COMPASS_Synoptic_TGW_2022: May

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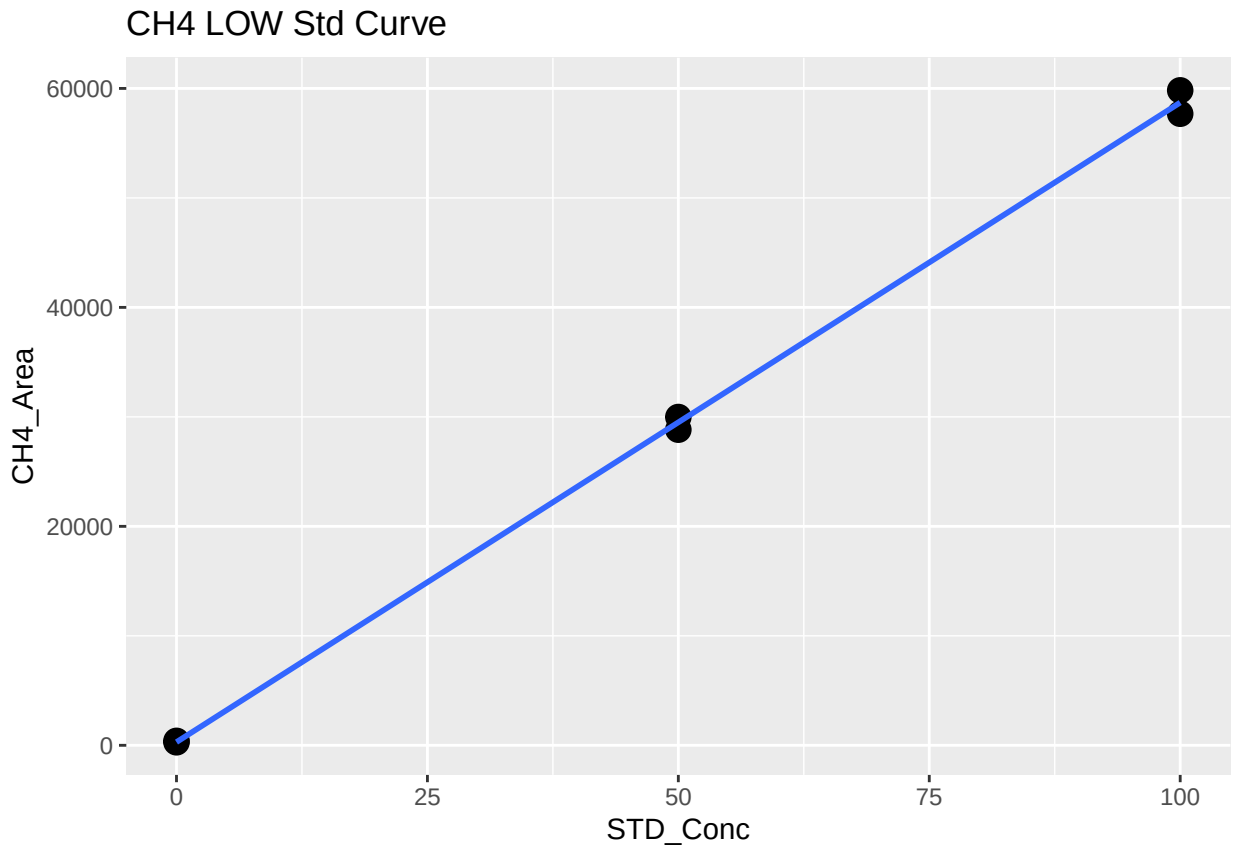
2023-01-14

##Set Up

Read in first data file and assess standard curves

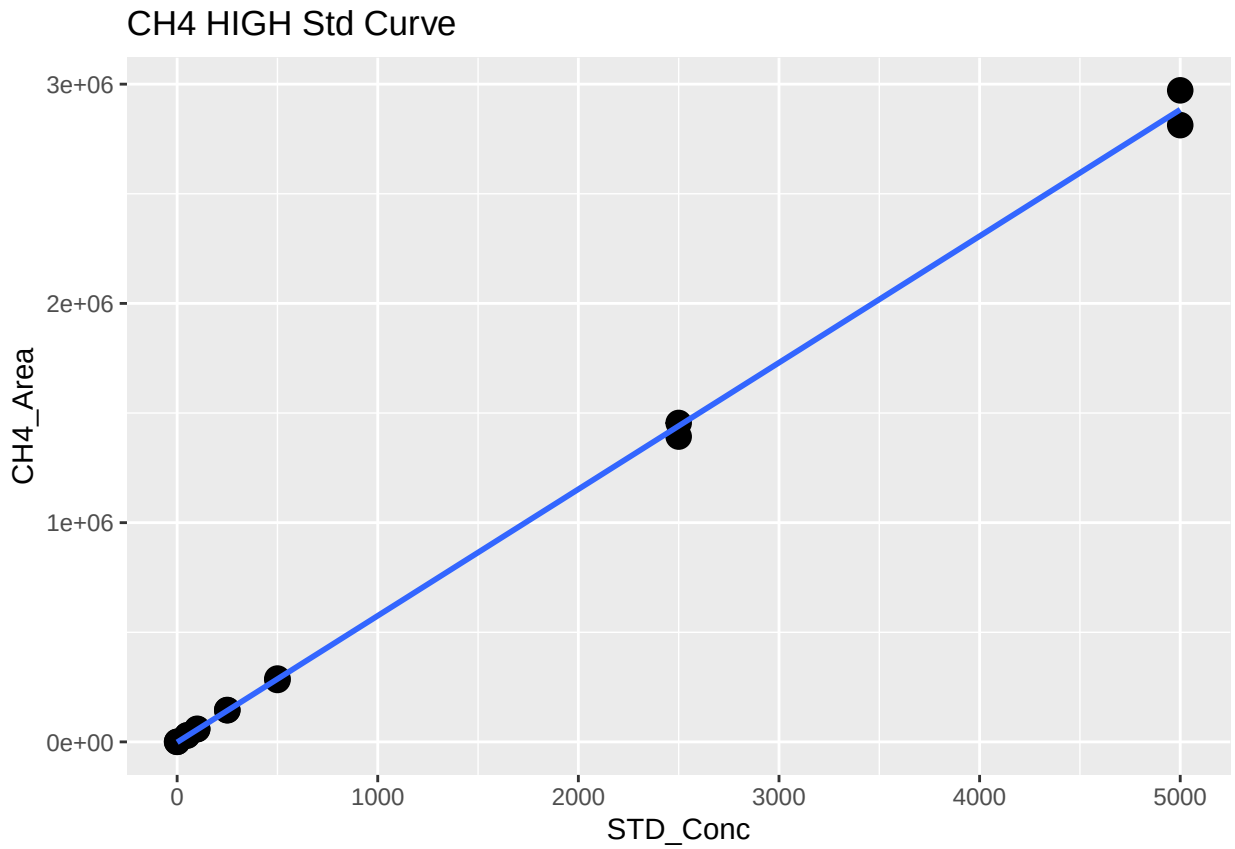
```
##     Machine                User Run_Date Sample_Type Type1 Sample_Year
## 1 Varian GC Stephanie J. Wilson   202205     Unknown  TGAS        2022
## 2 Varian GC Stephanie J. Wilson   202205     Unknown  TGAS        2022
## 3 Varian GC Stephanie J. Wilson   202205     Unknown  TGAS        2022
## 4 Varian GC Stephanie J. Wilson   202205     Unknown  TGAS        2022
## 5 Varian GC Stephanie J. Wilson   202205     Unknown  TGAS        2022
## 6 Varian GC Stephanie J. Wilson   202205     Unknown  TGAS        2022
##   Sample_Month        Sample_ID Dilution_Factor STD_Conc CH4_Area CO2_Area
## 1          May GWI_TGAS_TR_DS_1               2       NA     1420   285551
## 2          May GWI_TGAS_TR_DS_2               2       NA     5068  1114202
