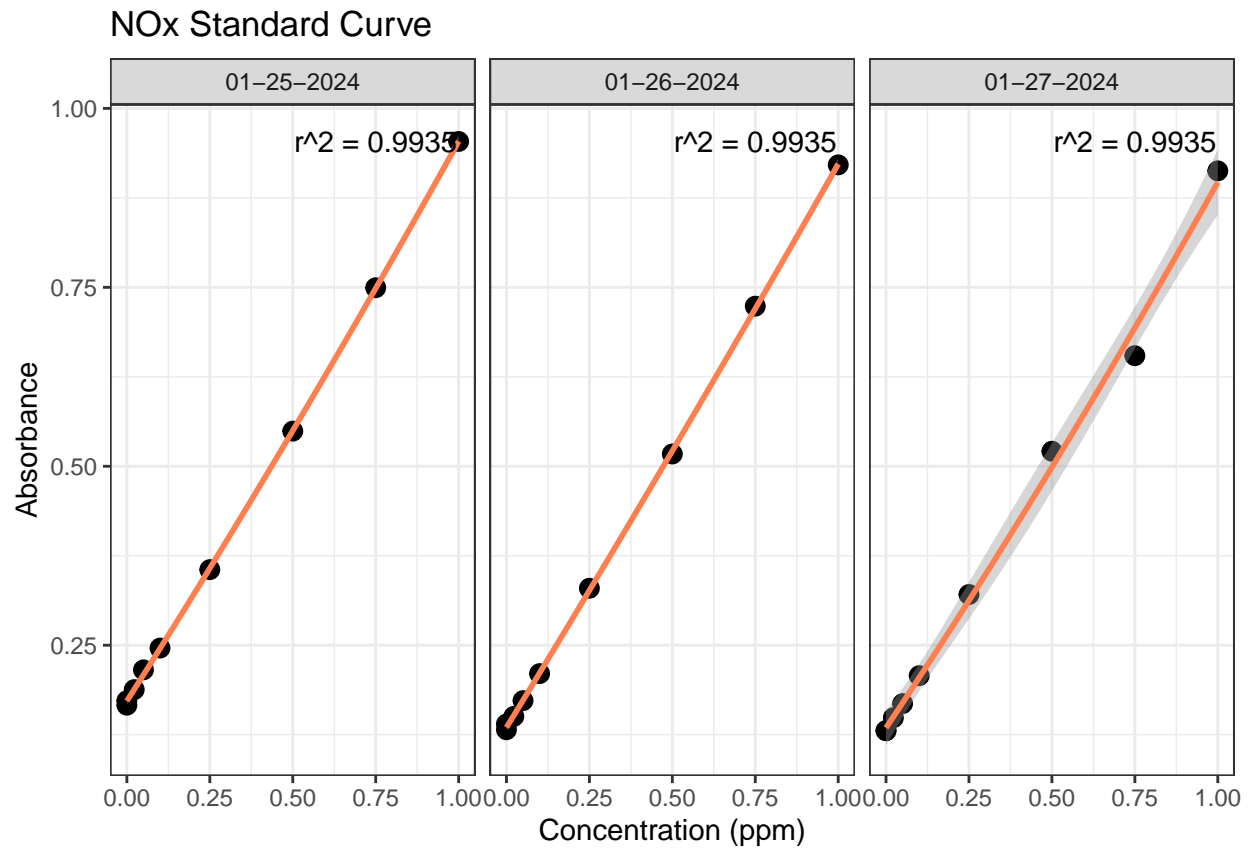
0.1 Import Data & Clean

0.2 Assessing standard Curves
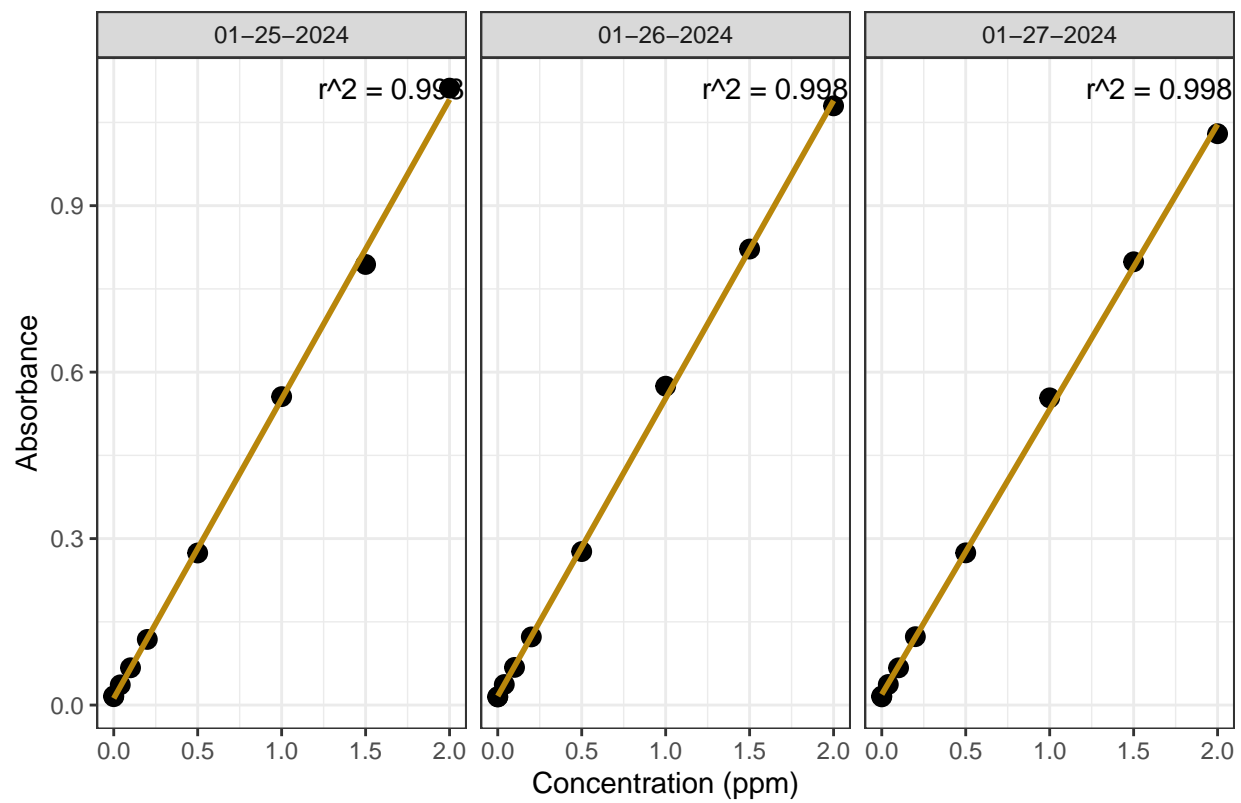
#Pull out standards data

Assess Standard Curves

#Plot standards data
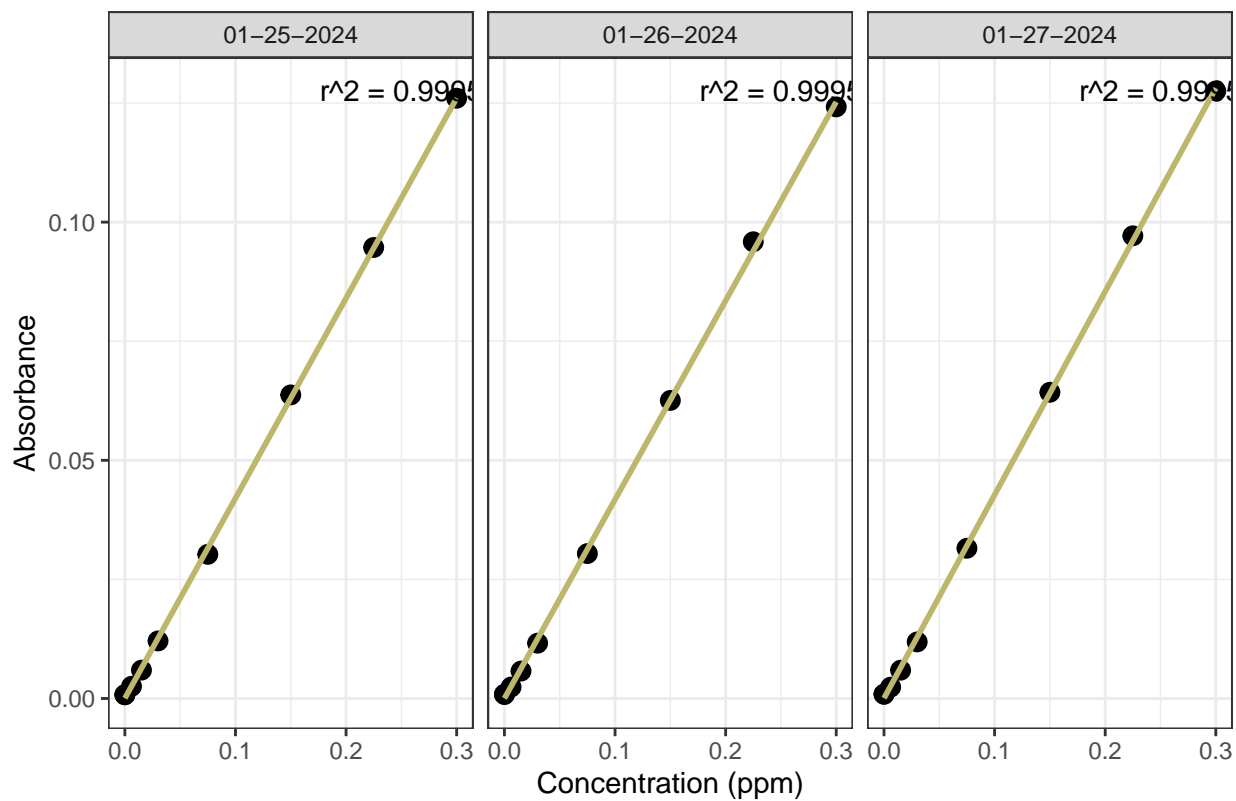
Assess Standard Curves

