COMPASS_Synoptic_TGW_2022: July

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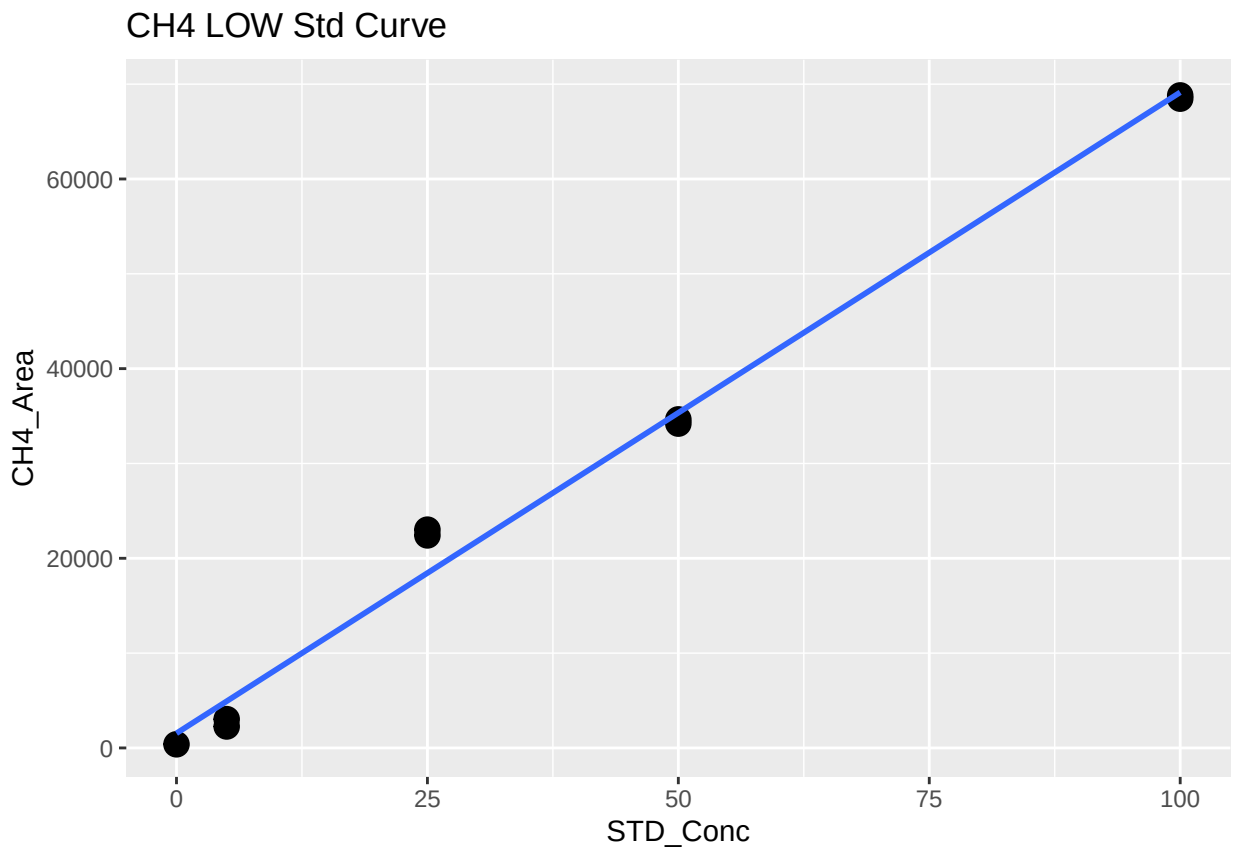
2023-01-14

##Set Up

Read in first data file and assess standard curves

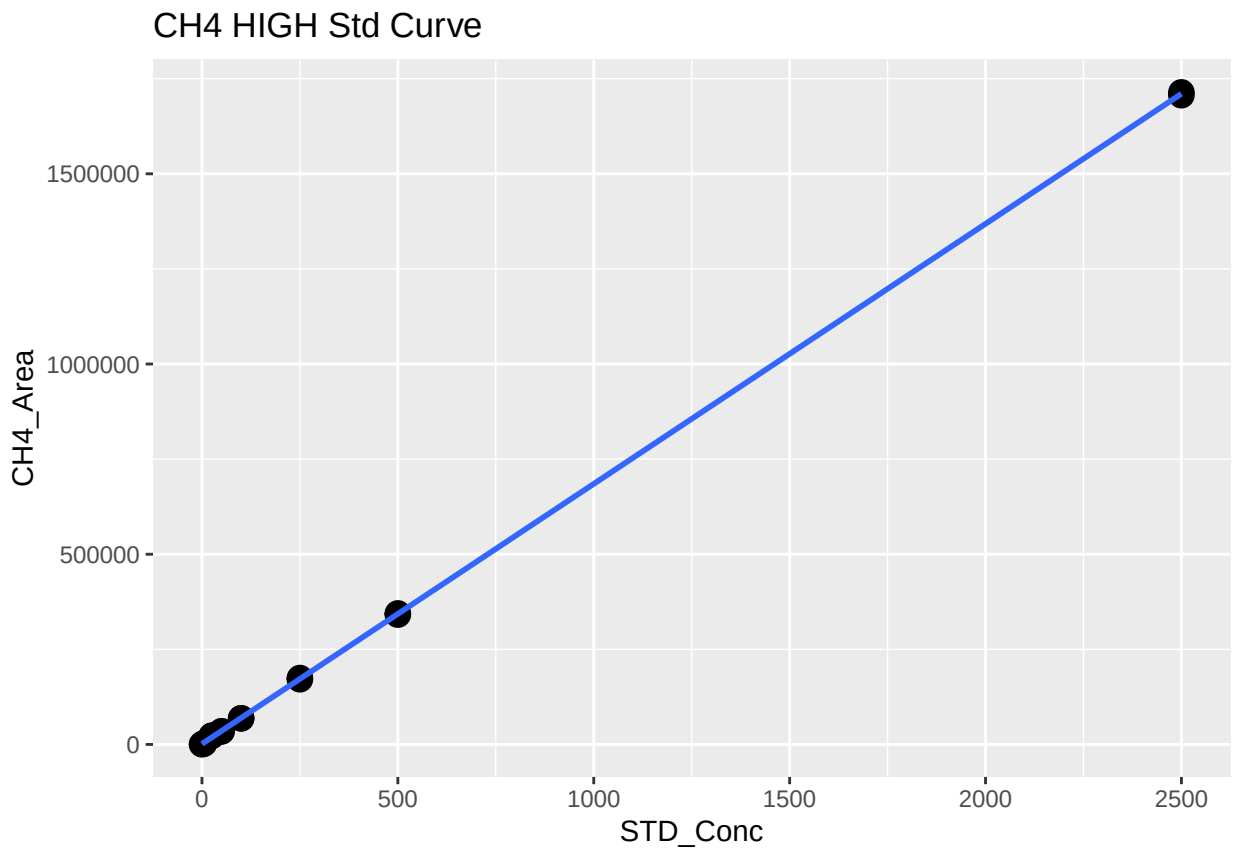
```
##     Machine                User Run_Date Sample_Type Type1 Sample_Year
## 1 Varian GC Stephanie J. Wilson   202207     Unknown  TGAS        2022
## 2 Varian GC Stephanie J. Wilson   202207     Unknown  TGAS        2022
## 3 Varian GC Stephanie J. Wilson   202207     Unknown  TGAS        2022
## 4 Varian GC Stephanie J. Wilson   202207     Unknown  TGAS        2022
## 5 Varian GC Stephanie J. Wilson   202207     Unknown  TGAS        2022
## 6 Varian GC Stephanie J. Wilson   202207     Unknown  TGAS        2022
##   Sample_Month          Sample_ID Dilution_Factor STD_Conc CH4_Area CO2_Area
## 1         July GCrew_Tgas_TR_SF_1               7       NA   387703  1228239
## 2         