COMPASS_Synoptic_TGW_2022: June

Stephanie J. Wilson

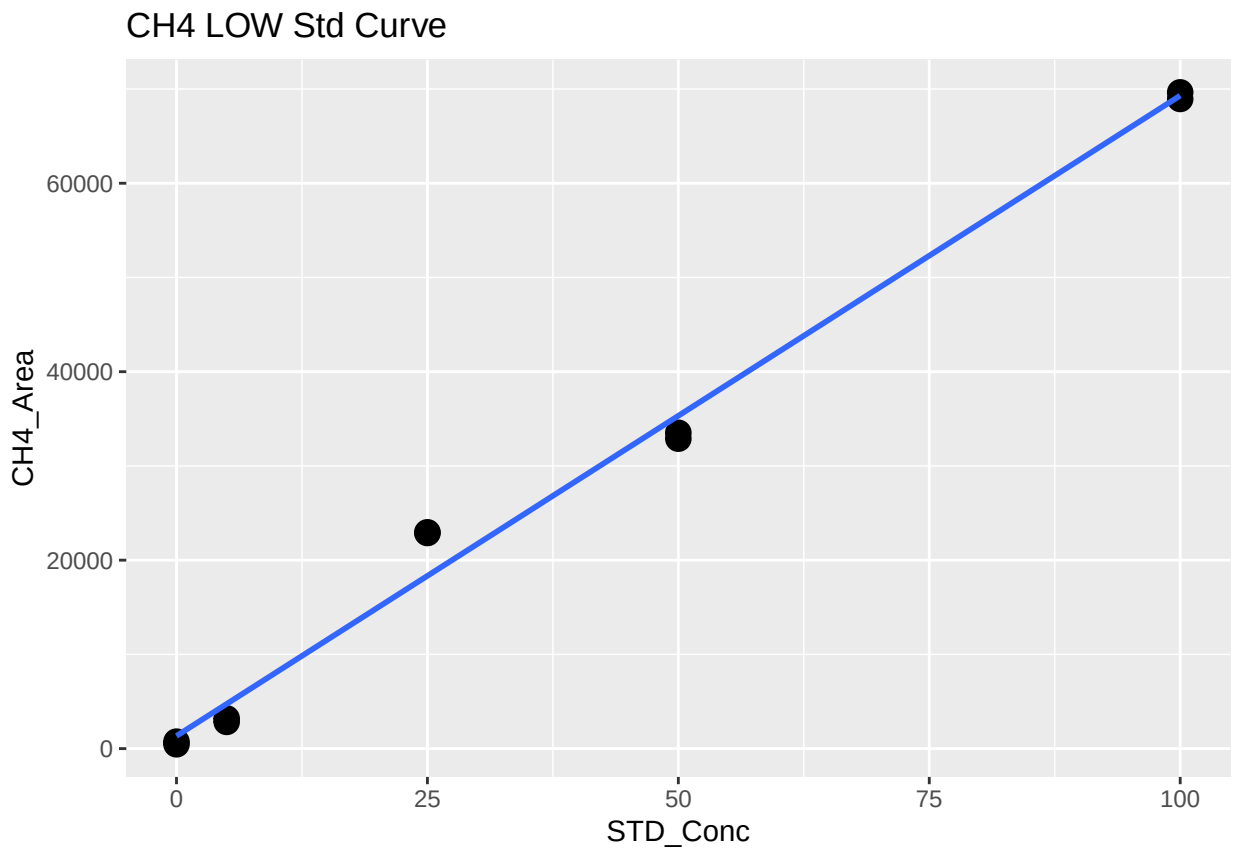
2023-01-14

##Set Up

Read in first data file and assess standard curves

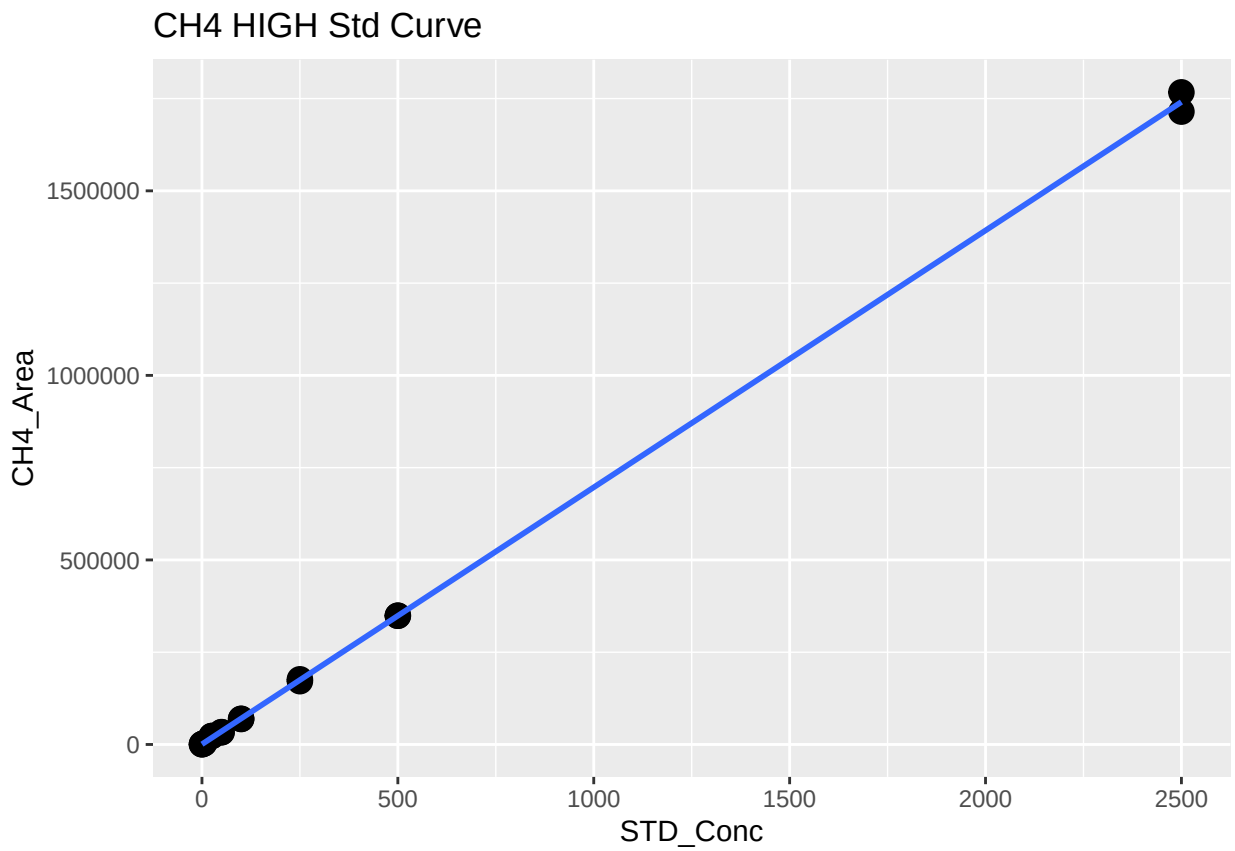
```
##     Machine                User Run_Date Sample_Type Type1 Sample_Year
## 1 Varian GC Stephanie J. Wilson   202206       Blank  TGAS        2022
## 2 Varian GC Stephanie J. Wilson   202206     Unknown  TGAS        2022
## 3 Varian GC Stephanie J. Wilson   202206     Unknown  TGAS        2022
## 4 Varian GC Stephanie J. Wilson   202206     Unknown  TGAS        2022
## 5 Varian GC Stephanie J. Wilson   202206     Unknown  TGAS        2022
## 6 Varian GC Stephanie J. Wilson   202206     Unknown  TGAS        2022
##   Sample_Month        Sample_ID Dilution_Factor STD_Conc CH4_Area CO2_Area
## 1         June          Blank_1               1       NA        0        0
## 2         June MSM_TGAS_UP_SF_1               2       NA    12697  1791814
## 3         June MSM_TGAS_UP_SF_2               2       NA    23232  5697789
## 4         June MSM_TGAS_UP_SF_3               2       NA     8442 10718524
## 5         June MSM_TGAS_UP_SF_4               2       NA     8731  6094426
## 6         June MSM_TGAS_UP_SF_5               2       NA    34611  8661859
##   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'
```