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
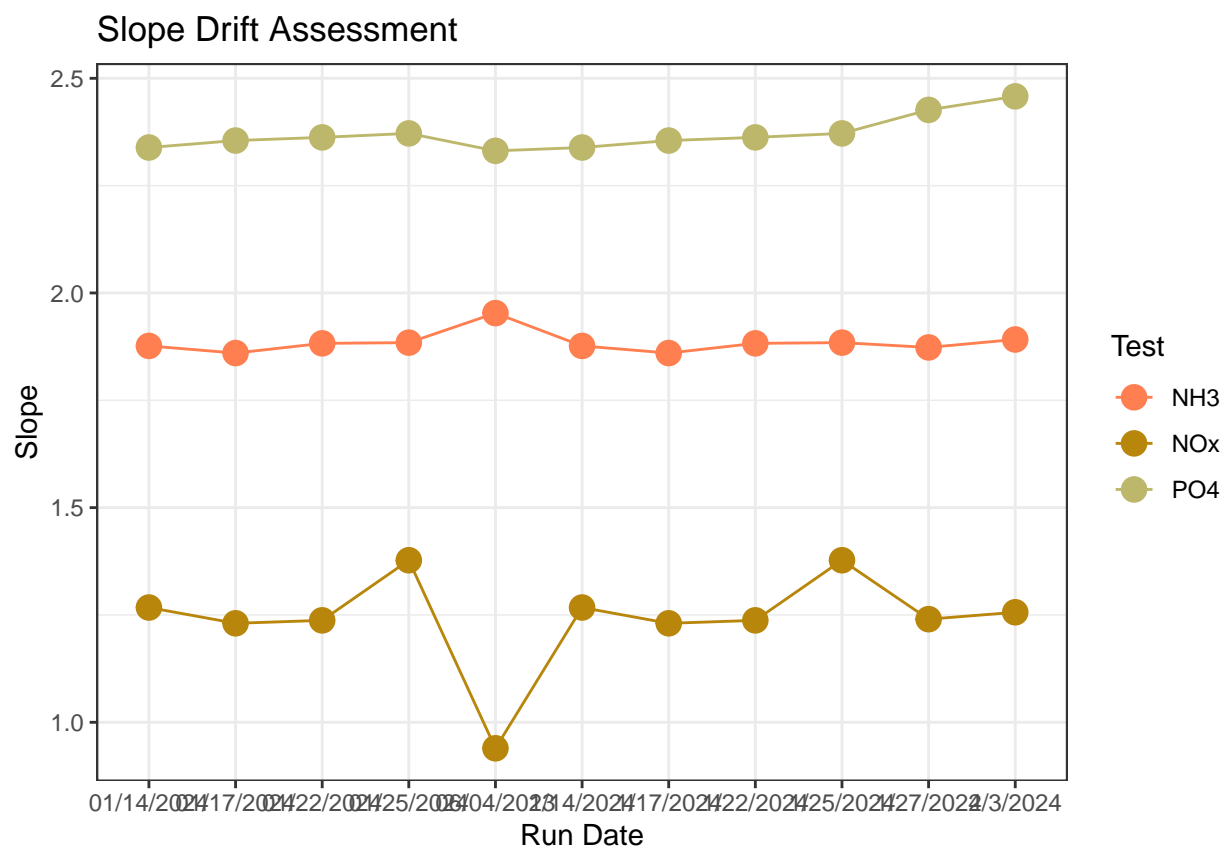

Table 1: Average Slope by Analyte

Test	avg_slope
NH3	1.884
NOx	1.242
PO4	2.370

0.3 TEMPORARY CHUNK FOR SEPT 2023 - Run finished then restarted for dilutions

0.4 Dilution Corrections - ensure the latest dilution is kept

```
## Dilution Corrections
```

```
## No duplicated samples.
```

0.5 Performance Check

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

```
## Run mean = 0.738716
```

```
## Expected  = 0.706
```

```
## [1] "NH3 pe Check has a % Difference >25% - REASSESS"
```

```
## Run mean = 1.531811
```

```
## Expected  = 0.948
```

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

```
## Run mean = 0.864723
```

```
## Expected  = 0.818
```