July GCrew_Tgas_TR_SF_2               7       NA   813894  1743563
## 3         July GCrew_Tgas_TR_SF_3               7       NA    98387  2163859
## 4         July GCrew_Tgas_TR_SF_4               7       NA   599507  2555958
## 5         July GCrew_Tgas_TR_SF_5               7       NA  8757124  1752010
## 6         July GCrew_Tgas_TR_SF_6               7       NA 13718650  1685685
##   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'
```



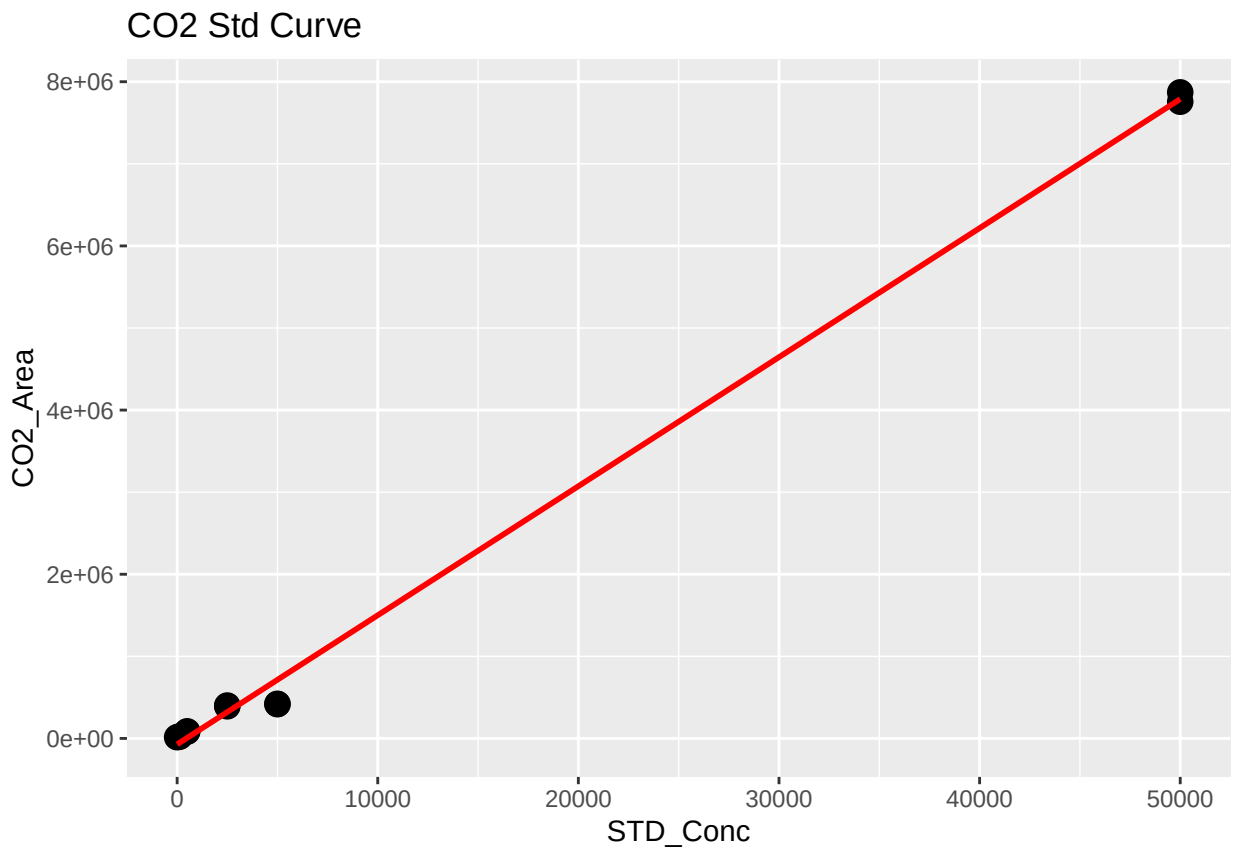

```
##
## Call:
## lm(formula = stds_ch4_low$CH4_Area ~ stds_ch4_low$STD_Conc)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -2663.1 -1163.6  -695.8  -324.1  4574.8
##
## Coefficients:
##                       Estimate Std. Error t value Pr(>|t|)
## (Intercept)            1547.59    1338.16   1.157    0.285
## stds_ch4_low$STD_Conc   675.90      24.75  27.304 2.27e-08 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2700 on 7 degrees