Synoptic_CB_Nutrients_2023_Sept

September

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 <- "20240125"
  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.xlsx"

#record any notes about the run or anything other info here:
  run_notes <- "NOx Blanks are out of range because of the slightly negative y intercept of the standar

#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

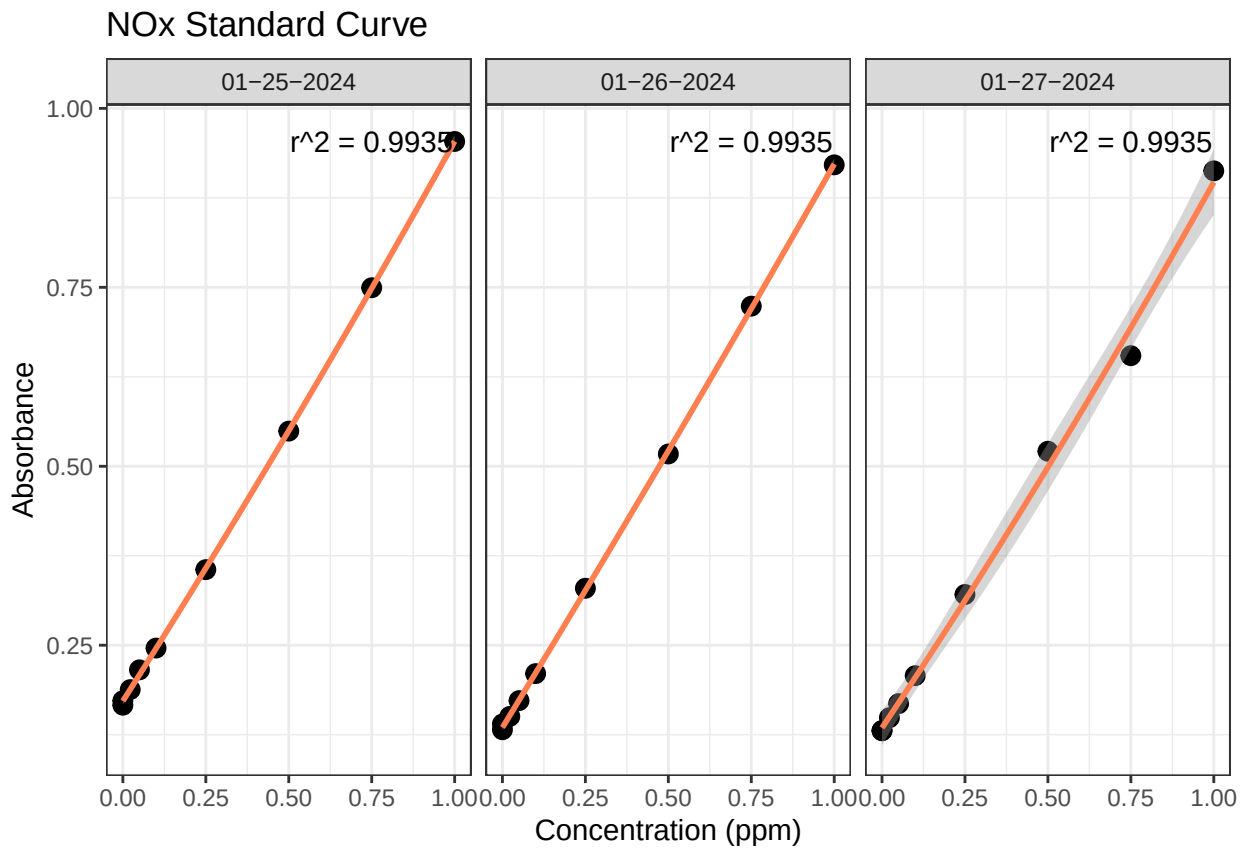
0.2 Assessing standard Curves

