COMPASS_Synoptic_TGW_2022: August- Run #2 (a)

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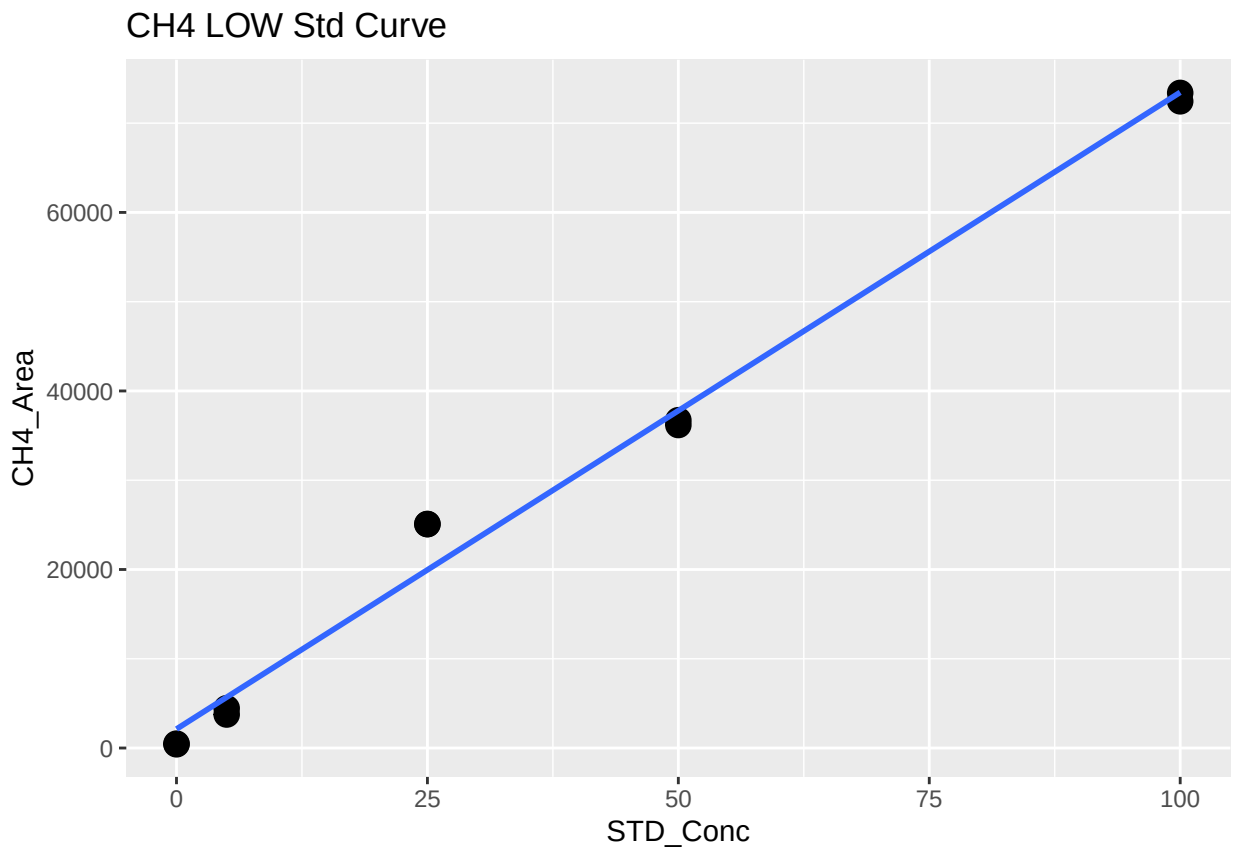
##Set Up

Read in first data file and assess standard curves

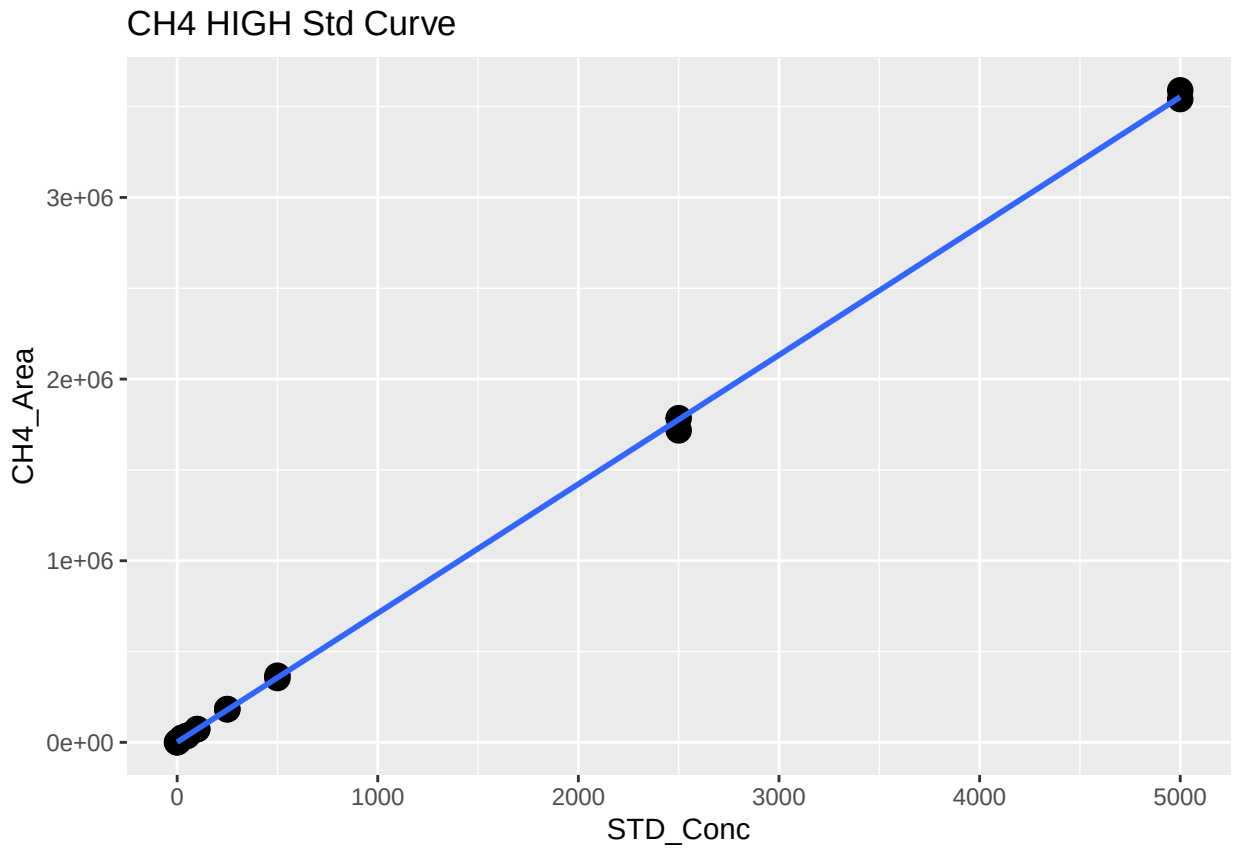
```
##     Machine                User Run_Date Sample_Type Type1 Sample_Year
## 1 Varian GC Stephanie J. Wilson   202208       Blank  TGAS        2022
## 2 Varian GC Stephanie J. Wilson   202208       Blank  TGAS        2022
## 3 Varian GC Stephanie J. Wilson   202208     Chk_STD  TGAS        2022
## 4 Varian GC Stephanie J. Wilson   202208     Chk_STD  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_1               1       NA    14802      418
## 2       August          Blank_2               1       NA    15298      492
## 3       August   CH4_Chk_100ppm               1      100        0    64136
## 4       August   CO2_Chk_500ppm               1      500    73831      209
## 5       August CH4_Chk_100ppm_1               1      100     