#Check NOx Reduction Efficiency

```
## Assess Reduction Efficiency
```

NOx (mg/L) plotted by sample for Nitrate Standard and Nitrite Standard. Legend: Reduction Efficiency >90% — YES (dark blue).

```
## [1] "Mean NOx Reduction Efficiency >95% - PROCEED"
```
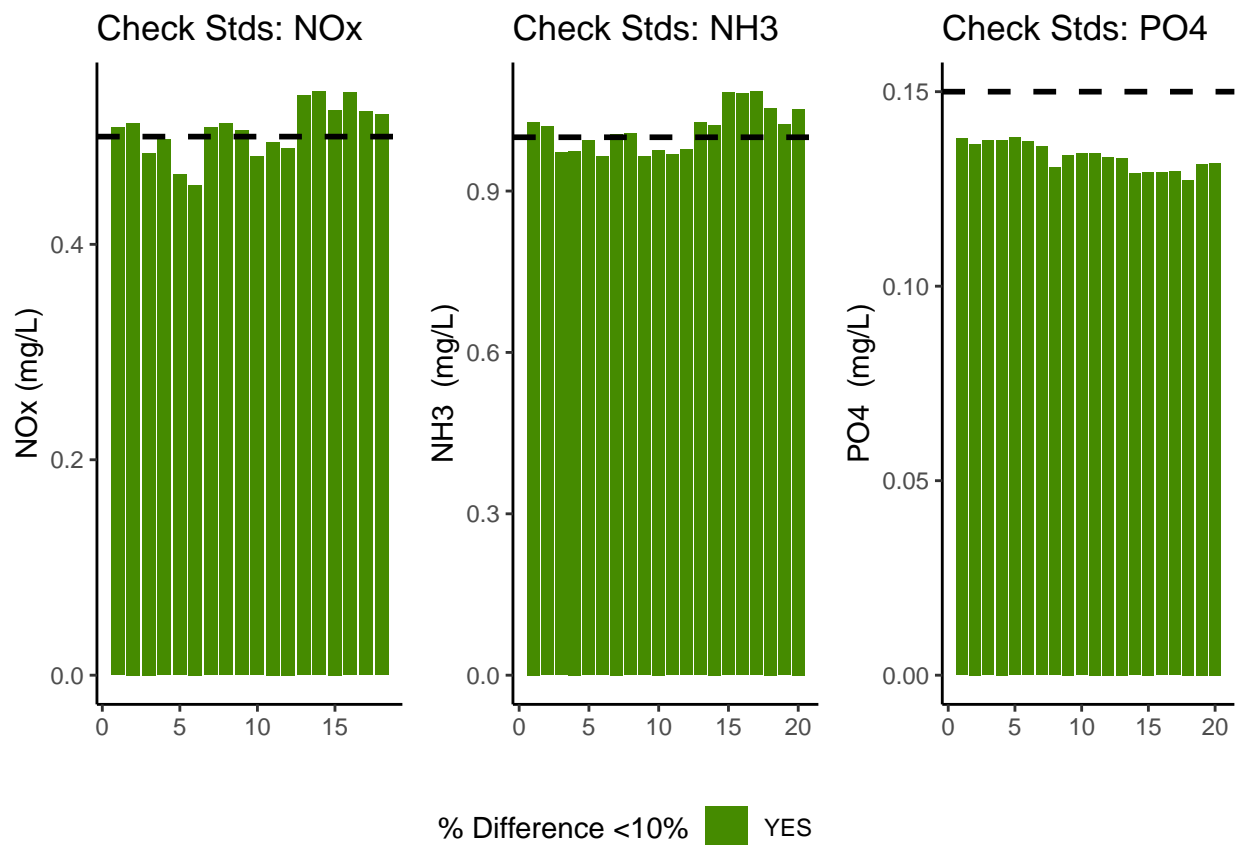
```
## [1] 98.47613
```

