

Synoptic CB: Porewater Nutrients

August 2024 Samples

2025-08-12

Contents

0.1	Import Data & Clean	3
0.2	Assessing standard Curves	3
0.3	Dilution Corrections - ensure the latest dilution is kept	7
0.4	Performance Check	7
0.5	Analyze the Check Standards	9
0.6	Analyze Blanks	10
0.7	Analyze Duplicates	11
0.8	Spikes	12
0.9	Matrix Effects	13
0.10	Unit Converted Data Column Added (mg/L to uM)	13
0.11	Sample Flagging - Within range of standard curve	13
0.12	Pull out sample id information	13
0.13	Check to see if samples run match metadata & merge info	13
0.14	Visualize Data	14
0.15	Export Processed Data	16

```

##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 <- "06/24/2025"
sample_year <- "2024"
sample_month <- "AUGUST"
user <- "Isabelle Van Benschoten"

#identify the files you want to read in
#read in as a list to accomodate ultiple runs in a month
NOx_files <- c("Raw Data/COMPASS_Synoptic_CB_202408_VNOx_1.csv")
NH3_P04_files <- c("Raw Data/COMPASS_Synoptic_CB_202408_NH3_P04_1.csv")

# Define the file path for QAQC log file - NO Need to change just check year
file_path <- "Raw Data/SEAL_COMPASS_Synoptic_QAAC_Log_2024.csv"
final_path <- "Processed Data/COMPASS_Synoptic_Nutrients_202408.csv"

#record any notes about the run or anything other info here:
run_notes <- "P04 pe check was out of range as well as it's duplicates and spikes.
Would reccommend rerunning the P04 for this SWH 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_2024.csv"

cat(run_notes)

## P04 pe check was out of range as well as it's duplicates and spikes.
## Would reccommend rerunning the P04 for this SWH run.

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

```

0.1 Import Data & Clean

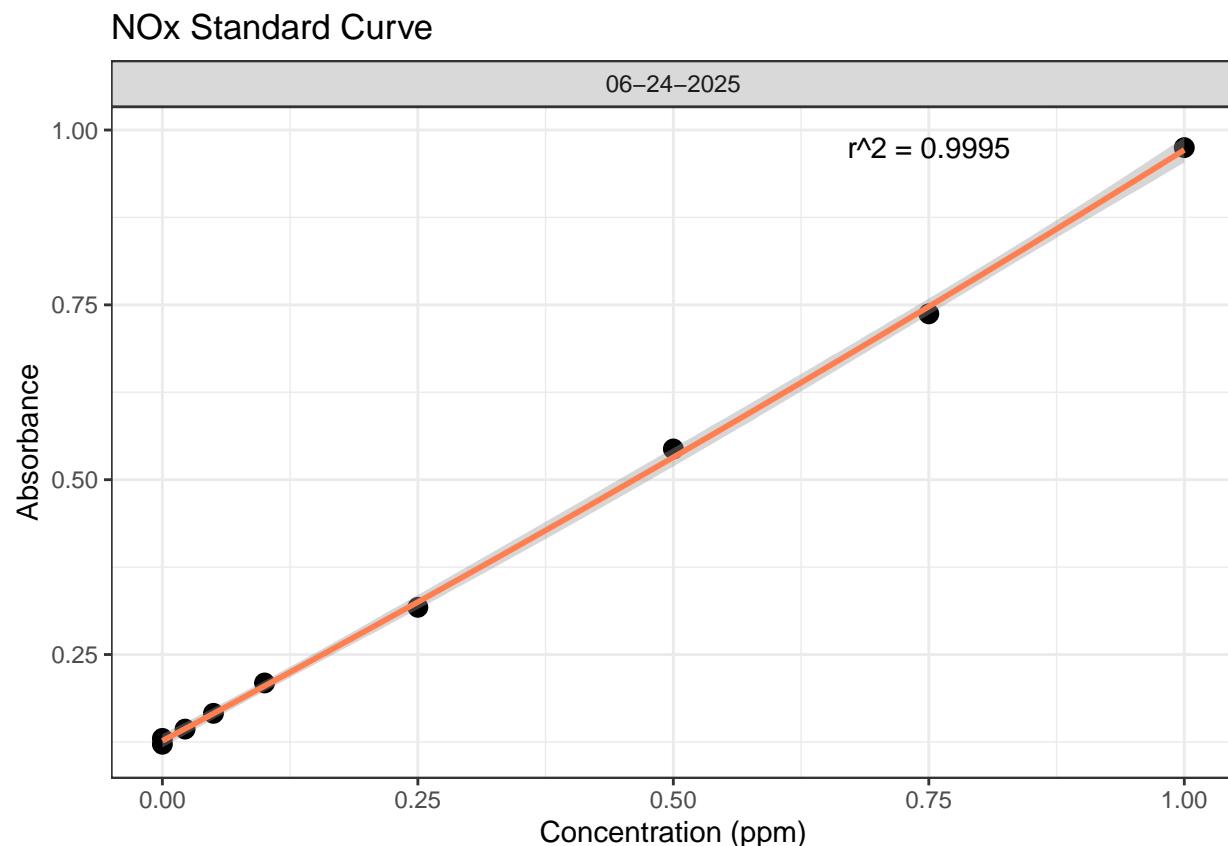
0.2 Assessing standard Curves

```
#Pull out standards data
```

```
## Assess Standard Curves
```

