Synoptic_CB_Nutrients_202305

May 2023

2025-07-01

Contents

##Run Information

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

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

```
#set the run date & user name
  run_date <- "20240114"
  sample_year <- 2023
  sample_month <- 05
  user <- "Stephanie Wilson"

#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/SEAL_COMPASS_Synoptic_NOx_May2023_1.csv",
                 "Raw Data/SEAL_COMPASS_Synoptic_NOx_May2023_2_redo.csv",
                 "Raw Data/SEAL_COMPASS_Synoptic_NOx_May2023_3_redoA.csv")
  NH3_PO4_files <- c("Raw Data/SEAL_COMPASS_Synoptic_NH3_PO4_May2023_1redopo4.csv",
                     "Raw Data/SEAL_COMPASS_Synoptic_NH3_PO4_May2023_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_202305.csv"

#record any notes about the run or anything other info here:
  run_notes <- "Autospikes for PO4 not included in this run. "

#duplicate sample names to be changed
  #list the sample iDs that are messed up and create a list
  #with run number as well so that we can change them below
  wrong_names <- c("GCW_202304_TR_LysC_45cm", "GCW_202304_TR_LysA_20cm_8",
                   "GWI_202304_UP_LysA_20cm", "GWI_202304_UP_LysA_20cm")
  wrong_nums <- c(20, 16, 46, 44)
  correct_names <- c("GCW_202304_TR_LysB_45cm", "GCW_202304_TR_LysA_20cm",
                     "GWI_202304_UP_LysA_10cm", "GWI_202304_UP_LysA_10cm")

  #can't determine from metadata - for now unsure
  remove_names <- c("GCW_202304_TR_LysA_20cm", "GCW_202304_TR_LysA_20cm",
                    "GCW_202304_TR_LysB_20cm_13", "GCW_202304_TR_LysB_20cm_13")
      #couldn't tell which onethis is from the metadata, no A_10cm which is what we thought
      #marked on the sheet, need to check sample vials in freezer
      #to see if we have a A_10cm from GCW_TR to be sure
  remove_nums <- c(15, 13, 21, 19 )

#Set up file path for metadata
  #downloaded metadata csv - downloaded from Google drive as csv for this year
  #https://docs.google.com/spreadsheets/d/1HCANO_q6y17xORUXVzID09hVal-RfwWc/edit?usp=sharing&ouid=10899
  Raw_Metadata = "Raw Data/COMPASS_SynopticCB_PW_SampleLog_2023.csv"
```

