COMPASS_Synoptic_TGW_2022: August

Stephanie J. Wilson

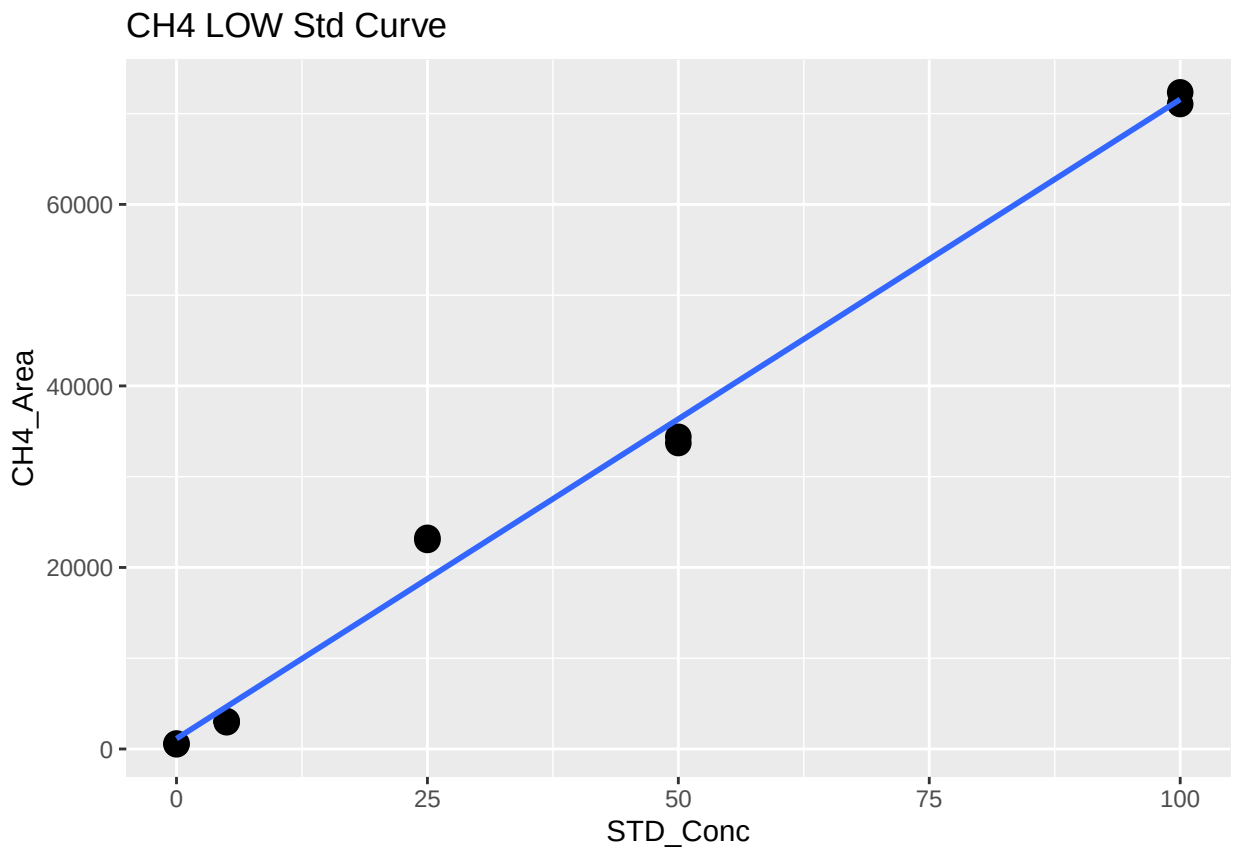
2023-01-14

##Set Up

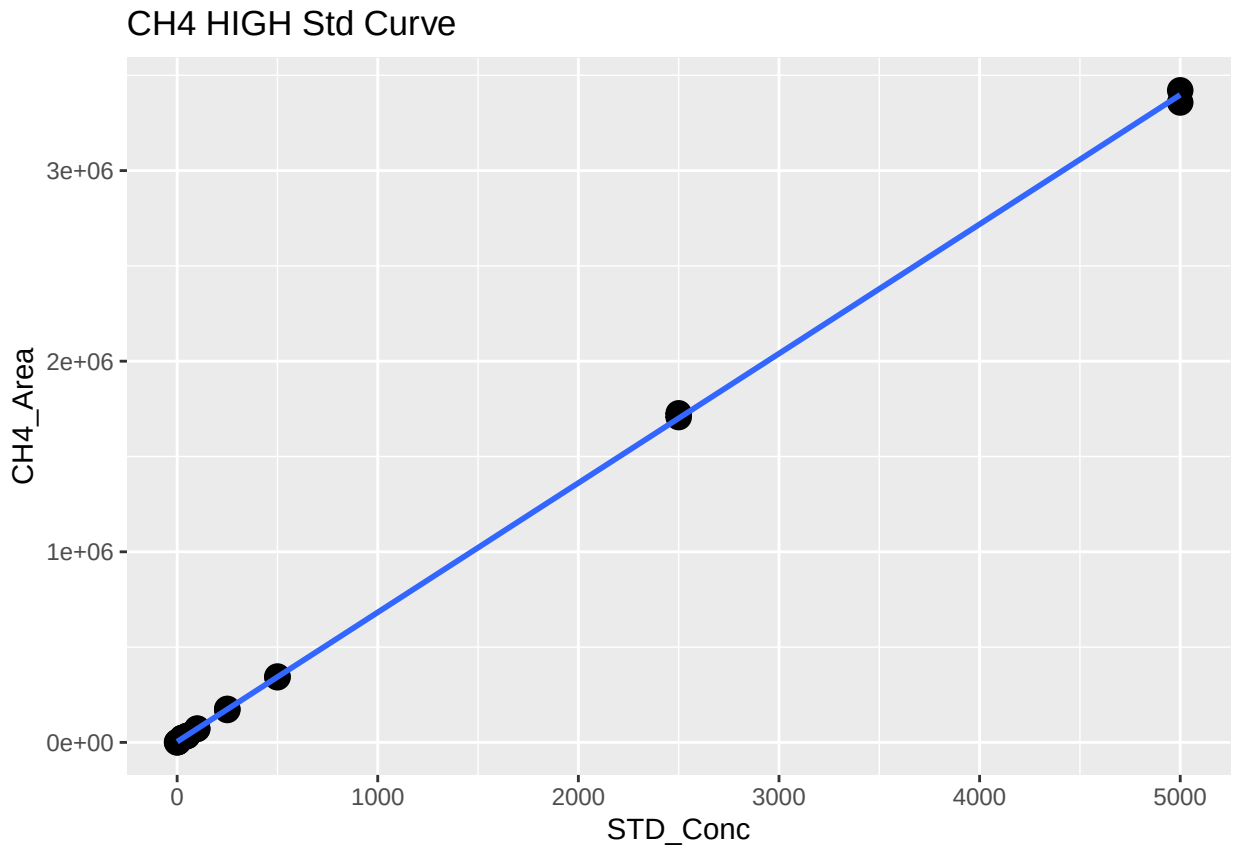
Read in first data file and assess standard curves

```
##     Machine                User Run_Date Sample_Type Type1 Sample_Year
## 1 Varian GC Stephanie J. Wilson   202208       Blank  TGAS        2022
## 2 Varian GC Stephanie J. Wilson   202208       Blank  TGAS        2022
## 3 Varian GC Stephanie J. Wilson   202208       Blank  TGAS        2022
## 4 Varian GC Stephanie J. Wilson   202208       Blank  TGAS        2022
## 5 Varian GC Stephanie J. Wilson   202208     Chk_STD  TGAS        2022
## 6 Varian GC Stephanie J. Wilson   202208     Chk_STD  TGAS        2022
##   Sample_Month        Sample_ID Dilution_Factor STD_Conc CO2_Area CH4_Area
## 1       August          Blank_2               1       NA    18795      607
## 2       August          Blank_3               1       NA    20159      516
## 3       August          Blank_4               1       NA    20414      634
## 4       August          Blank_5               1       NA    31001      723
## 5       August   100ppm_CH4_Chk               1       NA     1691    69235
## 6       August 100ppm_CH4_Chk_1               1       NA     9687    69584
##   Field.Notes Lab.Notes
## 1          NA        NA
## 2          NA        NA
## 3          NA        NA
## 4          NA        NA
## 5          NA        NA
## 6          NA        NA
```