of freedom
## Multiple R-squared:  0.9907, Adjusted R-squared:  0.9894
## F-statistic: 745.5 on 1 and 7 DF,  p-value: 2.267e-08

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



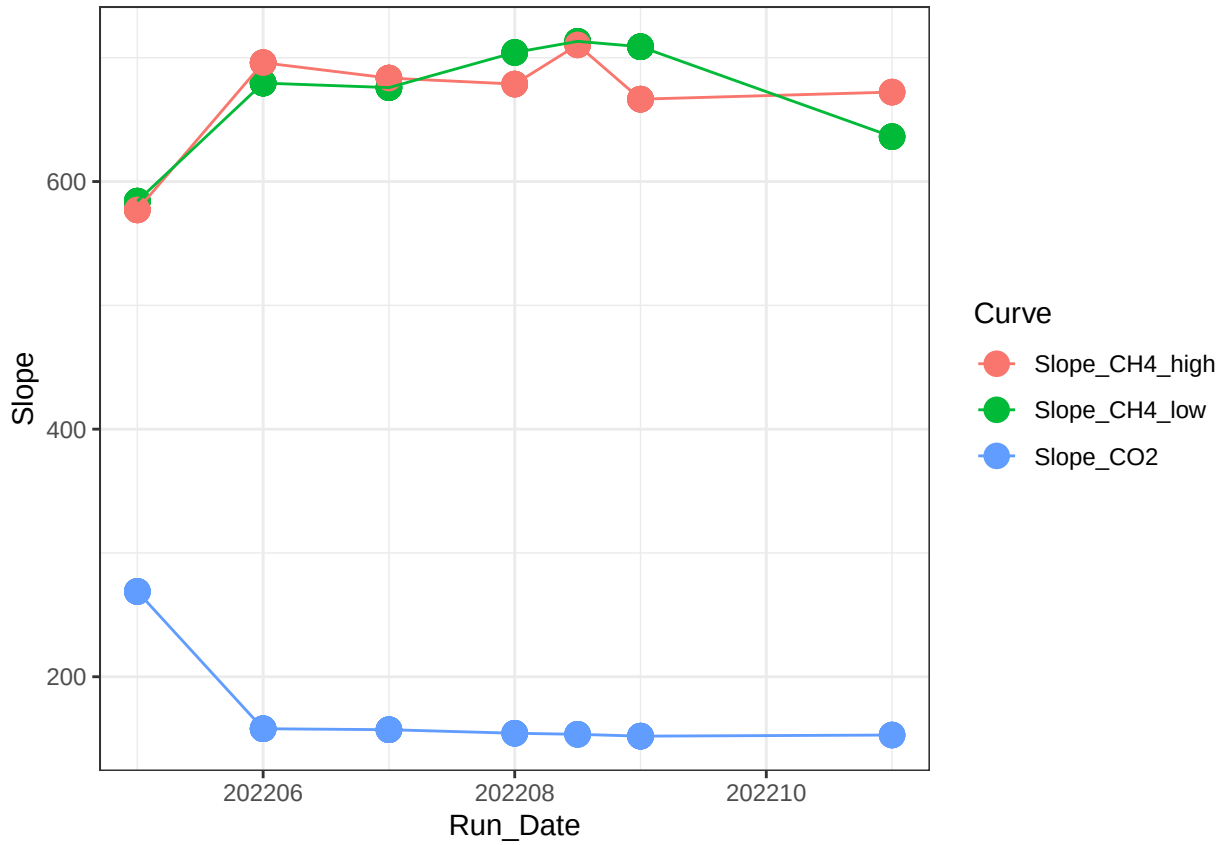

```
##
## Call:
## lm(formula = stds_ch4$CH4_Area ~ stds_ch4$STD_Conc)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -3795.6 -1512.2  -948.6  1849.4  4597.7
##
## Coefficients:
##                    Estimate Std. Error t value Pr(>|t|)
## (Intercept)       1332.5553   790.6757   1.685    0.116
## stds_ch4$STD_Conc  683.5880     0.8444 809.533   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2672 on 13 degrees of freedom
## Multiple R-squared:      1,  Adjusted R-squared:      1
## F-statistic: 6.553e+05 on 1 and 13 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
## -297324   18739   75227   78479   86329
##
## Coefficients:
##                      Estimate Std. Error t value Pr(>|t|)