##Setup

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

0.1 Import Data & Clean

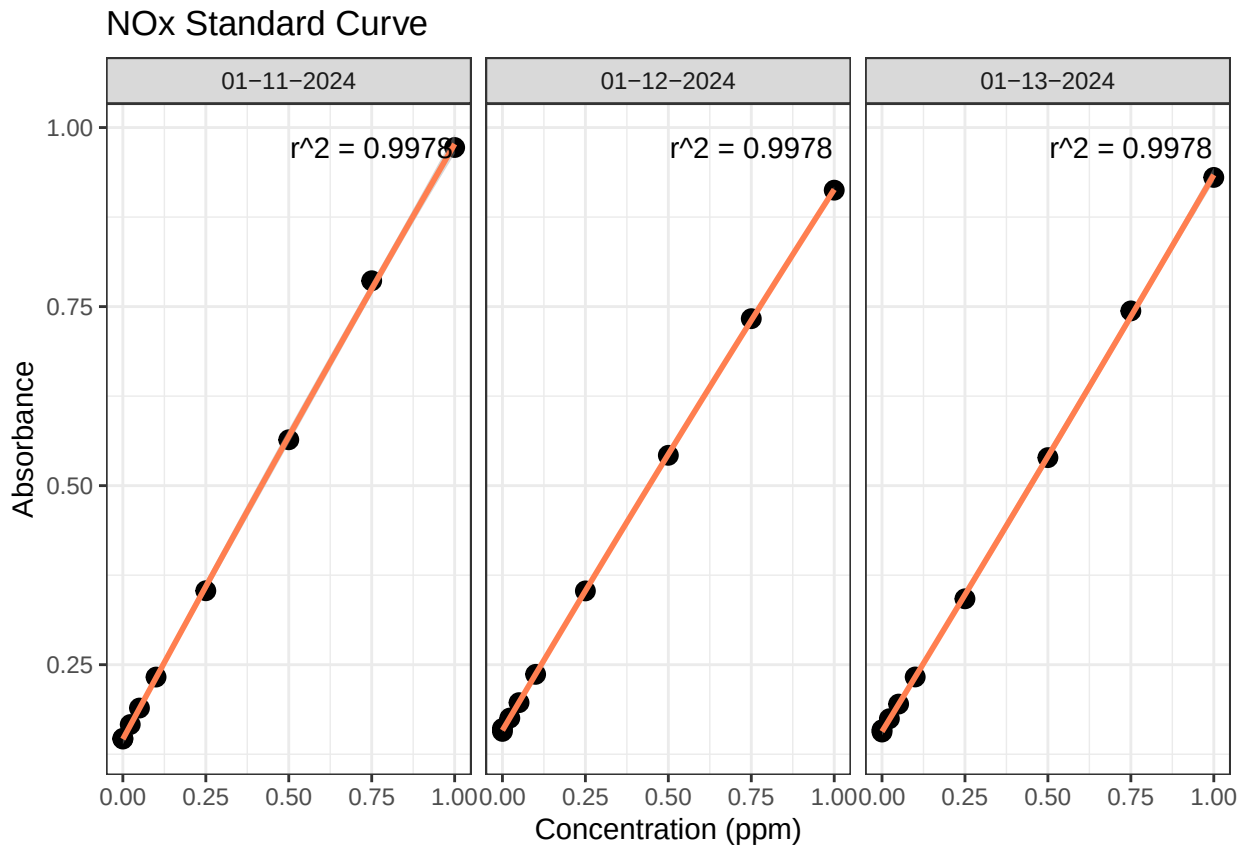
0.2 Assessing standard Curves

#Pull out standards data

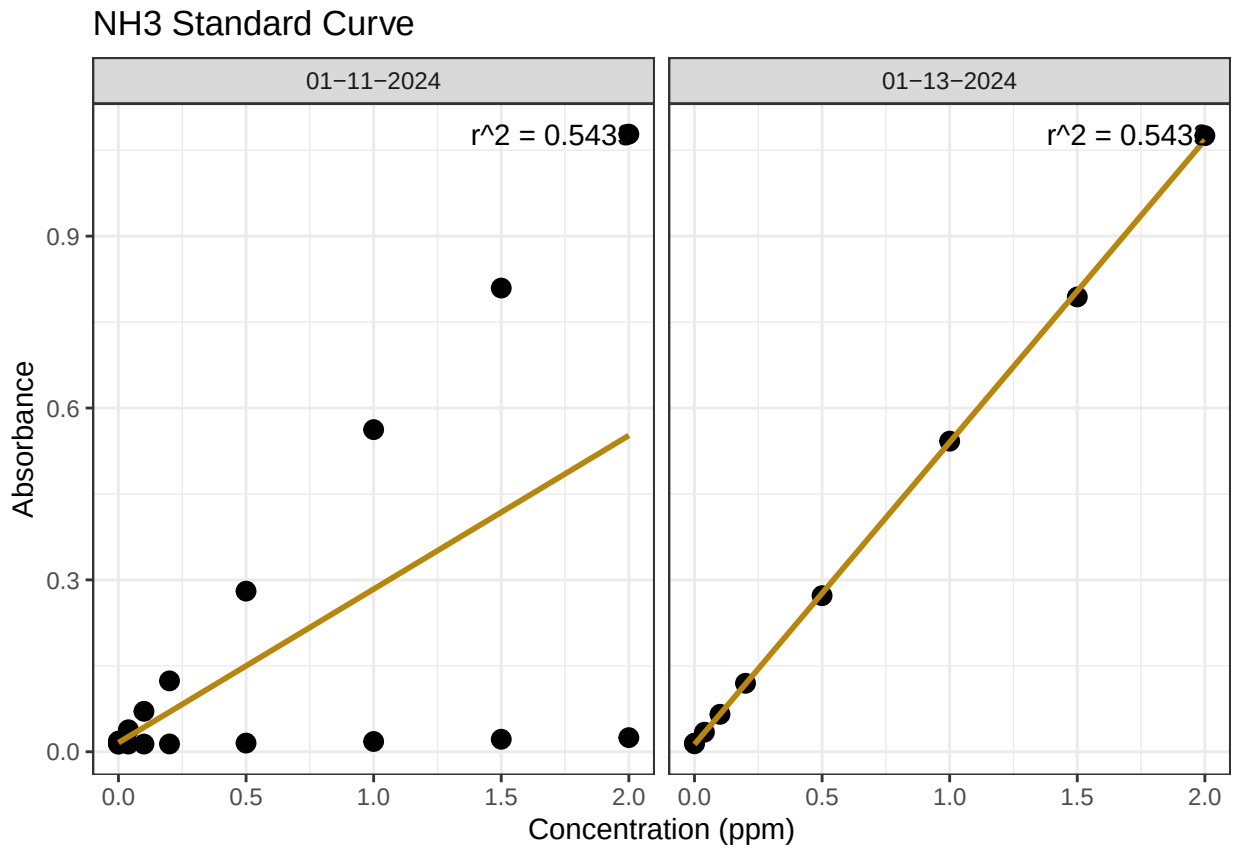
```
## Assess Standard Curves
```

#Plot standards data

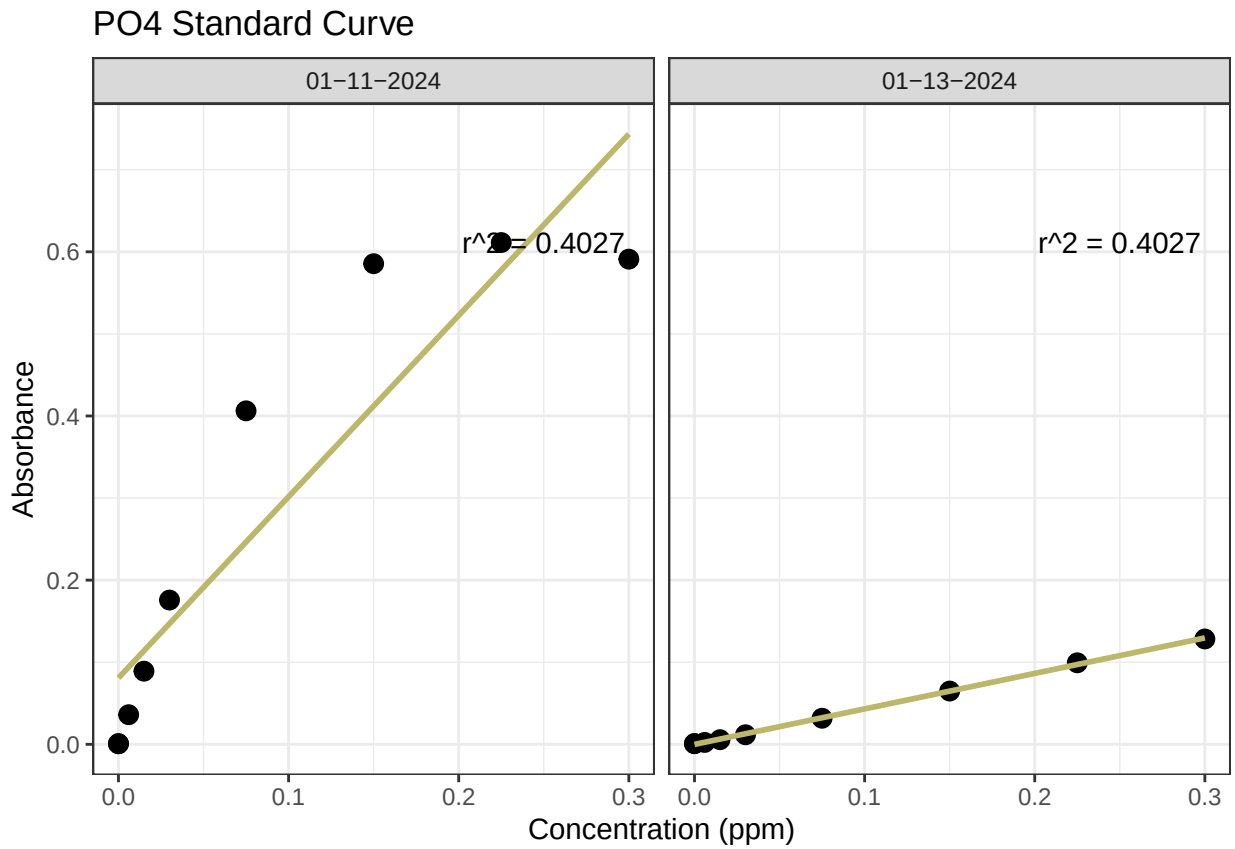
```
## Assess Standard Curves
```




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




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




```
## [1] "NOx Curve r2 GOOD - PROCEED"
```

```
## [1] "NH3 Curve r2 is below cutoff! - REASSESS"
```