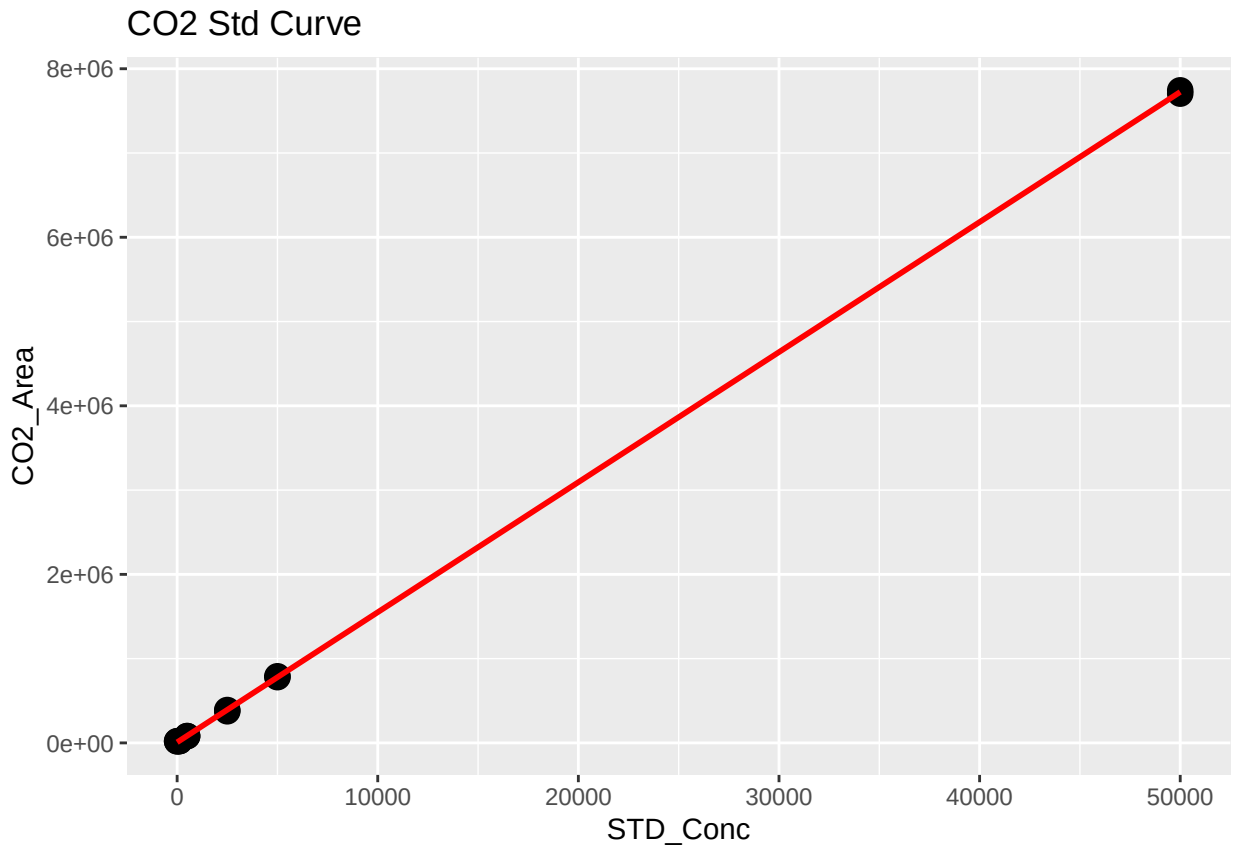
```
## `geom_smooth()` using formula = 'y ~ x'
```