#Pull out standards data

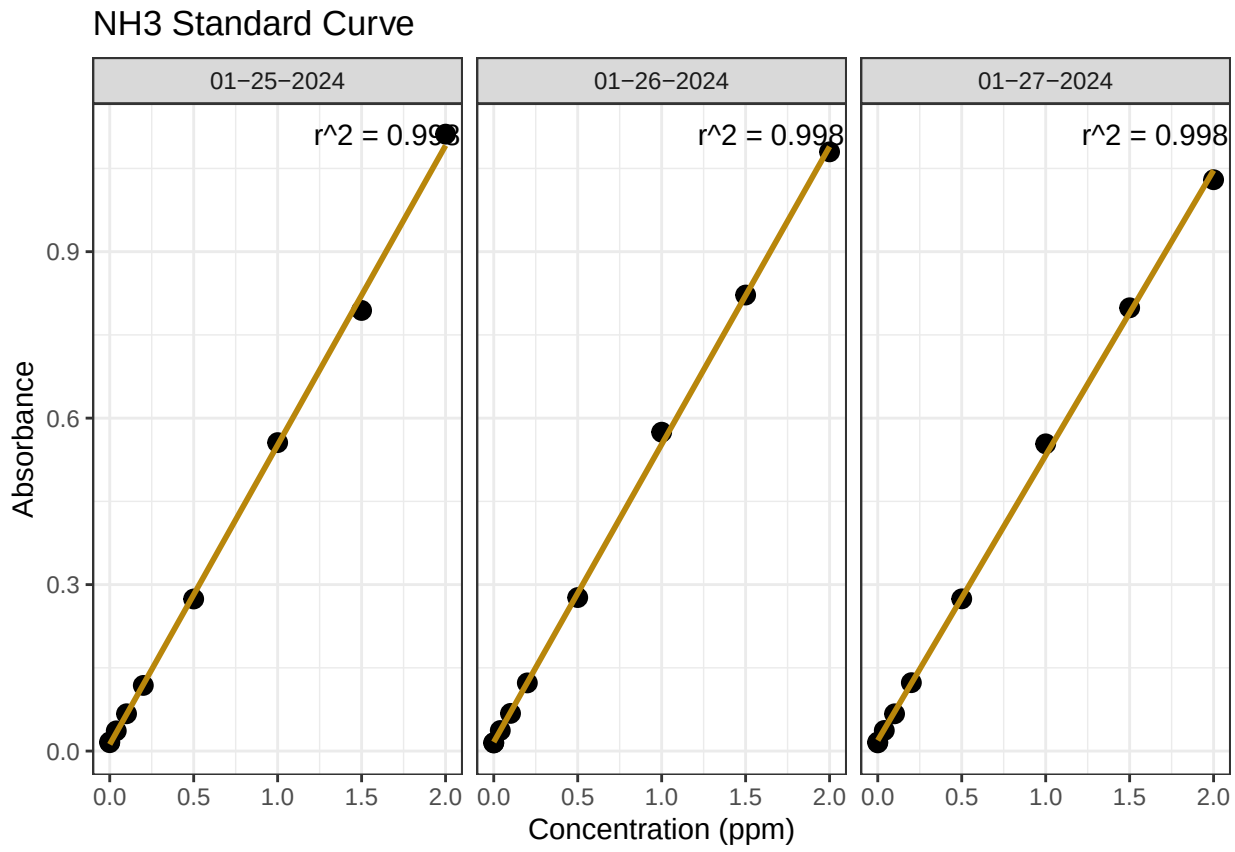
```
## Assess Standard Curves
```

#Plot standards data

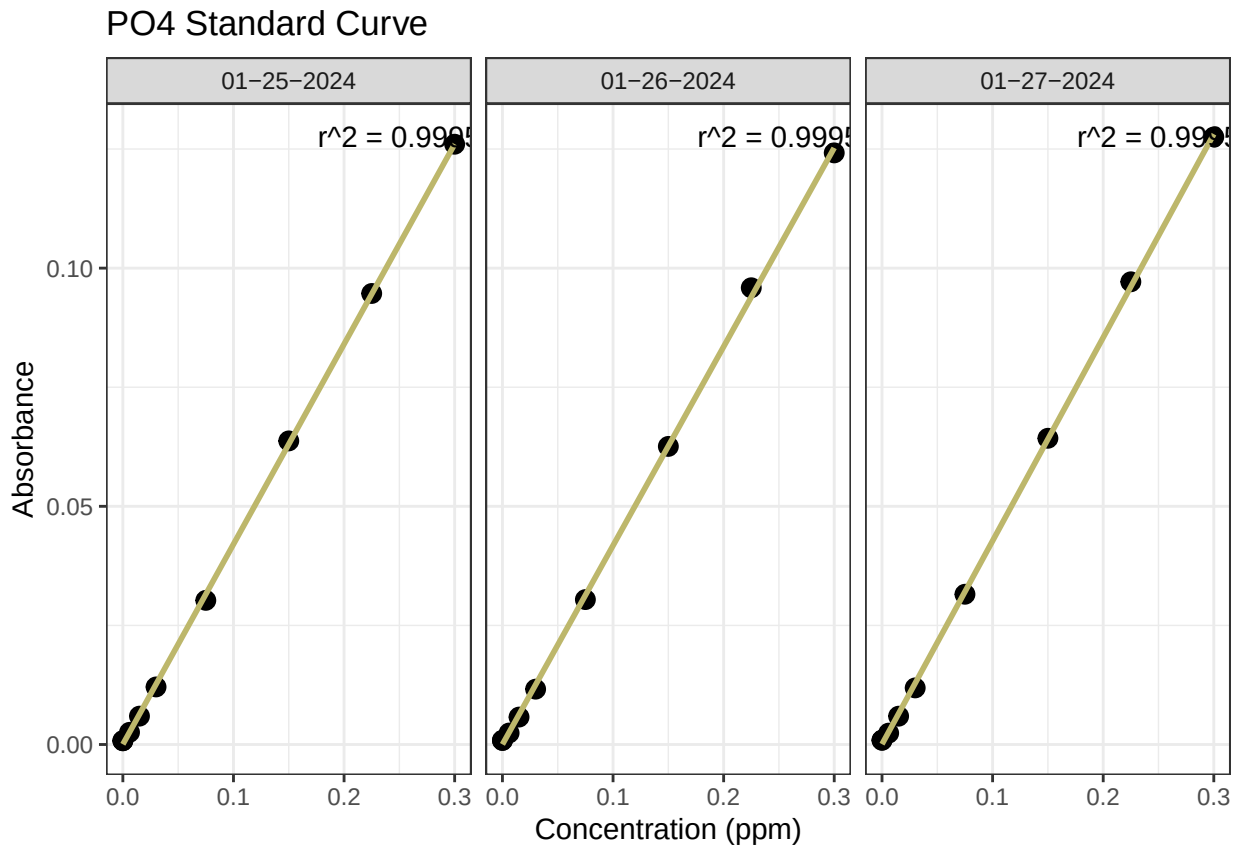
```
## Assess Standard Curves
```




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




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




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

```
## [1] "NH3 Curve r2 GOOD - PROCEED"
```

```
## [1] "PO4 Curve r2 GOOD - PROCEED"
```