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 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"
```
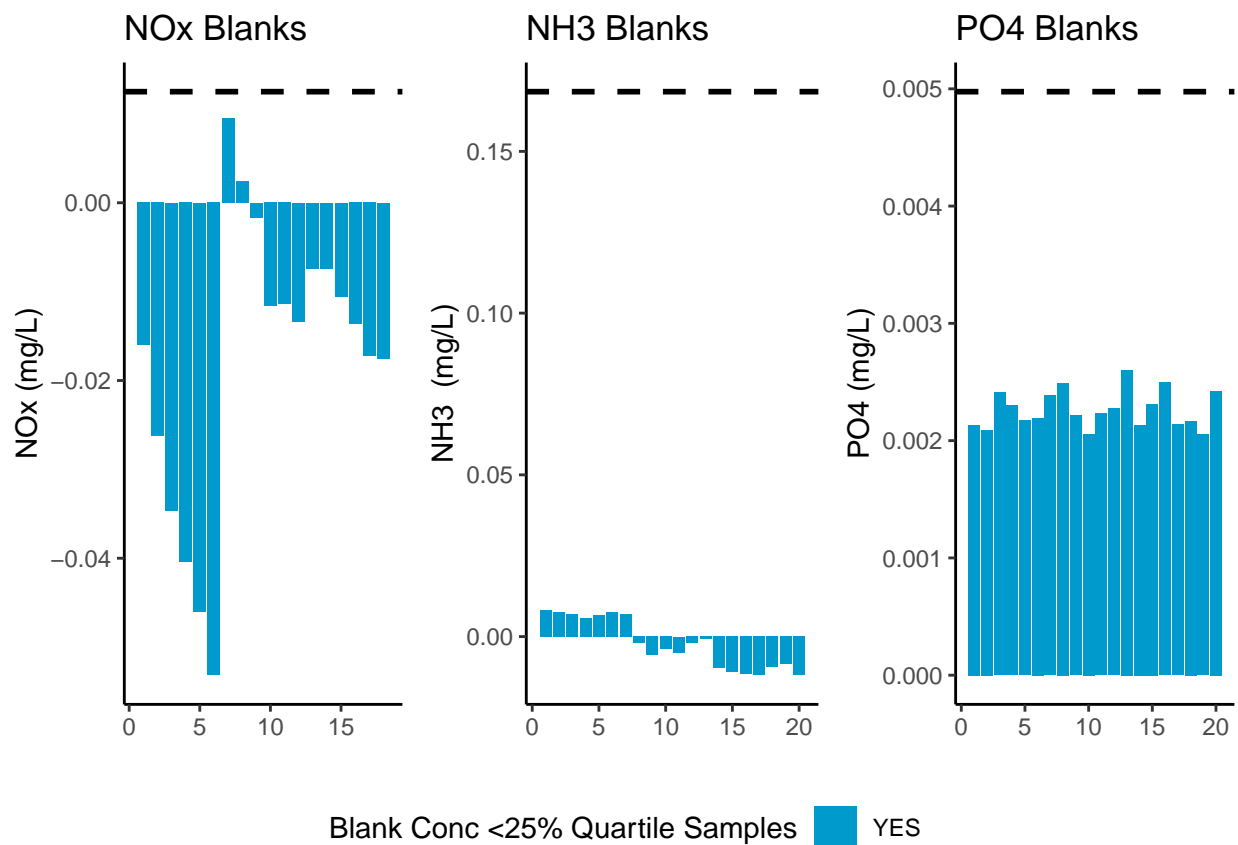

Table 2: Mean Concentration of Blanks

Test	Blank_Mean_Conc
NOx	-0.0176
NH3	-0.0022
PO4	0.0023