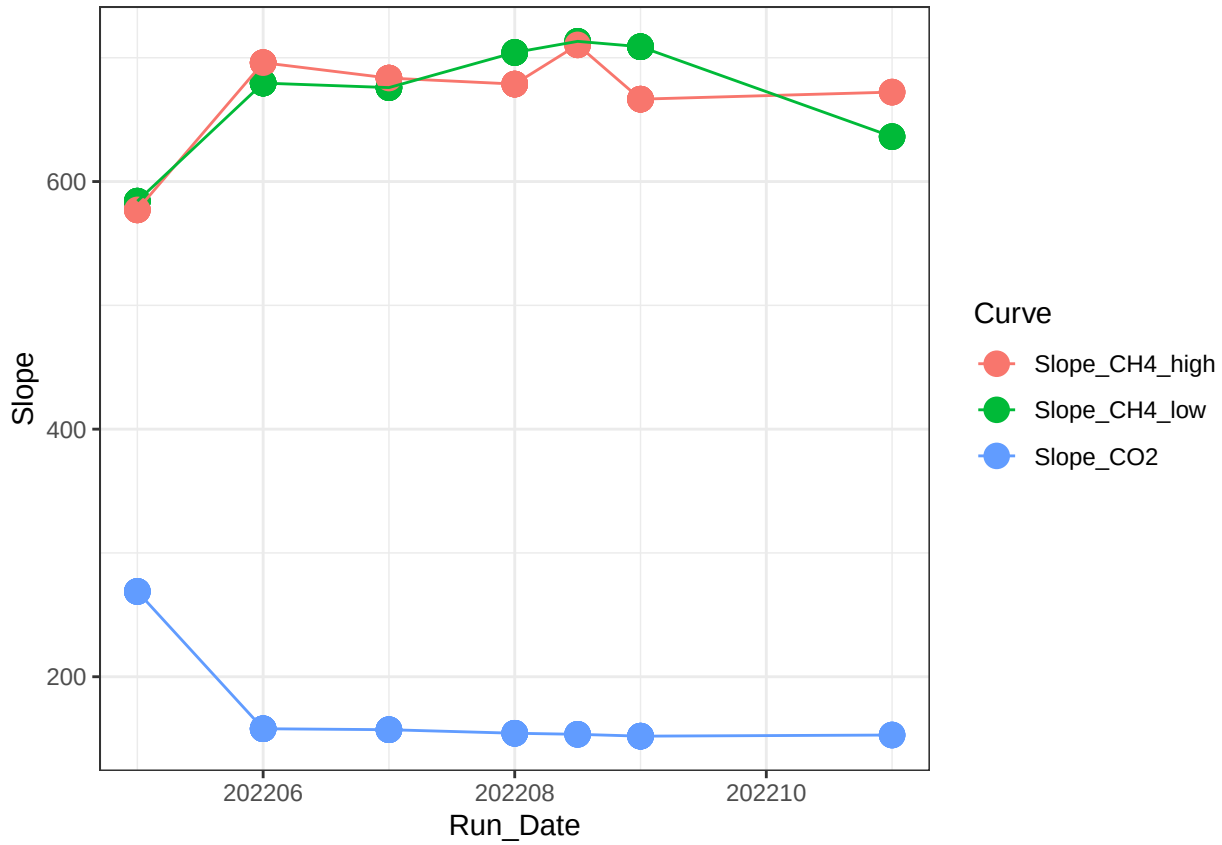

```
##
## Call:
## lm(formula = stds_ch4_low$CH4_Area ~ stds_ch4_low$STD_Conc)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -2647.9 -1684.5  -578.5   456.6  4516.6
##
## Coefficients:
##                       Estimate Std. Error t value Pr(>|t|)
## (Intercept)            1139.96    1181.10   0.965    0.363
## stds_ch4_low$STD_Conc   704.26      23.03  30.579 1.42e-09 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2660 on 8 degrees of freedom
## Multiple R-squared:  0.9915, Adjusted R-squared:  0.9905
## F-statistic: 935.1 on 1 and 8 DF,  p-value: 1.421e-09

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




```
##
## Call:
## lm(formula = stds_ch4$CH4_Area ~ stds_ch4$STD_Conc)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -39919  -3273   -890   2501  25949
##
## Coefficients:
##                   Estimate Std. Error t value Pr(>|t|)
## (Intercept)       3718.955   3719.318     1.0    0.332
## stds_ch4$STD_Conc  678.734      1.986   341.8   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 13670 on 16 degrees of freedom
## Multiple R-squared:  0.9999, Adjusted R-squared:  0.9999
## F-statistic: 1.168e+05 on 1 and 16 DF,  p-value: < 2.2e-16