## 3          May GWI_TGAS_TR_DS_3               2       NA     2119  4462563
## 4          May GWI_TGAS_TR_SF_1               2       NA     1847  3899395
## 5          May GWI_TGAS_TR_SF_2               2       NA     1424   856806
## 6          May GWI_TGAS_TR_SF_3               2       NA     3065  2703534
##   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'
```



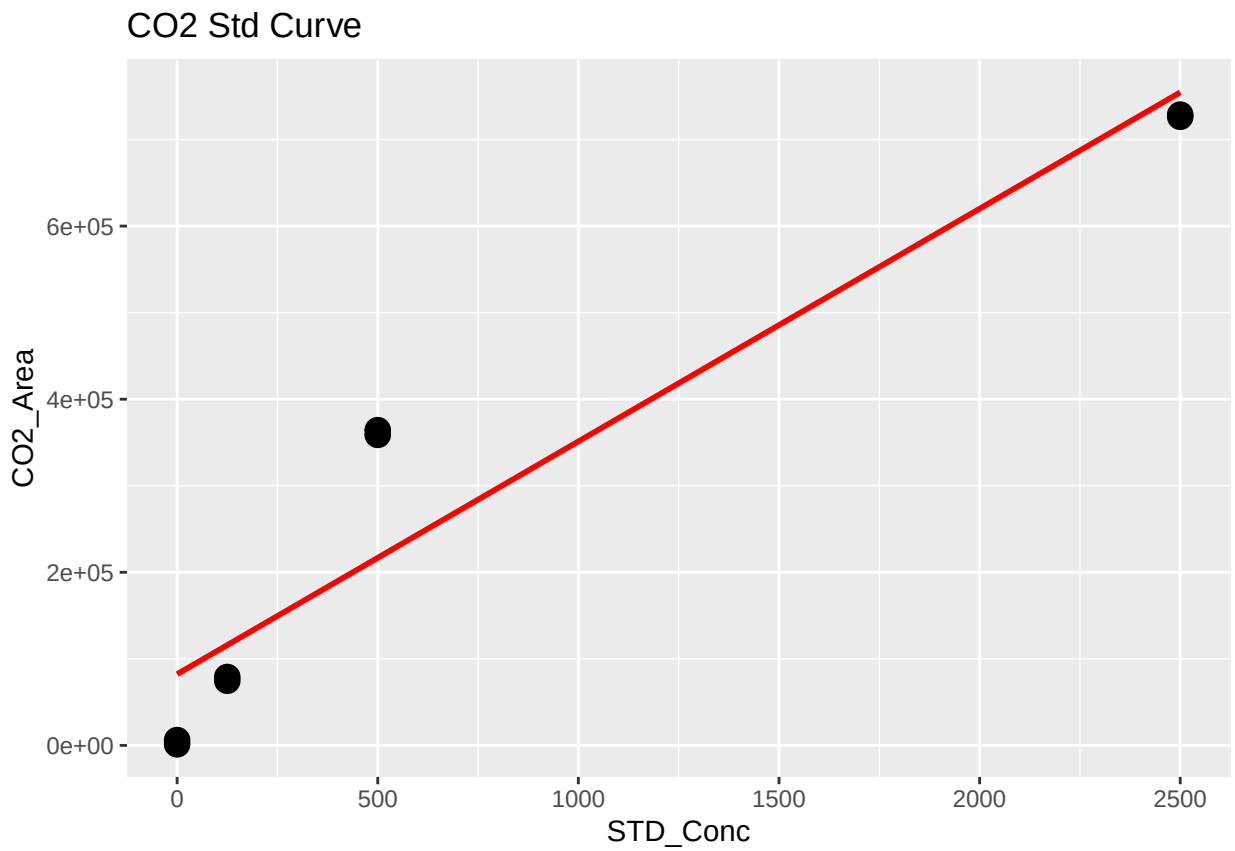

```
##
## Call:
## lm(formula = stds_ch4_low$CH4_Area ~ stds_ch4_low$STD_Conc)
##
## Residuals:
##        1        2        3        4        5        6
##   -18.67   112.33   484.83  -672.17  1116.33 -1022.67
##
## Coefficients:
##                       Estimate Std. Error t value Pr(>|t|)
## (Intercept)            292.667    558.260   0.524    0.628
## stds_ch4_low$STD_Conc  584.170      8.649  67.546 2.88e-07 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 864.9 on 4 degrees of freedom
## Multiple R-squared:  0.9991, Adjusted R-squared:  0.9989
## F-statistic:  4562 on 1 and 4 DF,  p-value: 2.878e-07

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