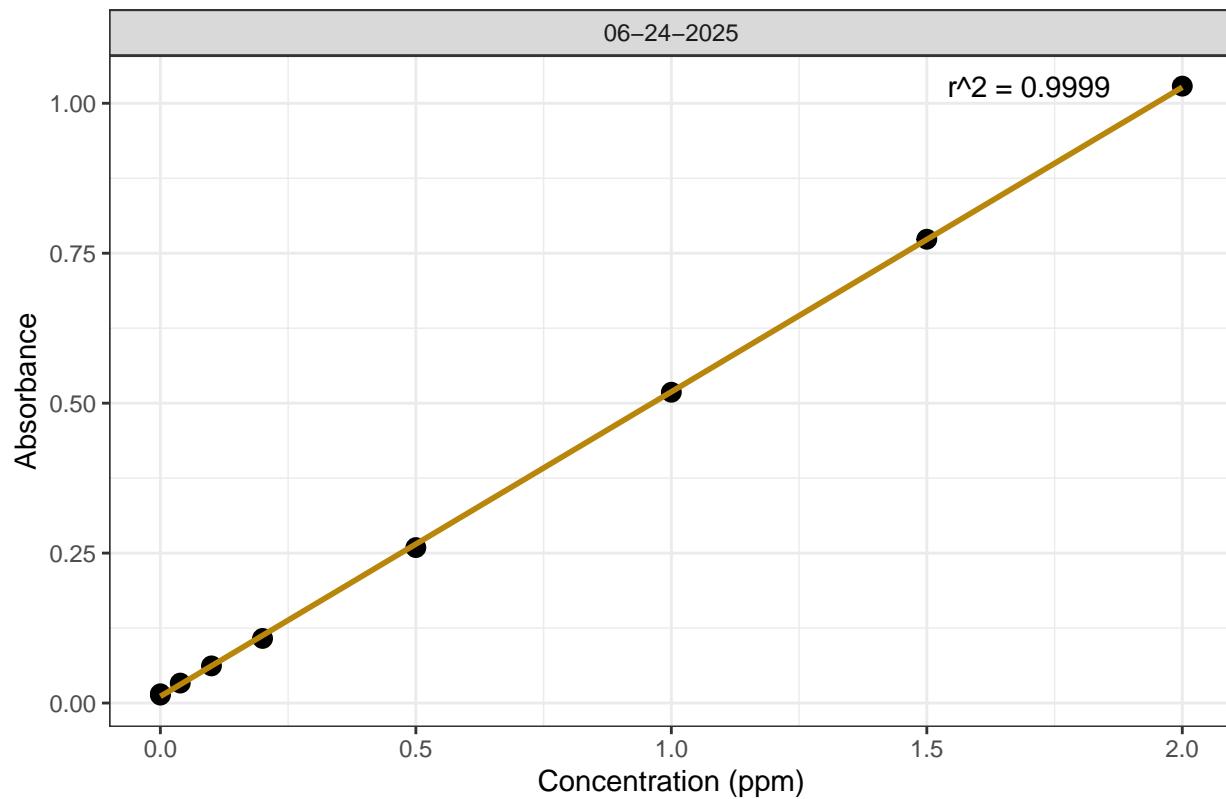
```
#Plot standards data
```

```
## Assess Standard Curves
```



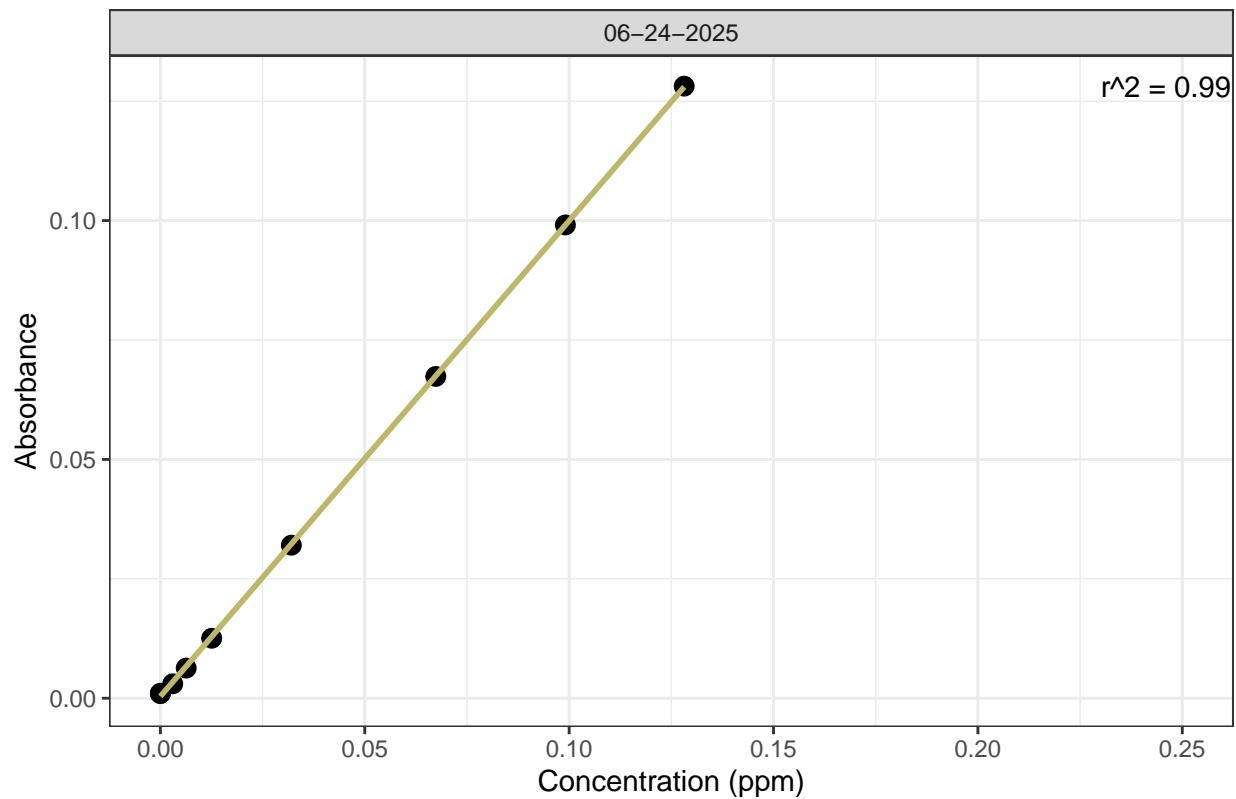
```
## 'geom_smooth()' using formula = 'y ~ x'
```