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




```
##
## Call:
## lm(formula = stds_co2$CO2_Area ~ stds_co2$STD_Conc)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -19667  -4847  -2794  11649  19476
##
## Coefficients:
##                     Estimate Std. Error t value Pr(>|t|)
## (Intercept)       7201.6545  4154.8720   1.733    0.114
## stds_co2$STD_Conc  154.3399     0.2023 763.019   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 12690 on 10 degrees of freedom
## Multiple R-squared:      1,  Adjusted R-squared:      1
## F-statistic: 5.822e+05 on 1 and 10 DF,  p-value: < 2.2e-16

##   X          Curve        R2    Slope  Intercept Run_Date
## 1 1  Slope_CH4_low 0.9989050 584.1700   292.6667   202205
## 2 2 Slope_CH4_high 0.9988404 577.1458 -1829.3469   202205
## 3 3      Slope_CO2 0.8941001 268.8803 82323.2843   202205
## 4 4  Slope_CH4_low 0.9989050 584.1700   292.6667   202205
## 5 5 Slope_CH4_high 0.9988404 577.1458 -1829.3469   202205
## 6 6      Slope_CO2 0.8941001 268.8803 82323.2843   202205
```



Now calculate the CH4 & CO2 concentrations in ppm

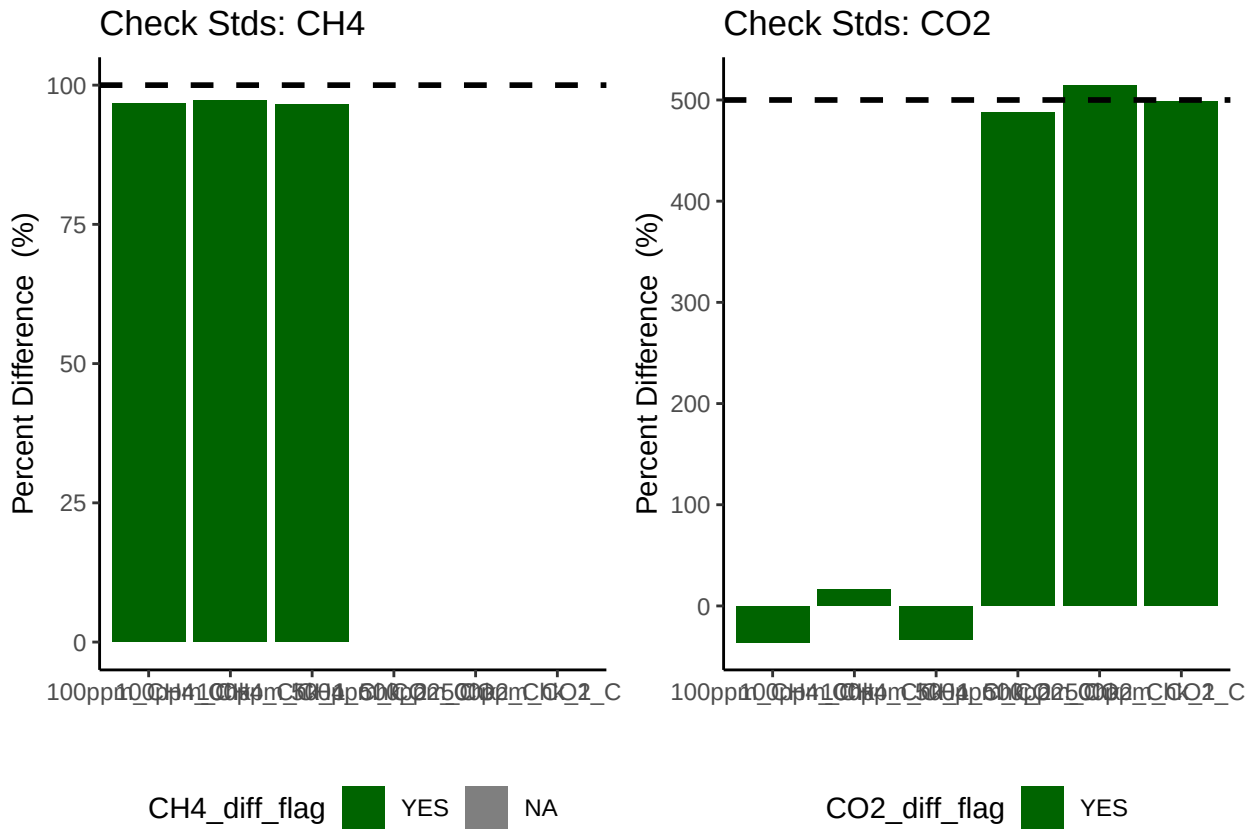
```
#head(raw)

#pull out methane standards
Samples <-  raw %>%
  filter(!str_detect(Sample_Type, "STD_CH4")) %>%
  filter(!str_detect(Sample_Type, "STD_CO2")) %>%
  filter(!str_detect(Sample_Type, "Blank")) %>%
  filter(!str_detect(Sample_Type, "Chk_STD")) %>%
   filter(!str_detect(Sample_Type, "CHKSTD")) %>%
  filter(!str_detect(Sample_Type, "CHK_STD")) %>%
  filter(!str_detect(Sample_Type, "NA"))
#head(Samples)

#Now flag any areas that are above the 100ppm area for CH4
Samples$CH4_Curve <- ifelse(Samples$CH4_Area >71000, "High", "Low")
#head(Samples)

#Calculate CH4 concentrations in ppm
Samples$CH4_Conc_ppm <- ifelse(Samples$CH4_Area >71000, (Samples$CH4_Area-Slope_CH4_high$Intercept)/Slo

#Calculate CO2 concentrations in ppm
Samples$CO2_Conc_ppm <- ((Samples$CO2_Area-Slope_CO2$Intercept)/Slope_CO2$Slope)
```

```r
#head(Samples)

##########make flags for any dilutions needed
#highest CH4 standard = 10000
#highest CO2 standard = 50000

Samples$CH4_Flag <- ifelse(Samples$CH4_Conc_ppm >10000, "Needs Dilution", "Within Range")
Samples$CO2_Flag <- ifelse(Samples$CO2_Conc_ppm >50000, "Needs Dilution", "Within Range")
#head(Samples)
```

