Synoptic CB: Porewater DIC

September 2024 Samples

2025-10-21

Contents

##Setup - Change things here & write any notes

```r
#identify section
cat("Setup Information")
```

```
## Setup Information
```

```r
###### Run information - PLEASE CHANGE
  Date_Run = "10/04/2024"   #Date that instrument was run
  Run_by = "Stephanie J. Wilson"   #Instrument user
  Script_run_by = "Stephanie J. Wilson" #Code user
  run_notes = "There is one sample: 202409_GWI_TR_LysA_45cm that is not in the metadata and
    There were no other samples collected from that lysimeter, so it cannot be that sample.
    There are two other lysimeters that could have yielded this sample, but no way to tell so
    we will remove this sample from the analysis - this is done in this code."   #any notes from the run
  samples <- c("GCW", "GWI", "MSM", "SWH") #whatever identifies your samples within the same names
  samples_pattern <- paste(samples, collapse = "|")
    #samples_pattern <- "GCW" #use this instead of the line above if you have only one site code
  chks_name = "Chk_Std_"   #what did you name your check standards?
  crm_name = "CRM|crm"     #what did you name your CRMS?

###### File Names - PLEASE CHANGE
#file path and name for raw summary data file
    raw_file_name = "Raw Data/TOCTN_COMPASS_Synoptic_DIC_202409.txt"

#file path and name for raw all peaks file
    raw_allpeaks_name = "Raw Data/TOCTN_COMPASS_Synoptic_DIC_202409_allpeaks.txt"

#file path and name of processed data file
    processed_file_name = "Processed Data/COMPASS_SynopticCB_PW_Processed_DIC_202409.csv"


###### Log Files - PLEASE CHECK
#downloaded metadata csv - downloaded from Google drive as csv for this year
  Raw_Metadata = "Raw Data/COMPASS_SynopticCB_PW_SampleLog_2024.csv"

#qaqc log file path for this year
  Log_path = "Raw Data/COMPASS_Synoptic_DIC_QAQClog_2024.csv"
```

