PROJECT: Porewater Nutrients

Month YEAR Samples

2026-02-25

Contents

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 accommadate ultiple runs in a month
NH3_PO4_files<- c("Raw Data/20260120_Tempest2024_NH3_PO4_Run1.csv", "Raw Data/20260209_Tempest2024_NH4P
  NOx_files    <- c("Raw Data/20260209_Tempest2024_VNOx_Run1.csv","Raw Data/20260213_Tempest2024_VNOx_R

# 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)
```

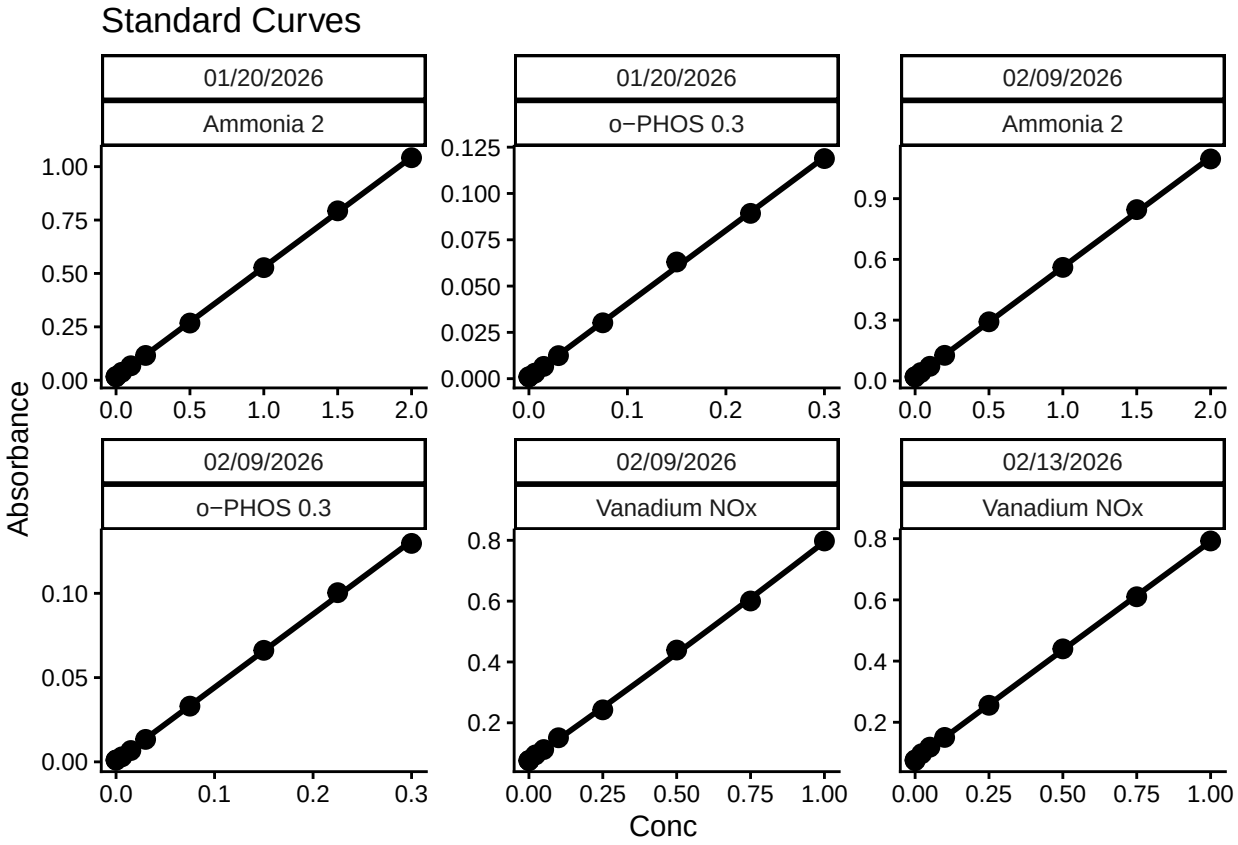