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

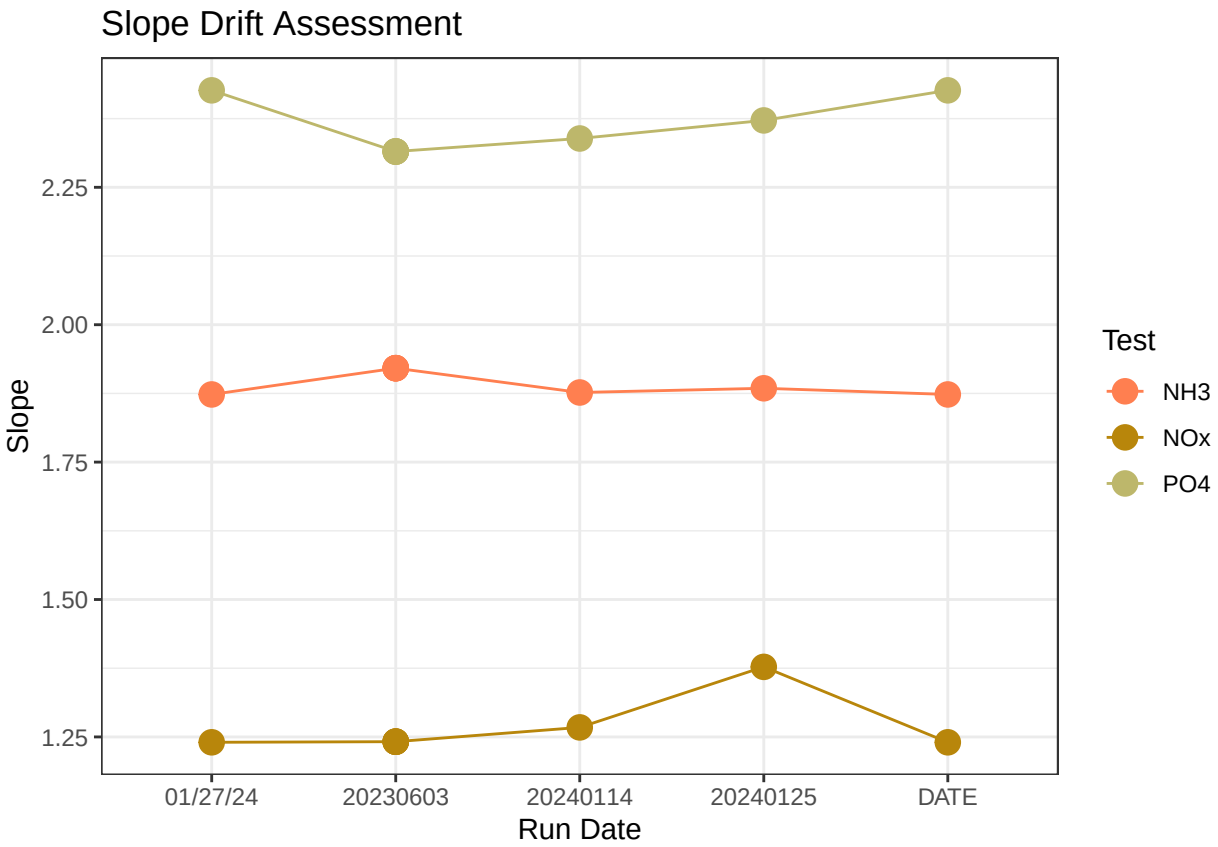


Table 1: Average Slope by Analyte

Test	avg_slope
NH3	1.899
NOx	1.261
PO4	2.353

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

0.4 Dilution Corrections - ensure the latest dilution is kept

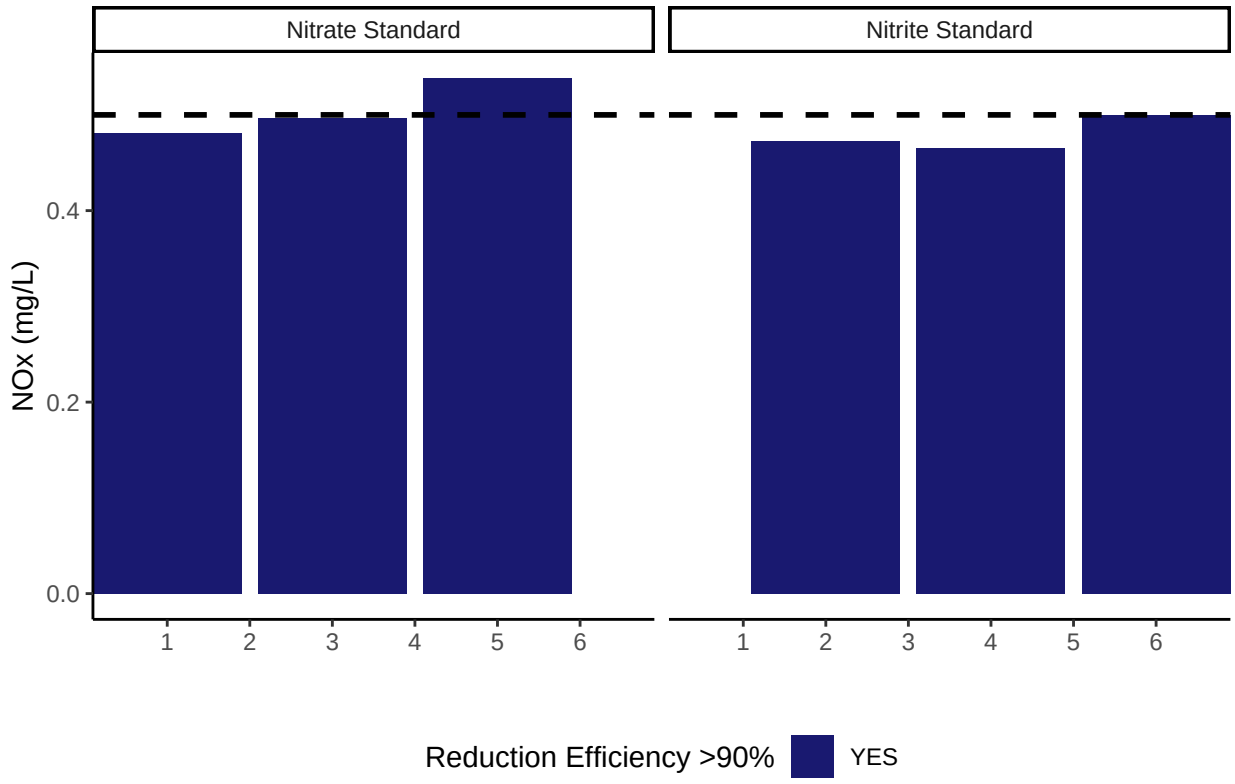
```
## Dilution Corrections

## Duplicated samples: MSM_202309_TR_LysA_20cm, MSM_202309_TR_LysB_10cm, MSM_202309_TR_LysB_20cm, MSM_2

## Duplicated samples with NO dilution present (possible input error): MSM_202309_UP_LysB_10cm
```

