

PROJECT: Porewater Nutrients

Month YEAR Samples

2026-02-25

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0.1 Run Information

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

## Run Information: NAME

#set the run date & user name
sample_year <- "2024"
user <- "NAME"

#identify the files you want to read in
#read in as a list to accomodate ultiple runs in a month
NH3_P04_files<- c("Raw Data/20260120_Tempest2024_NH3_P04_Run1.csv", "Raw Data/20260209_Tempest2024_NH4P04_Run1.csv")
NOx_files     <- c("Raw Data/20260209_Tempest2024_VNOx_Run1.csv", "Raw Data/20260213_Tempest2024_VNOx_Run1.csv")

# Define the file path for QAQC log file - NO Need to change just check year
file_path <- "Raw Data/SEAL_TEMPEST_QAQC_Log_2024.csv"
final_path <- "Processed Data/COMPASS_Synoptic_Nutrients_202407a.csv"

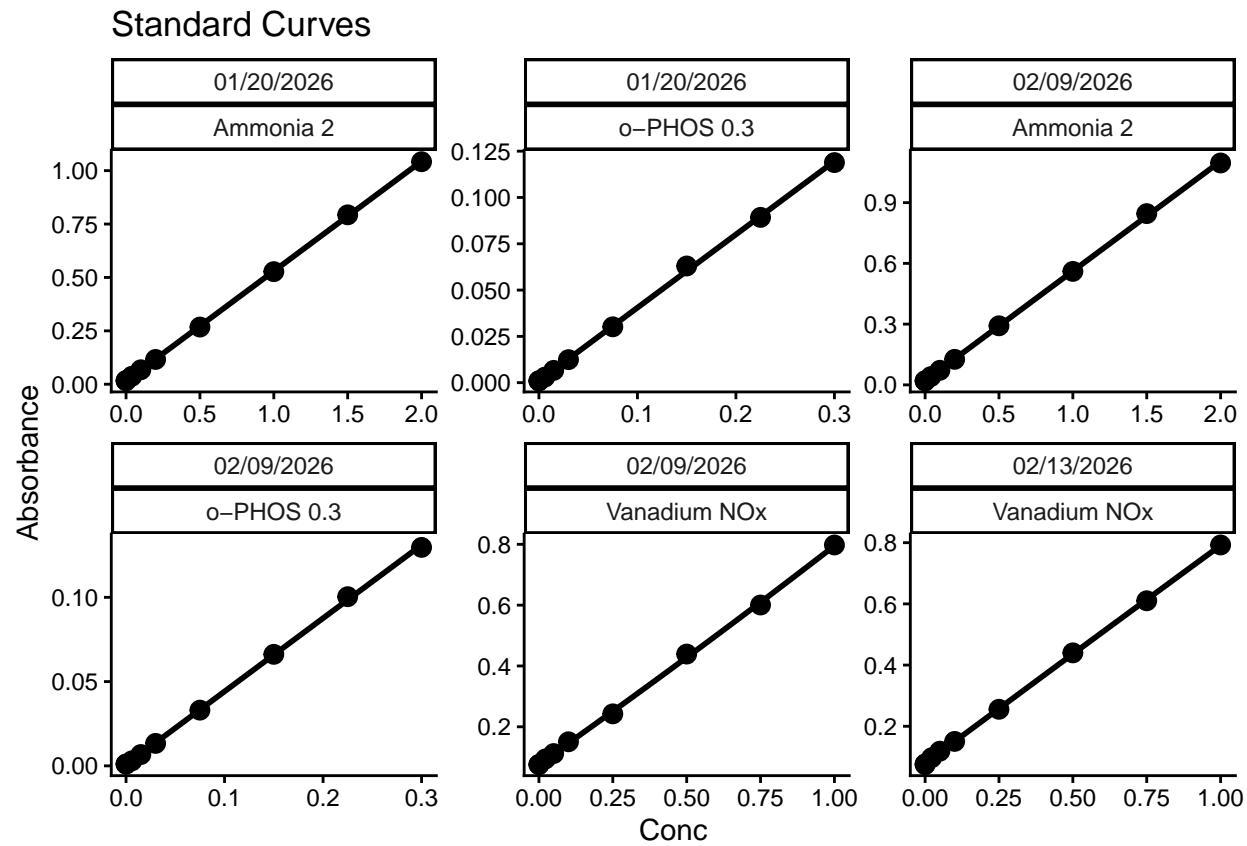
#record any notes about the run or anything other info here:
run_notes <- ""

#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)