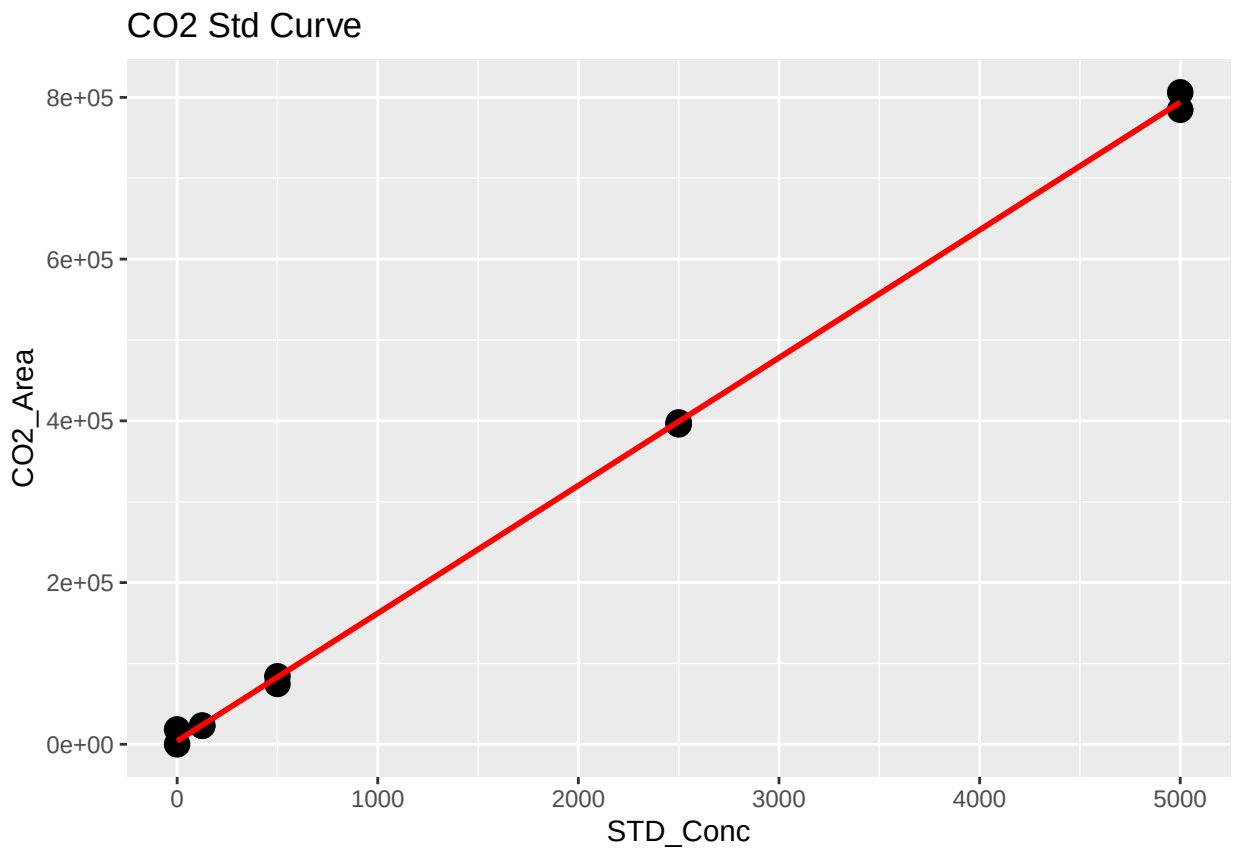

```
##
## Call:
## lm(formula = stds_ch4_low$CH4_Area ~ stds_ch4_low$STD_Conc)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -2430.8 -1733.7  -744.1   173.6  4623.8
##
## Coefficients:
##                       Estimate Std. Error t value Pr(>|t|)
## (Intercept)            1342.56    1201.65   1.117    0.296