Check the Check Standards

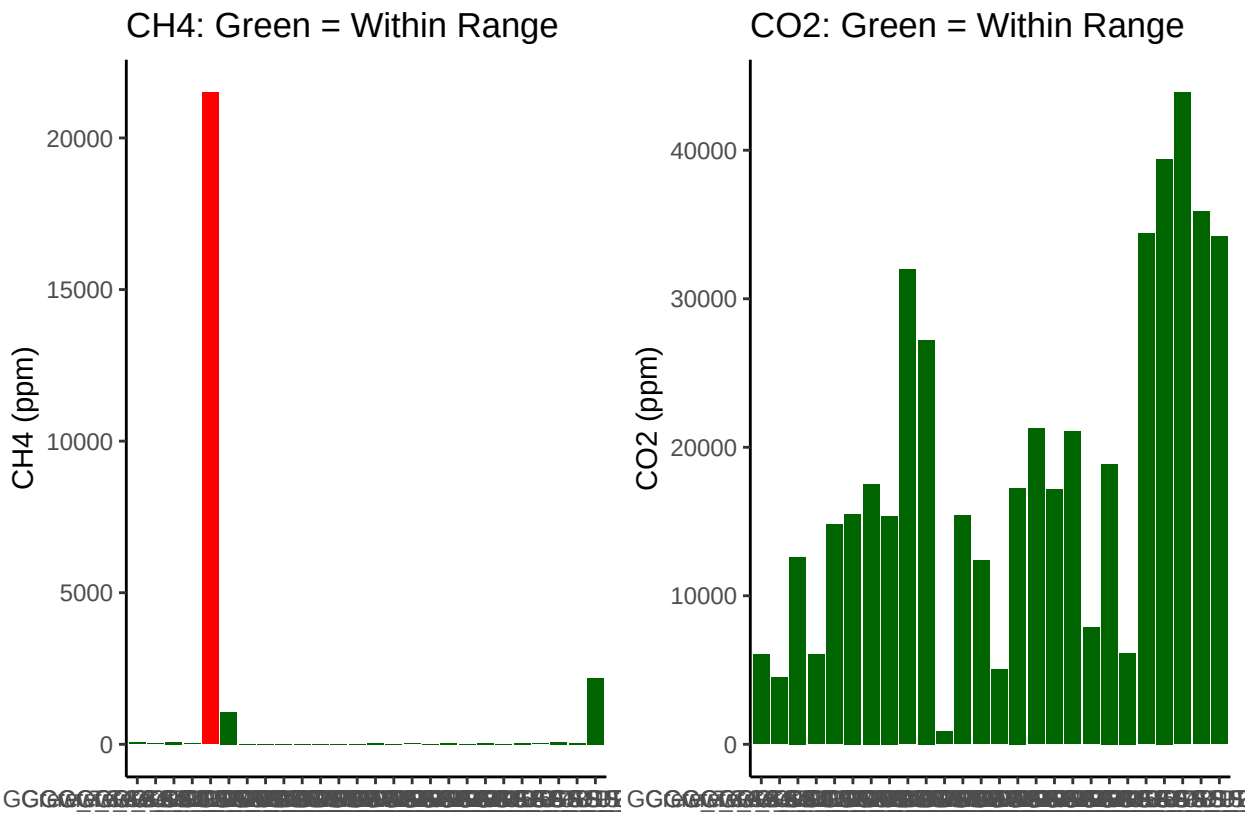
```
## Warning: Using 'size' aesthetic for lines was deprecated in ggplot2 3.4.0.
## i Please use 'linewidth' instead.
## This warning is displayed once every 8 hours.
## Call 'lifecycle::last_lifecycle_warnings()' to see where this warning was
## generated.
```

```
## Warning: Removed 3 rows containing missing values or values outside the scale range
## ('geom_bar()').
```