##Setup

##Pull in active porewater tracking inventory sheet from Google Drive:

##Create similar sample IDs to match with run samples

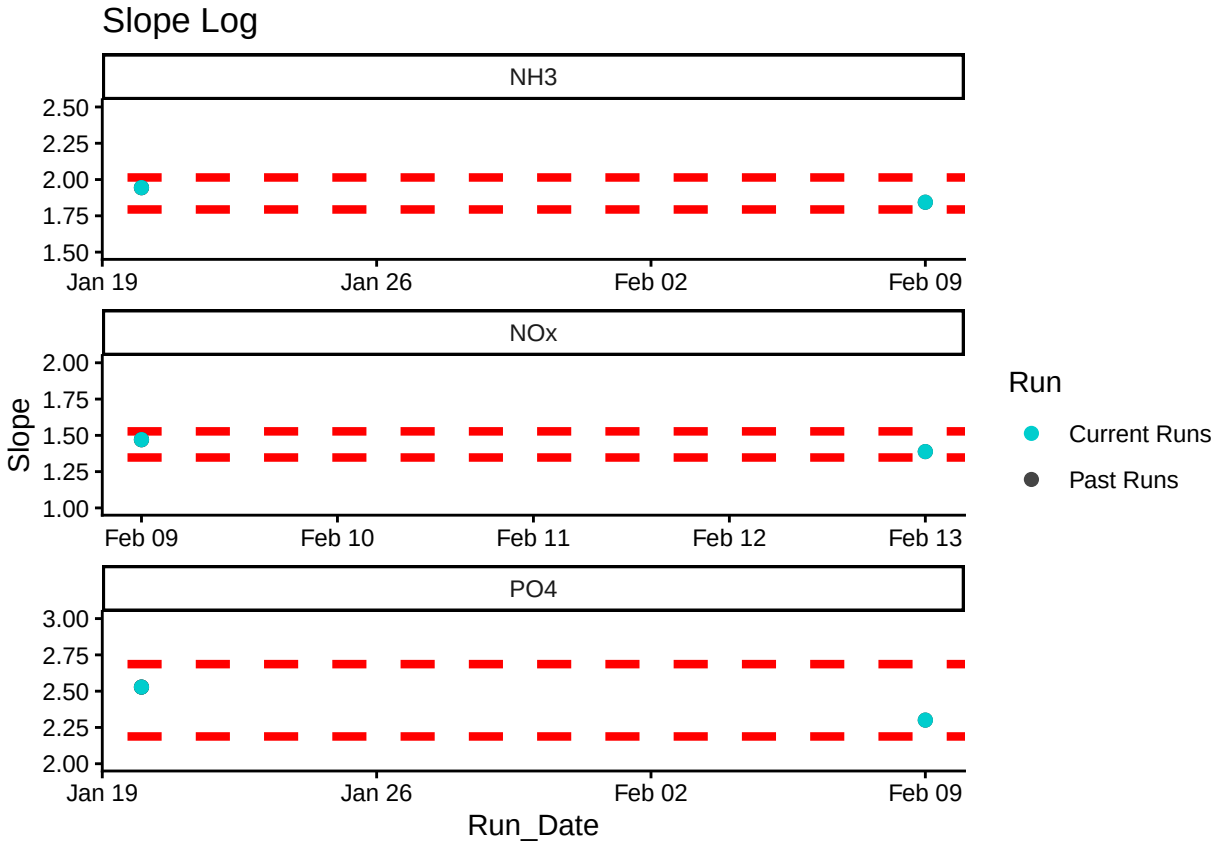
##Import Data & Clean

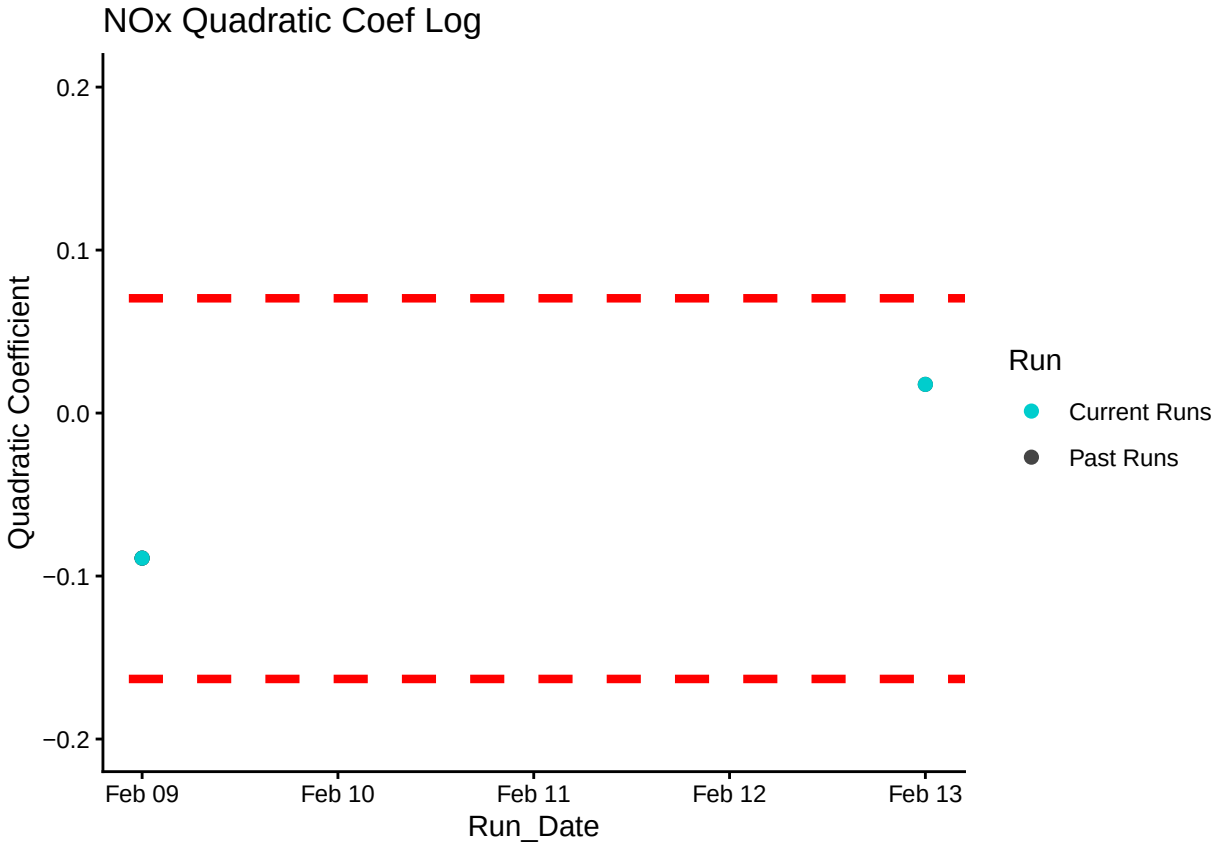
0.2 Assessing standard Curves

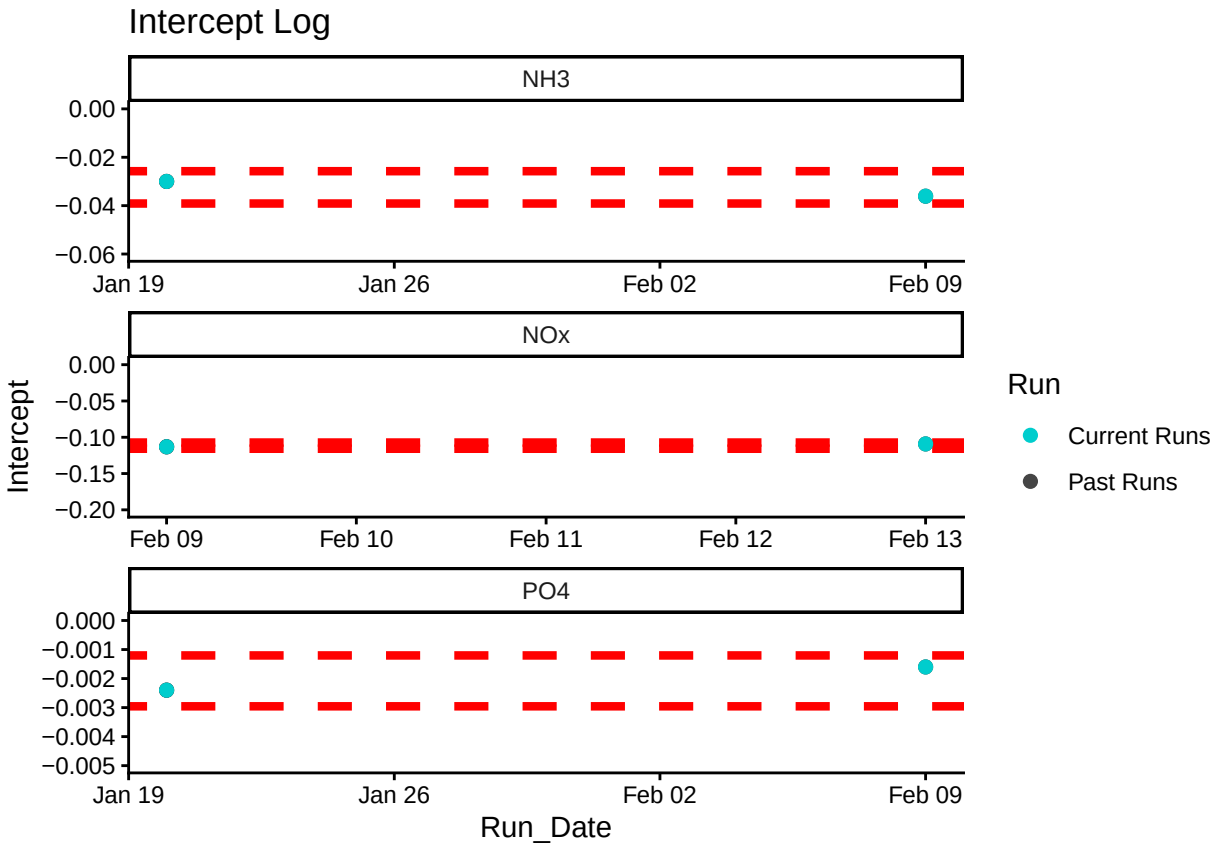


Test	Run_Date	R2_Flag	R2
Ammonia 2	01/20/2026	R2_Pass	0.9999133
o-PHOS 0.3	01/20/2026	R2_Pass	0.9993311
Ammonia 2	02/09/2026	R2_Pass	0.9997854
Vanadium NOx	02/09/2026	R2_Pass	0.9992713
o-PHOS 0.3	02/09/2026	R2_Pass	0.9995925
Vanadium NOx	02/13/2026	R2_Pass	0.9998115

0.3 Update Standard Log






Intercept Log
NH3
0.00
−0.02
−0.04
−0.06
Jan 19
Jan 26
Feb 02
Feb 09
NOx
0.00
−0.05
−0.10
−0.15
−0.20
Feb 09
Feb 10
Feb 11
Feb 12
Feb 13
PO4
0.000
−0.001
−0.002
−0.003
−0.004
−0.005
Jan 19
Jan 26
Feb 02
Feb 09
Intercept
Run_Date
Run
Current Runs
Past Runs

0.4 Dilution Corrections - ensure the latest dilution is kept