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"


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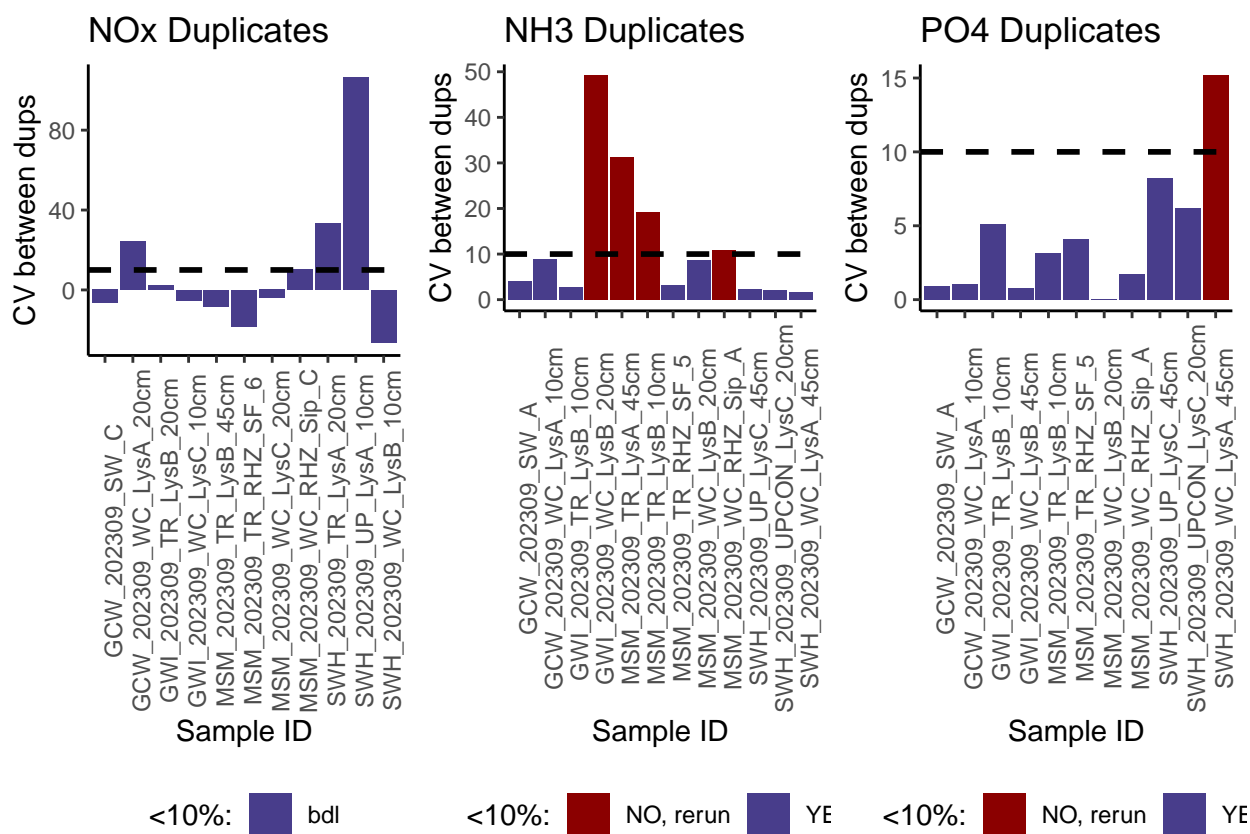
0.9   Spikes
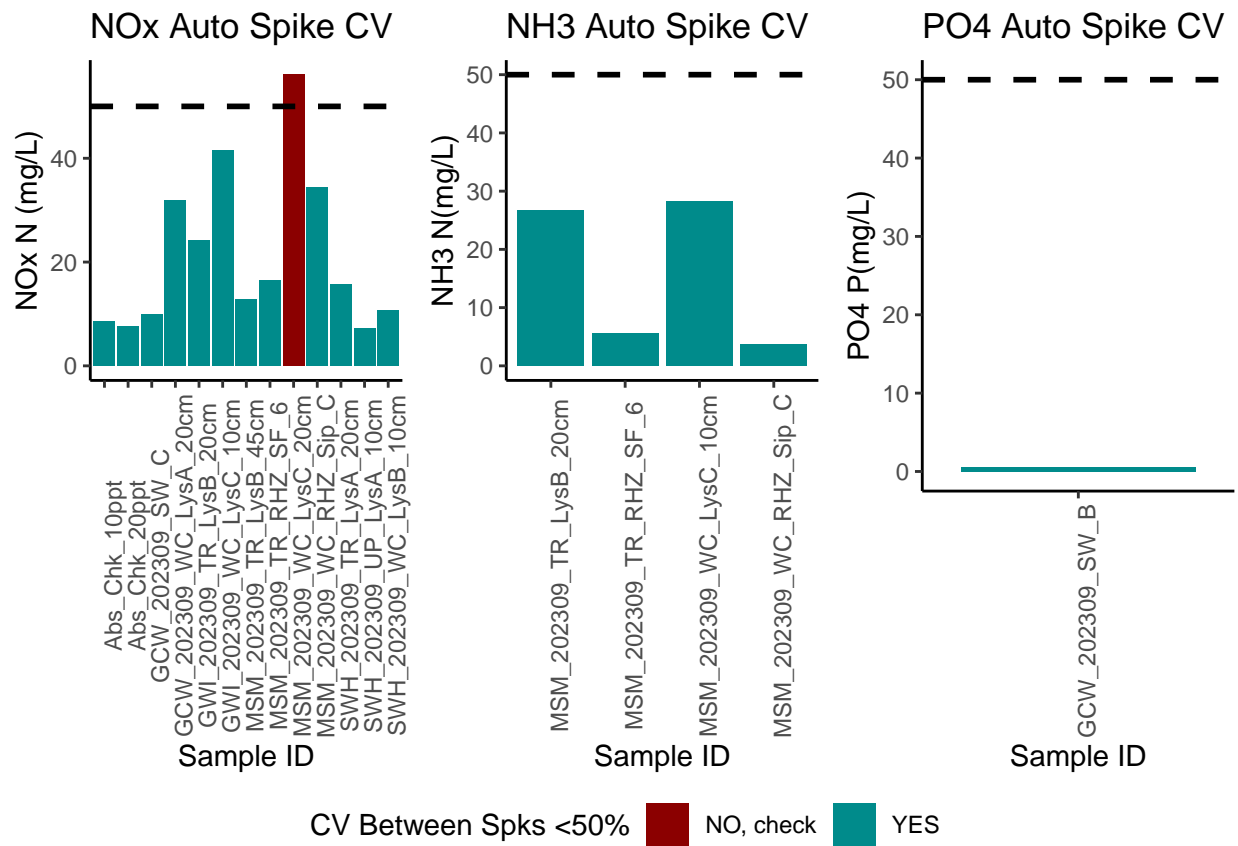
```
## [1] ">60% of Spikes have a CV <50% - PROCEED"