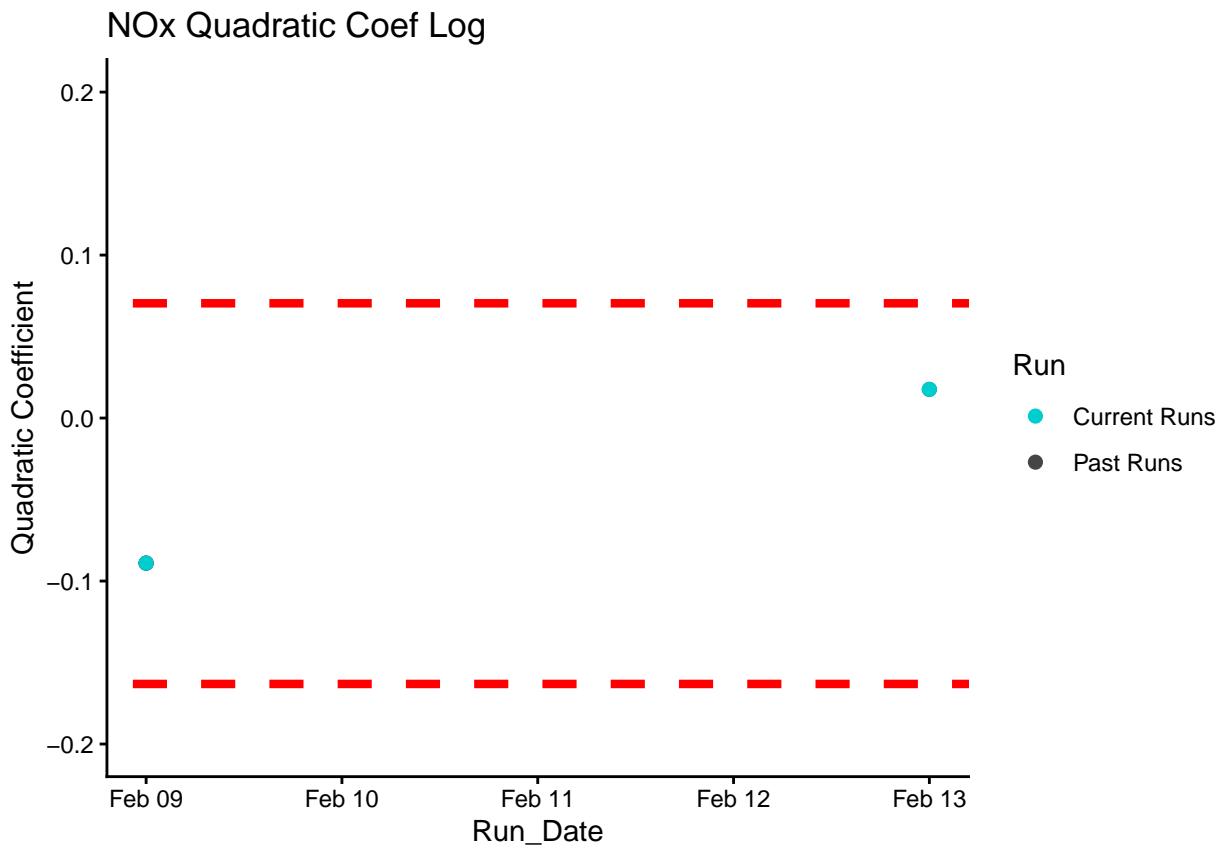
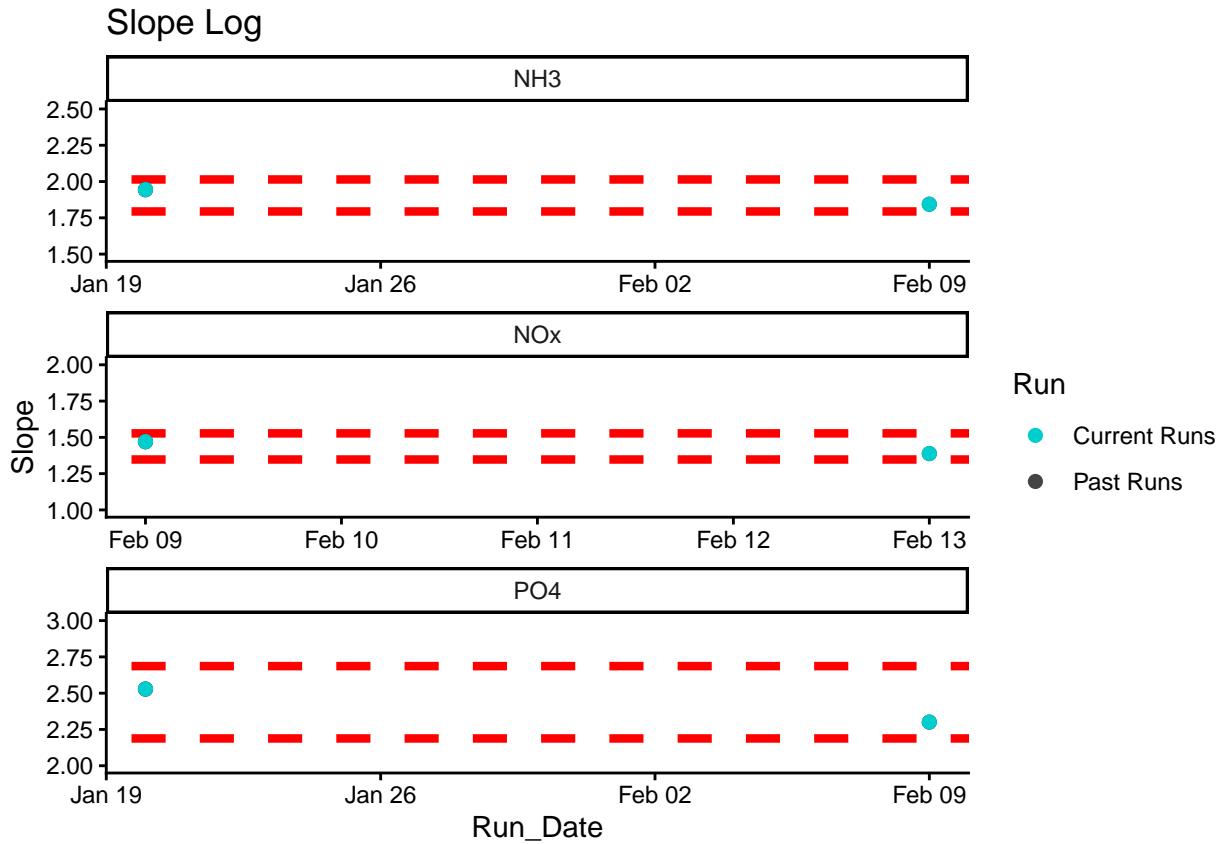
##Setup
##Pull in active porewater tracking inventory sheet from Google Drive:
##Create similar sample IDs to match with run samples
##Import Data & Clean
```

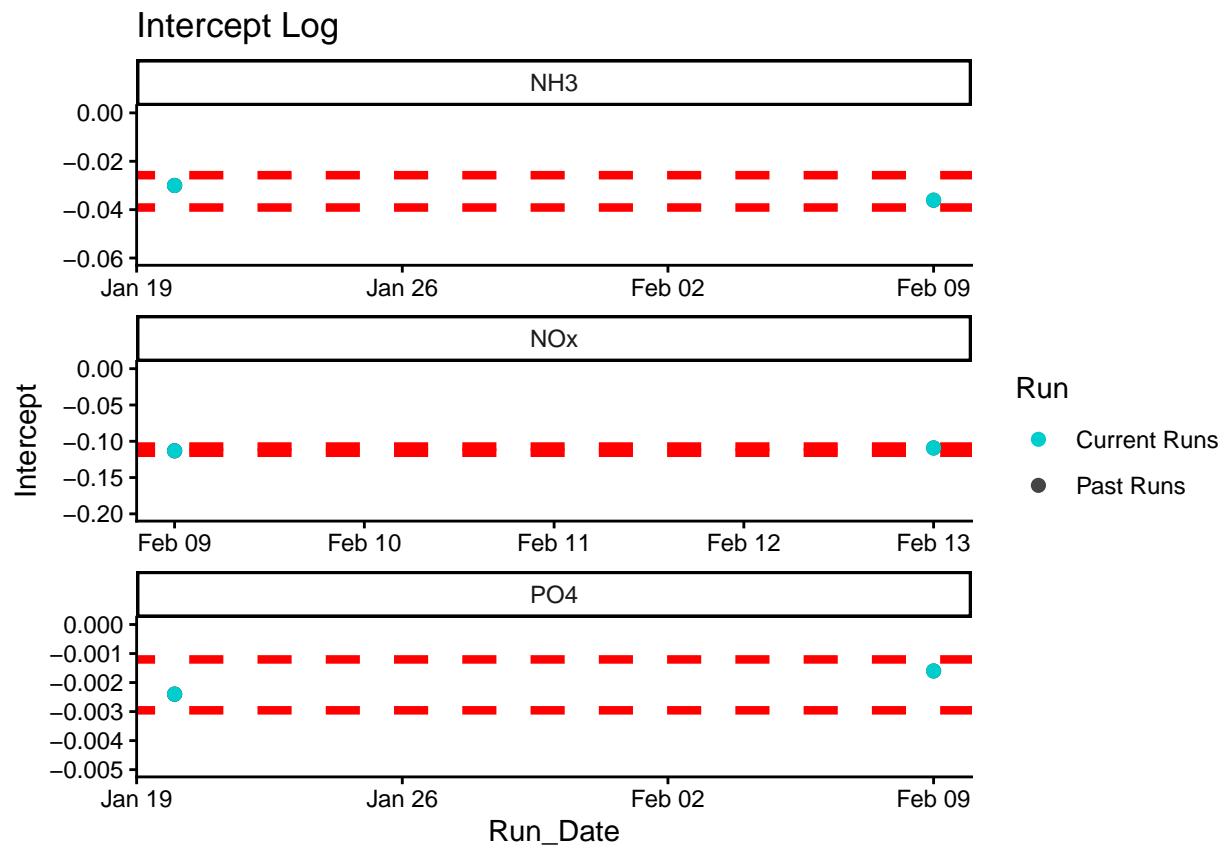
0.2 Assessing standard Curves



Test	Run_Date	R2_Flag	R2
