COMPASS_Synoptic_TGW_2023: May

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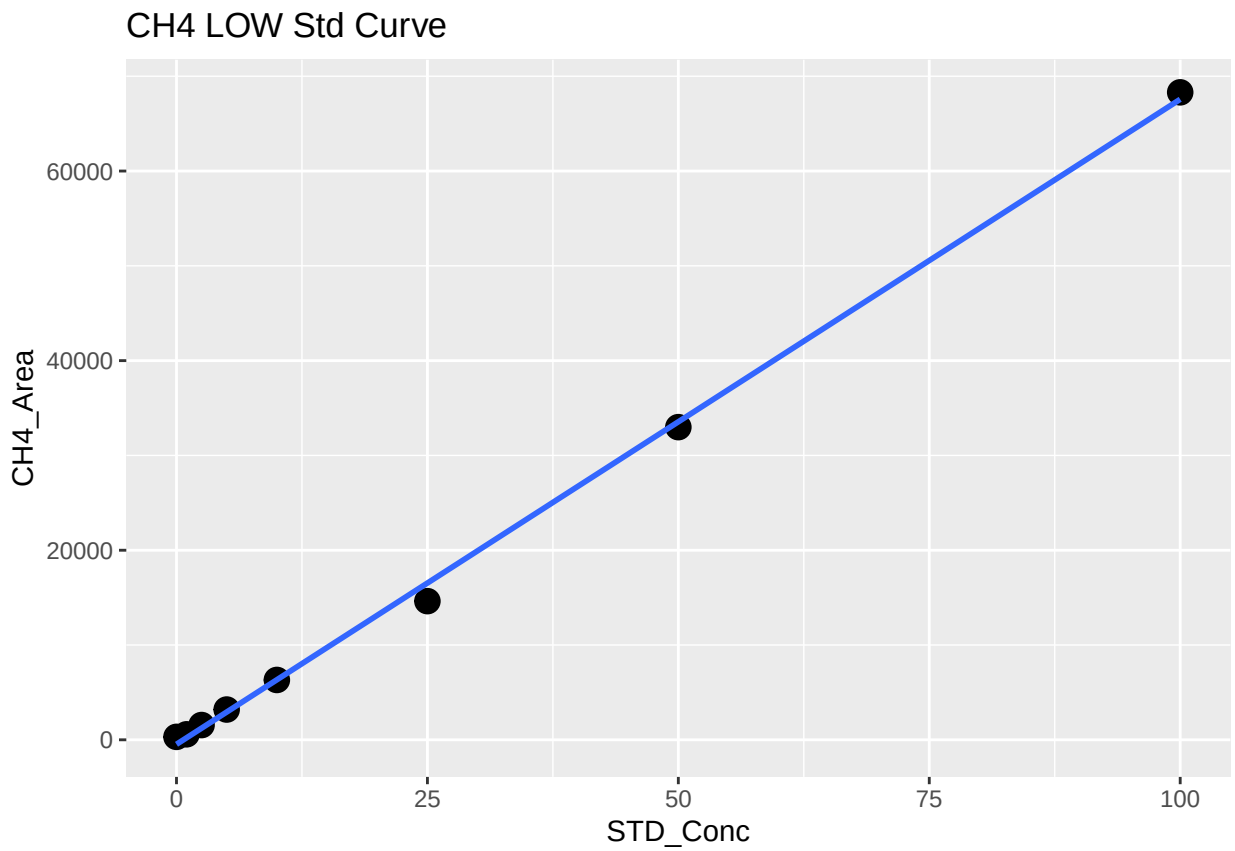
##Set Up

Read in first data file and assess standard curves

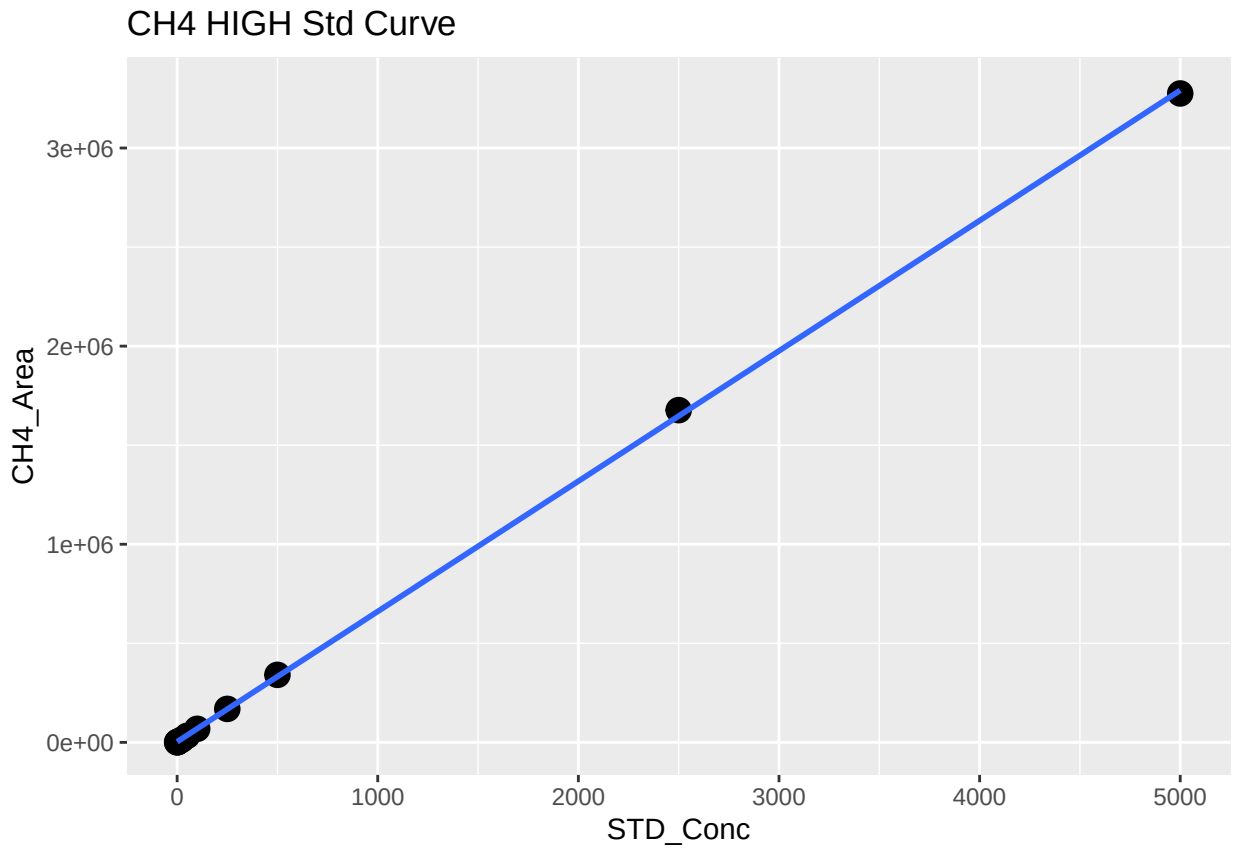
```
##     Machine   User Run_Date Sample_Type   Type1 Sample_Year Sample_Month
## 1 Varian GC Wegner 20240228       Blank   Blank        2024         <NA>
## 2 Varian GC Wegner 20240228     STD_CH4 STD_CH4        2024         <NA>
## 3 Varian GC Wegner 20240228     STD_CO2 STD_CO2        2024         <NA>
## 4 Varian GC Wegner 20240228     STD_CH4 STD_CH4        2023          May
## 5 Varian GC Wegner 20240228     STD_CH4 STD_CH4        2023          May
## 6 Varian GC Wegner 20240228     STD_CH4 STD_CH4        2023          May
##                Sample_ID Dilution_Factor STD_Conc CO2_Area CH4_Area Field.Notes
## 1                Blank_0               1      0.0    14889      311          NA
## 2   Blank_0_repeatforCH4               1      0.0    14889      311          NA
## 3 Blank_0_repeat for CO2               1      0.0    