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

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

0.10 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
```

```
## Warning: There was 1 warning in 'mutate()'.
## i In argument: 'Run_Time = lubridate::mdy_hm(Run_Time)'.
## Caused by warning:
## ! All formats failed to parse. No formats found.
```

```
## Warning: Expected 5 pieces. Missing pieces filled with 'NA' in 36 rows [18, 19, 20, 42,
## 43, 44, 77, 78, 79, 101, 102, 103, 121, 122, 123, 138, 139, 140, 157, 158,
## ...].
```

0.14 Pulling Rhizon Samples

```r
# Filter rhizon and peeper samples
df_rhizon <- df_all %>%
  filter(str_detect(Sample_Name, "RHZ"))
df_peep <- df_all %>%
  filter(str_detect(Sample_Name, "PPR"))

# Timestamp for backups
timestamp <- format(Sys.time(), "%Y-%m-%d_%H%M")

# Paths
folder_path <- file.path("Raw Data", "Rhizon+Peeper")
dir.create(folder_path, recursive = TRUE, showWarnings = FALSE)

rhizon_main <- file.path(folder_path, "rhizon_data.csv")
peeper_main <- file.path(folder_path, "peeper_data.csv")

rhizon_backup <- file.path(folder_path, paste0("rhizon_data_", timestamp, ".csv"))
peeper_backup <- file.path(folder_path, paste0("peeper_data_", timestamp, ".csv"))

# Write timestamped backups
```

```r
write.csv(df_rhizon, rhizon_backup, row.names = FALSE)
write.csv(df_peep, peeper_backup, row.names = FALSE)

# Overwrite the main files with latest data
write.csv(df_rhizon, rhizon_main, row.names = FALSE)
write.csv(df_peep, peeper_main, row.names = FALSE)