2124    72730
## 6       August CO2_Chk_500ppm_1               1      500    84203      275
##   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'
```



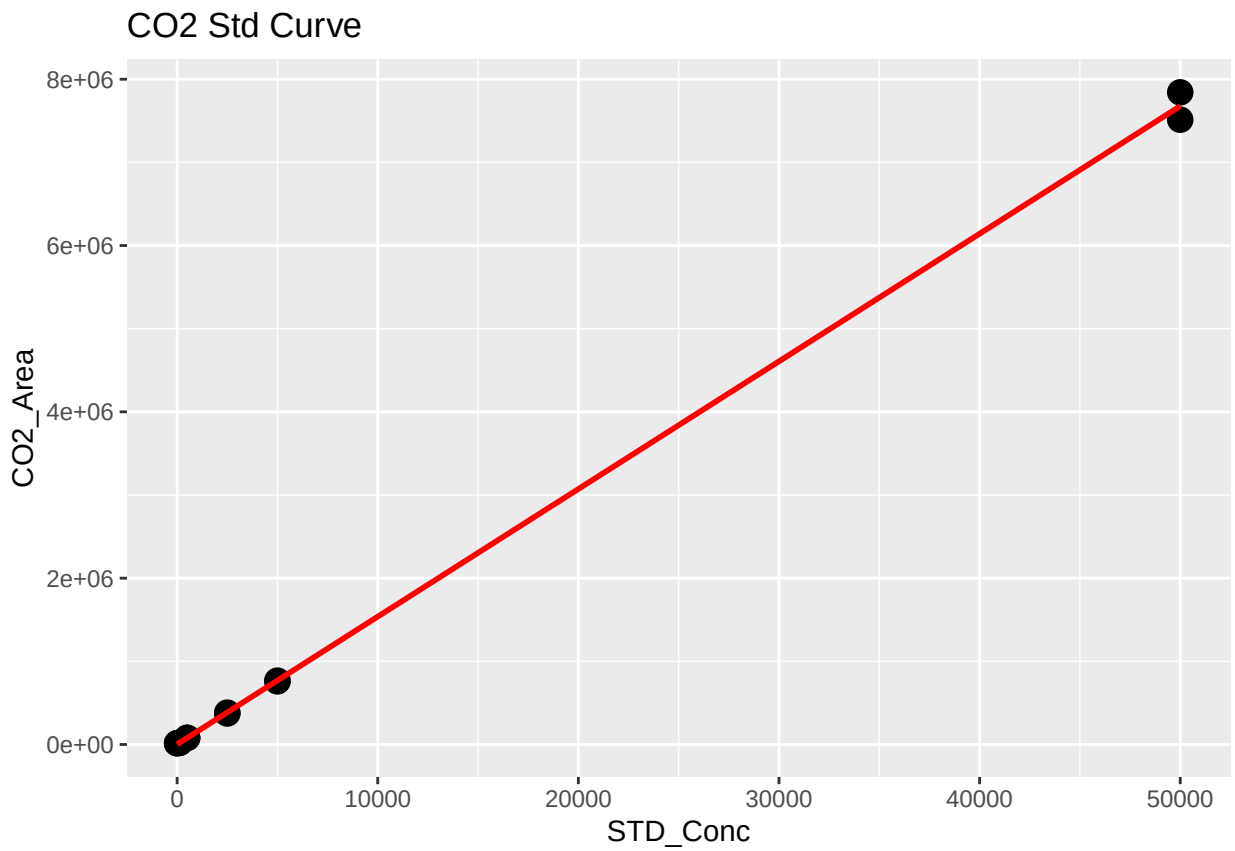

```
##
## Call:
## lm(formula = stds_ch4_low$CH4_Area ~ stds_ch4_low$STD_Conc)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -1939.9 -1627.9 -1149.2  -299.4  5139.9
##
## Coefficients:
##                       Estimate Std. Error t value Pr(>|t|)
## (Intercept)            2126.64    1296.86    1.64     0.14
## stds_ch4_low$STD_Conc   713.26      25.29   28.20  2.7e-09 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2921 on 8 degrees of freedom
## Multiple R-squared:   0.99,  Adjusted R-squared:  0.9888
## F-statistic: 795.5 on 1 and 8 DF,  p-value: 2.697e-09

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



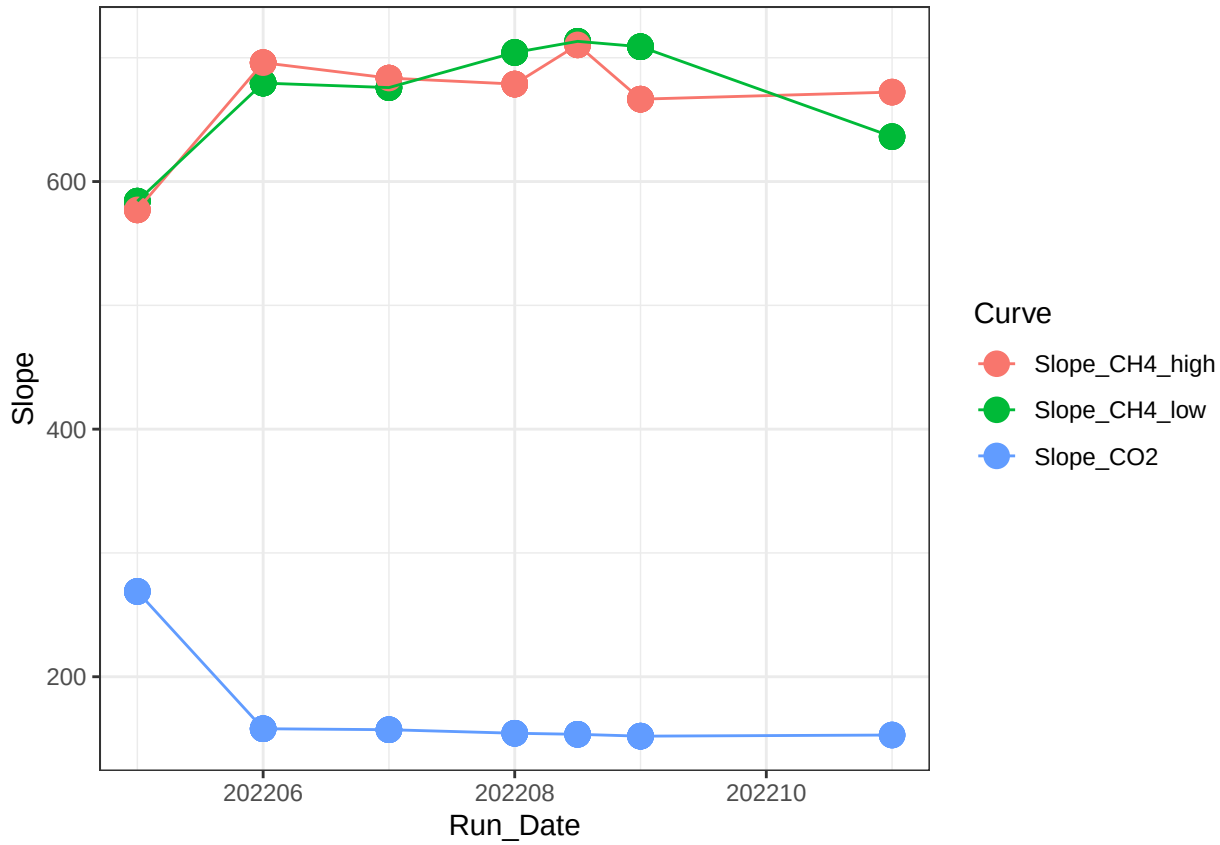

```