```
## [1] "No Reruns"
```

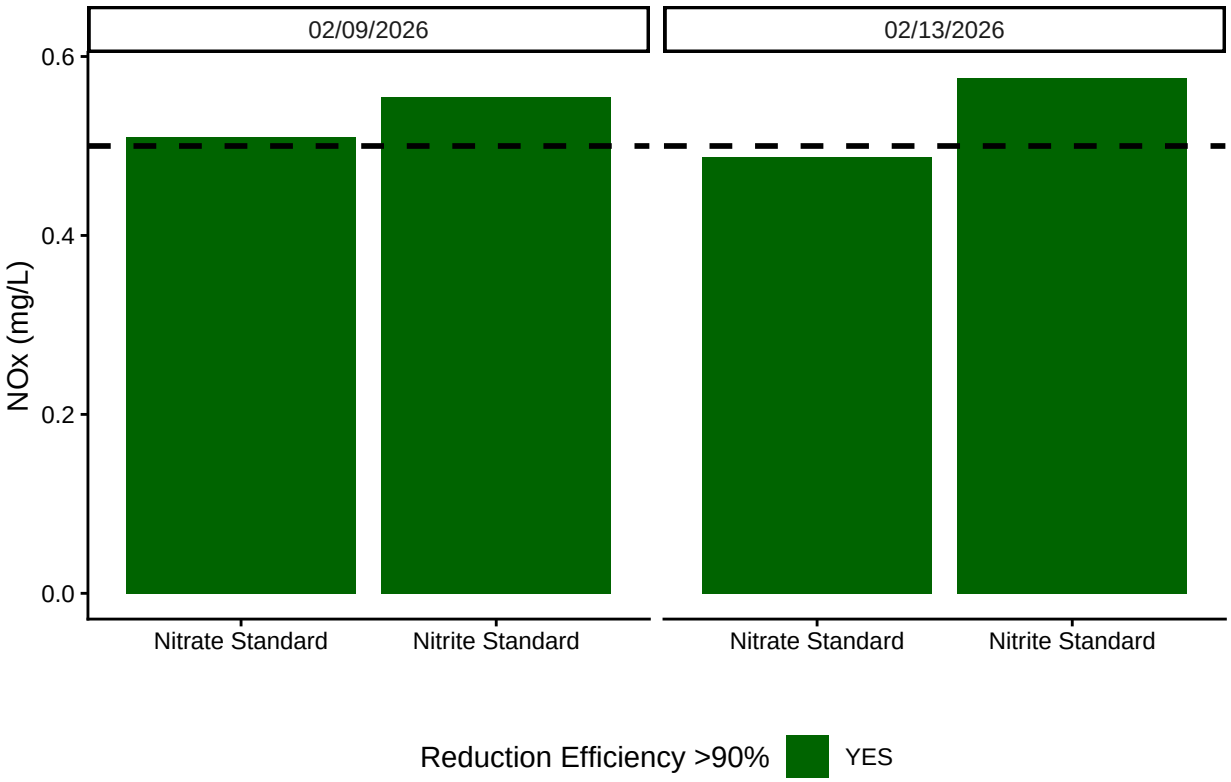
```
## [1] "No Dilutions"
```