##Set Up Code

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

0.1   Import Data Functions
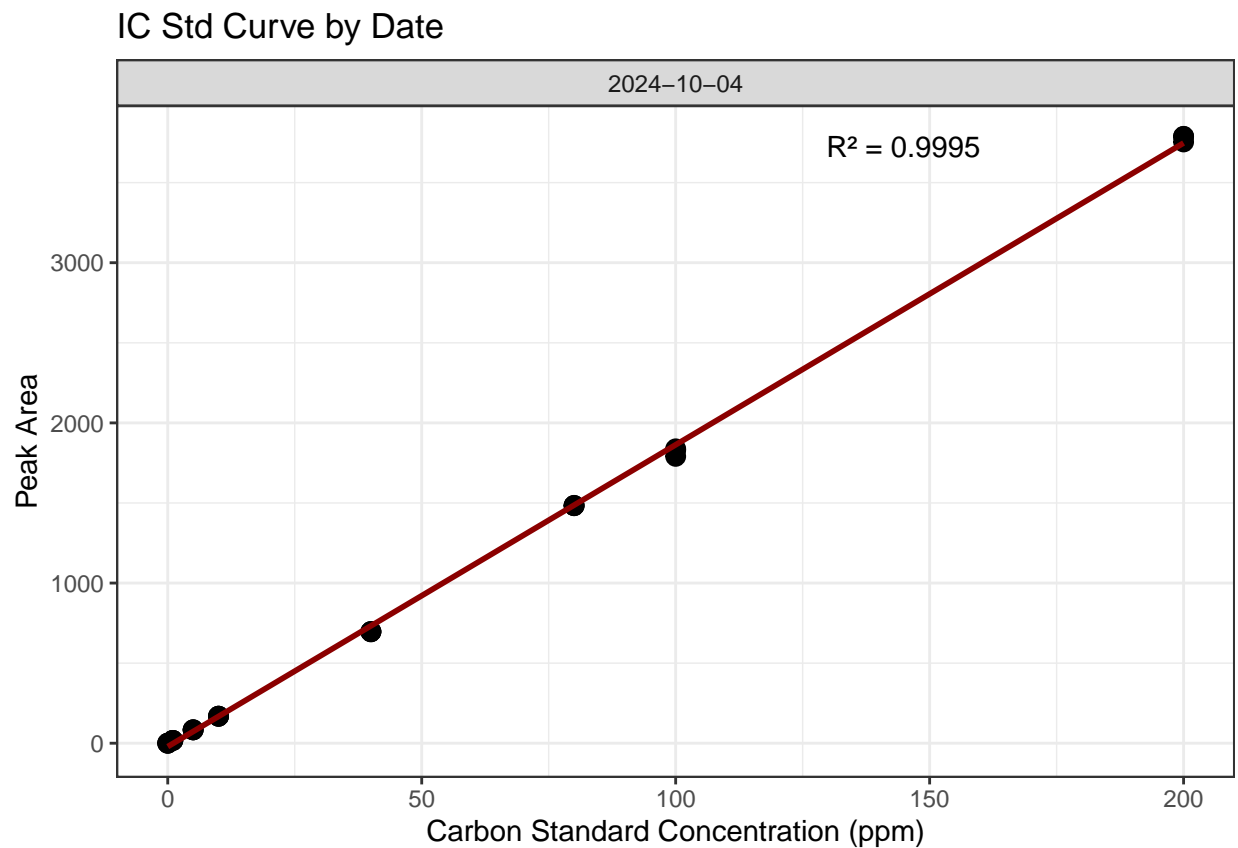
0.2   Import Sample Data

```
## Import Sample Data
```

```
## New names:
## * `` -> `...14`
```
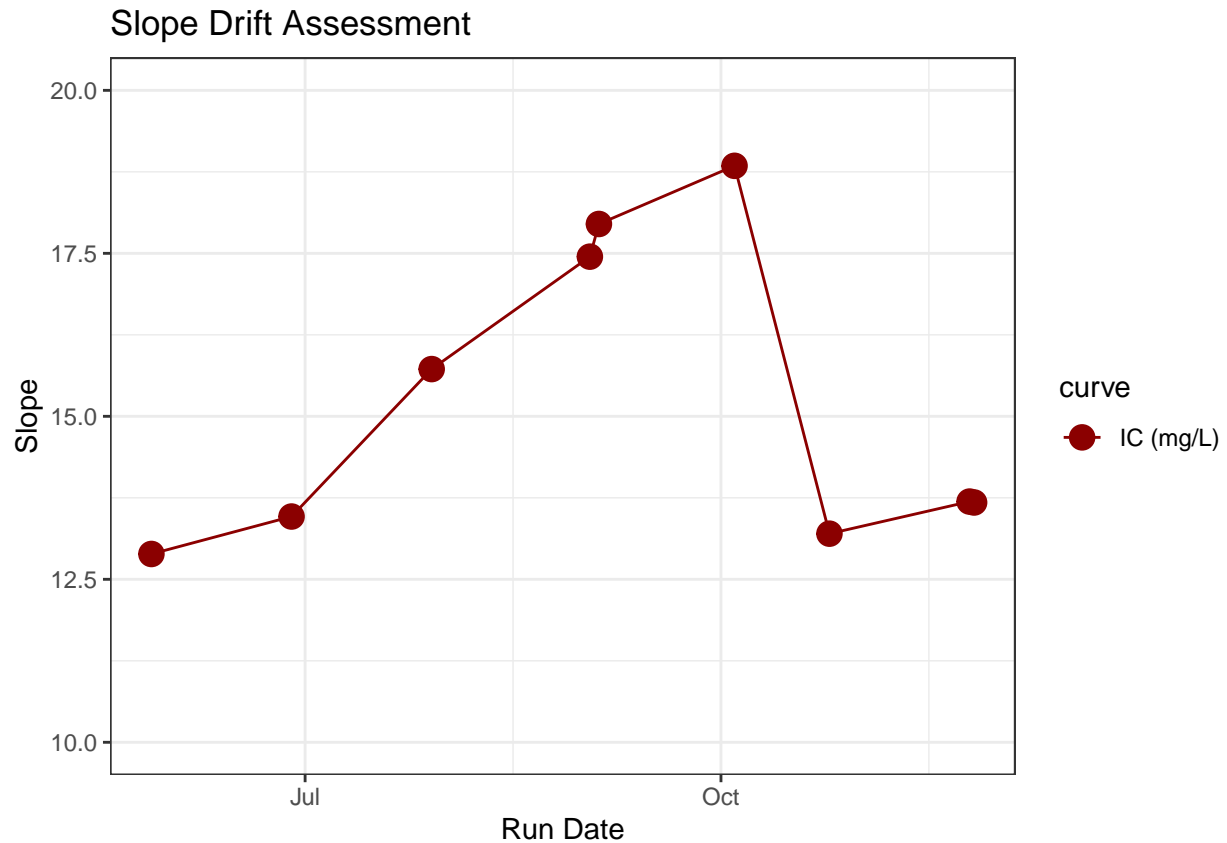
```
## # A tibble: 6 x 3
##   sample_name              ic_raw run_datetime
##   <chr>                     <dbl> <chr>
## 1 202409_GCW_TR_LysA_20cm   10.7  10/4/2024 8:52:54 PM
## 2 202409_GCW_TR_LysA_45cm   28.4  10/4/2024 9:07:20 PM
## 3 202409_GCW_TR_LysB_20cm   12.9  10/4/2024 9:20:58 PM
## 4 202409_GCW_TR_LysB_10cm    3.44 10/4/2024 10:16:41 PM
## 5 202409_GCW_TR_LysC_20cm    4.74 10/4/2024 10:29:03 PM
## 6 202409_GCW_WC_LysA_10cm  108.   10/4/2024 10:45:46 PM
```