## ^^ I think there is a cleaner way to write this out, but this should work for now ^^
```
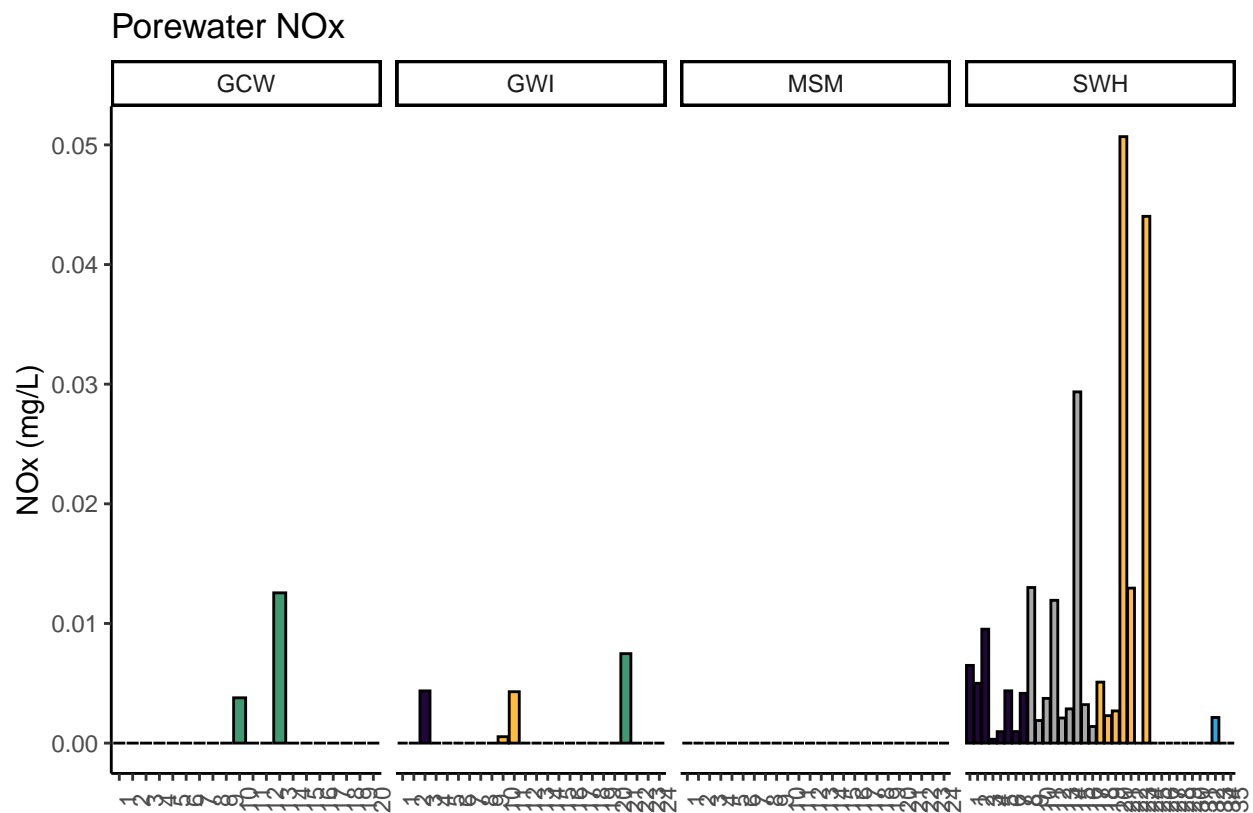
0.15 Check to see if samples run match metadata & merge info
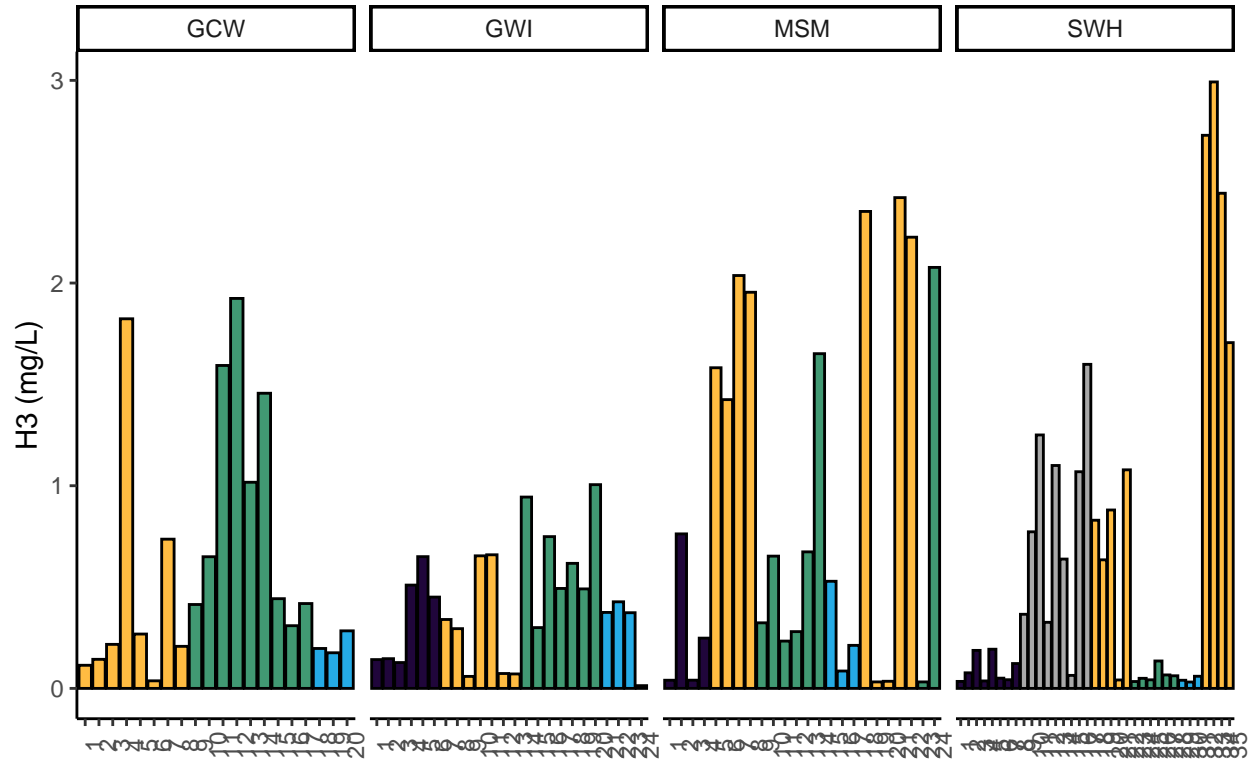
```
## Check Sample IDs with Metadata
```

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