```
## [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

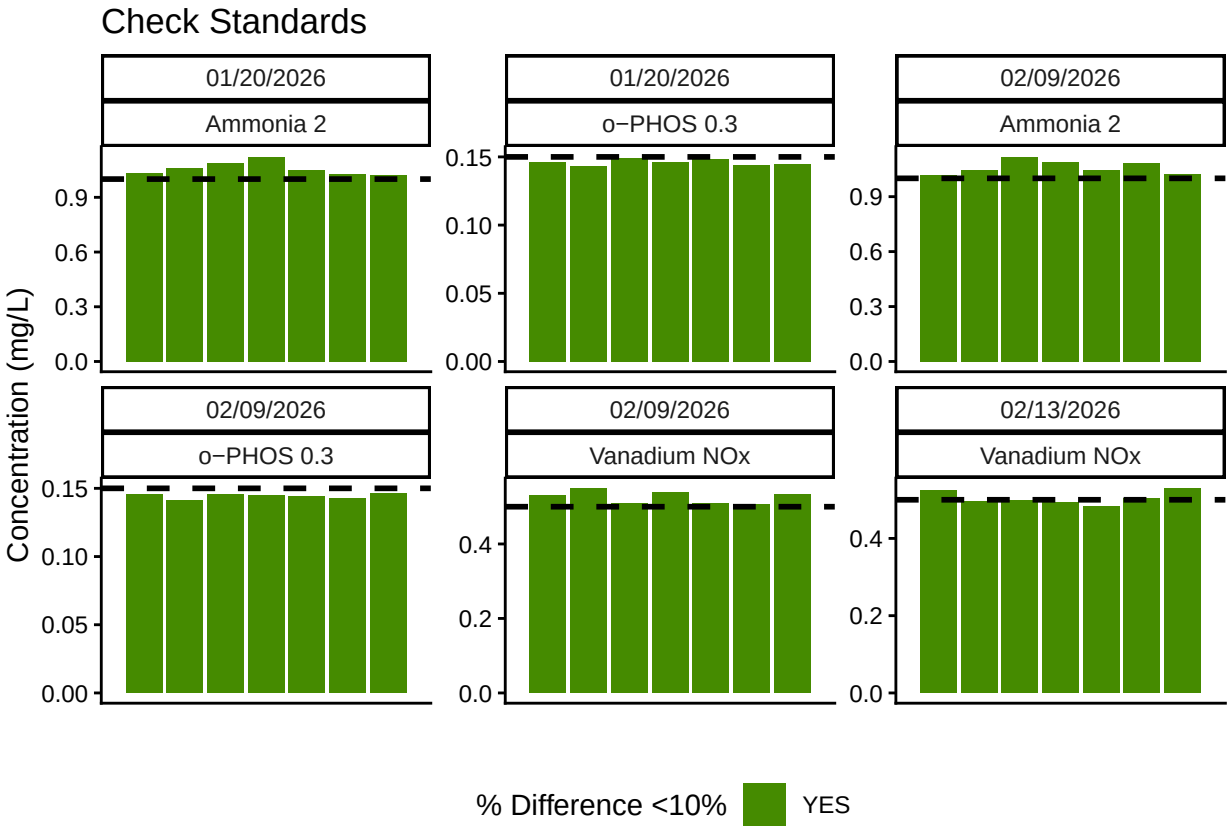
0.6 Check NOx Reduction Efficiency



Test	Run_Date	Red_Eff_Flag
Vanadium NOx	02/09/2026	Mean NOx Reduction Efficiency >95% - PROCEED
Vanadium NOx	02/13/2026	Mean NOx Reduction Efficiency >95% - PROCEED

0.7 Analyze the Check Standards

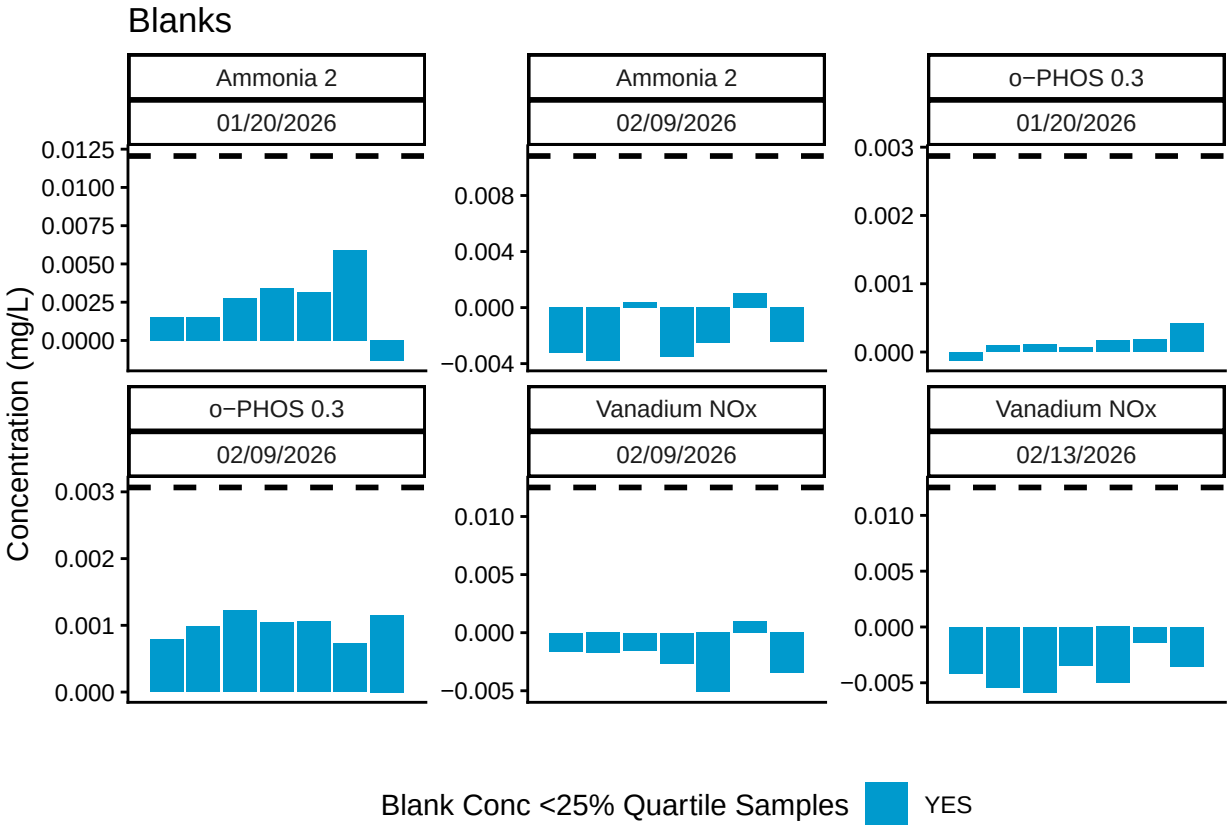
Test	Run_Date	RSV_Flag	RSV	RSV_Cutoff
Vanadium NOx	02/09/2026	RSV WITHIN RANGE - PROCEED	0.0382322	0.25
Vanadium NOx	02/13/2026	RSV WITHIN RANGE - PROCEED	0.0382322	0.25
Ammonia 2	01/20/2026	RSV WITHIN RANGE - PROCEED	0.0329643	0.25
o-PHOS 0.3	01/20/2026	RSV WITHIN RANGE - PROCEED	0.0144344	0.25
Ammonia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