## stds_ch4_low$STD_Conc   679.55      23.43  29.001 2.16e-09 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2706 on 8 degrees of freedom
## Multiple R-squared:  0.9906, Adjusted R-squared:  0.9894
## F-statistic: 841.1 on 1 and 8 DF,  p-value: 2.163e-09

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



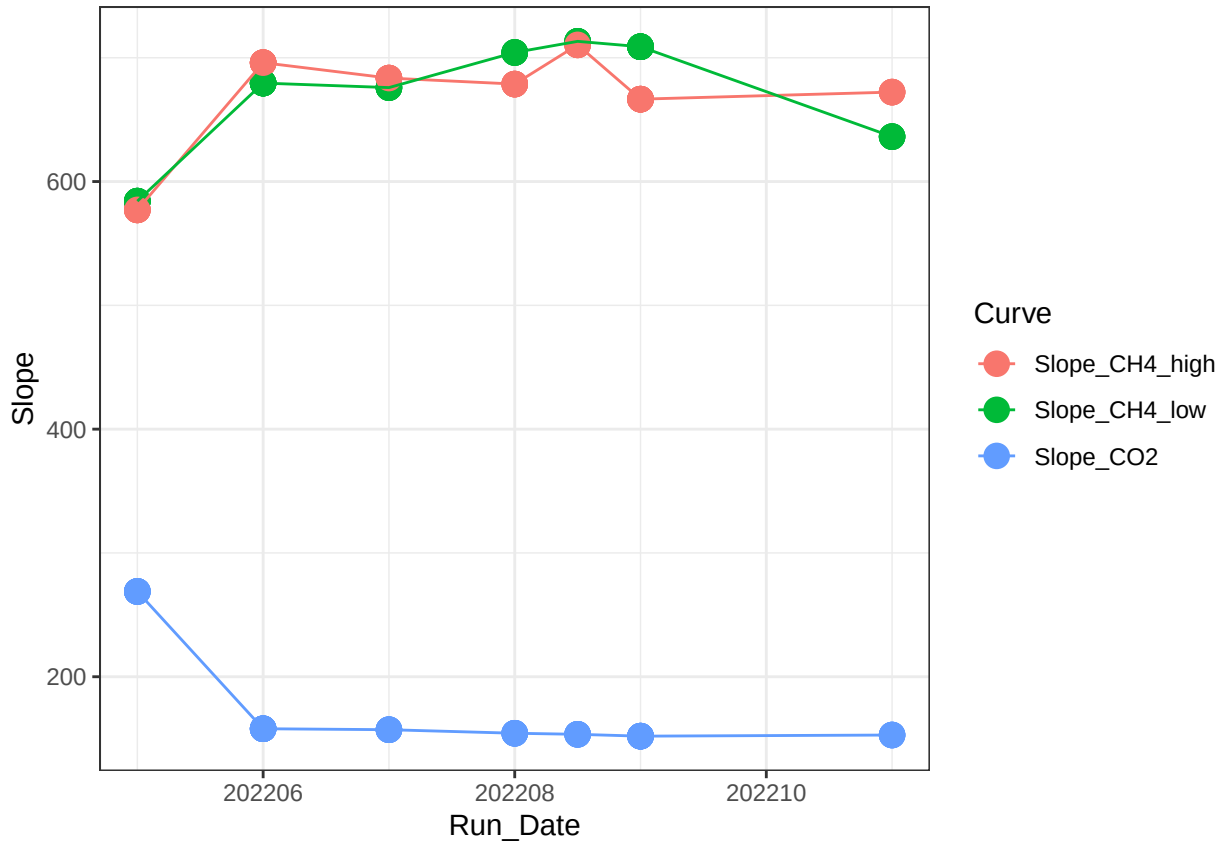