0.5 Performance Check

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

## Run mean = 0.738716

## Expected  = 0.706

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

## Run mean = 1.531811

## Expected  = 0.948

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

## Run mean = 0.864723

## Expected  = 0.818
```

#Check NOx Reduction Efficiency

```
## Assess Reduction Efficiency
```




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

```
## [1] 98.47613
```

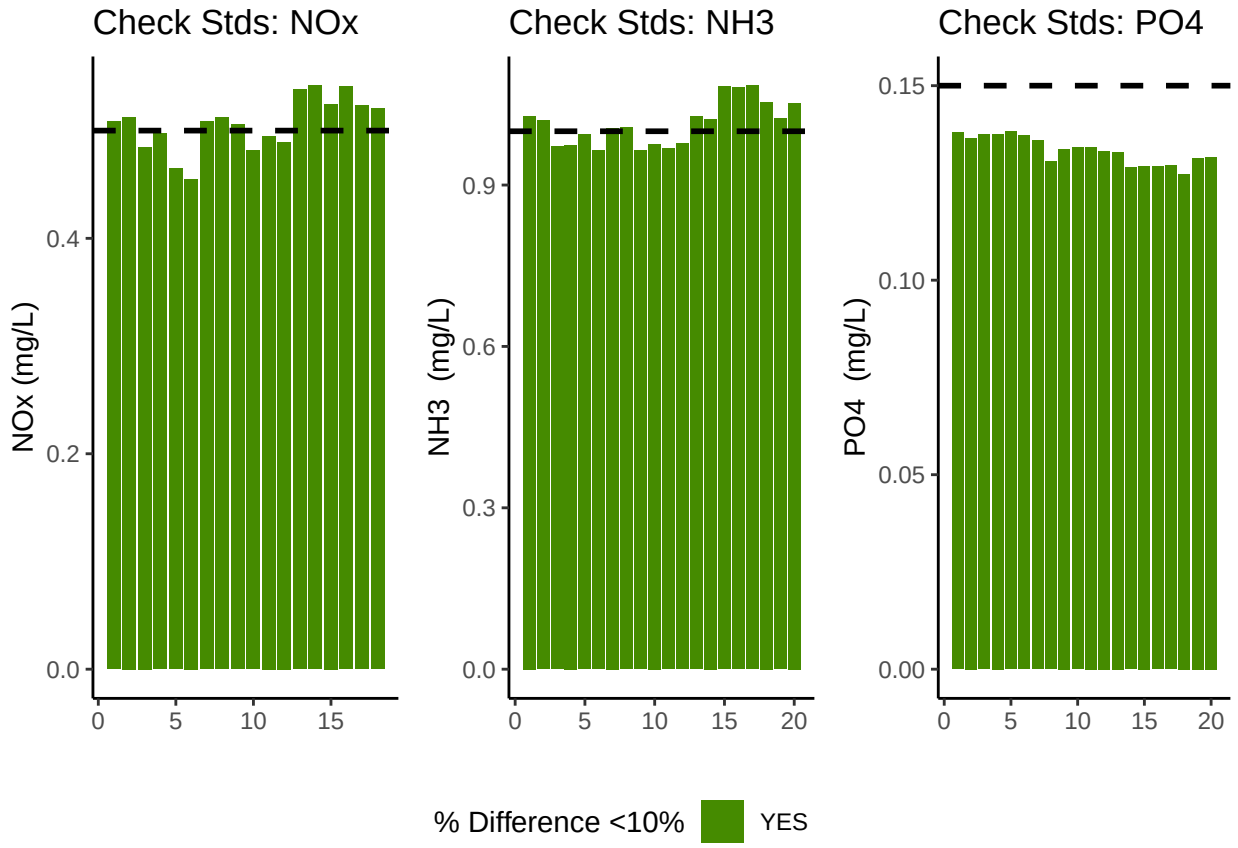
0.6 Analyze the Check Standards

```
## 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 blaks are lower 25% quartile of samples - REASSESS"