Ammonia 2	01/20/2026	R2_Pass	0.9999133
o-PHOS 0.3	01/20/2026	R2_Pass	0.9993311
Ammonia 2	02/09/2026	R2_Pass	0.9997854
Vanadium NOx	02/09/2026	R2_Pass	0.9992713
o-PHOS 0.3	02/09/2026	R2_Pass	0.9995925
Vanadium NOx	02/13/2026	R2_Pass	0.9998115

0.3 Update Standard Log





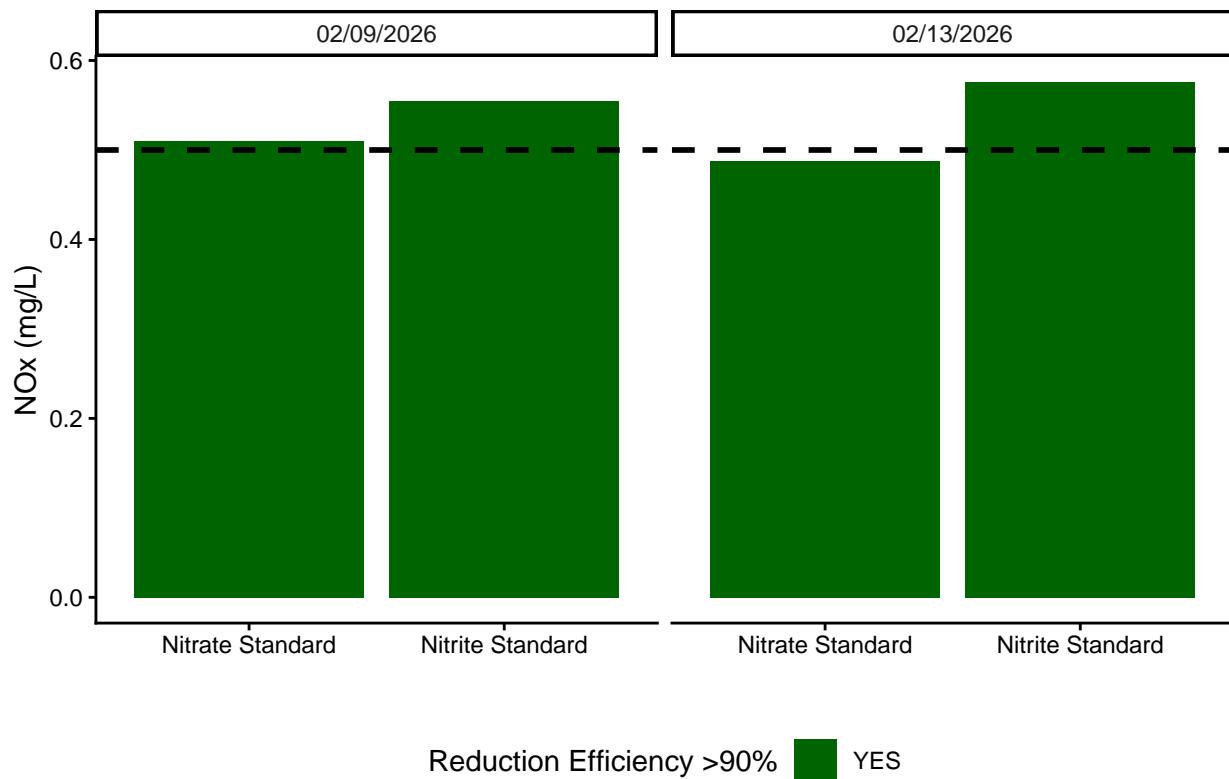
0.4 Dilution Corrections - ensure the latest dilution is kept