```
## [1] "PO4 Curve r2 is below cutoff! - REASSESS"
```

```
## [1] "QAQC log file exists and has been read into the code."
```

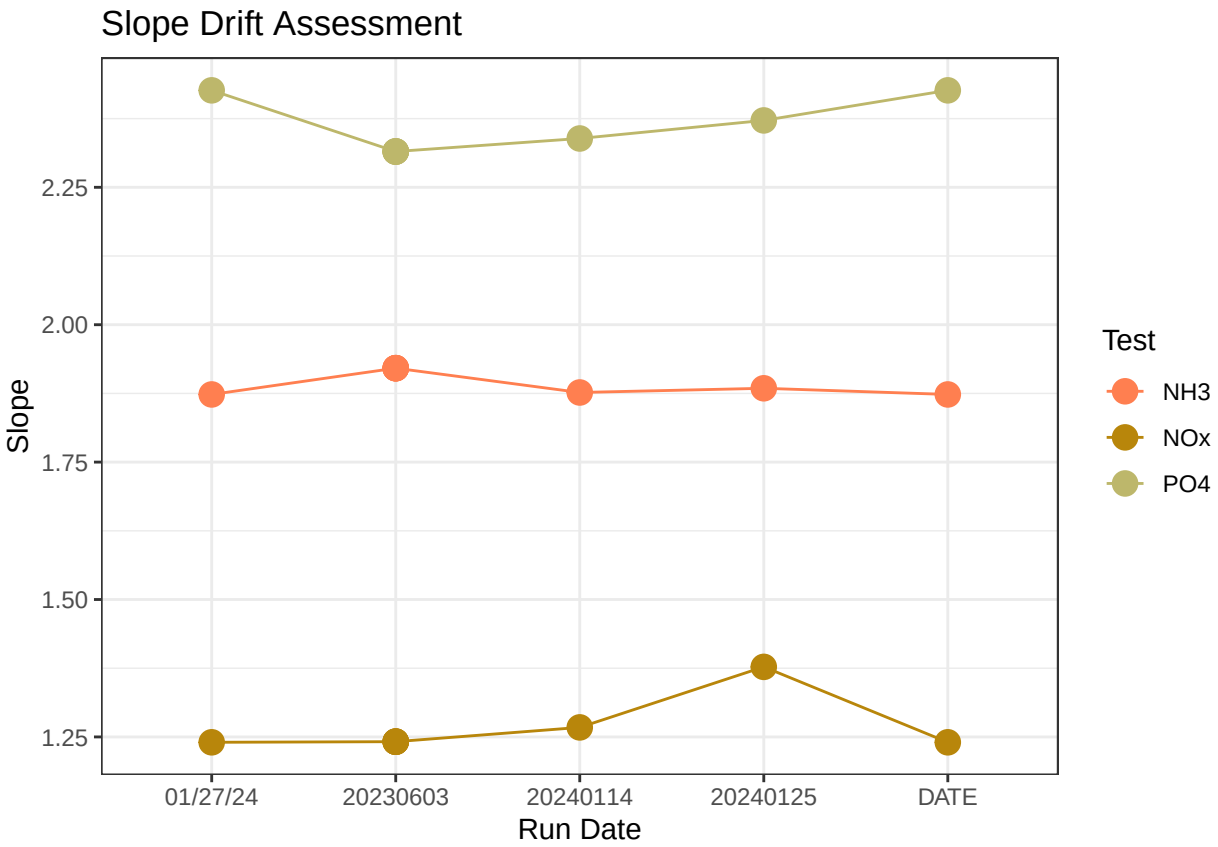


Table 1: Average Slope by Analyte

Test	avg_slope
NH3	1.899
NOx	1.261
PO4	2.353

0.3 Dilution Corrections - ensure the latest dilution is kept

```
## Dilution Corrections

## Duplicated samples: GCW_202305_UP_LysA_20cm, GCW_202305_UP_LysB_10cm, GCW_202305_UP_LysB_20cm, GCW_2

## Duplicated samples with NO dilution present (possible input error): GCW_202305_SW_A, GCW_202305_SW_B
```