## [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"

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

## Run mean = 0.738716

## Expected  = 0.706
```

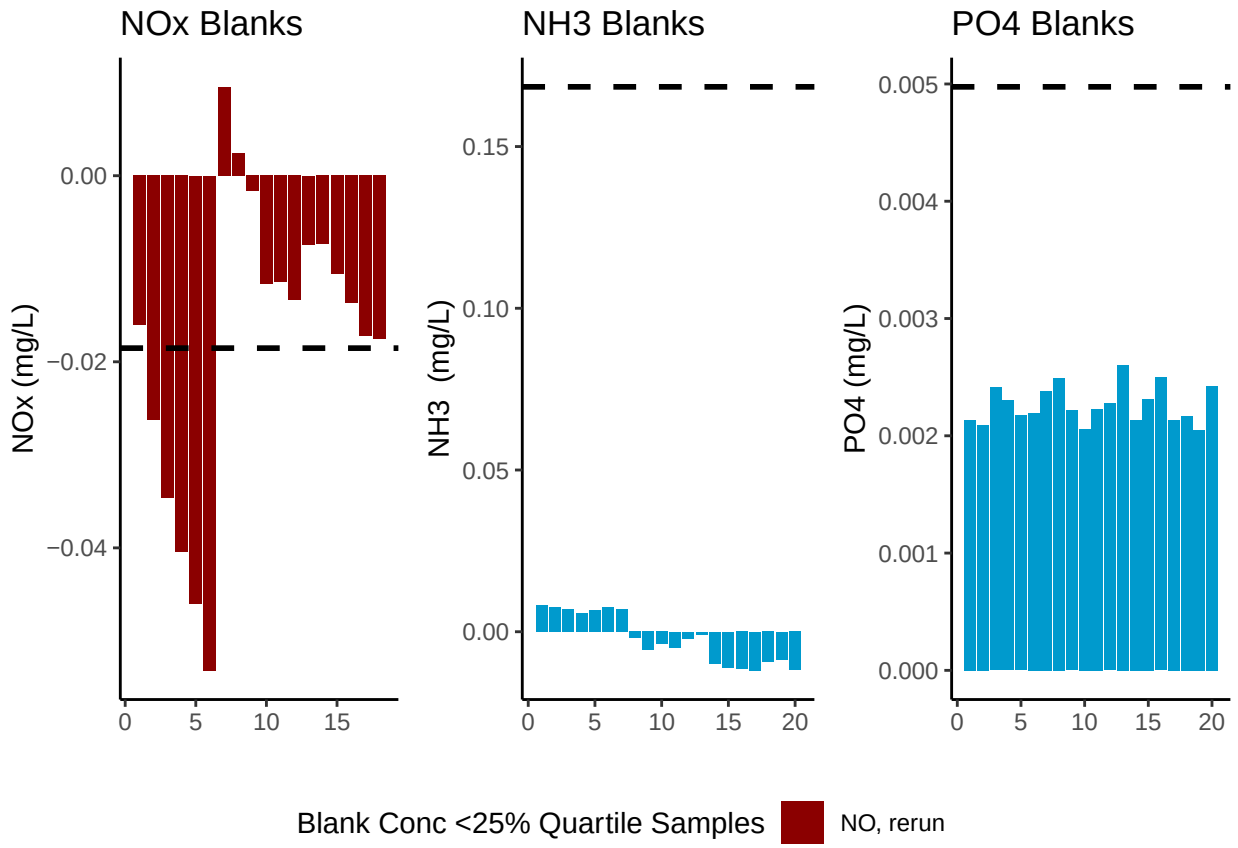


Table 2: Mean Concentration of Blanks

Test	Blank_Mean_Conc
NOx	-0.0176
NH3	-0.0022
PO4	0.0023

0.8 Analyze Duplicates

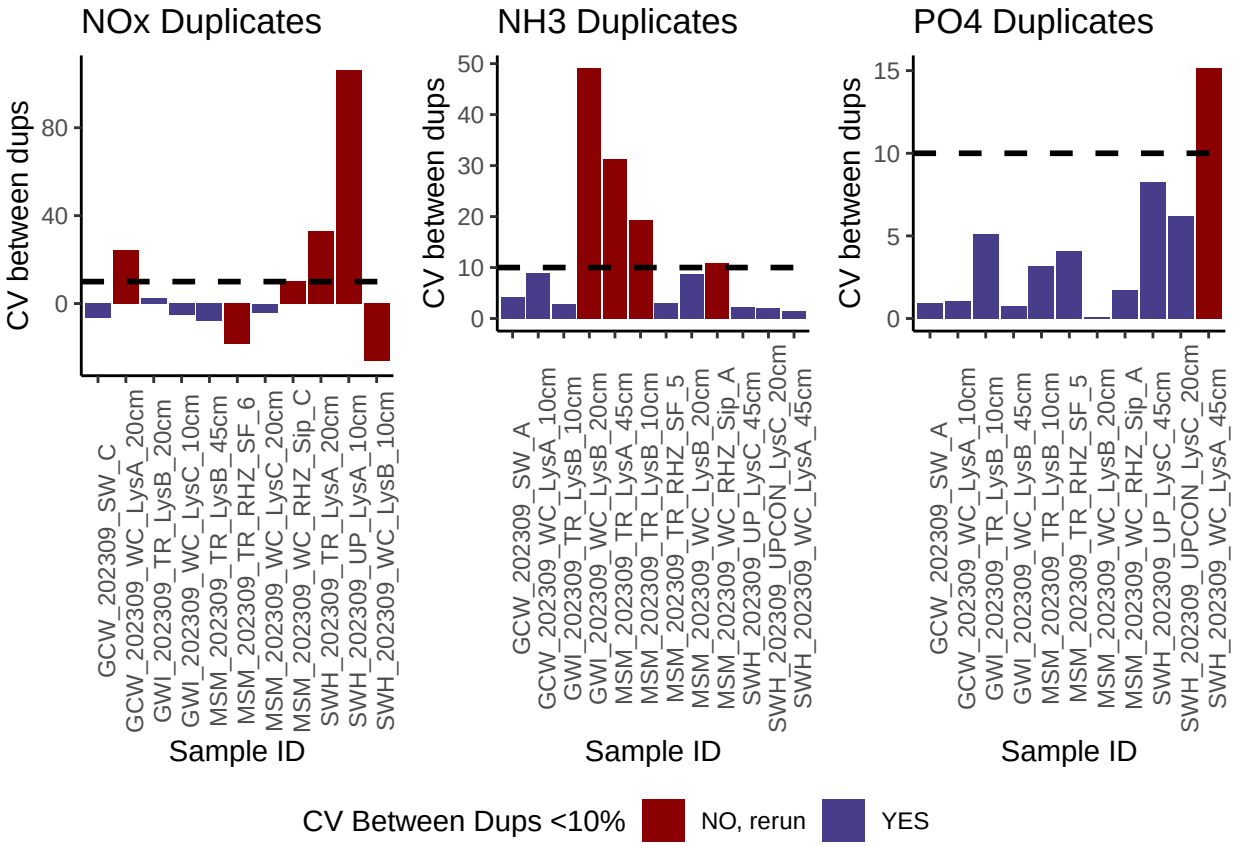
```
## Analyze Duplicates
```

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