```
## [1] "Reran Samples: TMP_SW_C3_T6_20240614"  
  
## [1] "Diluted Samples: TMP_SW_C3_T6_20240614"  
  
## [1] "No Naming Issues Detected"
```

0.5 Performance Check

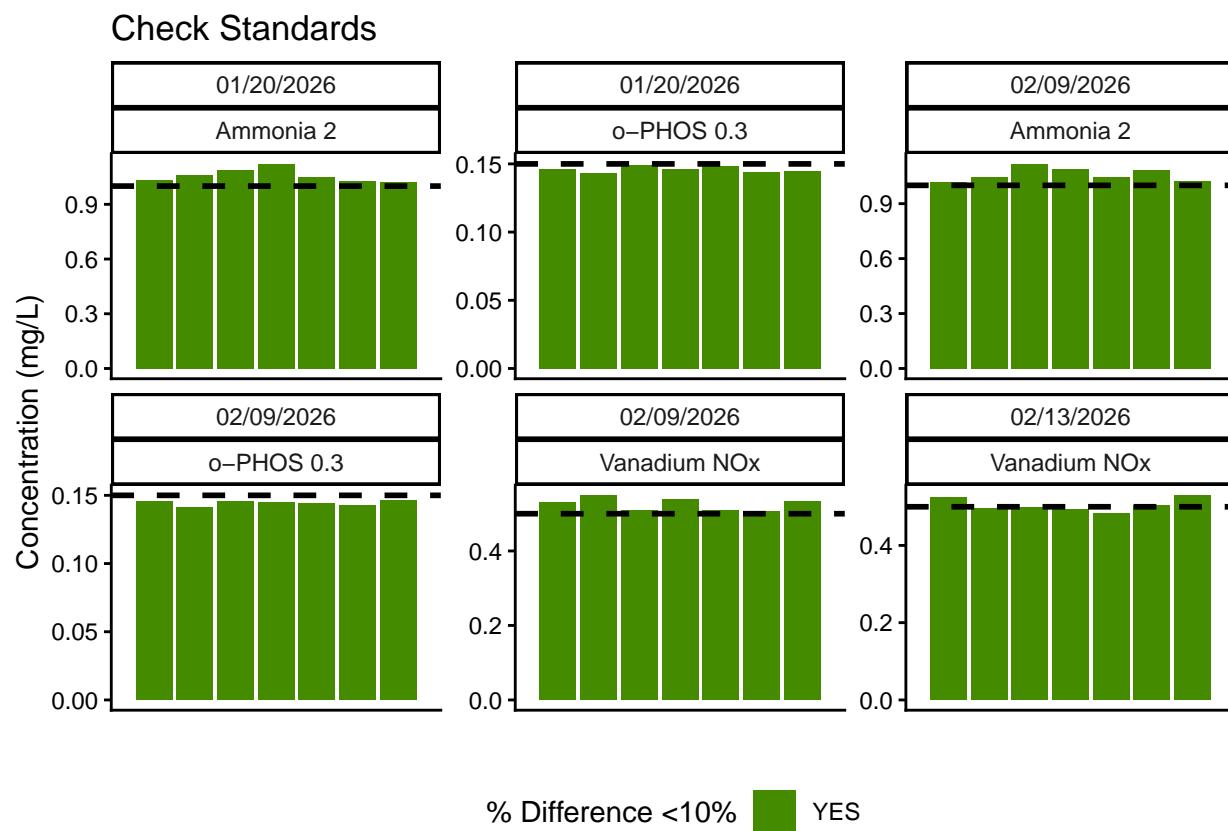
Test	Run_Date	PE_Flag	PE_Conc	PE_Target_Conc
o-PHOS 0.3	01/20/2026	Performance Check Within 25% - PROCEED	0.8646825	0.824
o-PHOS 0.3	02/09/2026	Performance Check Within 25% - PROCEED	0.8405030	0.824
Vanadium NOx	02/09/2026	Performance Check Within 25% - PROCEED	1.7939875	1.510
Vanadium NOx	02/13/2026	Performance Check Within 25% - PROCEED	1.6281090	1.510
Ammonia 2	01/20/2026	Performance Check Within 25% - PROCEED	1.1758200	1.034
Ammonia 2	02/09/2026	Performance Check Within 25% - PROCEED	1.1436275	1.034

0.6 Check NOx Reduction Efficiency



0.7 Analyze the Check Standards

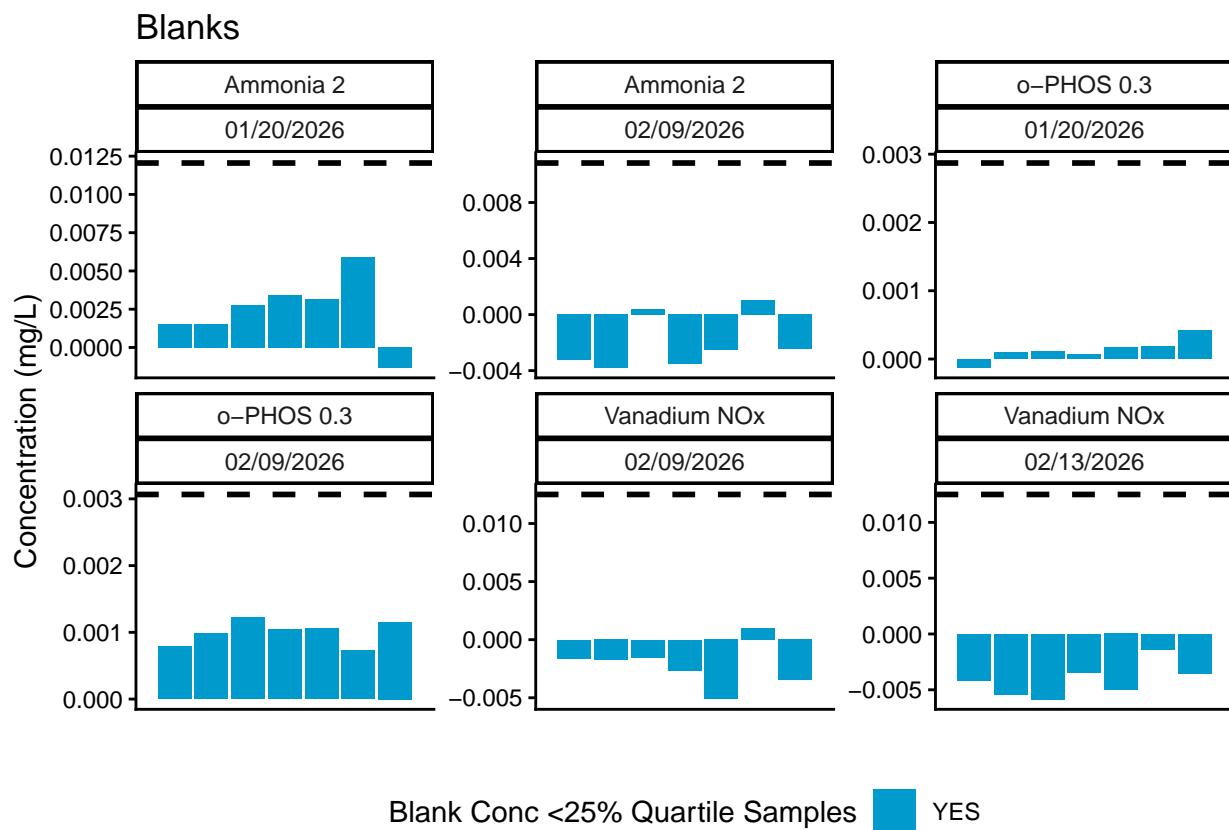