14889      311          NA
## 4         STD_2.5ppm_CH4               1      2.5    69708     1558          NA
## 5           STD_1ppm_CH4               1      1.0    25322      580          NA
## 6           STD_5ppm_CH4               1      5.0   140050     3194          NA
##   Lab.Notes
## 1
## 2
## 3
## 4
## 5
## 6
```

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



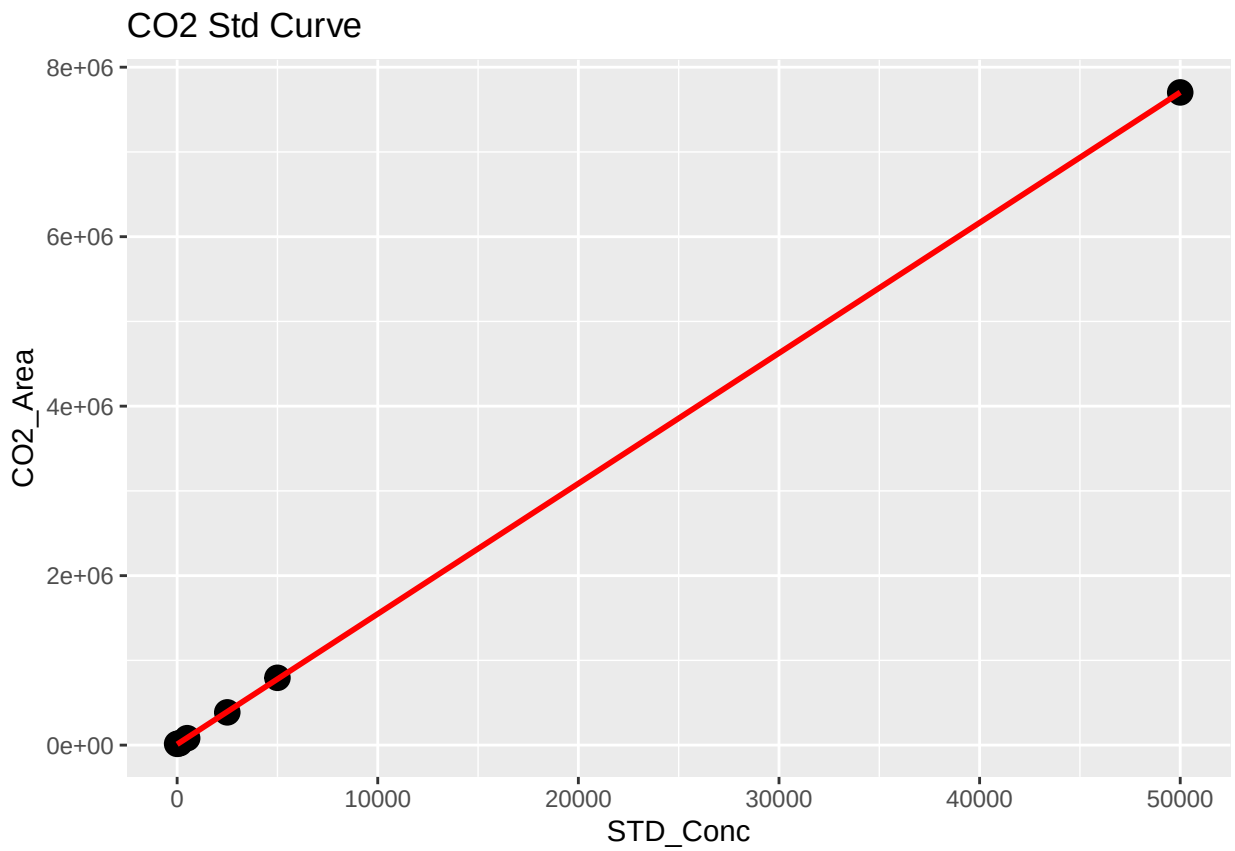

```
##
## Call:
## lm(formula = stds_ch4_low$CH4_Area ~ stds_ch4_low$STD_Conc)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -1908.0  -153.4   297.8   463.5   784.4
##
## Coefficients:
##                       Estimate Std. Error t value Pr(>|t|)
## (Intercept)           -473.37     418.23  -1.132    0.301
## stds_ch4_low$STD_Conc   680.41      10.27  66.227 7.97e-10 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 951.5 on 6 degrees of freedom
## Multiple R-squared:  0.9986, Adjusted R-squared:  0.9984
## F-statistic:  4386 on 1 and 6 DF,  p-value: 7.972e-10

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