## (Intercept)       -71502.431  54643.174  -1.309    0.223
## stds_co2$STD_Conc    157.207      2.547  61.723 3.88e-13 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 157700 on 9 degrees of freedom
## Multiple R-squared:  0.9976, Adjusted R-squared:  0.9974
## F-statistic:  3810 on 1 and 9 DF,  p-value: 3.879e-13

##   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)
```

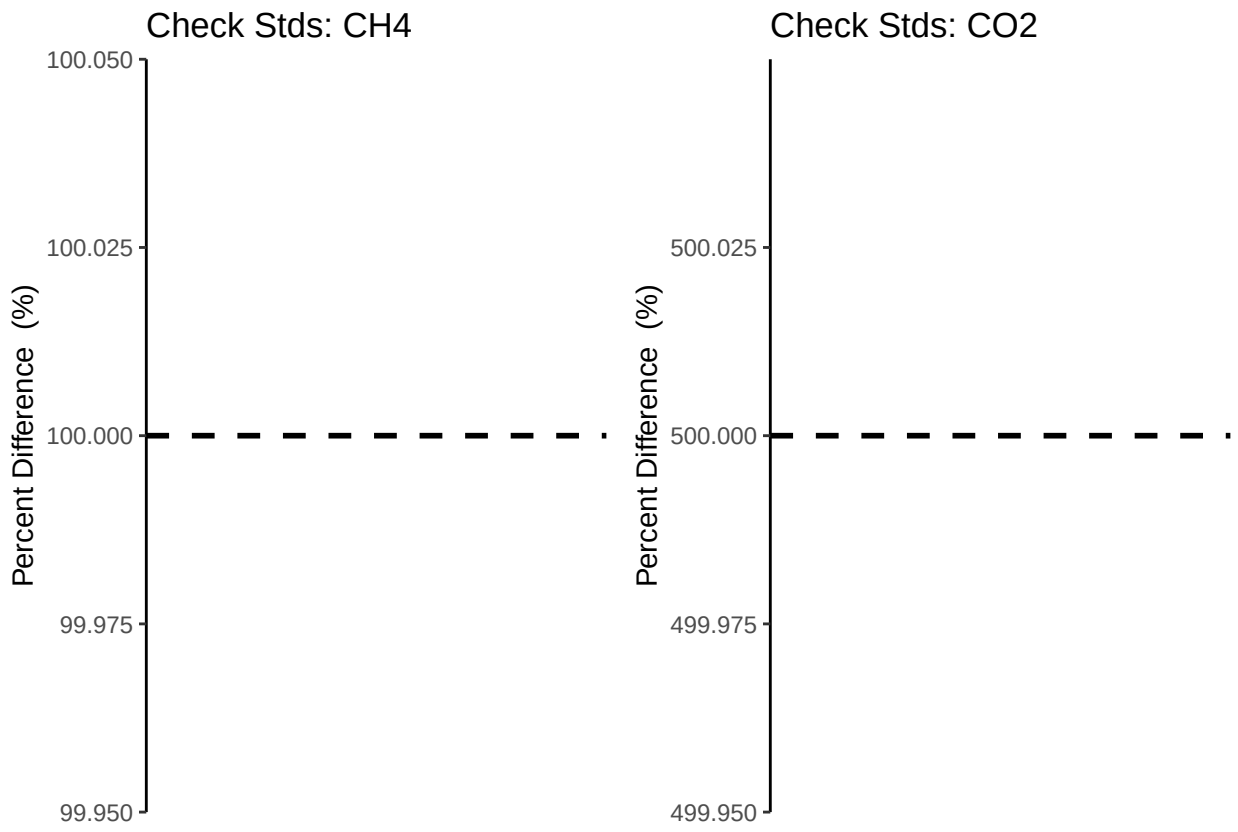
```
#head(Samples)

##########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

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

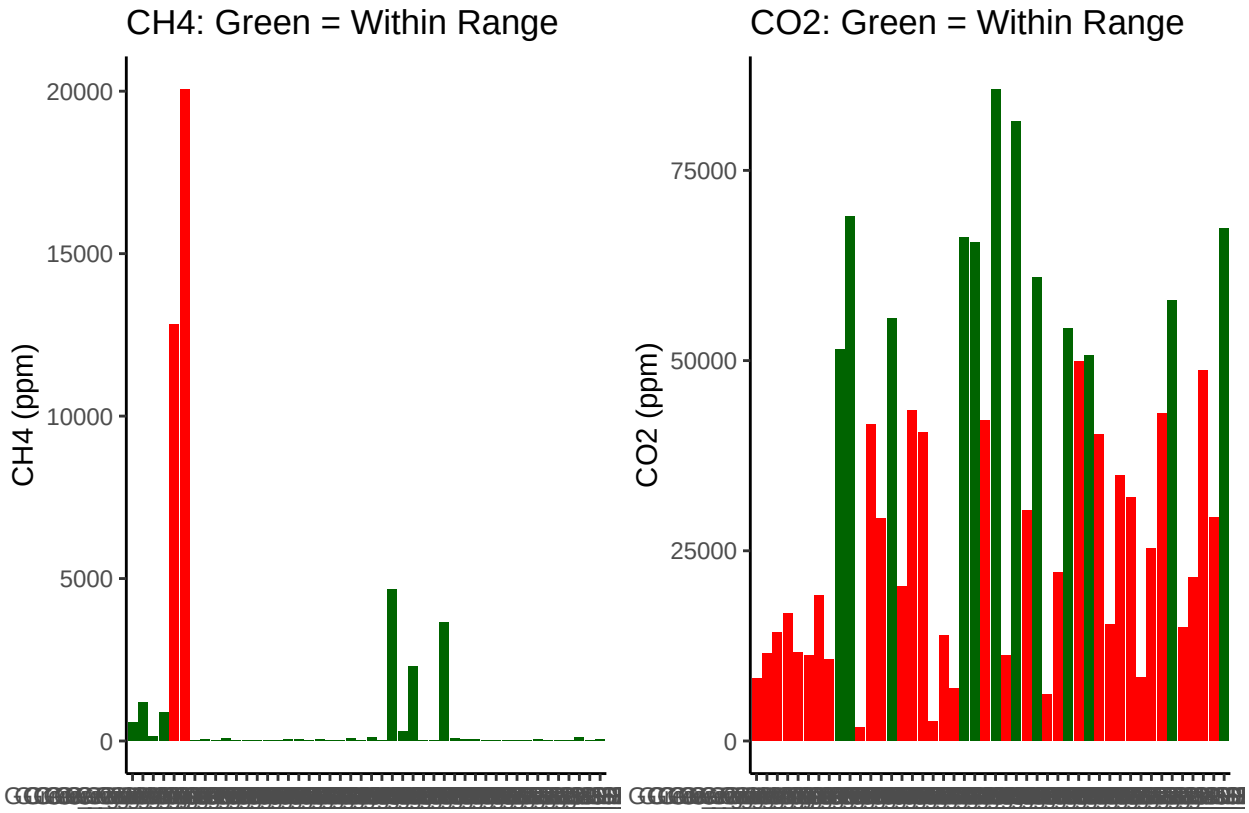
```r
Samples$CO2_Conc_ppm_dilcorr <- (Samples$CO2_Conc_ppm * Samples$Dilution_Factor)

#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( "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   202207     Unknown  TGAS        2022