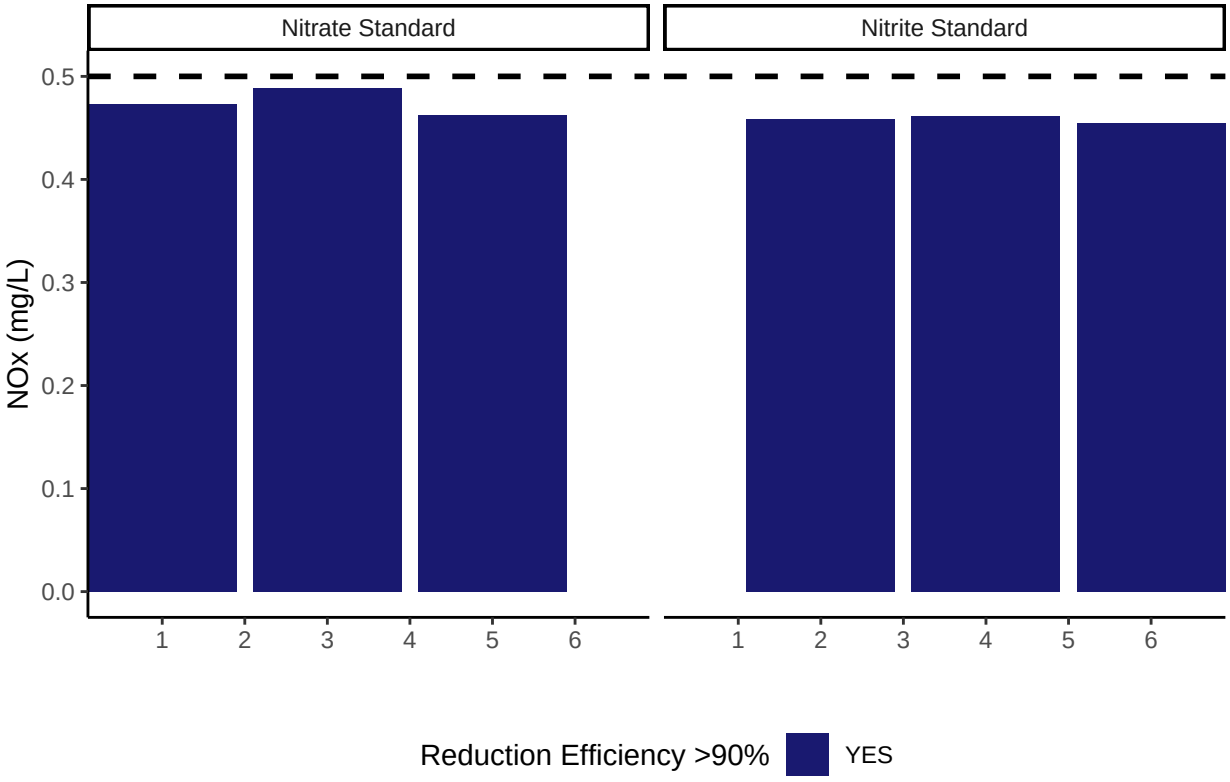
0.4 Temporary Chunk

0.5 Performance Check

```
## [1] "NOx pe Check has a % Difference <10% - PROCEED"

## Run mean = 0.712214

## Expected  = 0.706

## [1] "NH3 pe Check has a % Difference >10% - REASSESS"

## Run mean = 1.437577

## Expected  = 0.948

## [1] "PO4 pe Check has a % Difference <10% - PROCEED"

## Run mean = 0.893199

## Expected  = 0.818
```

#Check NOx Reduction Efficiency

```
## Assess Reduction Efficiency
```




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

```
## [1] 93.2968
```

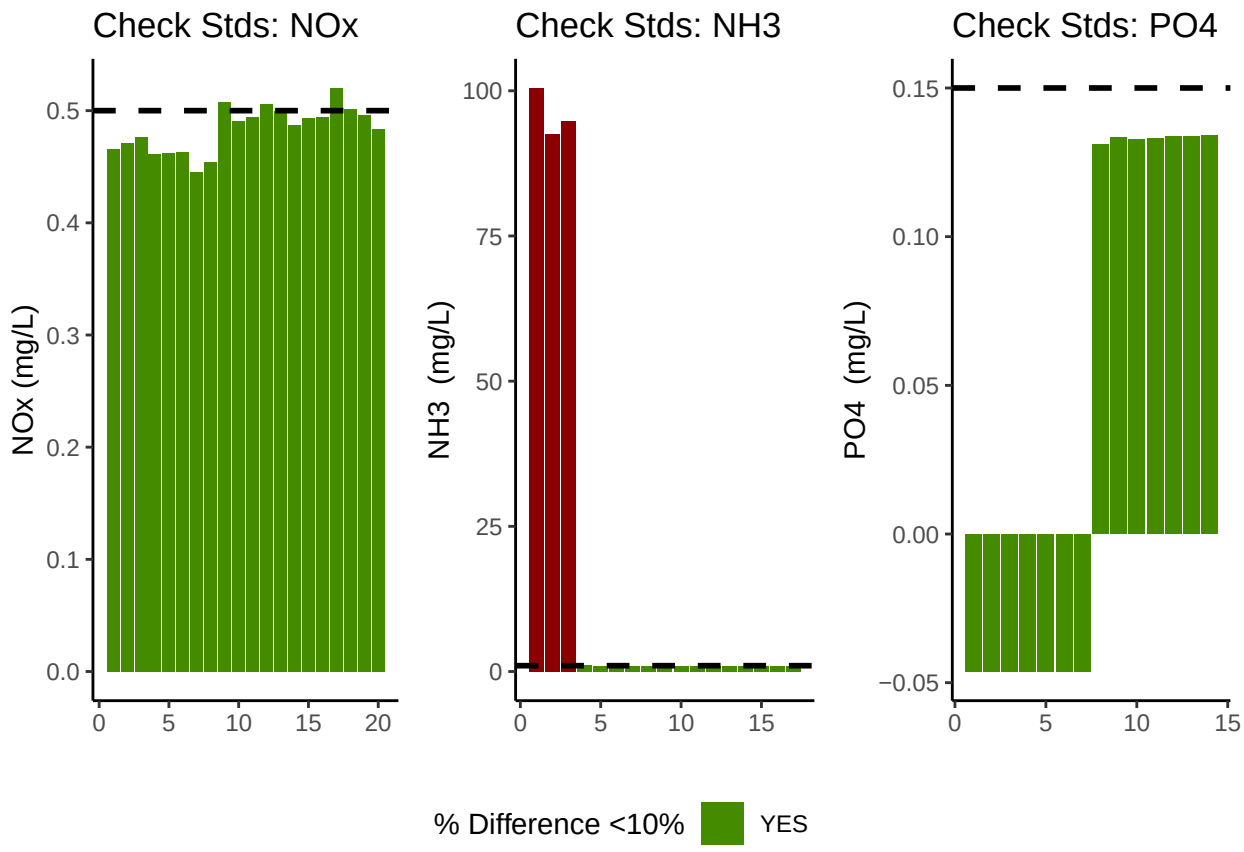
0.6 Analyze the Check Standards

```
## Analyze Check Standards
```