Dilution correct samples

```
#multiply the concentration by the dilution factor
Samples$CH4_Conc_ppm_dilcorr <- (Samples$CH4_Conc_ppm * Samples$Dilution_Factor)

Samples$CO2_Conc_ppm_dilcorr <- (Samples$CO2_Conc_ppm * Samples$Dilution_Factor)

#check results
#head(Samples)

#quick first look at the samples
ch4_samples <-  ggplot(data = Samples, aes(x = Sample_ID, y = CH4_Conc_ppm, fill=CH4_Flag)) +
       geom_bar(stat = 'identity') +
        scale_fill_manual(values=c( "red","darkgreen" ))+
        #scale_fill_gradient2(low='red', mid='white', high='blue', space='Lab') +
        theme_classic() + labs(x= " ", y="CH4 (ppm)", title="CH4: Green = Within Range") +
        theme(legend.position="none")


co2_samples <-  ggplot(data = Samples, aes(x = Sample_ID, y = CO2_Conc_ppm, fill=CO2_Flag)) +
       geom_bar(stat = 'identity') +
        scale_fill_manual(values=c( "darkgreen", "red"))+
        #scale_fill_gradient2(low='red', mid='white', high='blue', space='Lab') +
        theme_classic() + labs(x= " ", y="CO2 (ppm)", title="CO2: Green = Within Range") +
        theme(legend.position="none")

ggarrange(ch4_samples, co2_samples, nrow=1, ncol=2)
```