```
## Warning: Expected 5 pieces. Missing pieces filled with 'NA' in 36 rows [18, 19, 20, 42,
## 43, 44, 77, 78, 79, 101, 102, 103, 121, 122, 123, 138, 139, 140, 157, 158,
## ...].
```
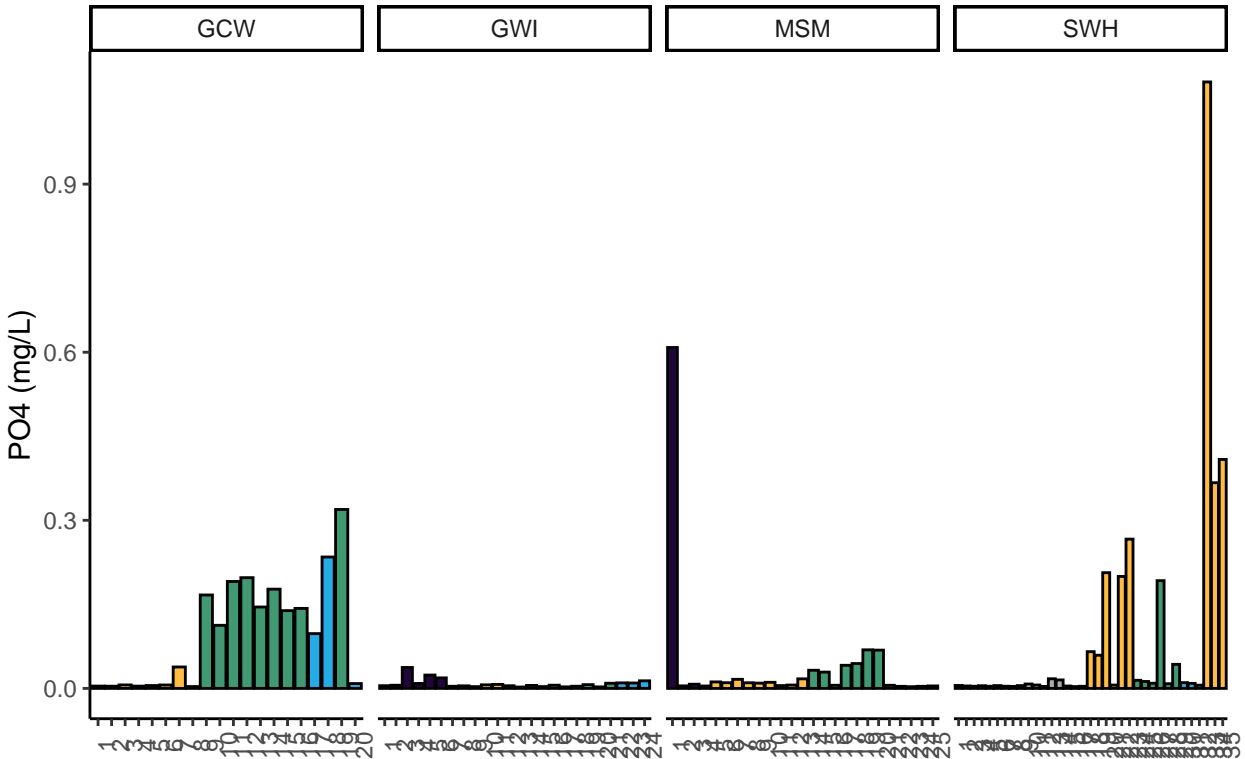
0.16 Visualize Data

```
## Visualize Data
```

Porewater NOx

Porewater NH3

Porewater PO4

0.17 Export Processed Data

#end