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

```
## [1] "NH3 CHECK STANDARD RSD TOO HIGH - REASSESS"
```

```
## [1] "PO4 CHECK STANDARD RSD 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"
```

0.7 Analyze Blanks

```
## Assess Blanks
```

```
## [1] ">60% of NOx Blank concentrations are lower than the lower 25% quartile of samples - PROCEED"
```

```
## [1] ">60% of NH3 Blank concentrations are lower than the lower 25% quartile of samples - PROCEED"
```

```
## [1] ">60% of PO4 Blank concentrations are lower than the lower 25% quartile of samples- PROCEED"
```

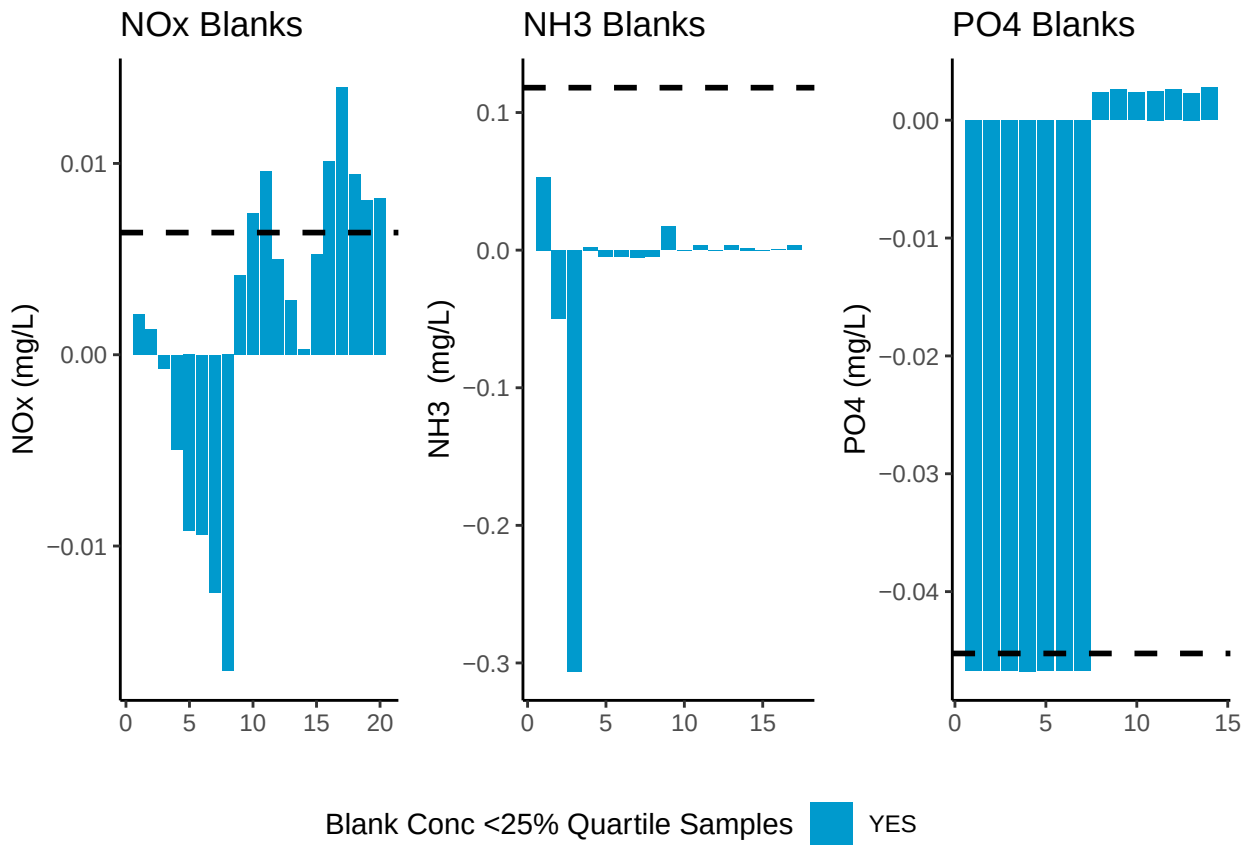


Table 2: Mean Concentration of Blanks

Test	Blank_Mean_Conc
NOx	0.0017
NH3	-0.0171
PO4	-0.0221

0.8 Analyze Duplicates

```
## Analyze Duplicates
```

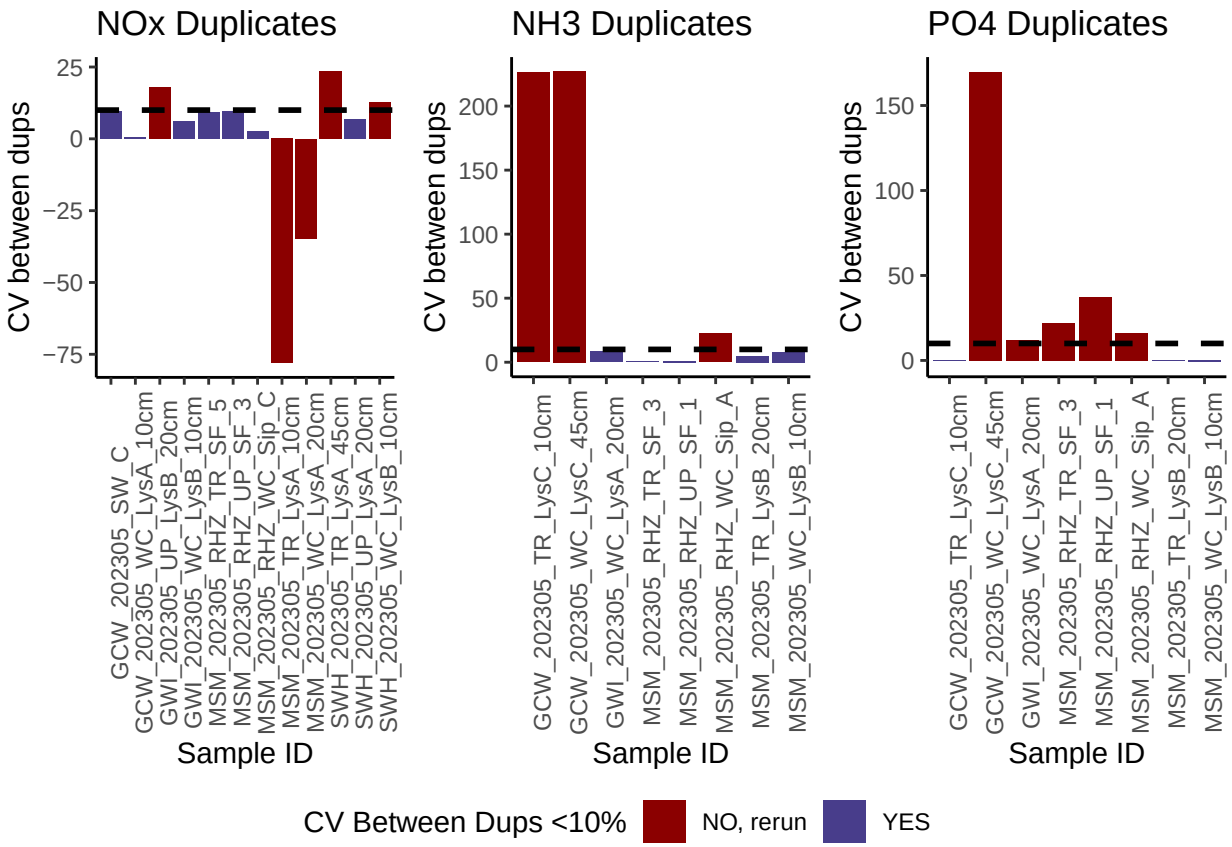
```