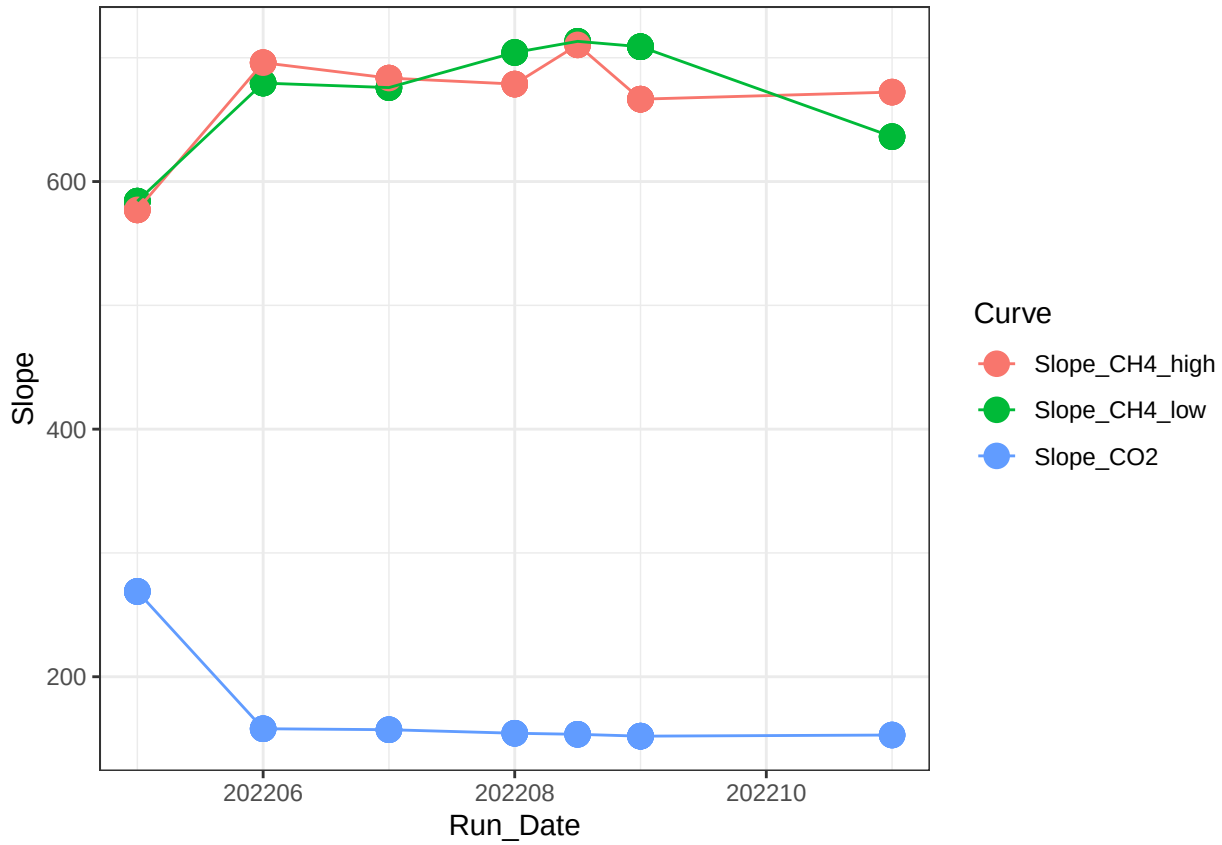

```
##
## Call:
## lm(formula = stds_ch4$CH4_Area ~ stds_ch4$STD_Conc)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -70767   1755   2118   3037  87949
##
## Coefficients:
##                    Estimate Std. Error t value Pr(>|t|)
## (Intercept)       -1829.347  11582.865  -0.158    0.877
## stds_ch4$STD_Conc   577.146      5.454 105.826   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 35760 on 12 degrees of freedom
## Multiple R-squared:  0.9989, Adjusted R-squared:  0.9988
## F-statistic: 1.12e+04 on 1 and 12 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
## -81062 -50011 -32599  16209 147447
##
## Coefficients:
##                   Estimate Std. Error t value Pr(>|t|)
## (Intercept)       82323.28   44265.89   1.860 0.112263
## stds_co2$STD_Conc   268.88      34.68   7.752 0.000242 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 