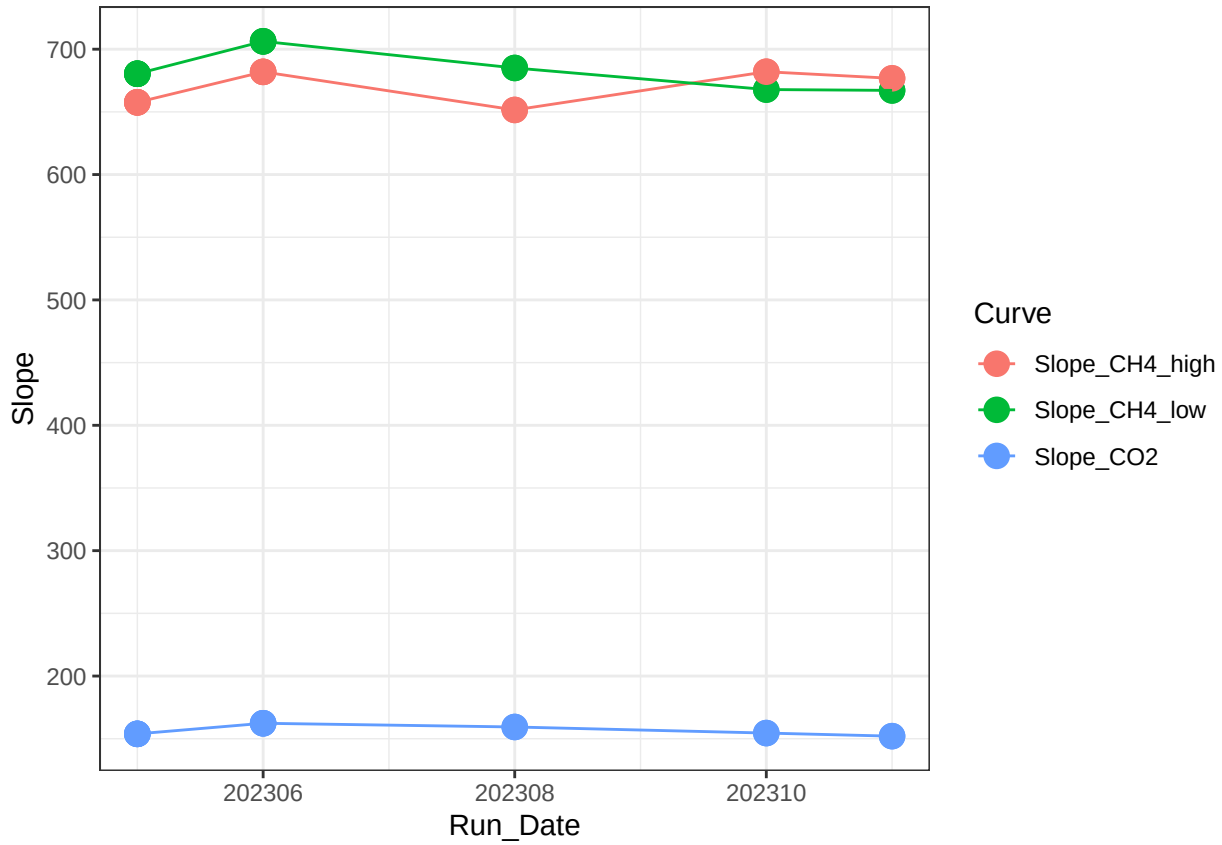

```
##
## Call:
## lm(formula = stds_ch4$CH4_Area ~ stds_ch4$STD_Conc)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -15778.7  -3255.2  -3106.3    -77.9  29794.1
##
## Coefficients:
##                   Estimate Std. Error t value Pr(>|t|)
## (Intercept)       3119.138   3655.225   0.853    0.413
## stds_ch4$STD_Conc  657.613      2.253 291.838   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 11410 on 10 degrees of freedom
## Multiple R-squared:  0.9999, Adjusted R-squared:  0.9999
## F-statistic: 8.517e+04 on 1 and 10 DF,  p-value: < 2.2e-16

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




```
##
## Call:
## lm(formula = stds_co2$CO2_Area ~ stds_co2$STD_Conc)
##
## Residuals:
##     1     2     3     4     5     6
##  5238 -6639 -4830 -7796 15080 -1053
##
## Coefficients:
##                     Estimate Std. Error t value Pr(>|t|)
## (Intercept)       9651.4986  4536.9799   2.127    0.101
## stds_co2$STD_Conc  153.8752     0.2209 696.653 2.55e-11 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 