0.3 Assessing Standard Curves

```
## Assess the Standard Curves
```

```
## New names:
## 'geom_smooth()' using formula = 'y ~ x'
## * '' -> '...18'
```


IC Std Curve by Date

Slope Drift Assessment


```
## [1] "IC Curve r2 GOOD"
```

0.4 CRM Check - Don't run chunk if no CRMs run

```
## Assess the CRMs
```

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

```
## [1] "IC crm has a % Difference <25% of expected - PROCEED"
```
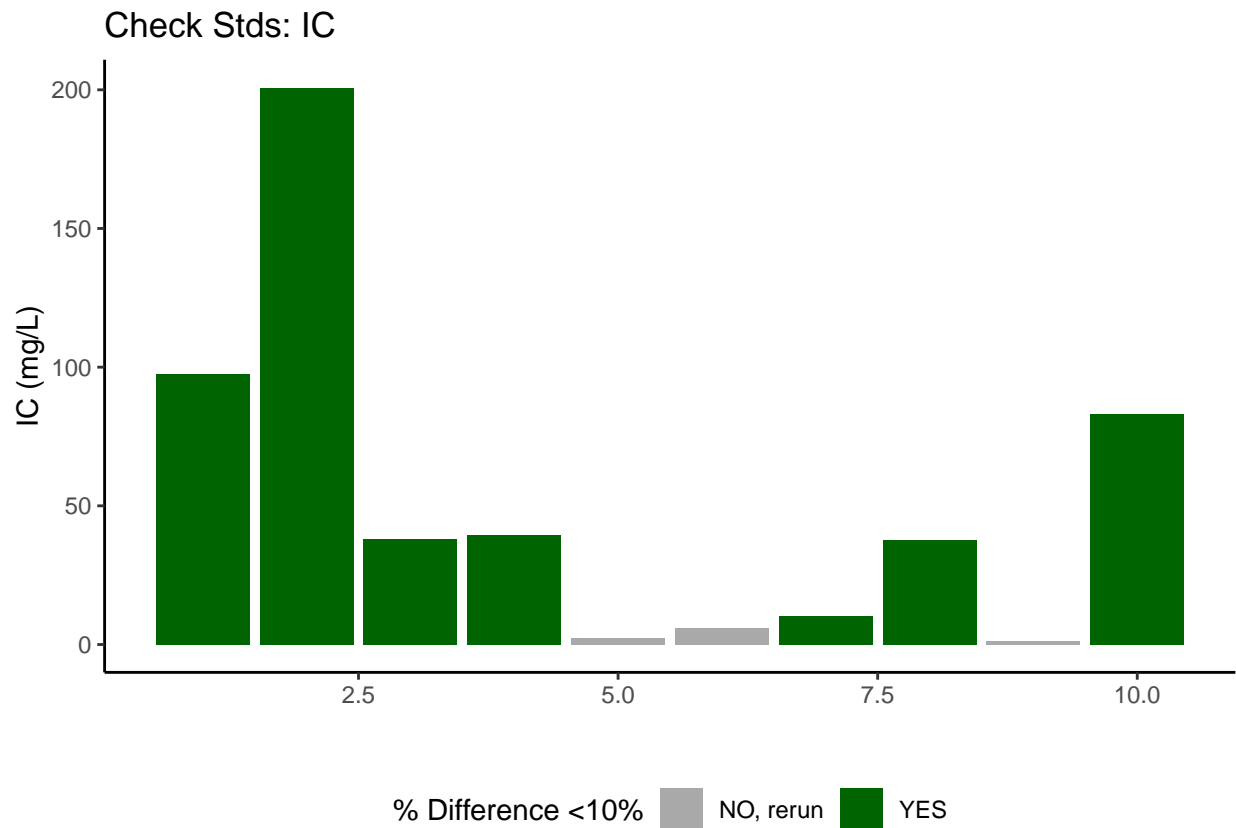
```
## Run mean = 22.25
```

```
## Expected  = 22.19
```