##
## Call:
## lm(formula = stds_ch4$CH4_Area ~ stds_ch4$STD_Conc)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -59583   -682    184   5799  36377
##
## Coefficients:
##                   Estimate Std. Error t value Pr(>|t|)
## (Intercept)       1118.715   4950.443   0.226    0.824
## stds_ch4$STD_Conc  710.435      2.643 268.804   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 18190 on 16 degrees of freedom
## Multiple R-squared:  0.9998, Adjusted R-squared:  0.9998
## F-statistic: 7.226e+04 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
## -163495   -5085      55    3750  165566
##
## Coefficients:
##                     Estimate Std. Error t value Pr(>|t|)
## (Intercept)         2267.436  24227.005   0.094    0.927
## stds_co2$STD_Conc    153.482      1.179 130.129   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 74000 on 10 degrees of freedom
## Multiple R-squared:  0.9994, Adjusted R-squared:  0.9994
## F-statistic: 1.693e+04 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)
```

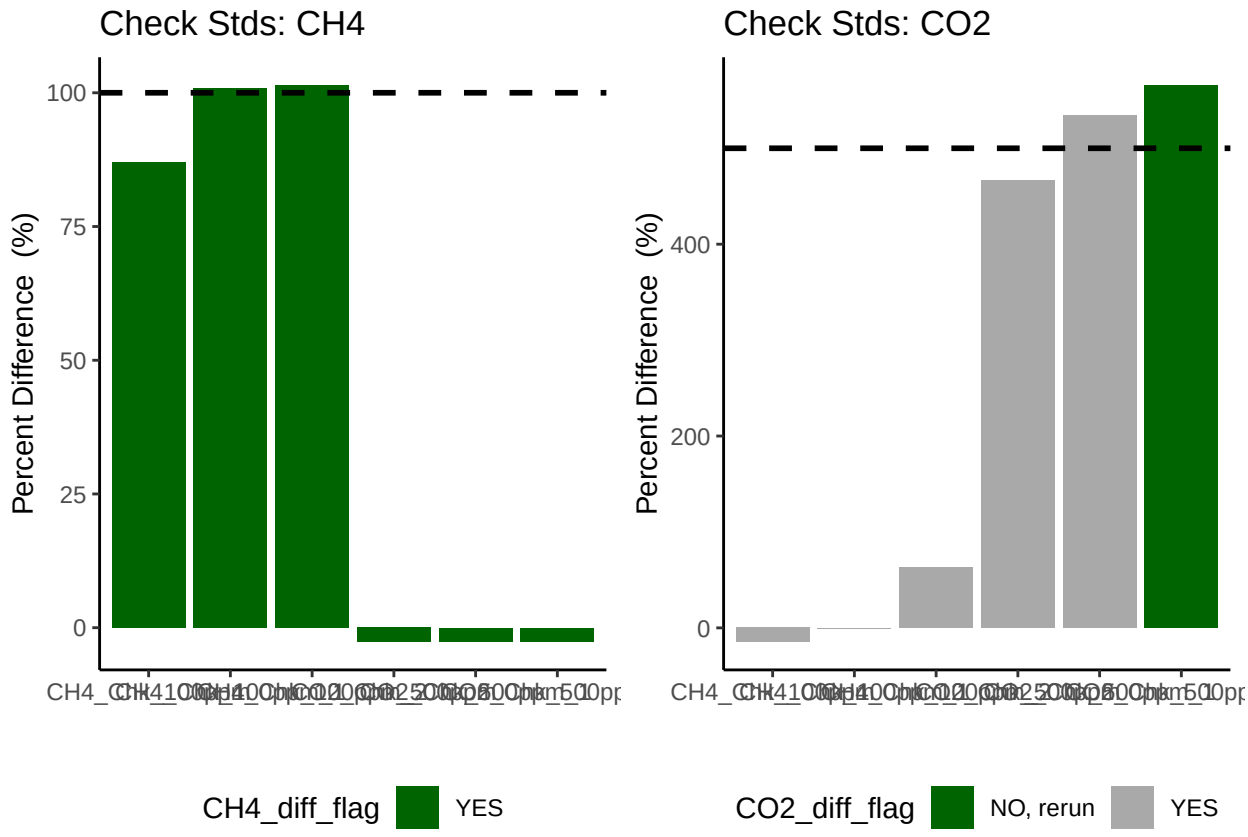
```r
#head(Samples)