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."
```

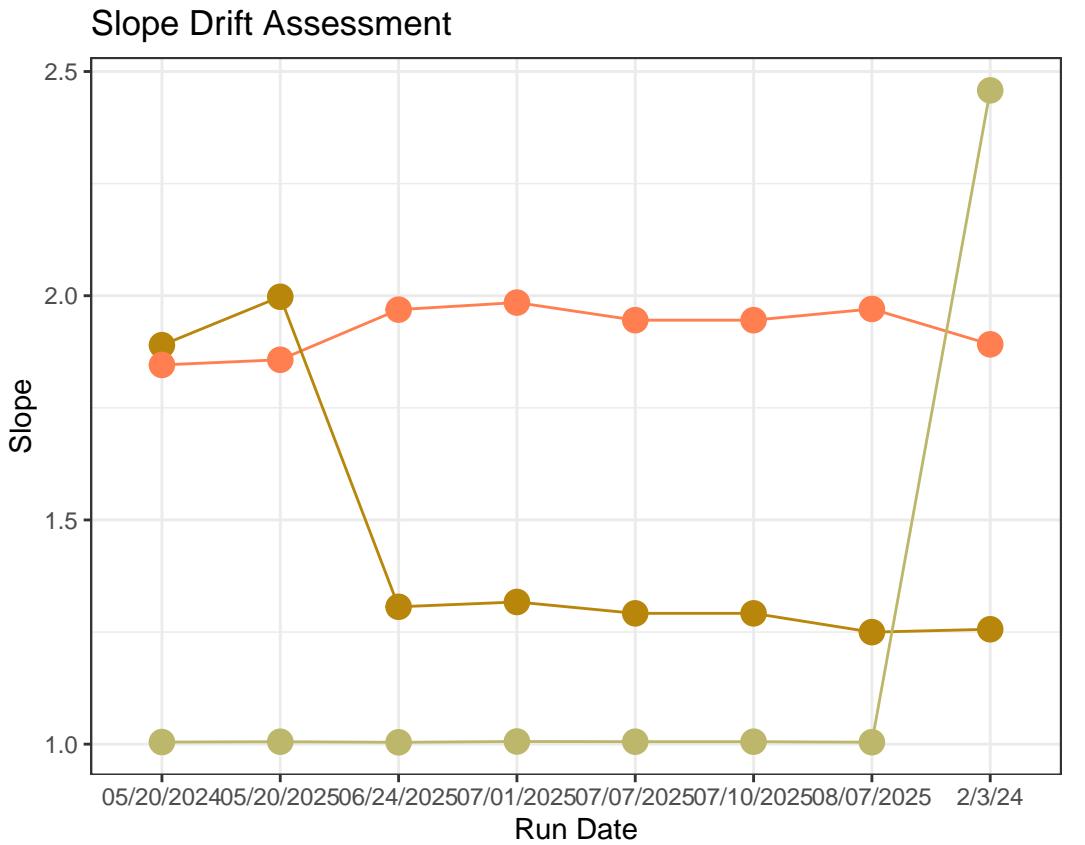


Table 1: Average Slope by Analyte

Test	avg_slope
NH3	1.926
NOx	1.450
PO4	1.187

0.3 Dilution Corrections - ensure the latest dilution is kept