Write out processed data & slopes

```
#check results
head(Samples)
```

```
##     Machine                User Run_Date Sample_Type Type1 Sample_Year
## 1 Varian GC Stephanie J. Wilson   202208     Unknown  TGAS        2022
## 2 Varian GC Stephanie J. Wilson   202208     Unknown  TGAS        2022
## 3 Varian GC Stephanie J. Wilson   202208     Unknown  TGAS        2022
## 4 Varian GC Stephanie J. Wilson   202208     Unknown  TGAS        2022
## 5 Varian GC Stephanie J. Wilson   202208     Unknown  TGAS        2022
## 6 Varian GC Stephanie J. Wilson   202208     Unknown  TGAS        2022
##   Sample_Month          Sample_ID Dilution_Factor STD_Conc CO2_Area CH4_Area
## 1       August GCrew_TGAS_TR_SF_1               7       NA   938587    41923
## 2       August GCrew_TGAS_TR_SF_2               7       NA   699652    21764
## 3       August GCrew_TGAS_TR_SF_3               7       NA  1952184    49939
## 4       August GCrew_TGAS_TR_SF_4               7       NA   941776    19526
## 5       August GCrew_TGAS_TR_SF_5               7       NA  2291292 14599628
## 6       August GCrew_TGAS_TR_SF_6               7       NA  2400385   730991
##   Field.Notes Lab.Notes CH4_Curve CH4_Conc_ppm CO2_Conc_ppm       CH4_Flag
## 1          NA        NA       Low     57.90911     6034.637   Within Range
## 2          NA        NA       Low     29.28472     4486.528   Within Range
## 3          NA        NA       Low     69.29128    12601.941   Within Range
## 4          NA        NA       Low     26.10691     6055.299   Within Range
```

```
## 5          NA        NA      High  21504.60758    14799.091 Needs Dilution
## 6          NA        NA      High   1071.51256    15505.927   Within Range
##       CO2_Flag CH4_Conc_ppm_dilcorr CO2_Conc_ppm_dilcorr
## 1 Within Range             405.3638             42242.46
## 2 Within Range             204.9930             31405.70
## 3 Within Range             485.0390             88213.58
## 4 Within Range             182.7484             42387.10
## 5 Within Range          150532.2531            103593.64
## 6 Within Range            7500.5879            108541.49
```

```
#pull out what we need
Samples1 <- Samples[ ,c(1:3,5:9,13, 18:21)]
head(Samples1)
```

```
##     Machine                User Run_Date Type1 Sample_Year Sample_Month
## 1 Varian GC Stephanie J. Wilson   202208  TGAS        2022       August
## 2 Varian GC Stephanie J. Wilson   202208  TGAS        2022       August
## 3 Varian GC Stephanie J. Wilson   202208  TGAS        2022       August
## 4 Varian GC Stephanie J. Wilson   202208  TGAS        2022       August
## 5 Varian GC Stephanie J. Wilson   202208  TGAS        2022       August
## 6 Varian GC Stephanie J. Wilson   202208  TGAS        2022       August
##            Sample_ID Dilution_Factor Field.Notes       CH4_Flag     CO2_Flag
## 1 GCrew_TGAS_TR_SF_1               7          NA   Within Range Within Range
## 2 GCrew_TGAS_TR_SF_2               7          NA   Within Range Within Range
## 3 GCrew_TGAS_TR_SF_3               7          NA   Within Range Within Range
## 4 GCrew_TGAS_TR_SF_4               7          NA   Within Range Within Range
## 5 GCrew_TGAS_TR_SF_5               7          NA Needs Dilution Within Range
## 6 GCrew_TGAS_TR_SF_6               7          NA   Within Range Within Range
##   CH4_Conc_ppm_dilcorr CO2_Conc_ppm_dilcorr
## 1             405.3638             42242.46
## 2             204.9930             31405.70
## 3             485.0390             88213.58
## 4             182.7484             42387.10
## 5          150532.2531            103593.64
## 6            7500.5879            108541.49
```

```
Samples1 <- Samples1 %>%
  separate(Sample_ID, into = c("Site", "Gas_Sample", "Zone", "Tree_Code", "Replicate"), sep = "_", remo
  mutate(Tree_Info = case_when(
    Tree_Code == "DS" ~ "Dead Standing",
    Tree_Code == "SF" ~ "Sapflow Monitoring",
    TRUE ~ "Other"  # Optional: handles any values that aren't DS or SF
  )) %>%
  mutate(Status = case_when(
    Tree_Code == "DS" ~ "Dead Standing",
    Tree_Code == "SF" ~ "Living",
    TRUE ~ "Other"
  )) %>%
  mutate(Project = "COMPASS: Synoptic",
         Region = "CB") %>%
  rename( Year = Sample_Year,
          Month = Sample_Month,
          CH4_ppm = CH4_Conc_ppm_dilcorr ,
```

```
          CO2_ppm = CO2_Conc_ppm_dilcorr )  %>%
  mutate(CH4_Flag = case_when(
    CH4_Flag == "Needs_Dilution" ~ "Over Std Curve Range",
    TRUE ~ "Within Std Curve Range"
  )) %>%
  mutate(CO2_Flag = case_when(
    CO2_Flag == "Needs_Dilution" ~ "Over Std Curve Range",
    TRUE ~ "Within Std Curve Range"
  ))

final <- Samples1 %>%
  select( "Project", "Region" , "Year","Month" ,"Site", "Zone", "Gas_Sample",
          "Sample_ID", "Tree_Code", "Replicate", "Status", "Tree_Info",
          "CH4_ppm", "CH4_Flag", "CO2_ppm", "CO2_Flag")

write.csv(final, "Processed Data/COMPASS_Synoptic_TGW_202208_Processed.csv")
```

#end