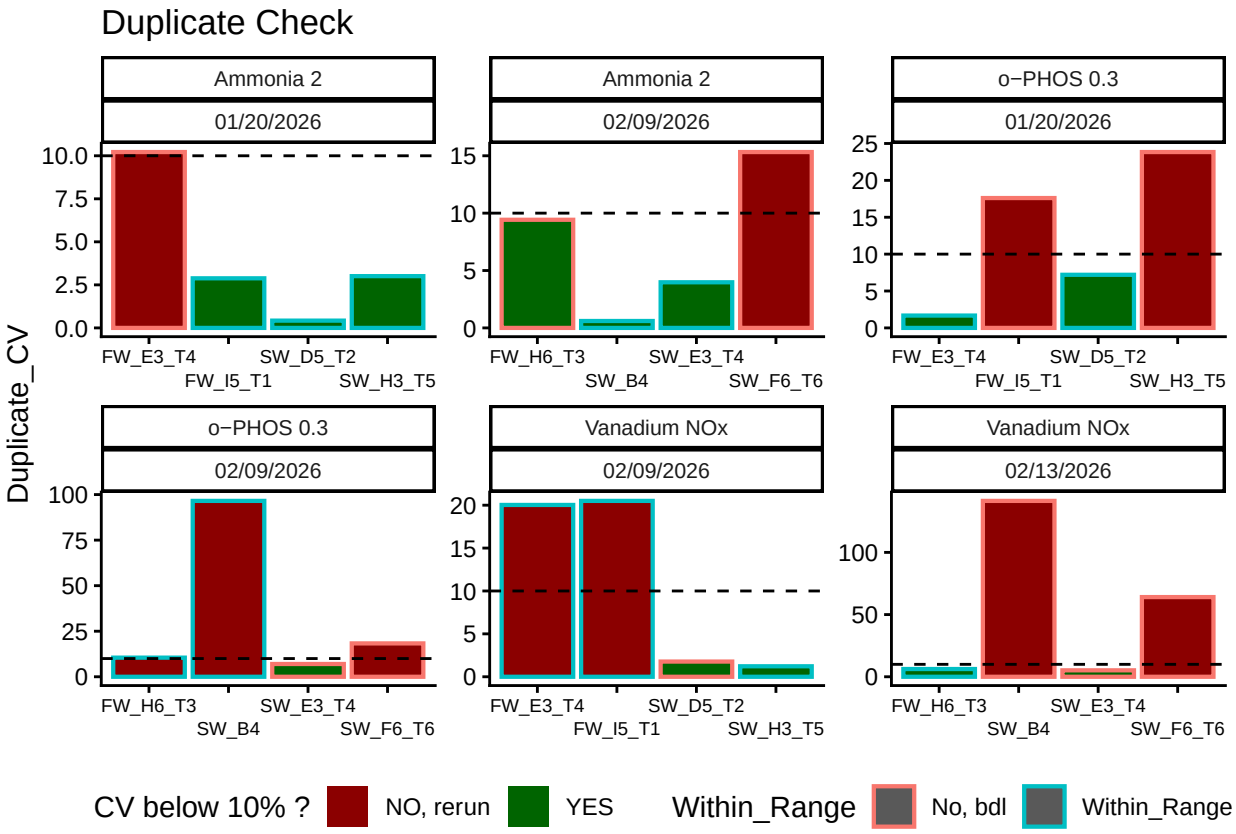
Test	Run_Date	CHK_Flag
Vanadium NOx	02/09/2026	>60% of Checks Pass - PROCEED
Vanadium NOx	02/13/2026	>60% of Checks Pass - PROCEED
Ammonia 2	01/20/2026	>60% of Checks Pass - PROCEED
o-PHOS 0.3	01/20/2026	>60% of Checks Pass - PROCEED
Ammonia 2	02/09/2026	>60% of Checks Pass - PROCEED
o-PHOS 0.3	02/09/2026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