```
## Dilution Corrections

## Duplicated samples: SWH_202408_TR_LysB_45cm, SWH_202408_TR_LysC_20cm, SWH_202408_TR_LysC_45, SWH_202408_TR_LysC_45

##  
## 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 = 1.619593

## Expected = 1.51

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

## Run mean = 1.157761

## Expected = 1.034

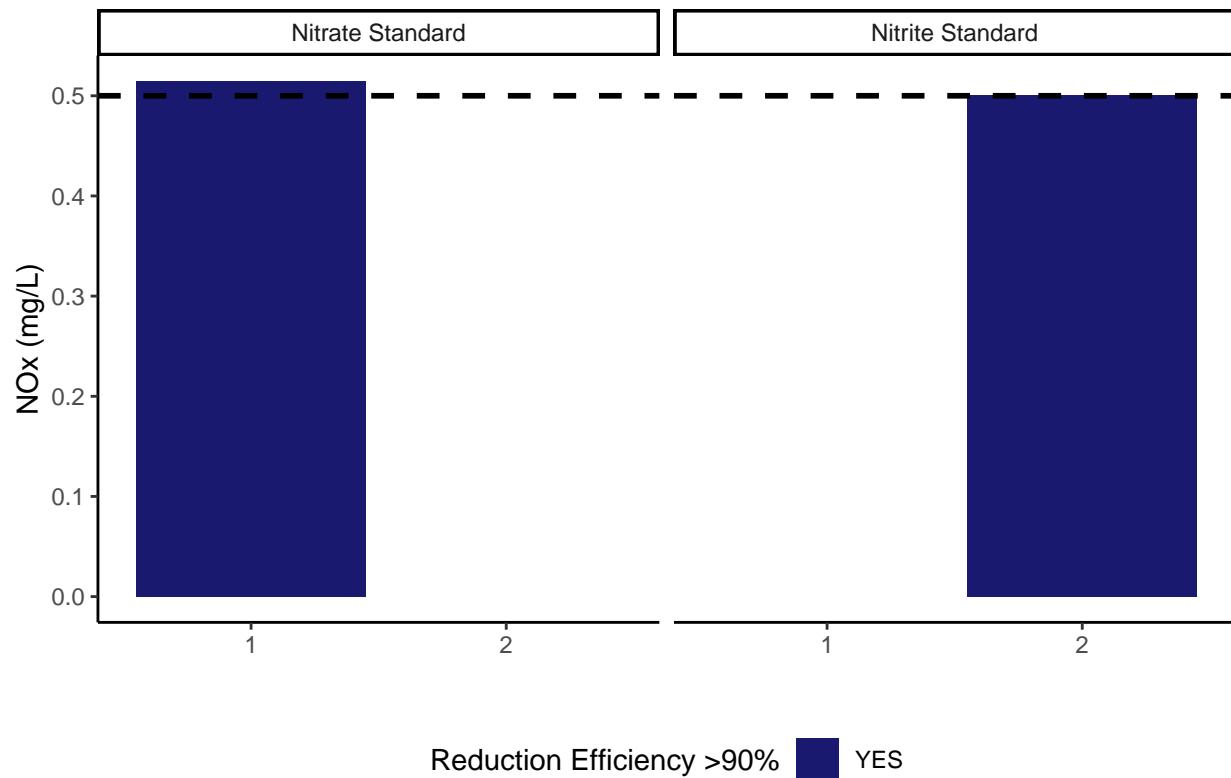
## [1] "PO4 pe Check has a % Difference >25% - REASSESS"

## Run mean = 0.27313

## Expected = 0.824

##Check NOx Reduction Efficiency

## Assess Reduction Efficiency
```



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

```
## [1] 101.5204
```

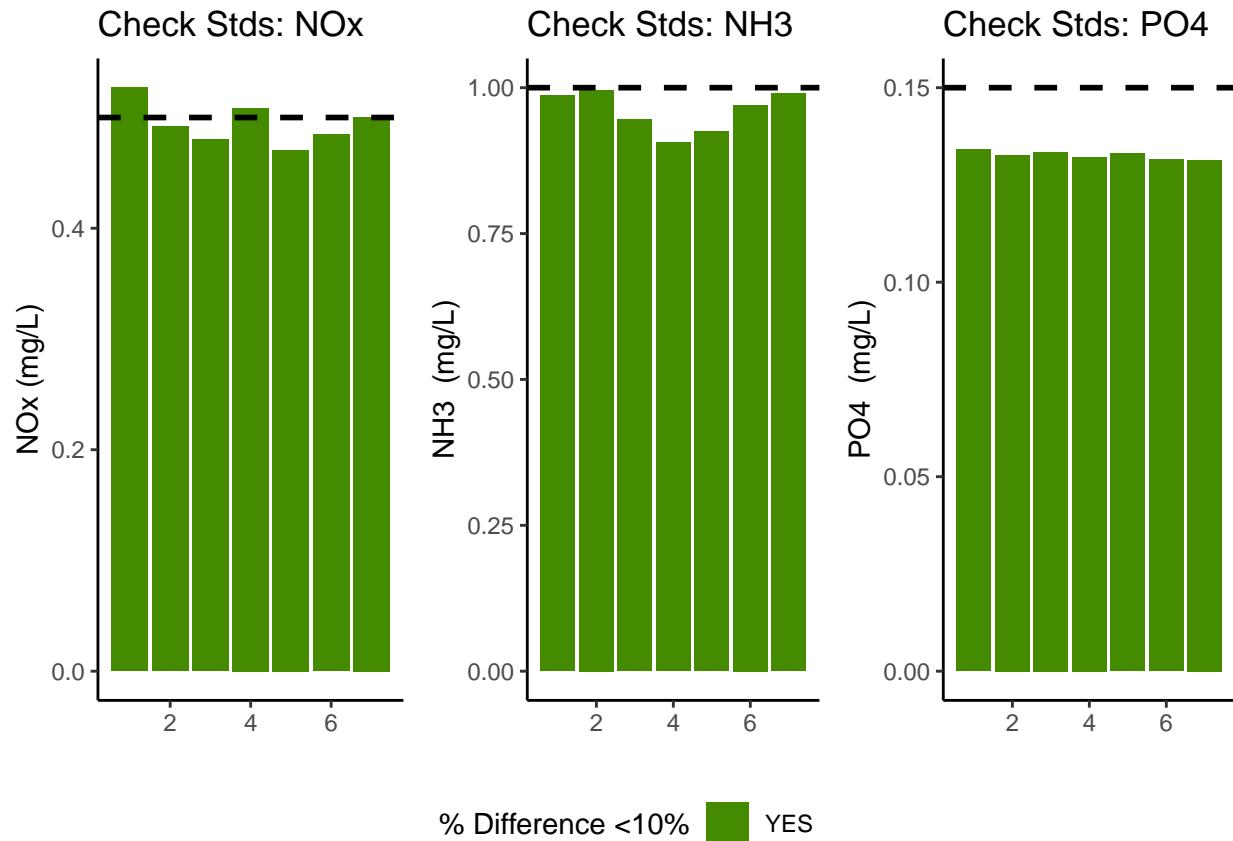
0.5 Analyze the Check Standards