##########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.
```



Dilution correct samples

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

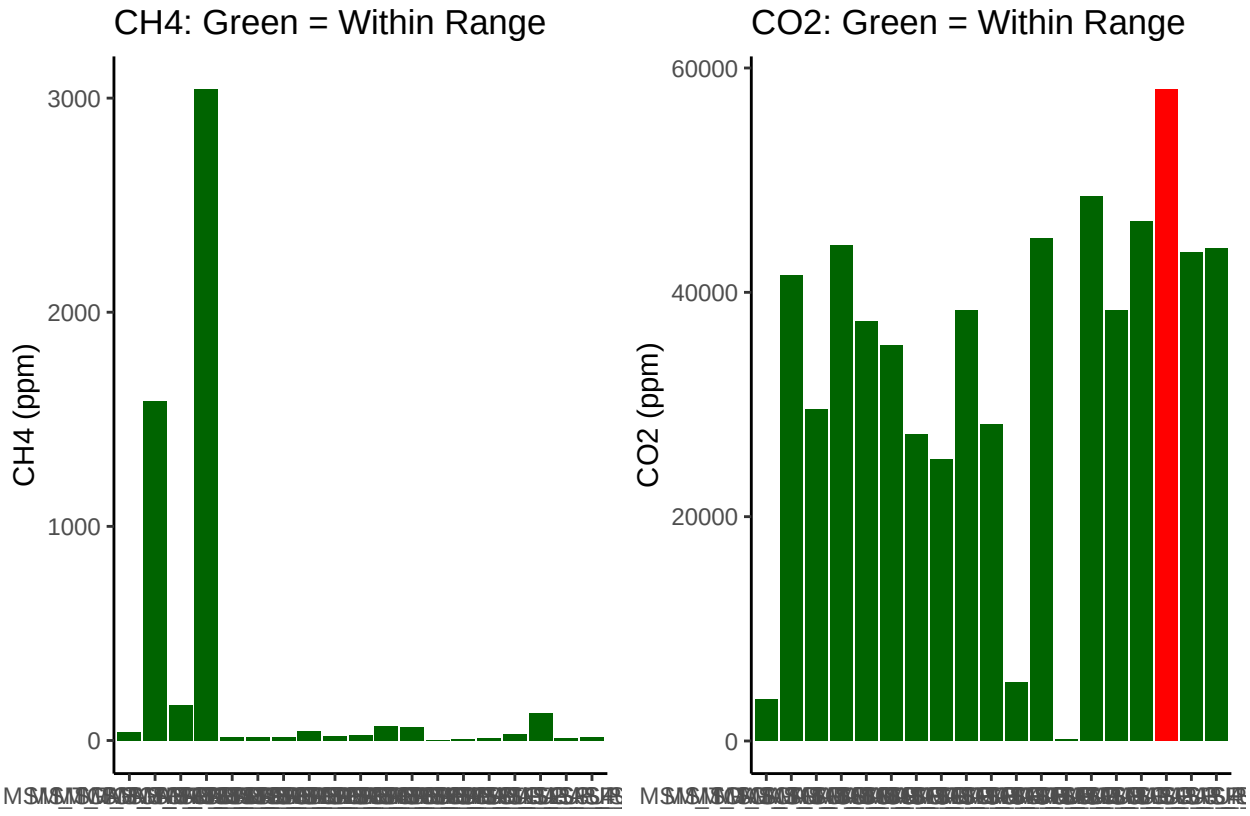
```
Samples$CO2_Conc_ppm_dilcorr <- (Samples$CO2_Conc_ppm * Samples$Dilution_Factor)

#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( "darkgreen", "red" ))+
        #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("red","darkgreen" ))+
        #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 MSM_TGAS_UP_SF_1               2       NA  6874162    46851
## 2       August MSM_TGAS_UP_SF_2               2       NA    24098      456
## 3       August MSM_TGAS_UP_SF_3               2       NA  7457774     8419
## 4       August MSM_TGAS_UP_SF_4               2       NA  5886606     9745
## 5       August MSM_TGAS_UP_SF_5               2       NA  7109680    24674
## 6       August MSM_TGAS_UP_SF_6               2       NA  8923495    91471
##   Field.Notes Lab.Notes CH4_Curve CH4_Conc_ppm CO2_Conc_ppm     