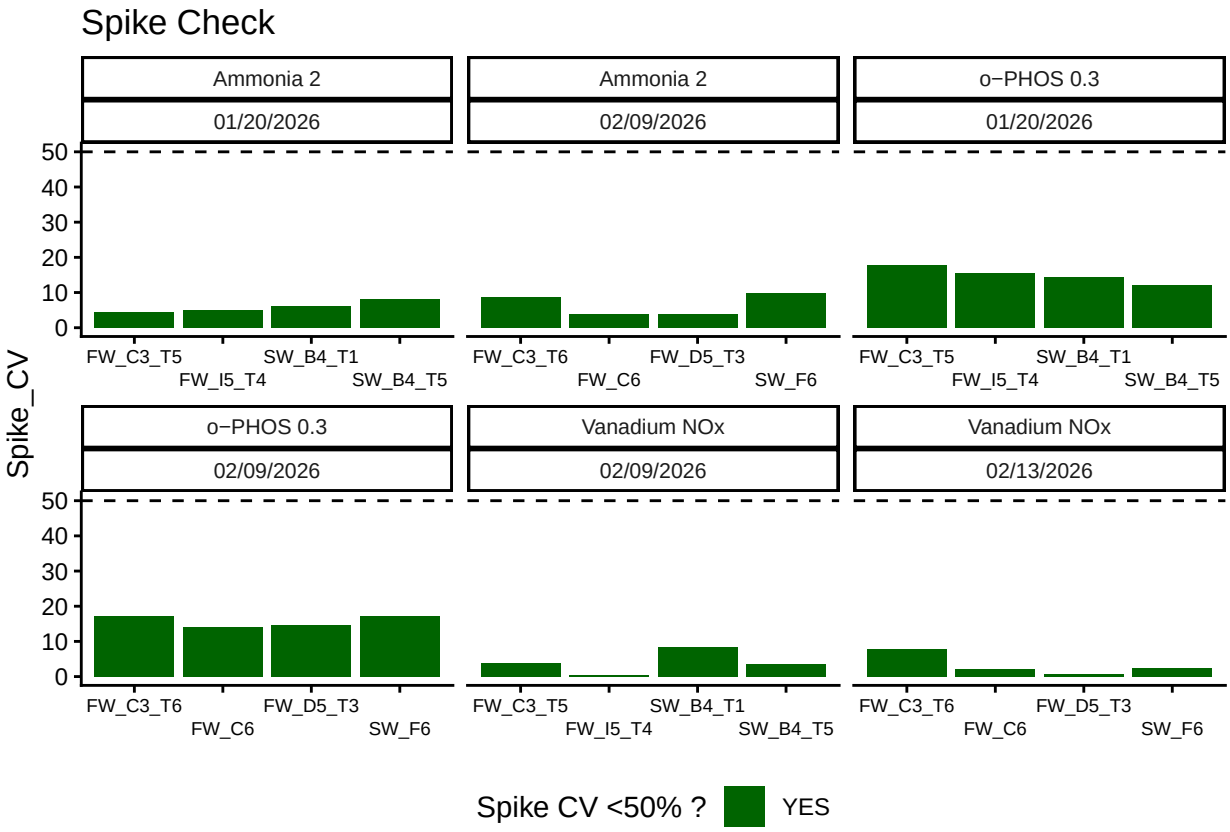


0.9 Analyze Duplicates



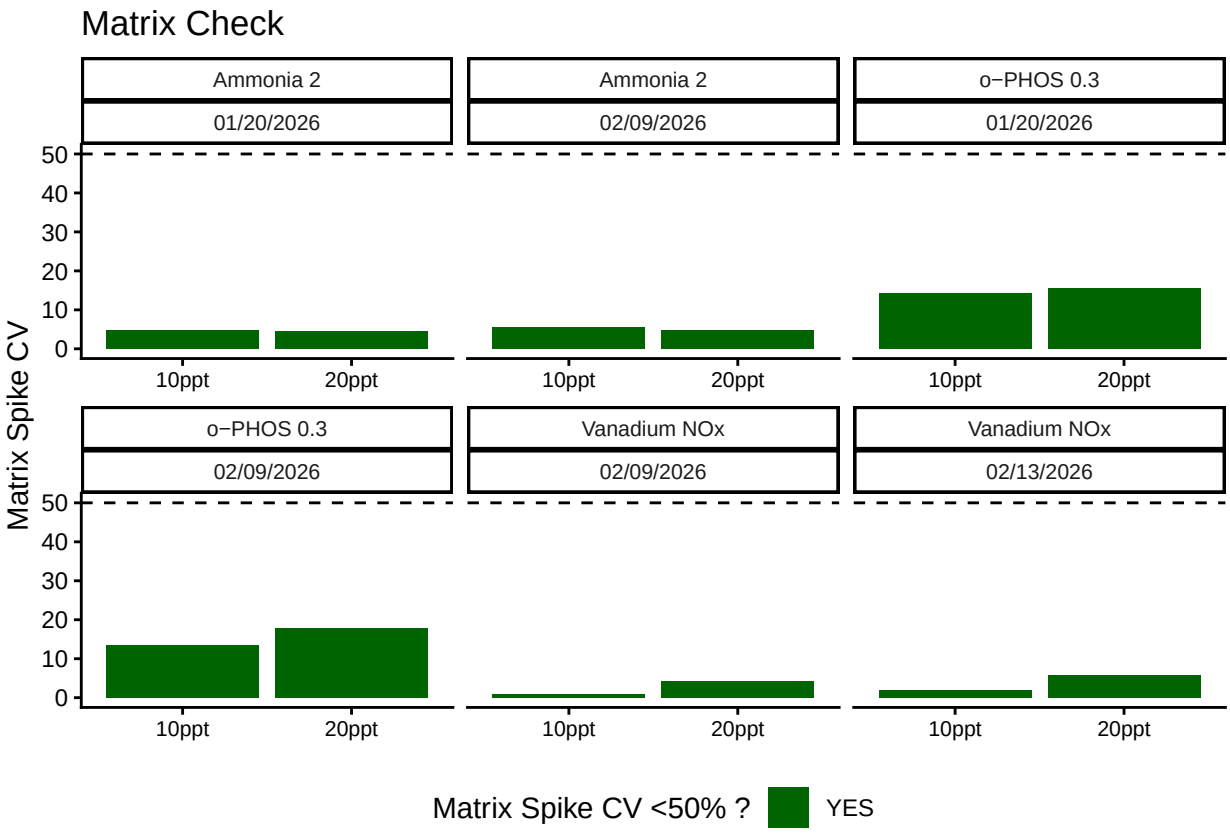
Test	Run_Date	Dup_Flags
Vanadium NOx	02/09/2026	<60% of Dups Pass - REASSESS
Vanadium NOx	02/13/2026	<60% of Dups Pass - REASSESS
Ammonia 2	01/20/2026	>60% of Dups Pass - PROCEED
o-PHOS 0.3	01/20/2026	<60% of Dups Pass - REASSESS
Ammonia 2	02/09/2026	>60% of Dups Pass - PROCEED
o-PHOS 0.3	02/09/2026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