Test	Run_Date	RSV_Flag	RSV	RSV_Cutoff
Vanadium NOx	02/09/2026	RSV WITHIN RANGE - PROCEED	0.0382322	0.25
Vanadium NOx	02/13/2026	RSV WITHIN RANGE - PROCEED	0.0382322	0.25
Ammonia 2	01/20/2026	RSV WITHIN RANGE - PROCEED	0.0329643	0.25
o-PHOS 0.3	01/20/2026	RSV WITHIN RANGE - PROCEED	0.0144344	0.25
Ammonia 2	02/09/2026	RSV WITHIN RANGE - PROCEED	0.0329643	0.25
o-PHOS 0.3	02/09/2026	RSV WITHIN RANGE - PROCEED	0.0144344	0.25



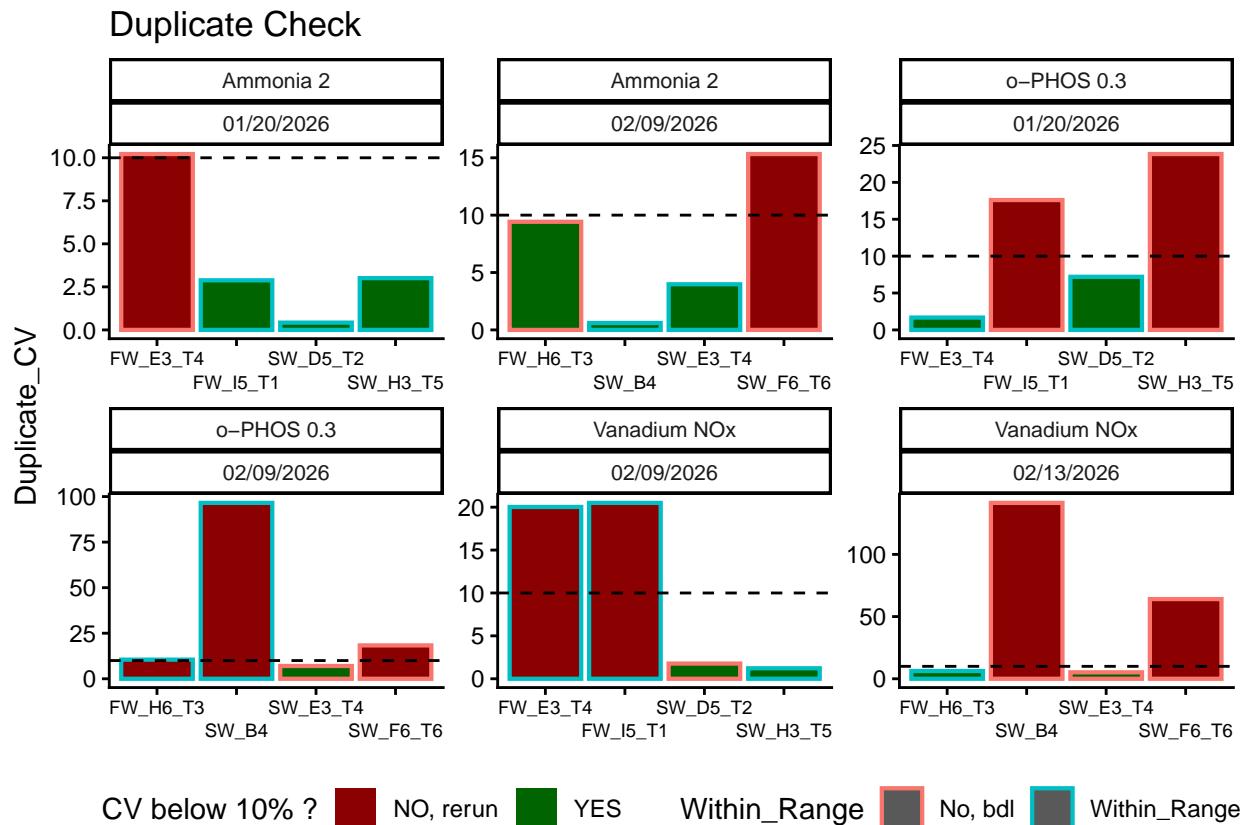
Test	Run_Date	CHK_Flag
Vanadium NOx	02/09/2026	>60% of Checks Pass - PROCEED
Vanadium NOx	02/13/2026	>60% of Checks Pass - PROCEED
Ammonia 2	01/20/2026	>60% of Checks Pass - PROCEED
o-PHOS 0.3	01/20/2026	>60% of Checks Pass - PROCEED
Ammonia 2	02/09/2026	>60% of Checks Pass - PROCEED
o-PHOS 0.3	02/09/2026	>60% of Checks Pass - PROCEED

0.8 Analyze Blanks

Test	Run_Date	BLK_Pct_Flag	Mean_Blk_Conc	Quantile_25