0.5 Assess Check Standards

```
## Assess the Check Standards
```

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

Check Stds: IC

% Difference <10%   NO, rerun   YES

[1] ">60% of IC Check Standards are within range of expected concentration"
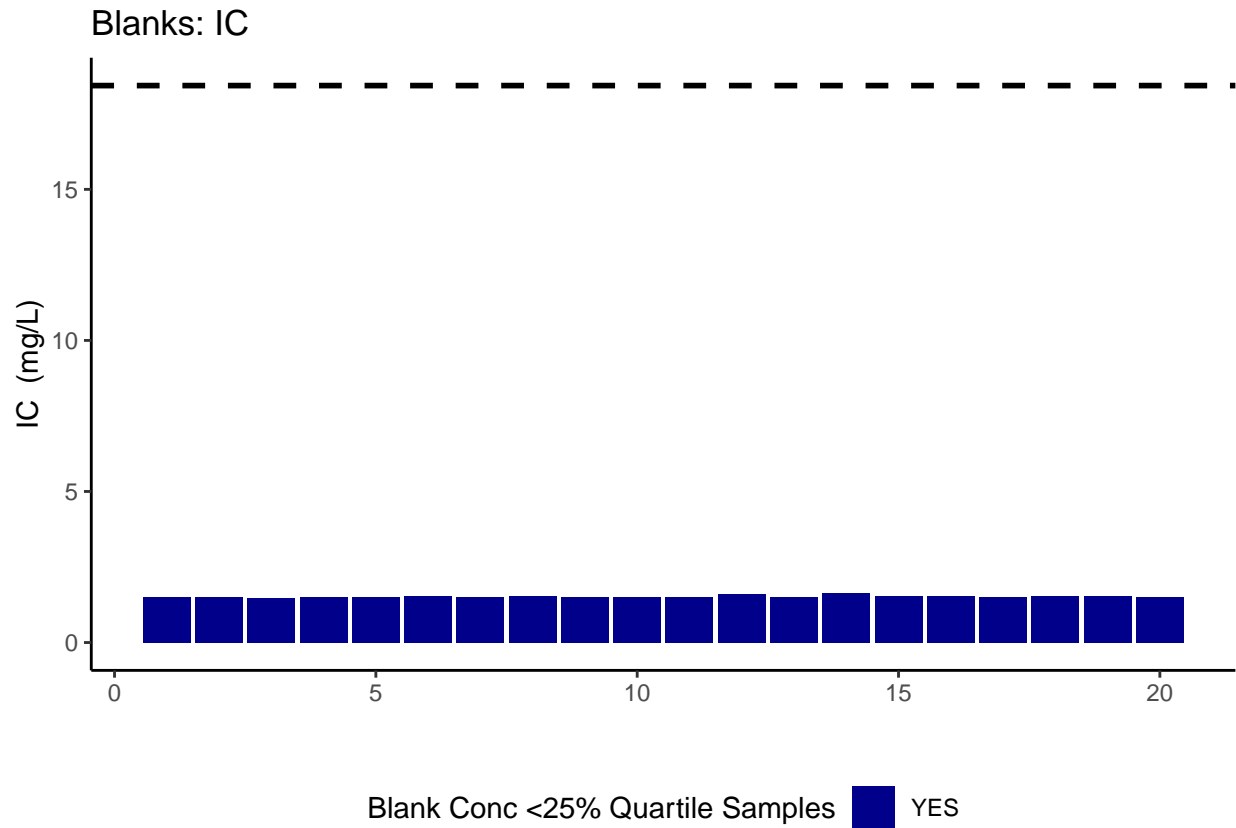
0.6   Assess Blanks

Assess Blanks

New names:
* `` -> `...14`

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

Blanks: IC

Blank Conc <25% Quartile Samples ■ YES

```
## carbon blanks:
```

```
## [1] 1.52715
```