## 2 Varian GC Stephanie J. Wilson   202207     Unknown  TGAS        2022
## 3 Varian GC Stephanie J. Wilson   202207     Unknown  TGAS        2022
## 4 Varian GC Stephanie J. Wilson   202207     Unknown  TGAS        2022
## 5 Varian GC Stephanie J. Wilson   202207     Unknown  TGAS        2022
## 6 Varian GC Stephanie J. Wilson   202207     Unknown  TGAS        2022
##   Sample_Month          Sample_ID Dilution_Factor STD_Conc CH4_Area CO2_Area
## 1         July GCrew_Tgas_TR_SF_1               7       NA   387703  1228239
## 2         July GCrew_Tgas_TR_SF_2               7       NA   813894  1743563
## 3         July GCrew_Tgas_TR_SF_3               7       NA    98387  2163859
## 4         July GCrew_Tgas_TR_SF_4               7       NA   599507  2555958
## 5         July GCrew_Tgas_TR_SF_5               7       NA  8757124  1752010
## 6         July GCrew_Tgas_TR_SF_6               7       NA 13718650  1685685
##   Field.Notes Lab.Notes CH4_Curve CH4_Conc_ppm CO2_Conc_ppm       CH4_Flag
## 1          NA        NA      High     565.2095     8267.732   Within Range
## 2          NA        NA      High    1188.6713    11545.738   Within Range
## 3          NA        NA      High     141.9780    14219.266   Within Range
## 4          NA        NA      High     875.0511    16713.431   Within Range
## 5          NA        NA      High   12808.5798    11599.470 Needs Dilution
## 6          NA        NA      High   20066.6446    11177.573 Needs Dilution
##       CO2_Flag CH4_Conc_ppm_dilcorr CO2_Conc_ppm_dilcorr
## 1 Within Range            3956.4666             57874.12
## 2 Within Range            8320.6992             80820.17
## 3 Within Range             993.8459             99534.86
## 4 Within Range            6125.3578            116994.02
## 5 Within Range           89660.0588             81196.29
## 6 Within Range          140466.5125             78243.01
```

```
#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   202207  TGAS        2022         July
## 2 Varian GC Stephanie J. Wilson   202207  TGAS        2022         July
## 3 Varian GC Stephanie J. Wilson   202207  TGAS        2022         July
## 4 Varian GC Stephanie J. Wilson   202207  TGAS        2022         July
## 5 Varian GC Stephanie J. Wilson   202207  TGAS        2022         July
## 6 Varian GC Stephanie J. Wilson   202207  TGAS        2022         July
##            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 Needs Dilution Within Range
```

```
##   CH4_Conc_ppm_dilcorr CO2_Conc_ppm_dilcorr
## 1            3956.4666             57874.12
## 2            8320.6992             80820.17
## 3             993.8459             99534.86
## 4            6125.3578            116994.02
## 5           89660.0588             81196.29
## 6          140466.5125             78243.01
```

```
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_202207_Processed.csv")
```

#end