```
## Analyze Check Standards

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

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

## [1] "PO4 Check Standard RSD 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"
```

0.6 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"
```

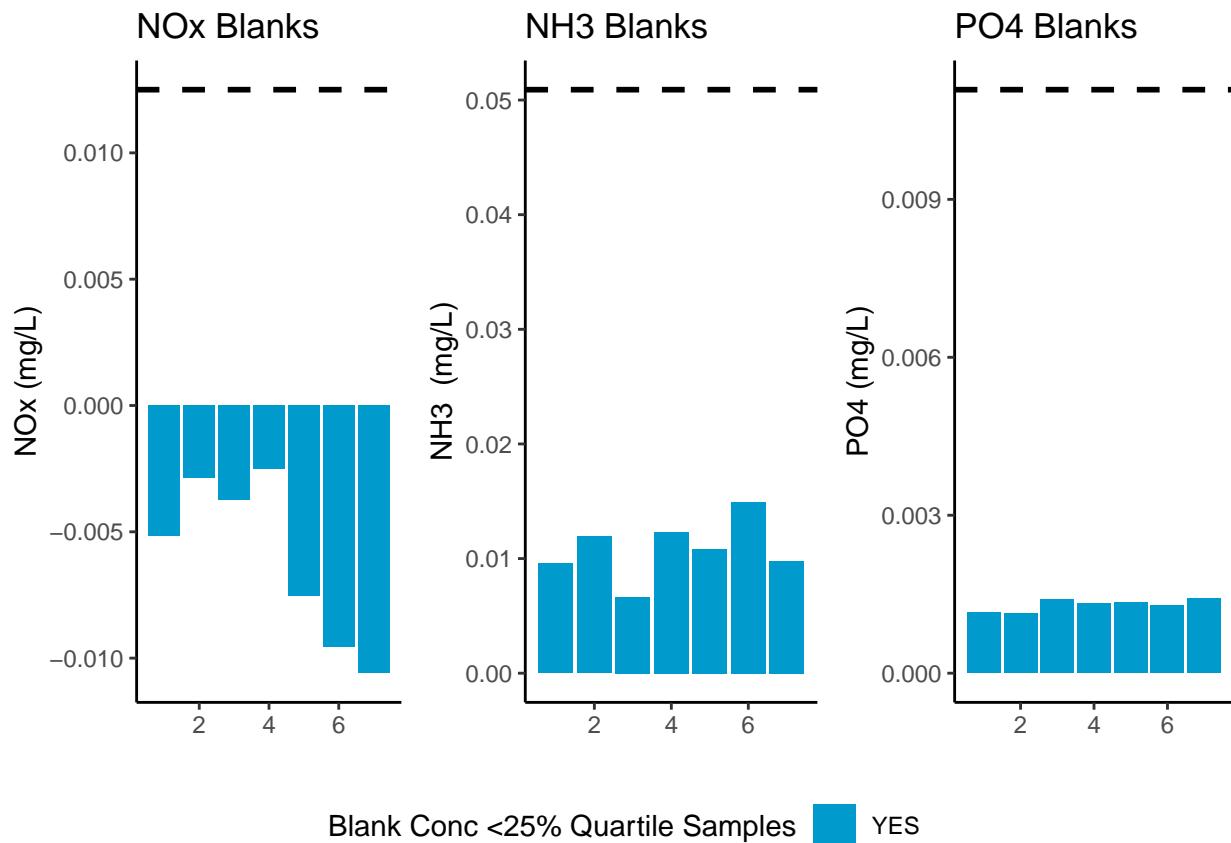


Table 2: Mean Concentration of Blanks

Test	Blank_Mean_Conc
NOx	-0.0060
NH3	0.0109
PO4	0.0013

0.7 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.