CH4_Flag
## 1          NA        NA       Low    62.704392    44773.192 Within Range
## 2          NA        NA       Low    -2.342270      142.235 Within Range
## 3          NA        NA       Low     8.822006    48575.662 Within Range
## 4          NA        NA       Low    10.681083    38338.862 Within Range
## 5          NA        NA       Low    31.611821    46307.688 Within Range
## 6          NA        NA      High   127.178863    58125.431 Within Range
##         CO2_Flag CH4_Conc_ppm_dilcorr CO2_Conc_ppm_dilcorr
## 1   Within Range            125.40878             89546.38
## 2   Within Range             -4.68454               284.47
## 3   Within Range             17.64401             97151.32
## 4   Within Range             21.36217             76677.72
## 5   Within Range             63.22364             92615.38
## 6 Needs Dilution            254.35773            116250.86
```

```
#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 MSM_TGAS_UP_SF_1               2          NA Within Range   Within Range
## 2 MSM_TGAS_UP_SF_2               2          NA Within Range   Within Range
## 3 MSM_TGAS_UP_SF_3               2          NA Within Range   Within Range
## 4 MSM_TGAS_UP_SF_4               2          NA Within Range   Within Range
## 5 MSM_TGAS_UP_SF_5               2          NA Within Range   Within Range
## 6 MSM_TGAS_UP_SF_6               2          NA Within Range Needs Dilution
```

```
##   CH4_Conc_ppm_dilcorr CO2_Conc_ppm_dilcorr
## 1            125.40878             89546.38
## 2             -4.68454               284.47
## 3             17.64401             97151.32
## 4             21.36217             76677.72
## 5             63.22364             92615.38
## 6            254.35773            116250.86
```

```
Samples1 <- Samples1 %>%
  separate(Sample_ID, into = c("Site", "Gas_Sample", "Zone", "Tree_Code", "Replicate"), sep = "_", remov
  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_202208a_Processed.csv")
```

#end