```
## [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.
```

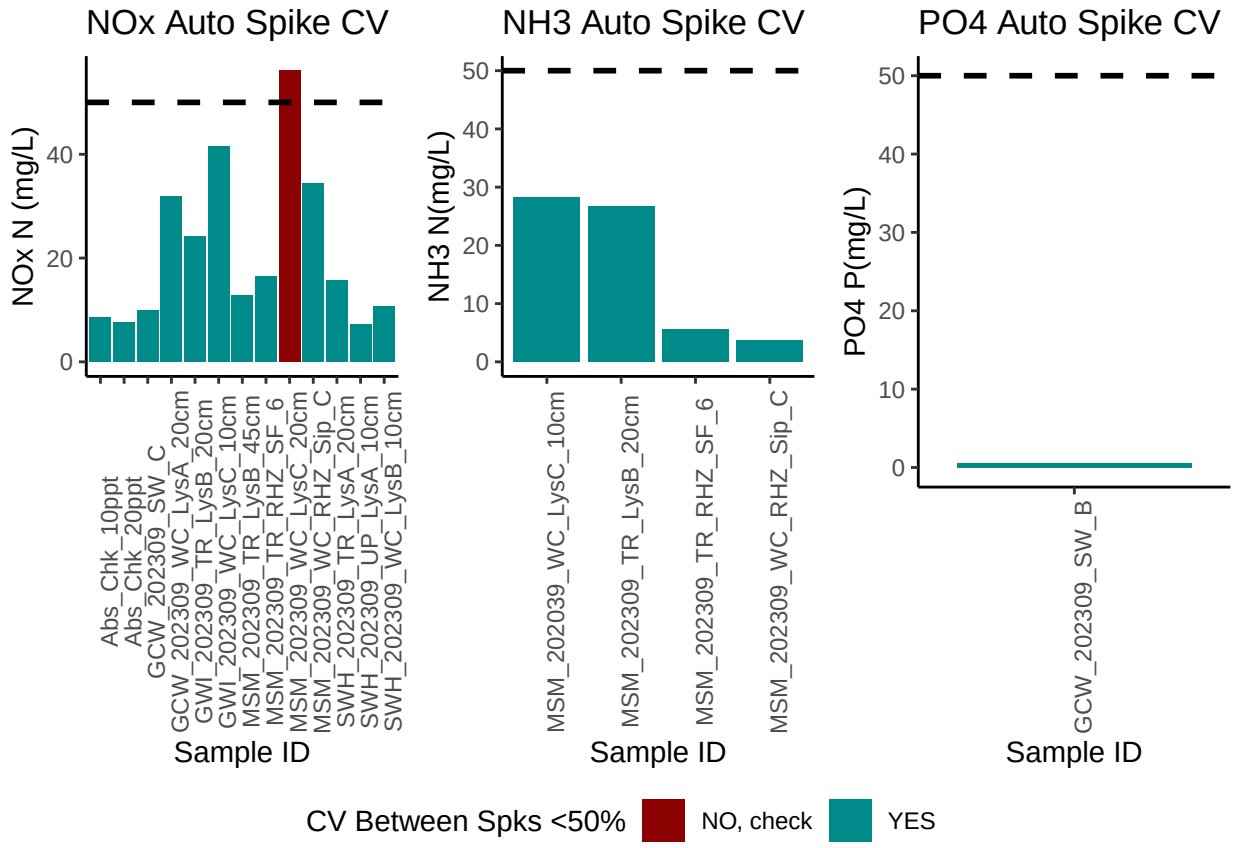


0.9 Spikes

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

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

```
## [1] "Flag not calculated for this run"
```



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 36 rows [18, 19, 20, 42,
## 43, 44, 77, 78, 79, 101, 102, 103, 121, 122, 123, 138, 139, 140, 157, 158,
## ...].
```

```
## Warning: There was 1 warning in `mutate()`.
## i In argument: `Samp_Time = ym(Samp_Time)`.
## Caused by warning:
## !  10 failed to parse.
```