```
##
## Call:
## lm(formula = stds_ch4$CH4_Area ~ stds_ch4$STD_Conc)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -26065.1  -1479.7   -414.3    670.4  26209.9
##
## Coefficients:
##                   Estimate Std. Error t value Pr(>|t|)
## (Intercept)        664.824   2880.168   0.231    0.821
## stds_ch4$STD_Conc  696.019      3.177 219.093   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 10150 on 14 degrees of freedom
## Multiple R-squared:  0.9997, Adjusted R-squared:  0.9997
## F-statistic: 4.8e+04 on 1 and 14 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
## -9295.7 -3873.2  -928.8   611.6 14324.4
##
## Coefficients:
##                    Estimate Std. Error t value Pr(>|t|)
## (Intercept)        4049.58    3415.57   1.186     0.27
## stds_co2$STD_Conc   157.99       1.36 116.130 3.38e-14 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 8233 on 8 degrees of freedom
## Multiple R-squared:  0.9994, Adjusted R-squared:  0.9993
## F-statistic: 1.349e+04 on 1 and 8 DF,  p-value: 3.379e-14

##   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)
```

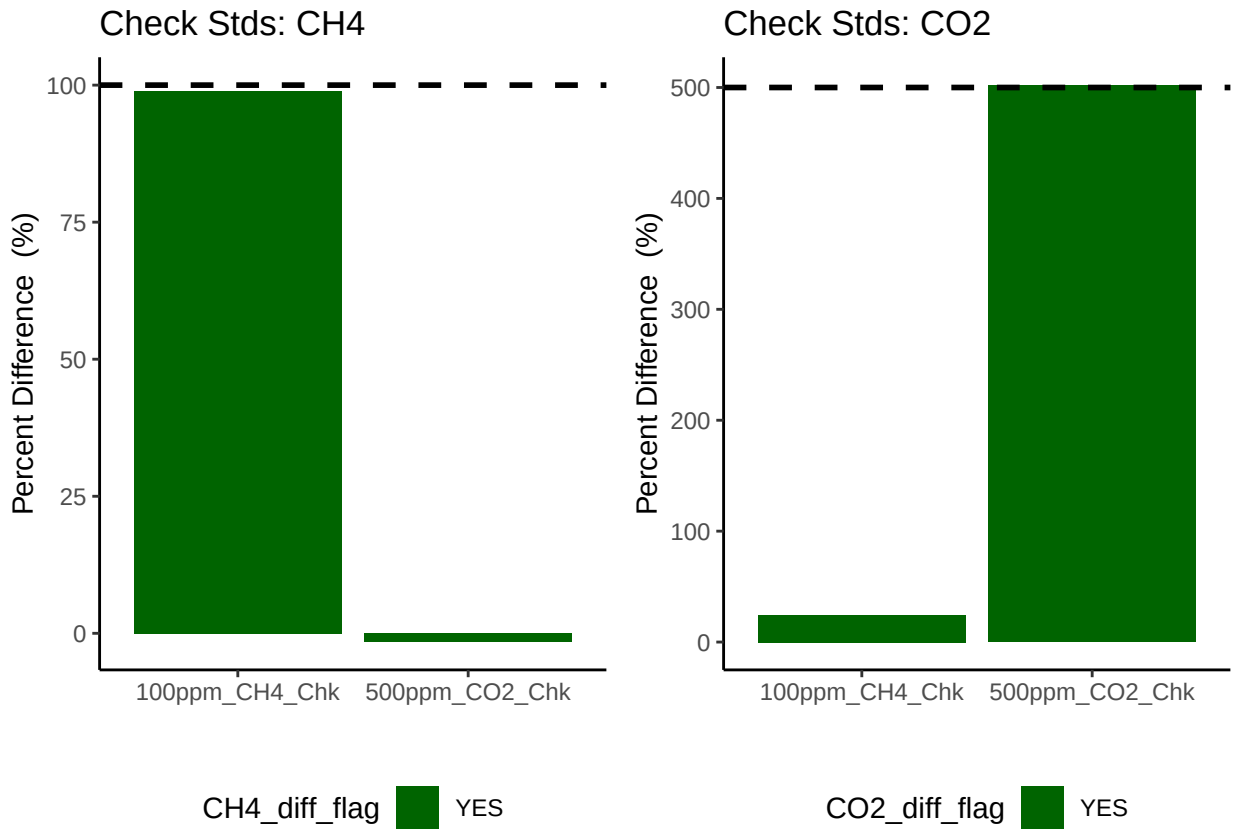
```r
#head(Samples)