## Warning: Returning more (or less) than 1 row per `summarise()` group was deprecated in
## dplyr 1.1.0.
## i Please use `reframe()` instead.
## i When switching from `summarise()` to `reframe()`, remember that `reframe()`
##   always returns an ungrouped data frame and adjust accordingly.
## Call `lifecycle::last_lifecycle_warnings()` to see where this warning was
## generated.
```

```
## [1] "<60% of NOx Duplicates have a CV <10% - REASSESS"
```

```
## [1] "<60% of NH3 Duplicates have a CV <10% - REASSESS"
```

```
## [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.
```

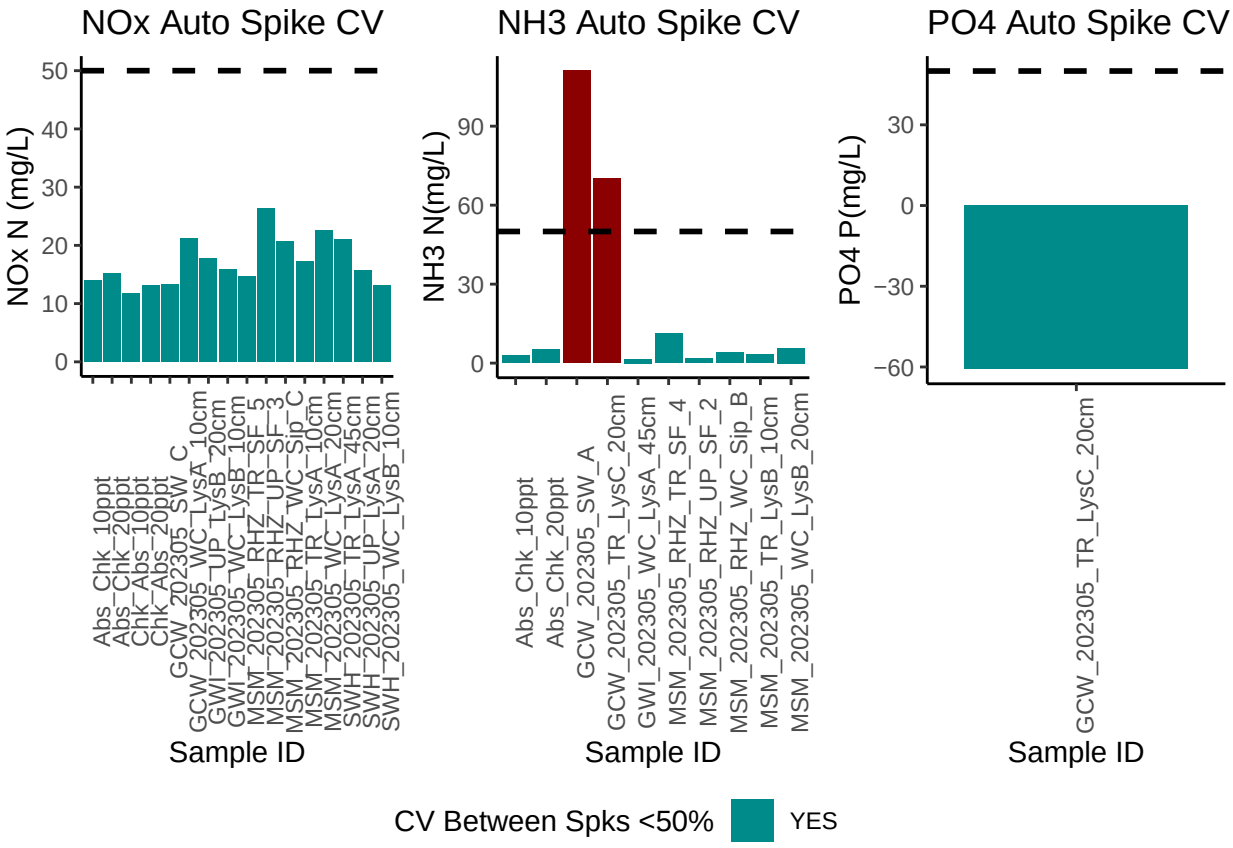


0.9 Spikes

```
## [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: Expected 5 pieces. Missing pieces filled with `NA` in 32 rows [19, 20, 21, 46,
## 47, 48, 83, 84, 108, 109, 110, 129, 130, 131, 150, 151, 152, 177, 178, 179,
## ...].
```