9800 on 4 degrees of freedom
## Multiple R-squared:      1,  Adjusted R-squared:      1
## F-statistic: 4.853e+05 on 1 and 4 DF,  p-value: 2.547e-11

##   X          Curve        R2    Slope Intercept Run_Date
## 1 1  Slope_CH4_low 0.9984062 680.4131 -473.3666   202305
## 2 2 Slope_CH4_high 0.9998709 657.6131 3119.1378   202305
## 3 3      Slope_CO2 0.9999897 153.8752 9651.4986   202305
## 4 4  Slope_CH4_low 0.9984062 680.4131 -473.3666   202305
## 5 5 Slope_CH4_high 0.9998709 657.6131 3119.1378   202305
## 6 6      Slope_CO2 0.9999897 153.8752 9651.4986   202305
```



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)
```

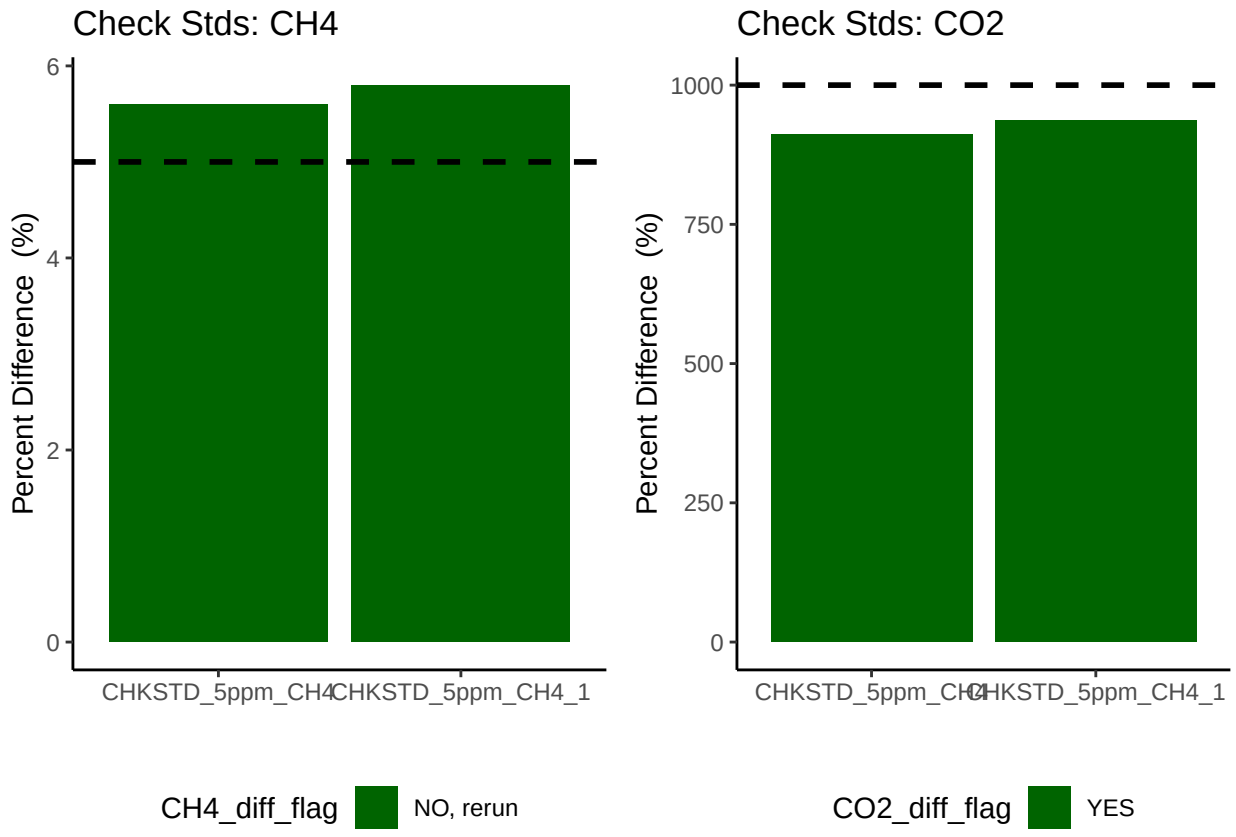
```r
#head(Samples)

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

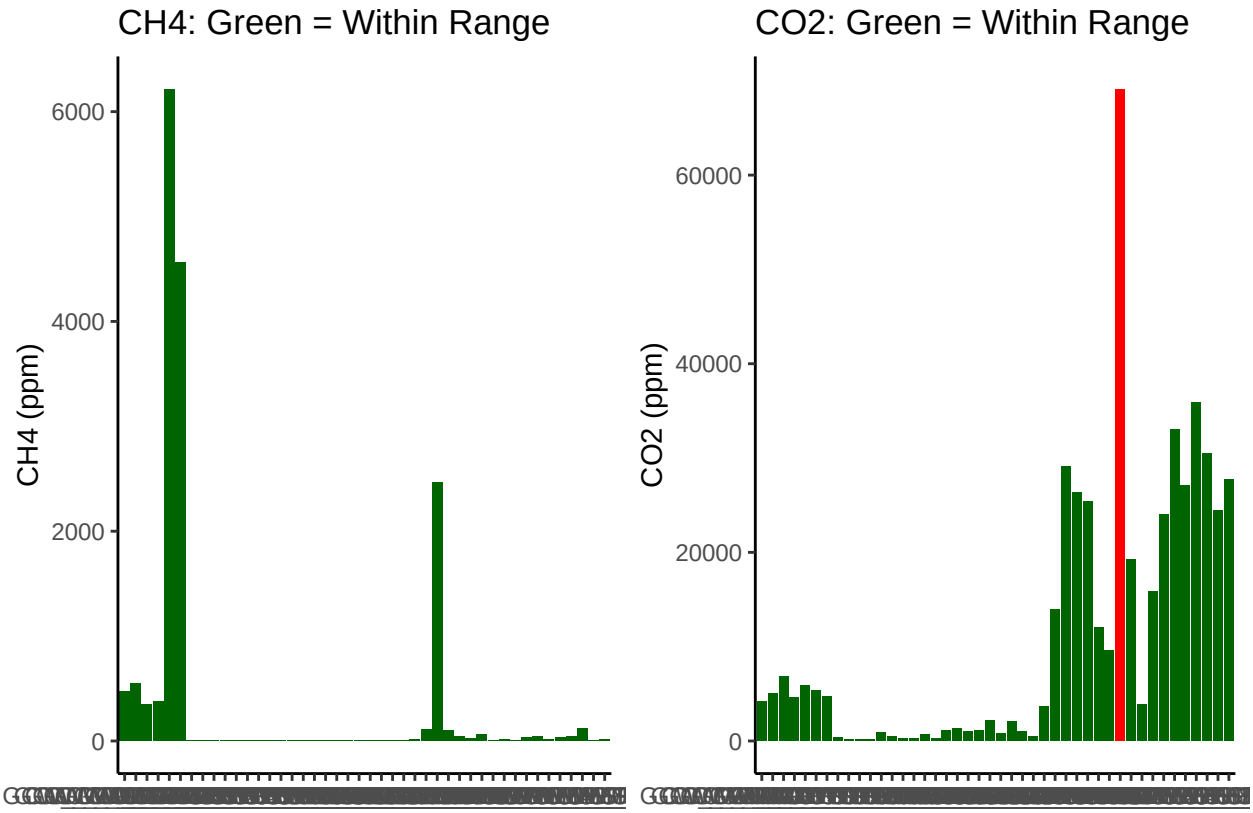
```r
Samples$CO2_Conc_ppm_dilcorr <- (Samples$CO2_Conc_ppm * Samples$Dilution_Factor)

#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 Sample_Month