0.14 Pulling Rhizon Samples

```
# 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
```

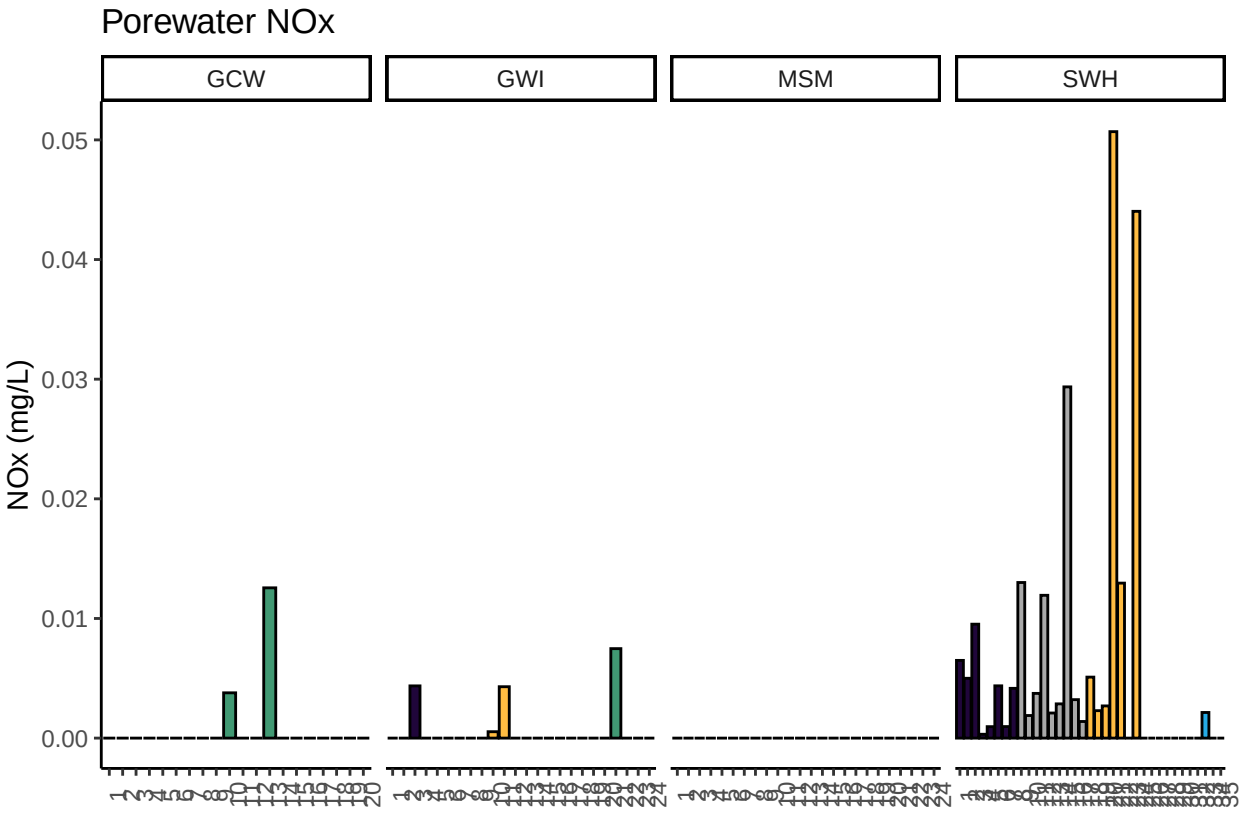
```r
write.csv(df_rhizon, rhizon_backup, row.names = FALSE)
write.csv(df_peep, peeper_backup, row.names = FALSE)

# 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 ^^
```

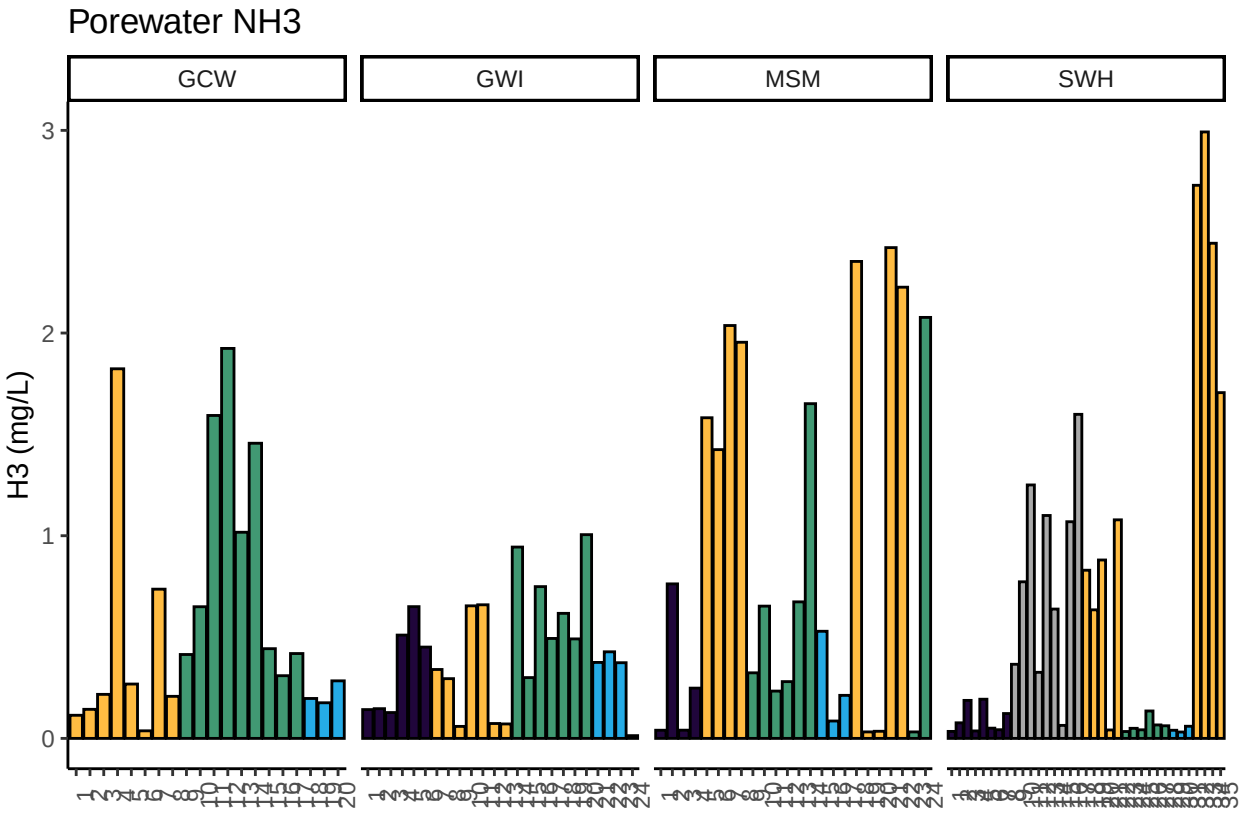
0.15 Check to see if samples run match metadata & merge info