0.10 Spikes



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



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

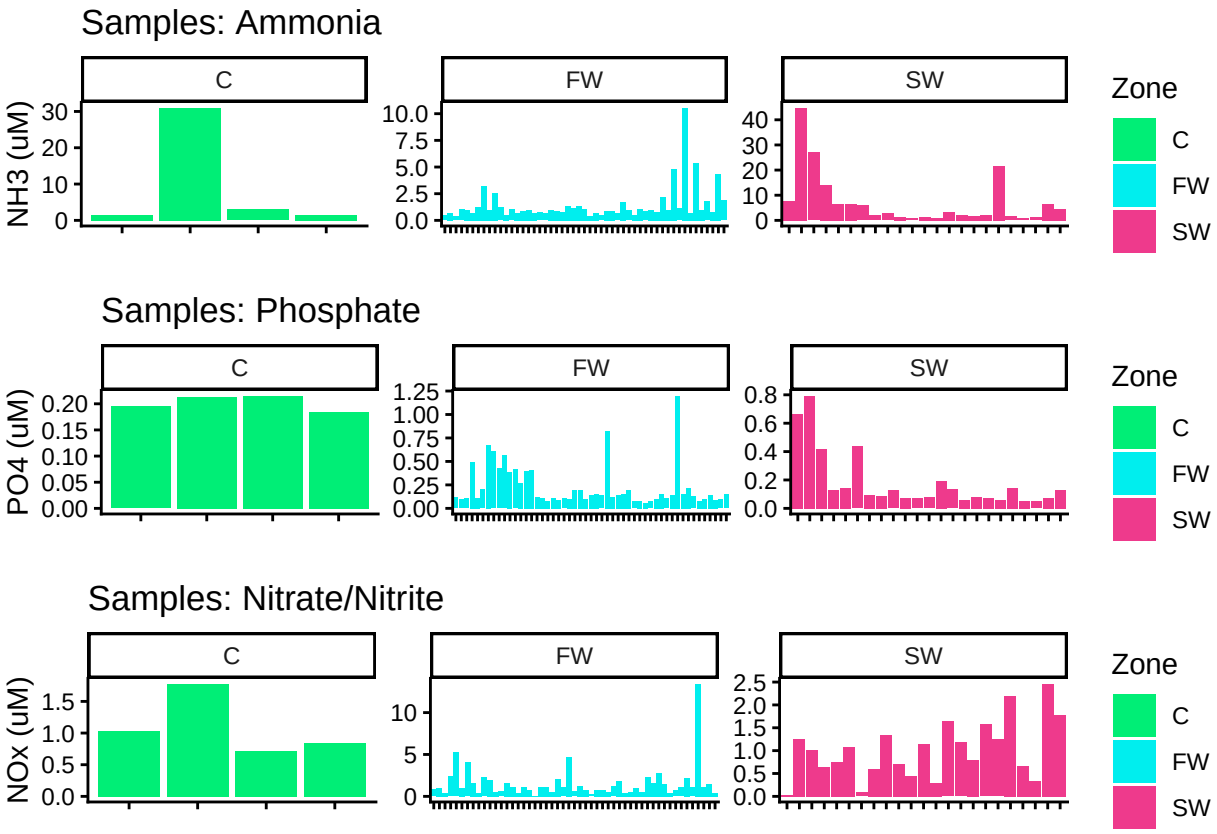
0.12 Check to see if samples run match metadata & merge info

```
## 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



##Write Out Data

#end