0.14 Pulling Out Rhizon Samples

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

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

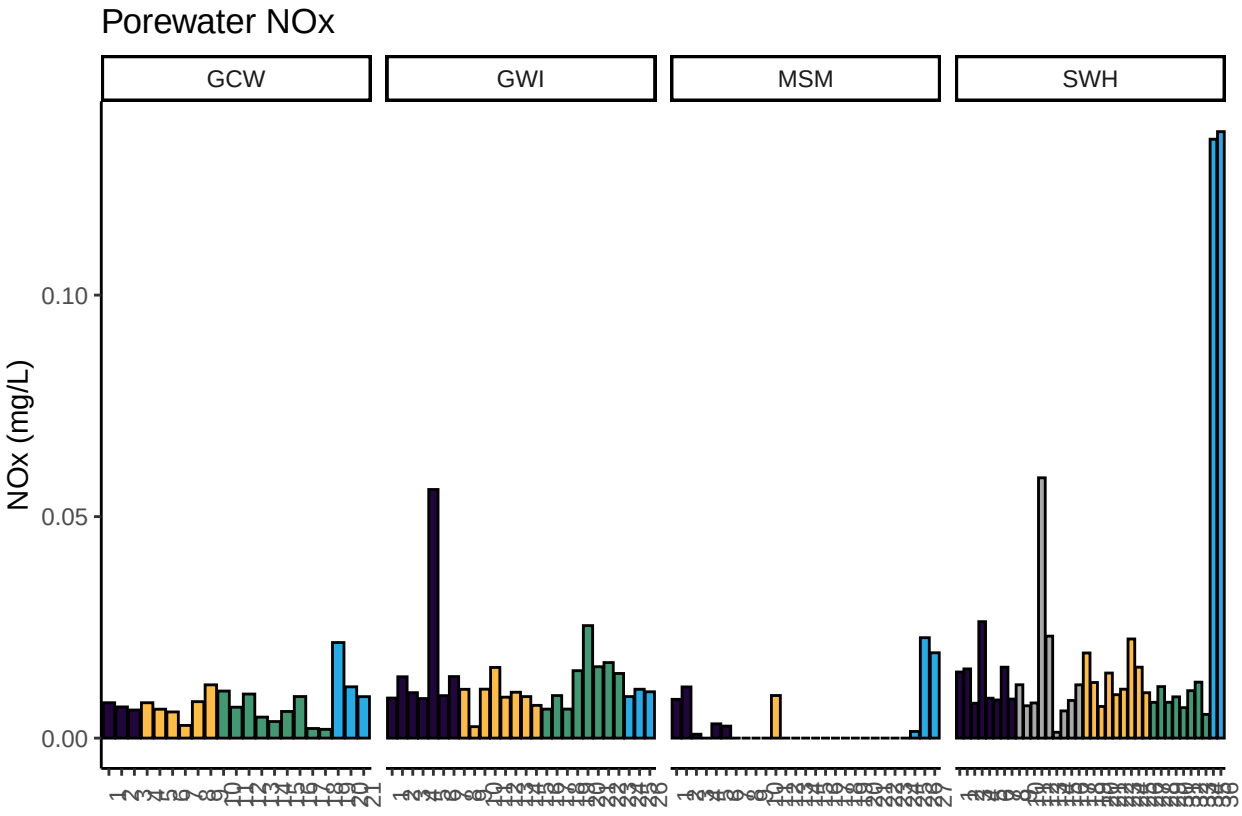
```
## Some sample IDs are missing from metadata.
```

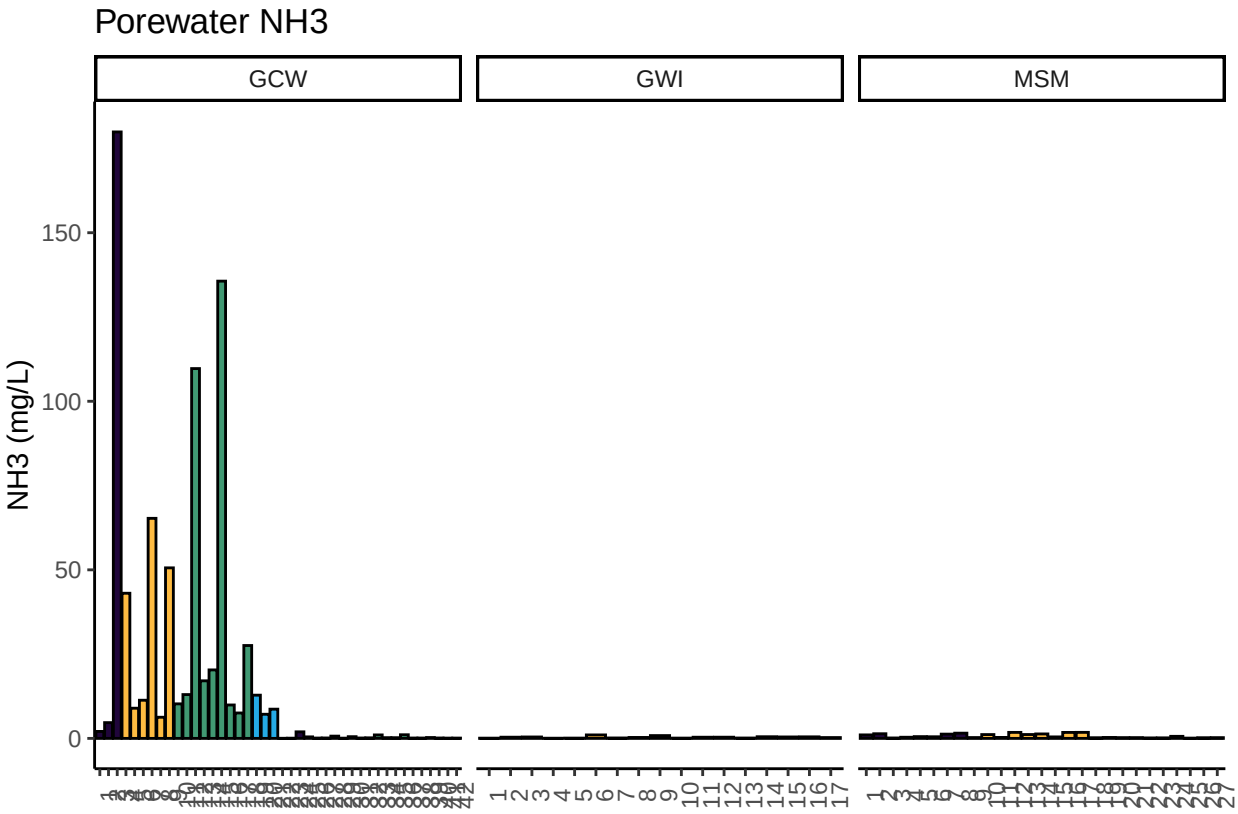
```
##  [1] "GCW_202305_UP_LysA_20cm"    "GCW_202305_UP_LysB_10cm"
##  [3] "GCW_202305_UP_LysB_20cm"    "MSM_202305_UP_LysC_45cm"
##  [5] "MSM_202305_TR_LysC_45cm"    "MSM_202305_WC_LysA_45cm"
##  [7] "SWH_202305_UPCON_LysA_10cm" "SWH_202305_UPCON_LysA_20cm"
##  [9] "SWH_202305_UPCON_LysA_45cm" "SWH_202305_UPCON_LysB_10cm"
## [11] "SWH_202305_UPCON_LysB_20cm" "SWH_202305_UPCON_LysB_45cm"
## [13] "SWH_202305_UPCON_LysC_20cm" "SWH_202305_UPCON_LysC_45cm"
## [15] "SWH_202305_UP_LysB_10cm"    "SWH_202305_WC_LysA_10cm"
## [17] "SWH_202305_WC_LysA_20cm"    "SWH_202305_WC_LysA_45cm"
## [19] "SWH_202305_WC_LysB_10cm"    "SWH_202305_WC_LysB_20cm"
## [21] "GWI_202305_TR_LysB_45cm"
```