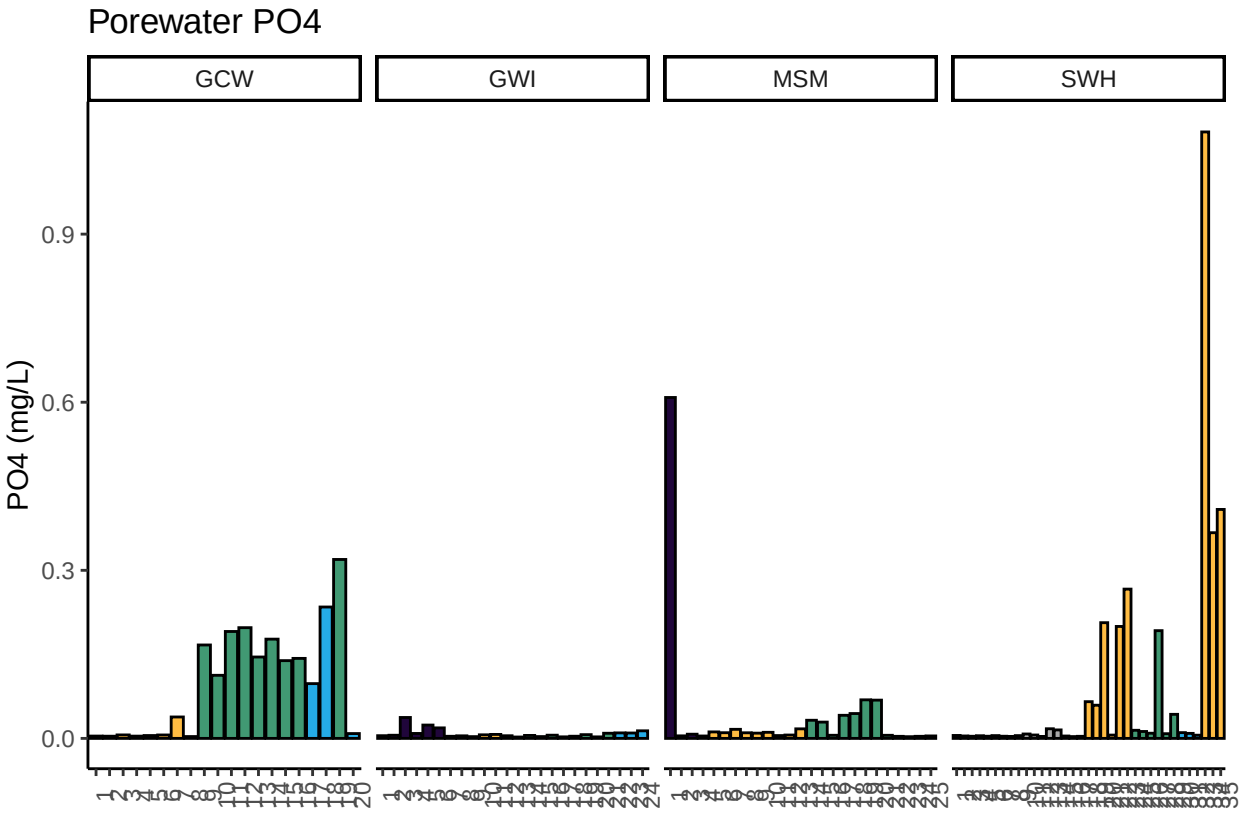
```
## Check Sample IDs with Metadata


## Some sample IDs are missing from metadata.


##  [1] "GCW_202039_SW_A"            "MSM_202309_TR_LysC_45cm"
##  [3] "SWH_202309_UPCON_LysA_10cm" "SWH_202309_UPCON_LysA_20cm"
##  [5] "SWH_202309_UPCON_LysA_45cm" "SWH_202309_UPCON_LysB_20cm"
##  [7] "SWH_202309_UPCON_LysB_45cm" "SWH_202309_UPCON_LysC_10cm"
##  [9] "SWH_202309_UPCON_LysC_20cm" "SWH_202309_UPCON_LysC_45cm"
## [11] "SWH_202039_TR_LysC_45cm"    "SWH_202309_WC_LysA_45cm"
## [13] "SWH_202309_WC_LysC_10cm"    "SWH_202309_WC_LysC_20cm"
## [15] "GWI_202039_WC_LysA_20cm"    "GWI_202039_WC_LysB_45cm"
## [17] "MSM_202039_WC_LysC_10cm"    "MSM_202039_WC_LysC_20cm"
## [19] "SWH_202039_TR_LysB_45cm"

## 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,
## ...].

## Warning: There was 1 warning in `mutate()`.
## i In argument: `Samp_Time = ym(Samp_Time)`.
## Caused by warning:
## !  10 failed to parse.
```

0.16 Visualize Data

```
## Visualize Data
```




Porewater NH3
GCW
GWI
MSM
SWH
H3 (mg/L)
0
1
2
3



0.17 Export Processed Data

#end