COMPASS: TEMPEST Discrete DOC Data QAQC

Freshwater Well Test: 2025-09-04

2025-09-18

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0.1 Run Information

```
#identify which section you are in
cat("Run Information")
```

Run Information

```
#a link to the Gitbook or whatever protocol you are using for this analysis
    #steph will add this soon

#anything that needs to be changed do this in the first chunk
Date_Run = "09/16/25"
Run_by = "Stephanie J. Wilson"
Script_run_by = "Stephanie J. Wilson"
run_notes = "No duplicates run, because field replicates collected. "

#file path and name for summary file
    raw_file_name = "Raw Data/TMP_20250904_FW_WellTest.txt"
#file path and name for the all peaks file
```

```
raw_allpeaks_name = "Raw Data/TMP_20250904_FW_WellTest_allpeaks.txt"
#file path and name for processed data after QAQC
processed_file_name = "Processed Data/TMP_20250904_FW_WellTest_DOC_Processed.csv"

#check standard concentrations - Update if running different checks:
    chk_std_c = 1
    chk_std_n = 1

#Log_path
Log_path = "Raw Data/COMPASS_TMP_TOCTN_QAQClog_2025.csv"
```

0.2 Setup

0.3 Import Data Functions

0.4 Import Sample Data

```
## Import Sample Data
## New names:
## * '' -> '...14'
## # A tibble: 6 x 4
   sample_name
                               npoc_raw tdn_raw run_datetime
##
    <chr>>
                                 <dbl> <dbl> <chr>
## 1 TMP_FW_Well_20250904_1225_A
                                  2.98 0.611 9/16/2025 10:03:05 PM
## 2 TMP_FW_Well_20250904_1225_B
                                  2.58 0.413 9/16/2025 10:25:04 PM
## 3 TMP_FW_Well_20250904_1225_C
                                  2.68 0.471 9/16/2025 10:51:00 PM
## 4 TMP_FW_Well_20250904_1300_A
                                         0.739 9/16/2025 11:13:51 PM
                                  2.19
## 5 TMP_FW_Well_20250904_1300_B
                                   2.22 0.744 9/16/2025 11:42:20 PM
## 6 TMP_FW_Well_20250904_1300_C 1.62 0.397 9/17/2025 12:08:12 AM
```

0.5 Assessing standard Curves

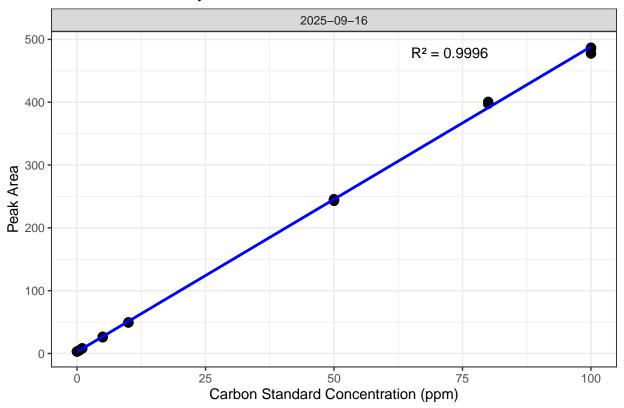
Assess the Standard Curve

```
## New names:
## * '' -> '...18'

## Warning: One or more parsing issues, call 'problems()' on your data frame for details,
## e.g.:
## dat <- vroom(...)
## problems(dat)</pre>
```

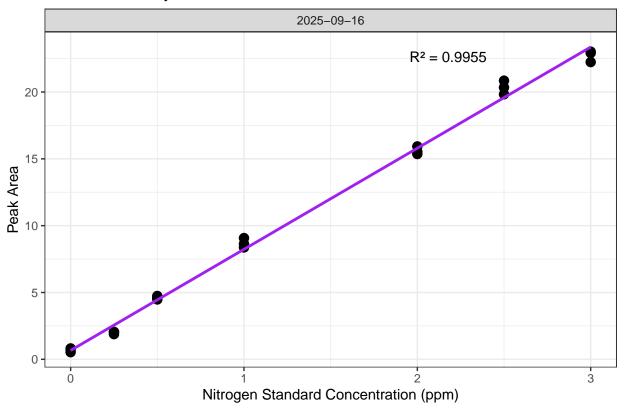
NPOC Std Curve by Date

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

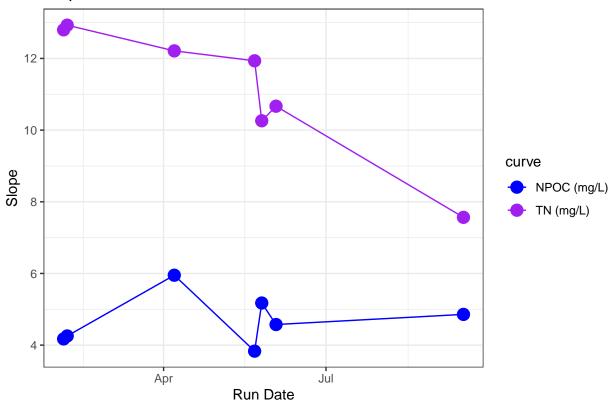


'geom_smooth()' using formula = 'y ~ x'