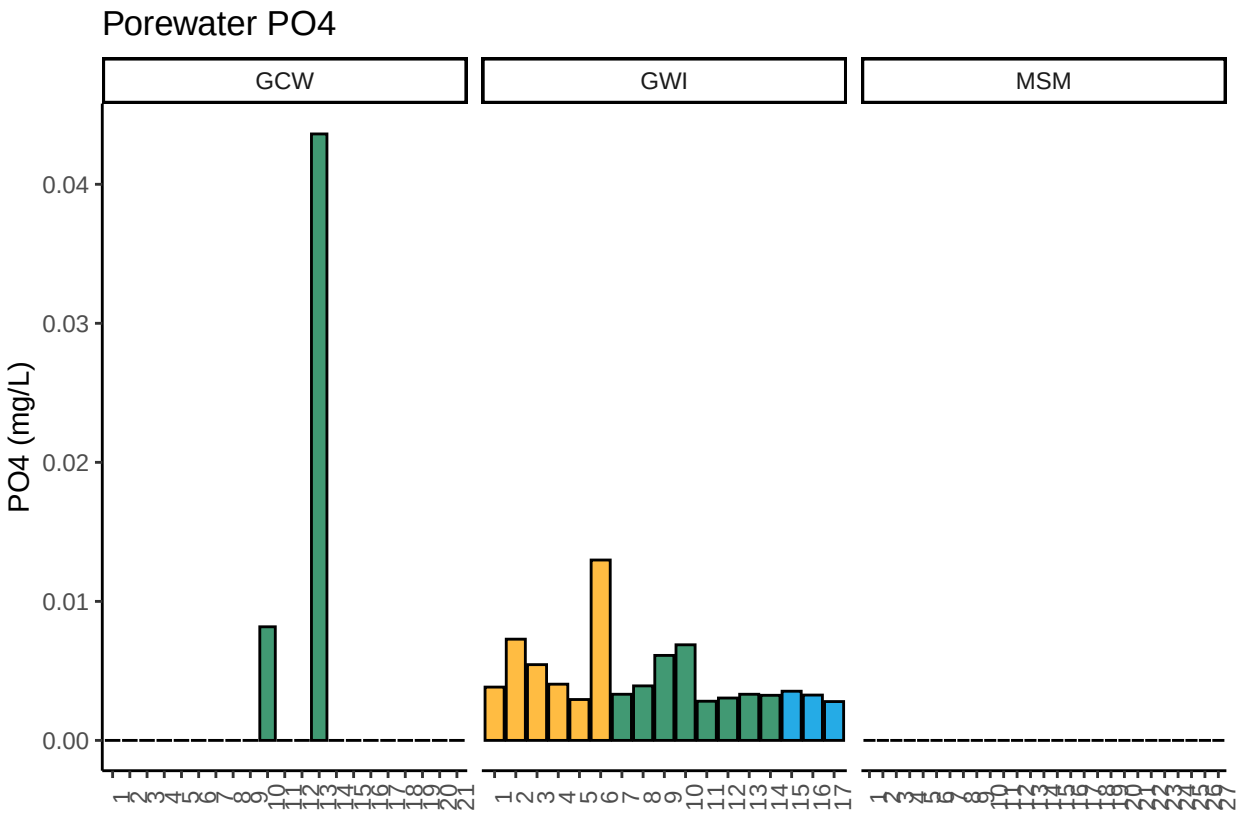
```
## Warning: Expected 5 pieces. Missing pieces filled with `NA` in 32 rows [19, 20, 21, 46,
## 47, 48, 83, 84, 108, 109, 110, 129, 130, 131, 150, 151, 152, 177, 178, 179,
## ...].
```

0.16 Visualize Data

```
## Visualize Data
```




Porewater NH3
GCW
GWI
MSM
NH3 (mg/L)
150
100
50
0



0.17 Export Processed Data

#end