##########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)
```

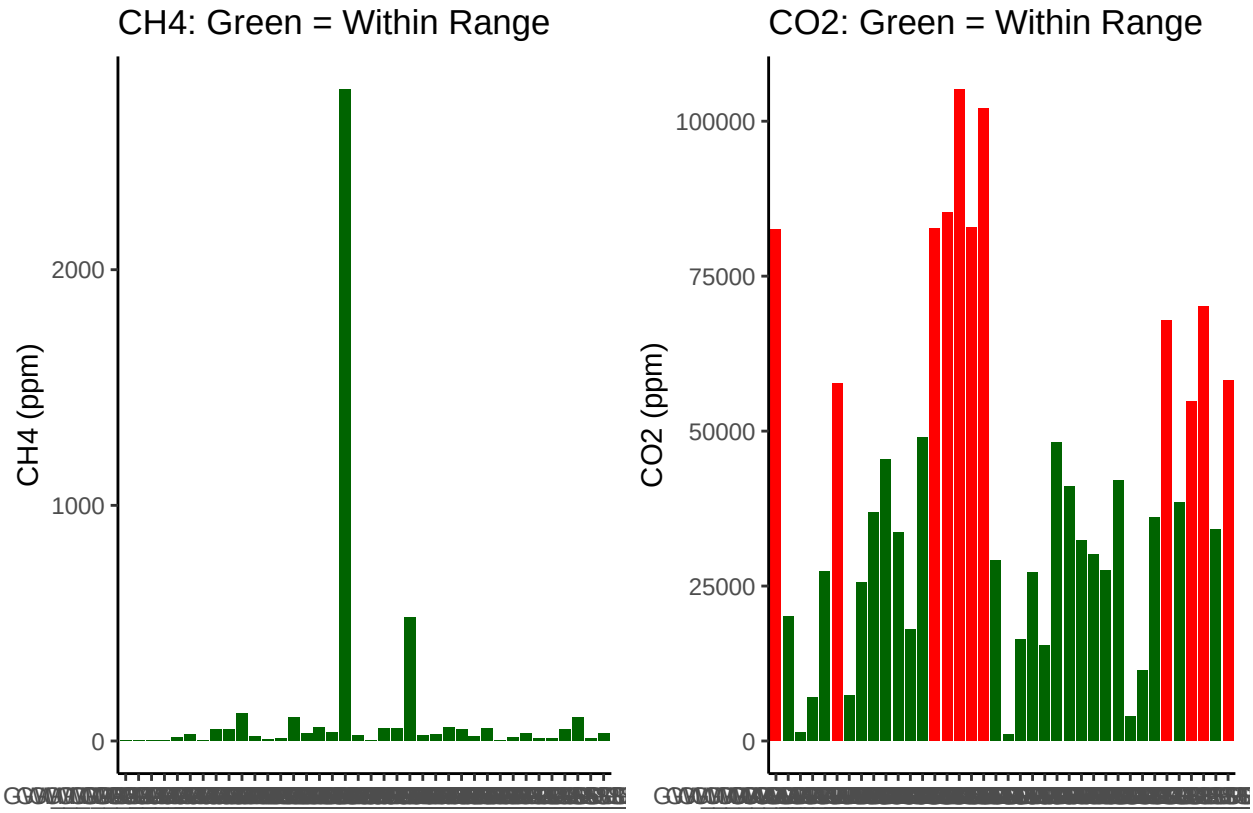
```r
Samples$CO2_Conc_ppm_dilcorr <- (Samples$CO2_Conc_ppm * Samples$Dilution_Factor)