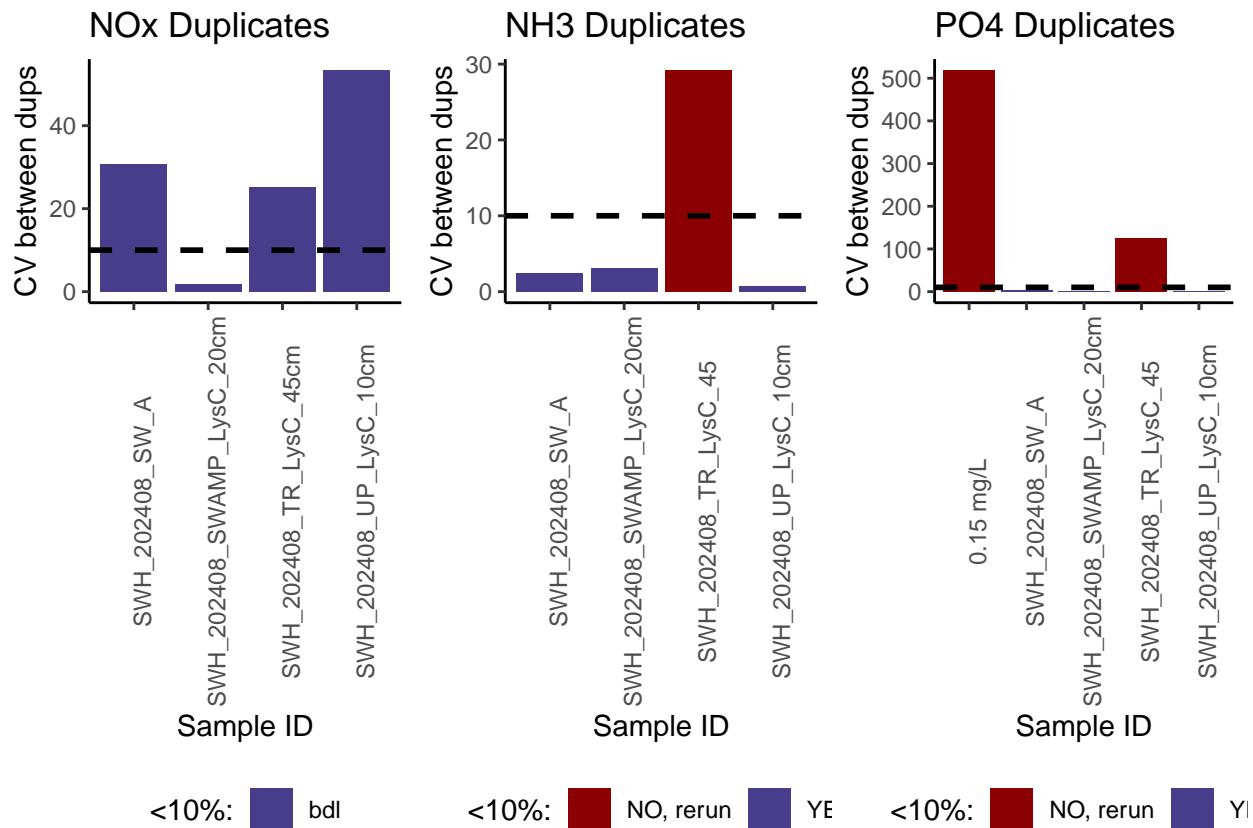
## [1] ">60% of NOx Duplicates have a CV <10% - PROCEED"

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

## [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.

```

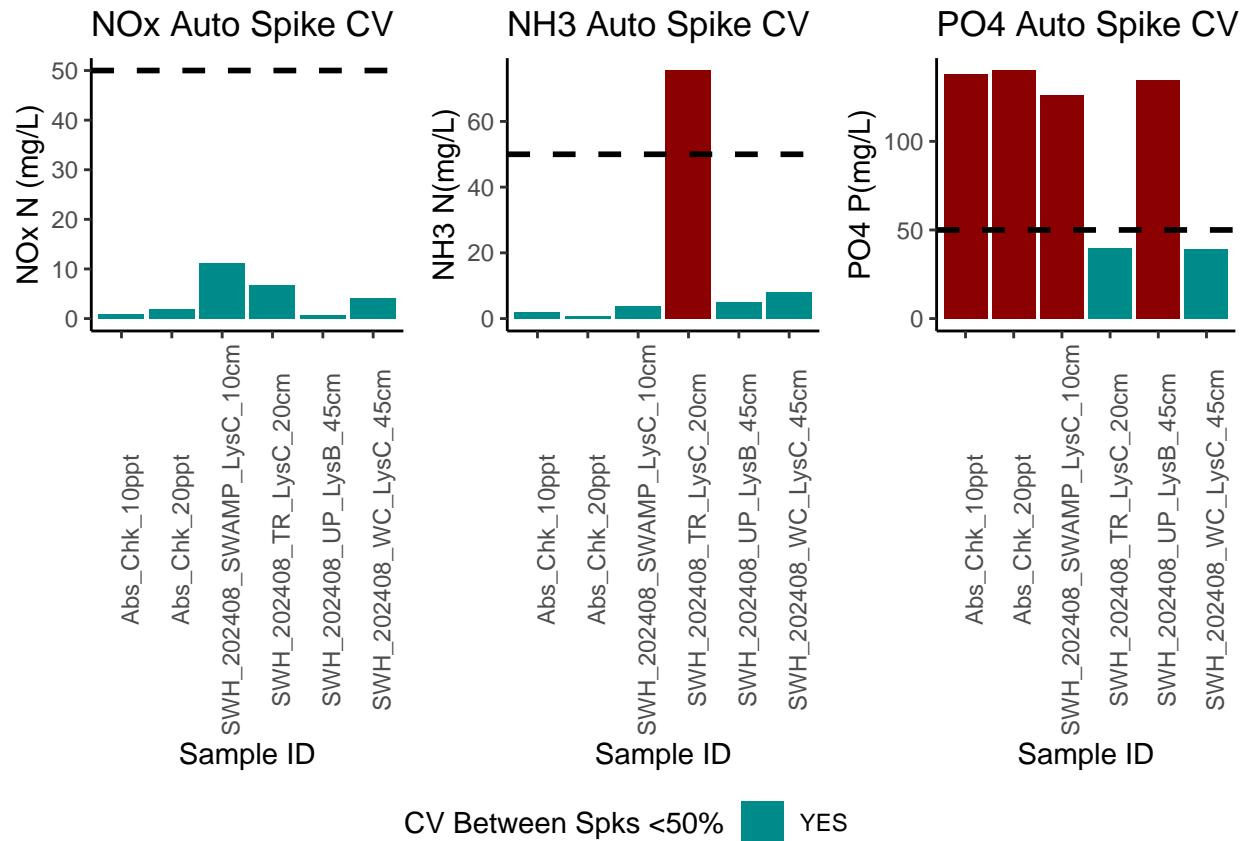


0.8 Spikes

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

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

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



0.9 Matrix Effects

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

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

## [1] ">20% CV in ASW P04 matrix effect checks - REASSESS"
```