## 1 Varian GC Wegner 20240228     Unknown   TGW        2023          May
## 2 Varian GC Wegner 20240228     Unknown   TGW        2023          May
## 3 Varian GC Wegner 20240228     Unknown   TGW        2023          May
## 4 Varian GC Wegner 20240228     Unknown   TGW        2023          May
## 5 Varian GC Wegner 20240228     Unknown   TGW        2023          May
## 6 Varian GC Wegner 20240228     Unknown   TGW        2023          May
##         Sample_ID Dilution_Factor STD_Conc CO2_Area CH4_Area Field.Notes
## 1 GCW_TGW_TR_SF_1              12       NA   658482   312134          NA
## 2 GCW_TGW_TR_SF_2              12       NA   777613   362443          NA
## 3 GCW_TGW_TR_SF_3              12       NA  1066233   229897          NA
## 4 GCW_TGW_TR_SF_4              12       NA   719637   250211          NA
## 5 GCW_TGW_TR_SF_5              12       NA   913981  4090681          NA
## 6 GCW_TGW_TR_SF_6              12       NA   834714  3000165          NA
##               Lab.Notes CH4_Curve CH4_Conc_ppm CO2_Conc_ppm     CH4_Flag
## 1 10mL N2 added in lab       High     469.9037     4216.602 Within Range
## 2 10mL N2 added in lab       High     546.4062     