99010 on 6 degrees of freedom
## Multiple R-squared:  0.9092, Adjusted R-squared:  0.8941
## F-statistic:  60.1 on 1 and 6 DF,  p-value: 0.0002421

##   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)
```

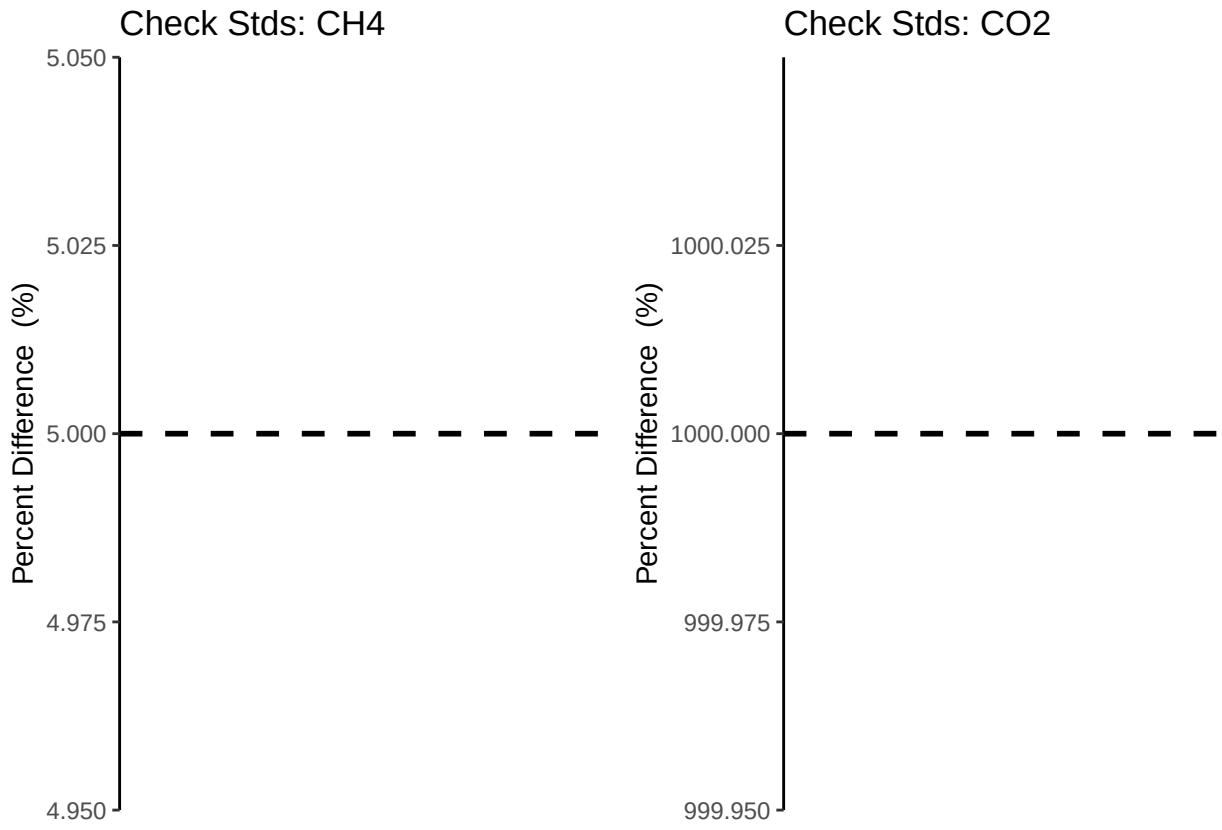
```
#head(Samples)

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

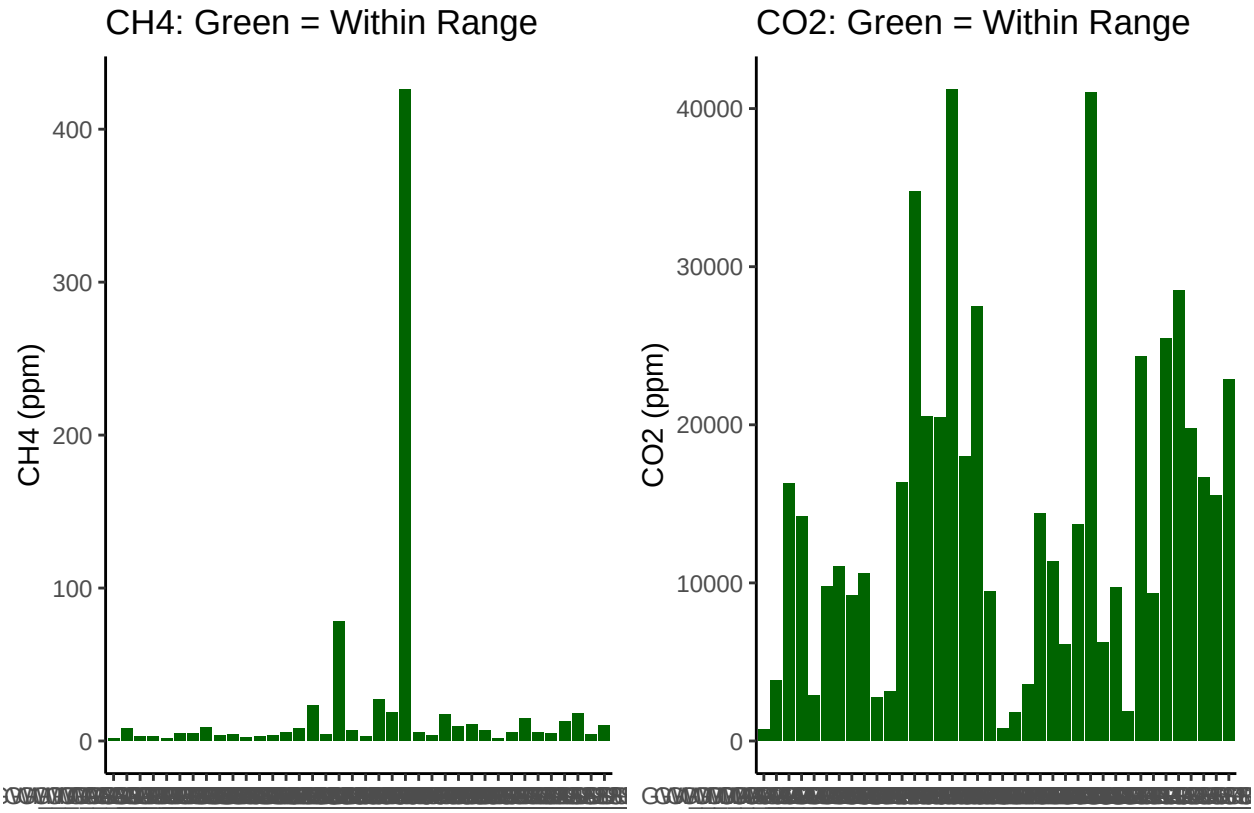
```r
Samples$CO2_Conc_ppm_dilcorr <- (Samples$CO2_Conc_ppm * Samples$Dilution_Factor)

#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( "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("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   202205     Unknown  TGAS        2022
## 2 Varian GC Stephanie J. Wilson   202205     Unknown  TGAS        2022
## 3 Varian GC Stephanie J. Wilson   202205     Unknown  TGAS        2022
## 4 Varian GC Stephanie J. Wilson   202205     Unknown  TGAS        2022
## 5 Varian GC Stephanie J. Wilson   202205     Unknown  TGAS        2022
## 6 Varian GC Stephanie