TN Std Curve by Date



Slope Drift Assessment



- ## [1] "NPOC Curve r2 GOOD"
- ## [1] "TN Curve r2 GOOD"

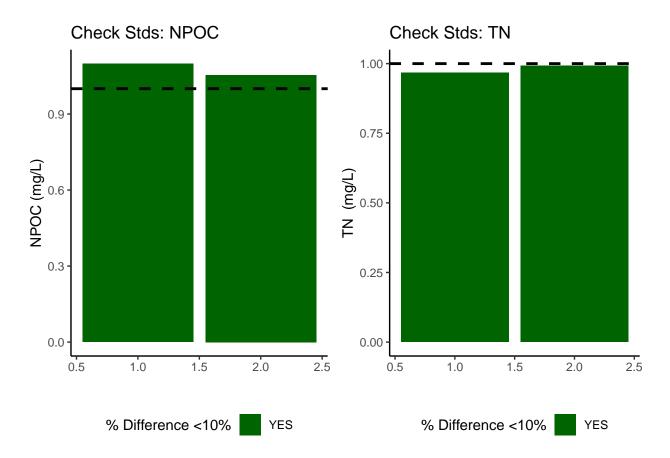
0.6 Assess Check Standards

Assess the Check Standards

New names: ## * '' -> '...14'

[1] "Carbon Check Standard RSD within Range"

[1] "Nitrogen Check Standard RSD within Range"



[1] ">60% of Carbon Check Standards are within range of the expected concentration"

[1] ">60% of Nitrogen Check Standards are within range of the expected concentration"

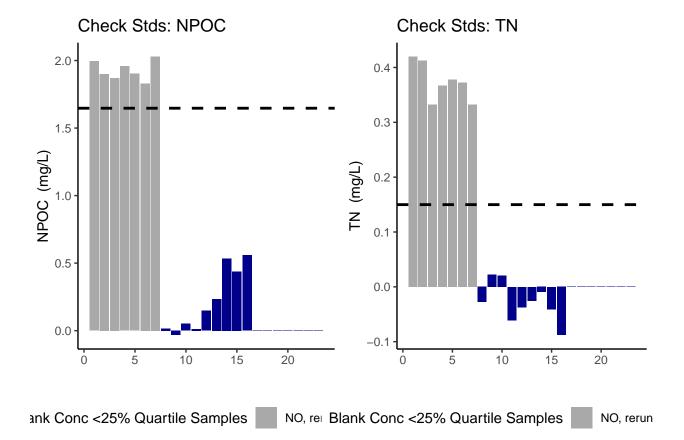
0.7 Assess Blanks

Assess Blanks

New names: ## * '' -> '...14'

[1] ">60% of Carbon Blank concentrations are below the lower 25% quartile of samples"

[1] ">60% of Nitrogen Blank concentrations are below the lower 25% quartile of samples"



carbon blanks:

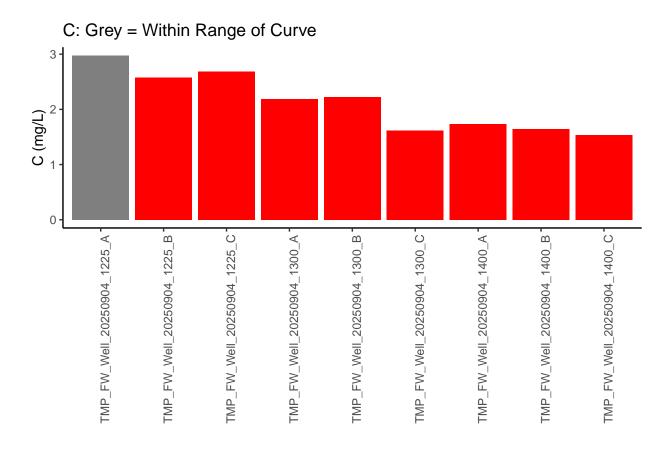
[1] 0.6713891

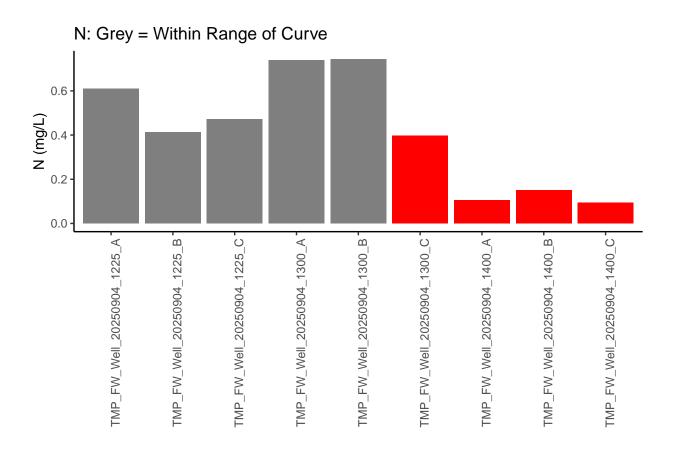
nitrogen blanks:

[1] 0.1029187

0.8 Sample Flagging

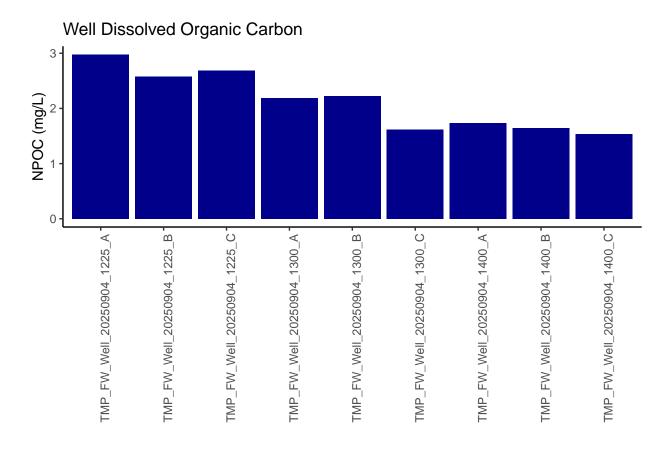
Sample Flagging

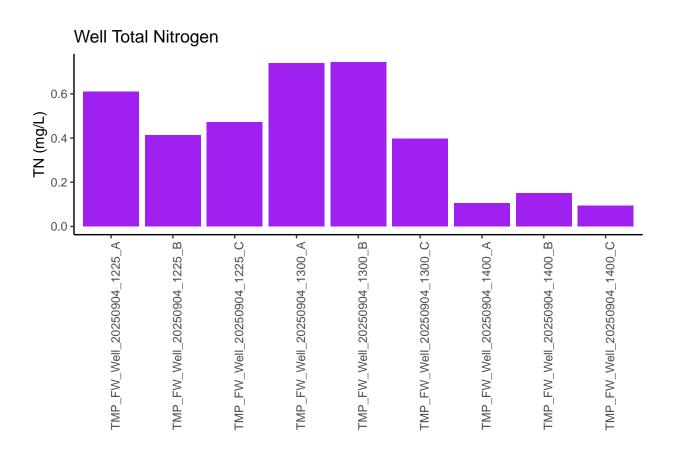




0.9 Visualize Data by Plot

Visualize Data





0.10 Convert data from mg/L to uMoles/L

0.11 Export Processed Data

Export Processed Data

```
## # A tibble: 6 x 14
##
    Project Experiment
                            Sample_Date Sample_Time Replicate sample_name npoc_mgL
                                                    <chr>
##
     <chr>
           <chr>
                            <chr>
                                         <chr>
                                                               <chr>
                                                                              <dbl>
## 1 COMPASS TEMPEST: Well ~ 2025-09-04 12:25
                                                               TMP_FW_Wel~
                                                    Α
                                                                              2.98
## 2 COMPASS TEMPEST: Well ~ 2025-09-04 12:25
                                                    В
                                                               TMP FW Wel~
                                                                              2.58
## 3 COMPASS TEMPEST: Well ~ 2025-09-04 12:25
                                                     С
                                                               TMP_FW_Wel~
                                                                              2.68
## 4 COMPASS TEMPEST: Well ~ 2025-09-04 13:00
                                                     Α
                                                               TMP_FW_Wel~
                                                                              2.19
## 5 COMPASS TEMPEST: Well ~ 2025-09-04 13:00
                                                     В
                                                               TMP_FW_Wel~
                                                                              2.22
                                                     С
## 6 COMPASS TEMPEST: Well ~ 2025-09-04 13:00
                                                               TMP_FW_Wel~
                                                                              1.62
## # i 7 more variables: npoc_uM <dbl>, npoc_flag <chr>, tdn_mgL <dbl>,
     tdn_uM <dbl>, tdn_flag <chr>, Analysis_runtime <chr>, Run_notes <chr>
```

 $\#\mathrm{end}$