Vanadium NOx	02/09/2026	>60% of Blanks Pass - PROCEED	-0.0021684	0.0125000
Vanadium NOx	02/13/2026	>60% of Blanks Pass - PROCEED	-0.0041230	0.0125000
Ammonia 2	01/20/2026	>60% of Blanks Pass - PROCEED	0.0024320	0.0120530
o-PHOS 0.3	01/20/2026	>60% of Blanks Pass - PROCEED	0.0001294	0.0028710
Ammonia 2	02/09/2026	>60% of Blanks Pass - PROCEED	-0.0020141	0.0108195
o-PHOS 0.3	02/09/2026	>60% of Blanks Pass - PROCEED	0.0009981	0.0030657



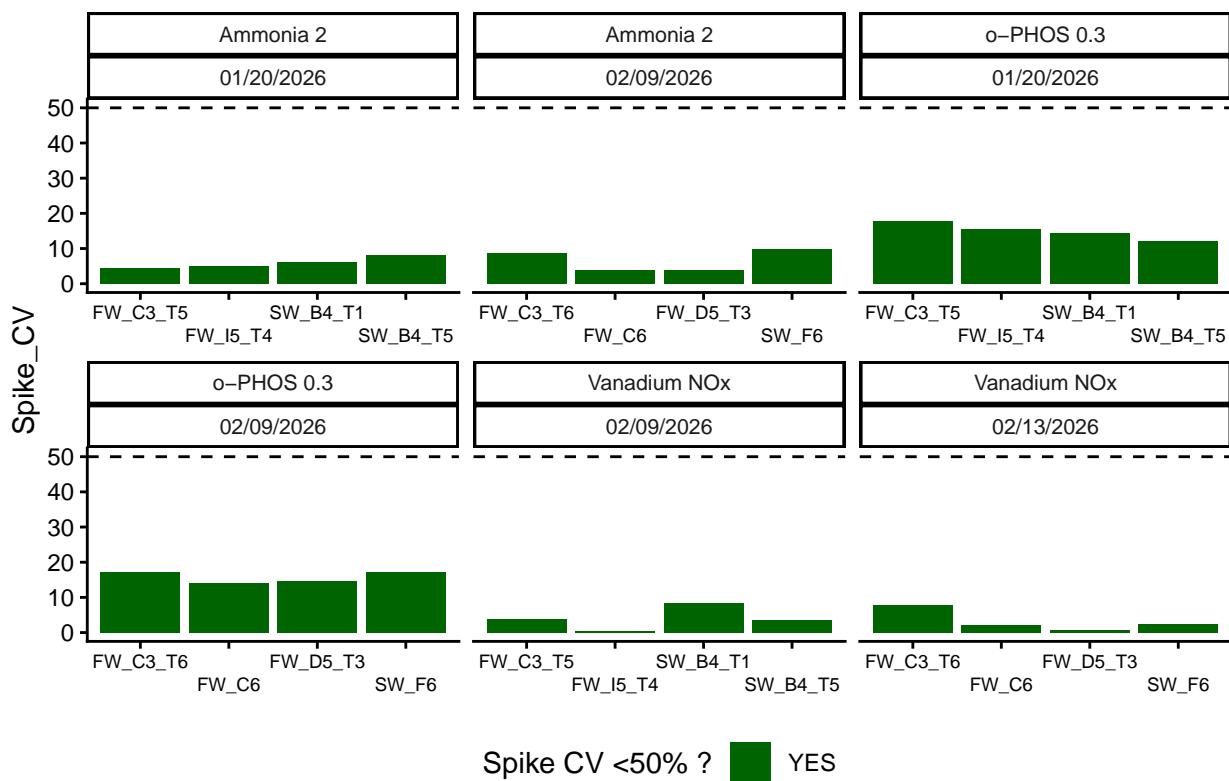
0.9 Analyze Duplicates



Test	Run_Date	Dup_Flags
Vanadium NOx	02/09/2026	<60% of Dups Pass - REASSESS
Vanadium NOx	02/13/2026	<60% of Dups Pass - REASSESS
Ammonia 2	01/20/2026	>60% of Dups Pass - PROCEED
o-PHOS 0.3	01/20/2026	<60% of Dups Pass - REASSESS
Ammonia 2	02/09/2026	>60% of Dups Pass - PROCEED
o-PHOS 0.3	02/09/2026	<60% of Dups Pass - REASSESS