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

## Warning: Expected 5 pieces. Missing pieces filled with 'NA' in 9 rows [37, 38, 39, 73,
## 74, 75, 106, 107, 108].
```

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

```
## Check Sample IDs with Metadata

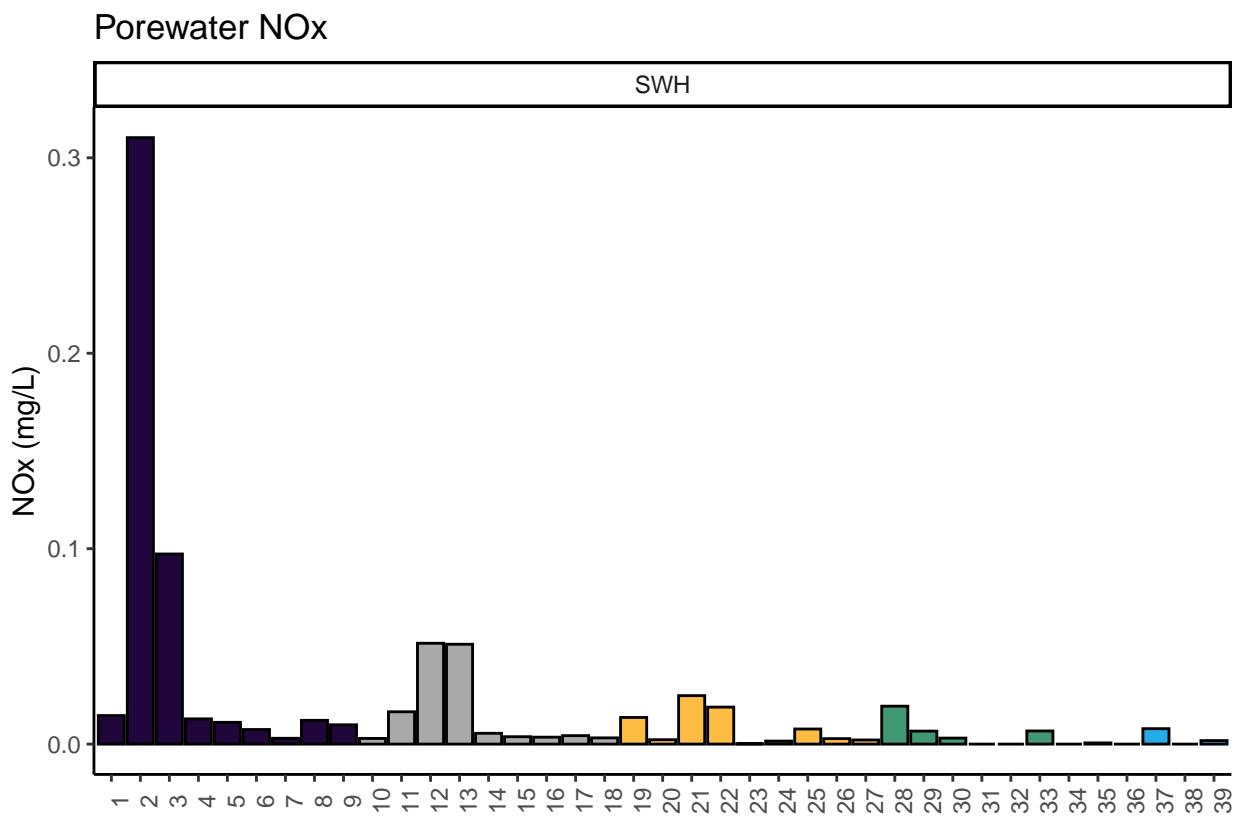
## Some sample IDs are missing from metadata.