4990.807 Within Range
## 3 10mL N2 added in lab       High     344.8500     6866.483 Within Range
## 4 10mL N2 added in lab       High     375.7405     4614.034 Within Range
## 5 10mL N2 added in lab       High    6215.7548     5877.032 Within Range
## 6 10mL N2 added in lab       High    4557.4606     5361.893 Within Range
##       CO2_Flag CH4_Conc_ppm_dilcorr CO2_Conc_ppm_dilcorr
## 1 Within Range             5638.845             50599.22
## 2 Within Range             6556.874             59889.68
## 3 Within Range             4138.200             82397.79
## 4 Within Range             4508.886             55368.41
## 5 Within Range            74589.057             70524.38
## 6 Within Range            54689.527             64342.72
```

```
#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       Sample_ID
## 1 Varian GC Wegner 20240228   TGW        2023          May GCW_TGW_TR_SF_1
## 2 Varian GC Wegner 20240228   TGW        2023          May GCW_TGW_TR_SF_2
## 3 Varian GC Wegner 20240228   TGW        2023          May GCW_TGW_TR_SF_3
## 4 Varian GC Wegner 20240228   TGW        2023          May GCW_TGW_TR_SF_4
## 5 Varian GC Wegner 20240228   TGW        2023          May GCW_TGW_TR_SF_5
## 6 Varian GC Wegner 20240228   TGW        2023          May GCW_TGW_TR_SF_6
##   Dilution_Factor Field.Notes     CH4_Flag     CO2_Flag CH4_Conc_ppm_dilcorr
## 1              12          NA Within Range Within Range             5638.845
## 2              12          NA Within Range Within Range             6556.874
## 3              12          NA Within Range Within Range             4138.200
## 4              12          NA Within Range Within Range             4508.886
## 5              12          NA Within Range Within Range            74589.057
## 6              12          NA Within Range Within Range            54689.527
```

```
##   CO2_Conc_ppm_dilcorr
## 1             50599.22
## 2             59889.68
## 3             82397.79
## 4             55368.41
## 5             70524.38
## 6             64342.72
```

```r
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_202305_Processed.csv")
```

#end