J. Wilson   202205     Unknown  TGAS        2022
##   Sample_Month        Sample_ID Dilution_Factor STD_Conc CH4_Area CO2_Area
## 1          May GWI_TGAS_TR_DS_1               2       NA     1420   285551
## 2          May GWI_TGAS_TR_DS_2               2       NA     5068  1114202
## 3          May GWI_TGAS_TR_DS_3               2       NA     2119  4462563
## 4          May GWI_TGAS_TR_SF_1               2       NA     1847  3899395
## 5          May GWI_TGAS_TR_SF_2               2       NA     1424   856806
## 6          May GWI_TGAS_TR_SF_3               2       NA     3065  2703534
##   Field.Notes Lab.Notes CH4_Curve CH4_Conc_ppm CO2_Conc_ppm     CH4_Flag
## 1          NA        NA       Low     1.929804     755.8298 Within Range
## 2          NA        NA       Low     8.174561    3837.6884 Within Range
## 3          NA        NA       Low     3.126373   16290.6695 Within Range
## 4          NA        NA       Low     2.660755   14196.1760 Within Range
## 5          NA        NA       Low     1.936651    2880.3999 Within Range
## 6          NA        NA       Low     4.745765    9748.6166 Within Range
##       CO2_Flag CH4_Conc_ppm_dilcorr CO2_Conc_ppm_dilcorr
## 1 Within Range             3.859607             1511.660
## 2 Within Range            16.349122             7675.377
## 3 Within Range             6.252746            32581.339
## 4 Within Range             5.321510            28392.352
## 5 Within Range             3.873302             5760.800
## 6 Within Range             9.491529            19497.233
```

```
#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   202205  TGAS        2022          May
## 2 Varian GC Stephanie J. Wilson   202205  TGAS        2022          May
## 3 Varian GC Stephanie J. Wilson   202205  TGAS        2022          May
## 4 Varian GC Stephanie J. Wilson   202205  TGAS        2022          May
## 5 Varian GC Stephanie J. Wilson   202205  TGAS        2022          May
## 6 Varian GC Stephanie J. Wilson   202205  TGAS        2022          May
##          Sample_ID Dilution_Factor Field.Notes     CH4_Flag     CO2_Flag
## 1 GWI_TGAS_TR_DS_1               2          NA Within Range Within Range
## 2 GWI_TGAS_TR_DS_2               2          NA Within Range Within Range
## 3 GWI_TGAS_TR_DS_3               2          NA Within Range Within Range
## 4 GWI_TGAS_TR_SF_1               2          NA Within Range Within Range
## 5 GWI_TGAS_TR_SF_2               2          NA Within Range Within Range
## 6 GWI_TGAS_TR_SF_3               2          NA Within Range Within Range
```

```
##   CH4_Conc_ppm_dilcorr CO2_Conc_ppm_dilcorr
## 1             3.859607             1511.660
## 2            16.349122             7675.377
## 3             6.252746            32581.339
## 4             5.321510            28392.352
## 5             3.873302             5760.800
## 6             9.491529            19497.233
```

```
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_202205_Processed.csv")
```

#end