#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   202206     Unknown  TGAS        2022
## 2 Varian GC Stephanie J. Wilson   202206     Unknown  TGAS        2022
## 3 Varian GC Stephanie J. Wilson   202206     Unknown  TGAS        2022
## 4 Varian GC Stephanie J. Wilson   202206     Unknown  TGAS        2022
## 5 Varian GC Stephanie J. Wilson   202206     Unknown  TGAS        2022
## 6 Varian GC Stephanie J. Wilson   202206     Unknown  TGAS        2022
##   Sample_Month        Sample_ID Dilution_Factor STD_Conc CH4_Area CO2_Area
## 1         June MSM_TGAS_UP_SF_1               2       NA    12697  1791814
## 2         June MSM_TGAS_UP_SF_2               2       NA    23232  5697789
## 3         June MSM_TGAS_UP_SF_3               2       NA     8442 10718524
## 4         June MSM_TGAS_UP_SF_4               2       NA     8731  6094426
## 5         June MSM_TGAS_UP_SF_5               2       NA    34611  8661859
## 6         June MSM_TGAS_UP_SF_6               2       NA    68050 11080250
##   Field.Notes Lab.Notes CH4_Curve CH4_Conc_ppm CO2_Conc_ppm     CH4_Flag
## 1          NA        NA       Low     16.70887     11315.66 Within Range
## 2          NA        NA       Low     32.21188     36038.55 Within Range
## 3          NA        NA       Low     10.44734     67817.32 Within Range
## 4          NA        NA       Low     10.87262     38549.07 Within Range
## 5          NA        NA       Low     48.95689     54799.65 Within Range
## 6          NA        NA       Low     98.16478     70106.87 Within Range
##         CO2_Flag CH4_Conc_ppm_dilcorr CO2_Conc_ppm_dilcorr
## 1   Within Range             33.41775             22631.33
## 2   Within Range             64.42376             72077.11
## 3 Needs Dilution             20.89467            135634.65
## 4   Within Range             21.74524             77098.14
## 5 Needs Dilution             97.91379            109599.30
## 6 Needs Dilution            196.32956            140213.74
```

```
#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   202206  TGAS        2022         June
## 2 Varian GC Stephanie J. Wilson   202206  TGAS        2022         June
## 3 Varian GC Stephanie J. Wilson   202206  TGAS        2022         June
## 4 Varian GC Stephanie J. Wilson   202206  TGAS        2022         June
## 5 Varian GC Stephanie J. Wilson   202206  TGAS        2022         June
## 6 Varian GC Stephanie J. Wilson   202206  TGAS        2022         June
##          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 Needs Dilution
## 4 MSM_TGAS_UP_SF_4               2          NA Within Range   Within Range
## 5 MSM_TGAS_UP_SF_5               2          NA Within Range Needs Dilution
## 6 MSM_TGAS_UP_SF_6               2          NA Within Range Needs Dilution
```

```
##   CH4_Conc_ppm_dilcorr CO2_Conc_ppm_dilcorr
## 1             33.41775             22631.33
## 2             64.42376             72077.11
## 3             20.89467            135634.65
## 4             21.74524             77098.14
## 5             97.91379            109599.30
## 6            196.32956            140213.74
```

```
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_202206_Processed.csv")
```

#end