0.10 Spikes

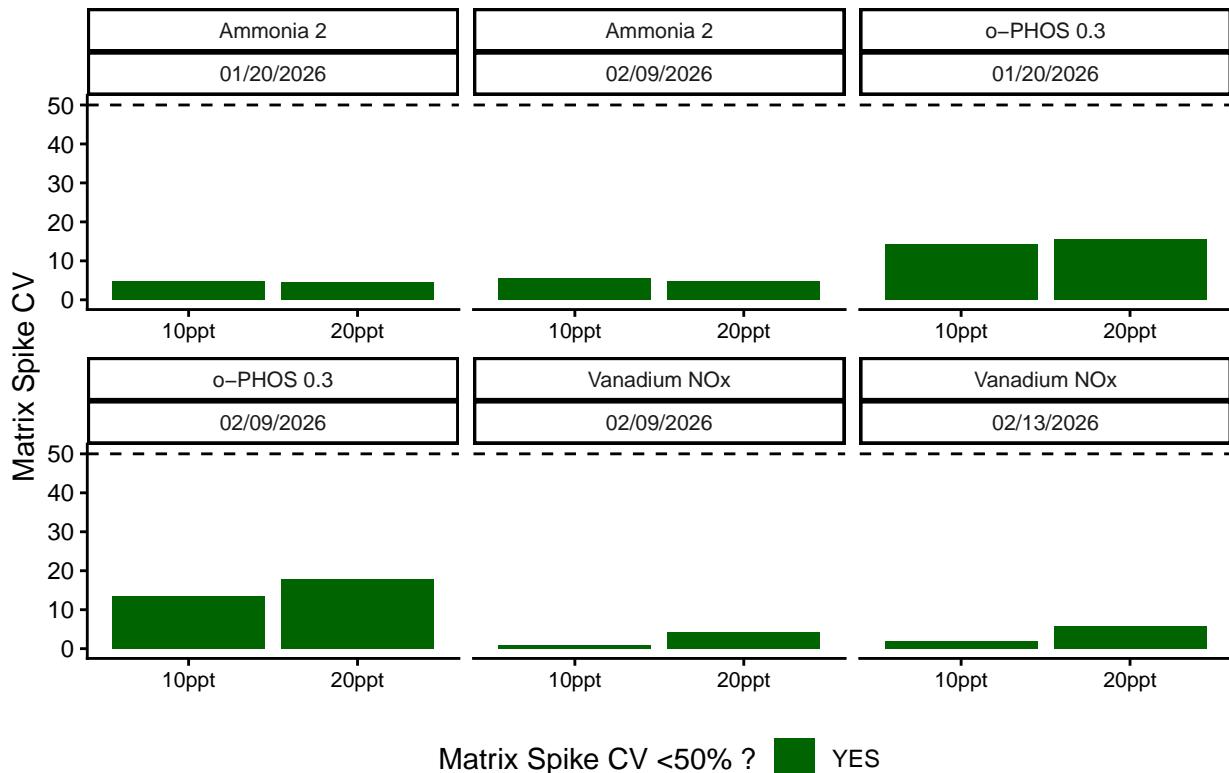
Spike Check



Test	Run_Date	Spike_Flags
Vanadium NOx	02/09/2026	>60% of Spikes have a CV <50% - PROCEED
Vanadium NOx	02/13/2026	>60% of Spikes have a CV <50% - PROCEED
Ammonia 2	01/20/2026	>60% of Spikes have a CV <50% - PROCEED
o-PHOS 0.3	01/20/2026	>60% of Spikes have a CV <50% - PROCEED
Ammonia 2	02/09/2026	>60% of Spikes have a CV <50% - PROCEED
o-PHOS 0.3	02/09/2026	>60% of Spikes have a CV <50% - PROCEED

0.11 Matrix Effects

Matrix Check



Test	Run_Date	Matrix_Flags
Vanadium NOx	02/09/2026	Matrix Has CV <50% - PROCEED
Vanadium NOx	02/13/2026	Matrix Has CV <50% - PROCEED
Ammonia 2	01/20/2026	Matrix Has CV <50% - PROCEED
o-PHOS 0.3	01/20/2026	Matrix Has CV <50% - PROCEED
Ammonia 2	02/09/2026	Matrix Has CV <50% - PROCEED
o-PHOS 0.3	02/09/2026	Matrix Has CV <50% - PROCEED