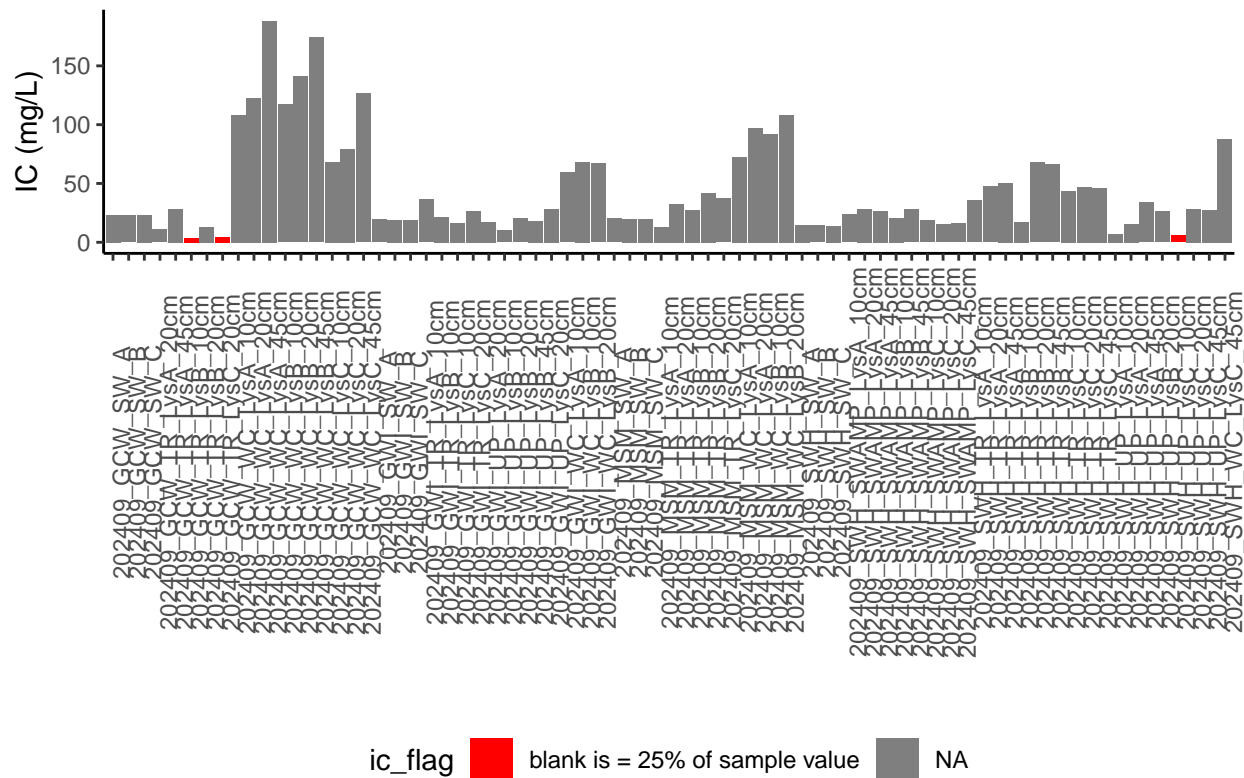## 0.7 Assess Duplicates - no duplicates included on this run

0.8 Sample Flagging - Are samples Within the range of the curve?

```
## Sample Flagging
```

C: Grey = Within Range of Curve

ic_flag [red] blank is = 25% of sample value [grey] NA

0.9 Visualize Data by Plot

```
## Visualize Data
```

```
## Warning in rbind(c("202409", "GCW", "TR", "LysA", "20cm"), c("202409", "GCW", :
## number of columns of result is not a multiple of vector length (arg 15)
```

Samples: DIC

0.10 Convert data from mg/L to uMoles/L

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

```
## Check Sample IDs with Metadata

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

0.12 Export Processed Data

```
## Export Processed Data

## # A tibble: 6 x 18
##   Project       Region Site  Zone  Replicate Depth_cm Sample_ID Year Month   Day
##   <chr>         <chr>  <chr> <fct> <chr>         <int> <chr>    <int> <int> <int>
## 1 COMPASS: Sy~  CB     SWH   UP    A                10 202409_S~ 2024     9    24
## 2 COMPASS: Sy~  CB     SWH   UP    A                20 202409_S~ 2024     9    24
## 3 COMPASS: Sy~  CB     SWH   UP    A                45 202409_S~ 2024     9    24
## 4 COMPASS: Sy~  CB     SWH   UP    B                20 202409_S~ 2024     9    24
## 5 COMPASS: Sy~  CB     SWH   UP    C                10 202409_S~ 2024     9    24
## 6 COMPASS: Sy~  CB     SWH   UP    C                20 202409_S~ 2024     9    24
## # i 8 more variables: Time <chr>, Time_Zone <chr>, ic_mgL <dbl>, ic_uM <dbl>,
## #   ic_flag <chr>, Analysis_runtime <chr>, Run_notes <chr>, Field_notes <chr>
```

#end