## [1] "SWH_202408_SWAMP_LycC_45cm" "SWH_202408_TR_LysC_45"

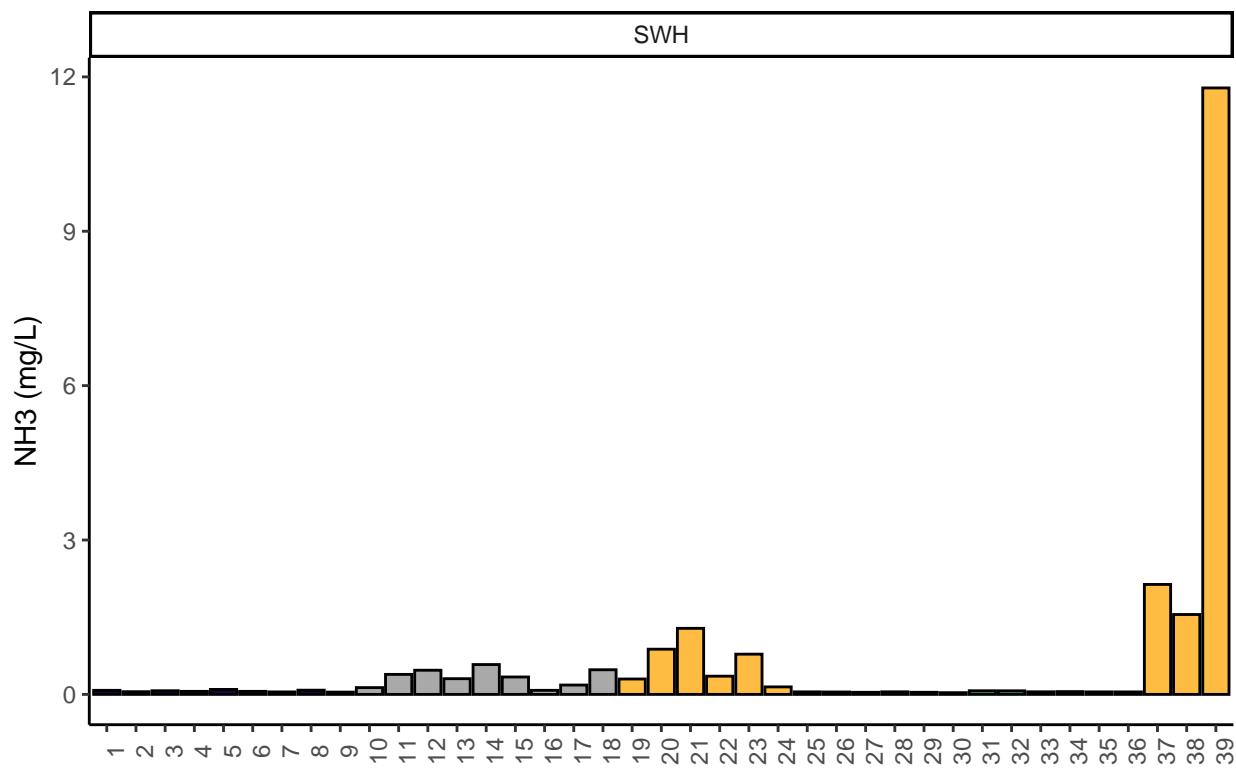
## Warning: Expected 5 pieces. Missing pieces filled with 'NA' in 9 rows [37, 38, 39, 73,
## 74, 75, 106, 107, 108].
```

0.14 Visualize Data

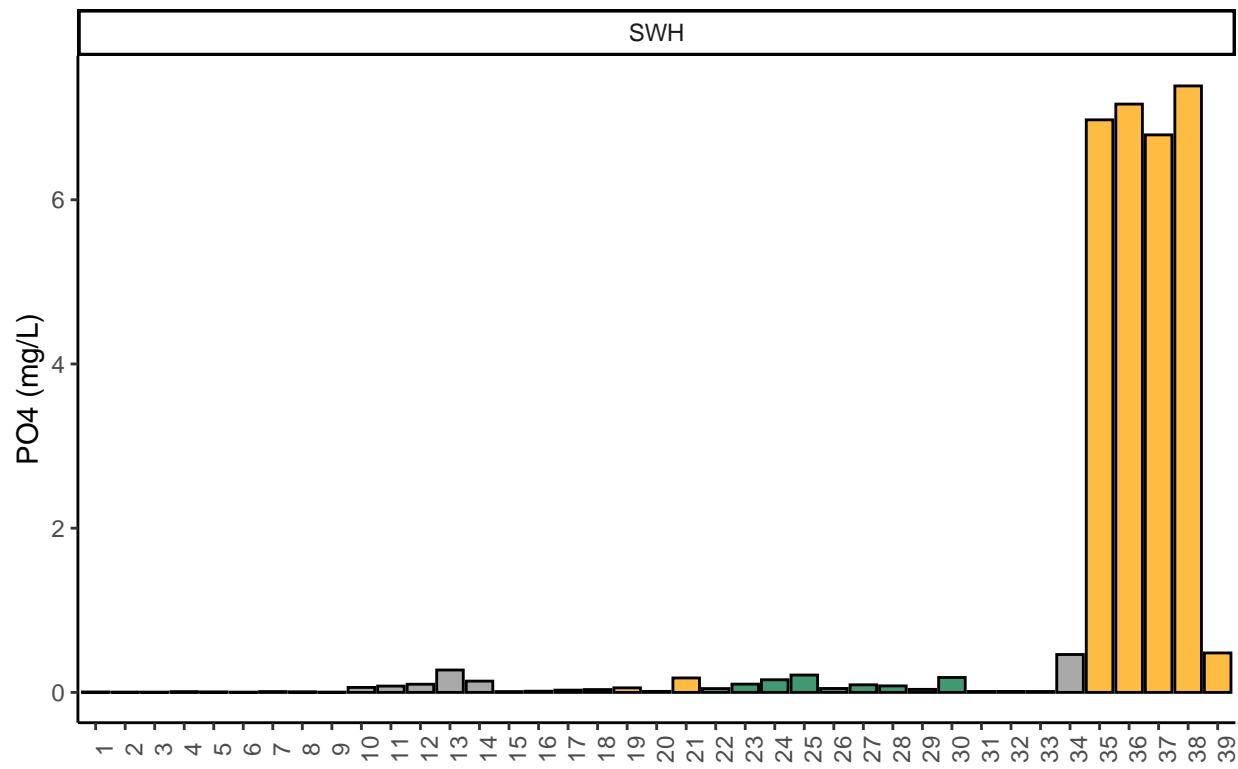
```
## Visualize Data
```



Porewater NH₃



Porewater PO4



0.15 Export Processed Data

```
#end
```