```
##Sample Flagging - Within range of standard curve
```

```
##Add QAQC Flags
```

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

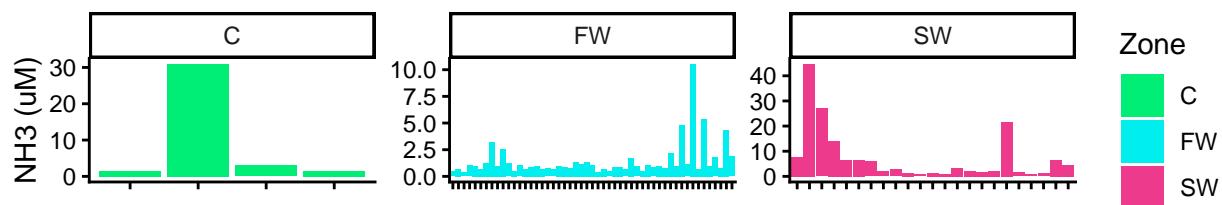
```
## All sample IDs are present in metadata.
```

```
## [1] "Sample_Name"   "Run_Number"    "Conc"          "Absorbance"    "Dilution"
## [6] "Unit"          "Test"          "Run_Time"      "Run_Date"      "Keep"
## [11] "Pair_ID"       "Conc_uM"       "Conc_flag"
```

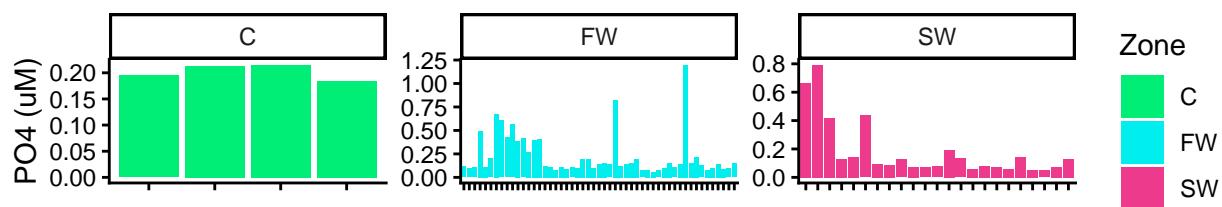
```
##Format Data
```

0.13 Visualize Data by Plot

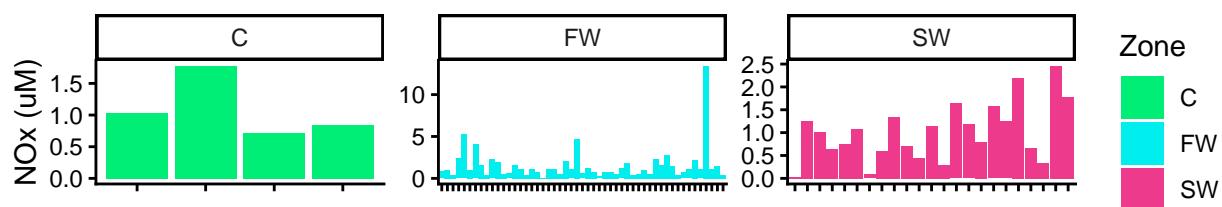
Samples: Ammonia



Samples: Phosphate



Samples: Nitrate/Nitrite



```
##Write Out Data  
#end
```