COMPASS_Synoptic_TGW_2023: Oct & Nov

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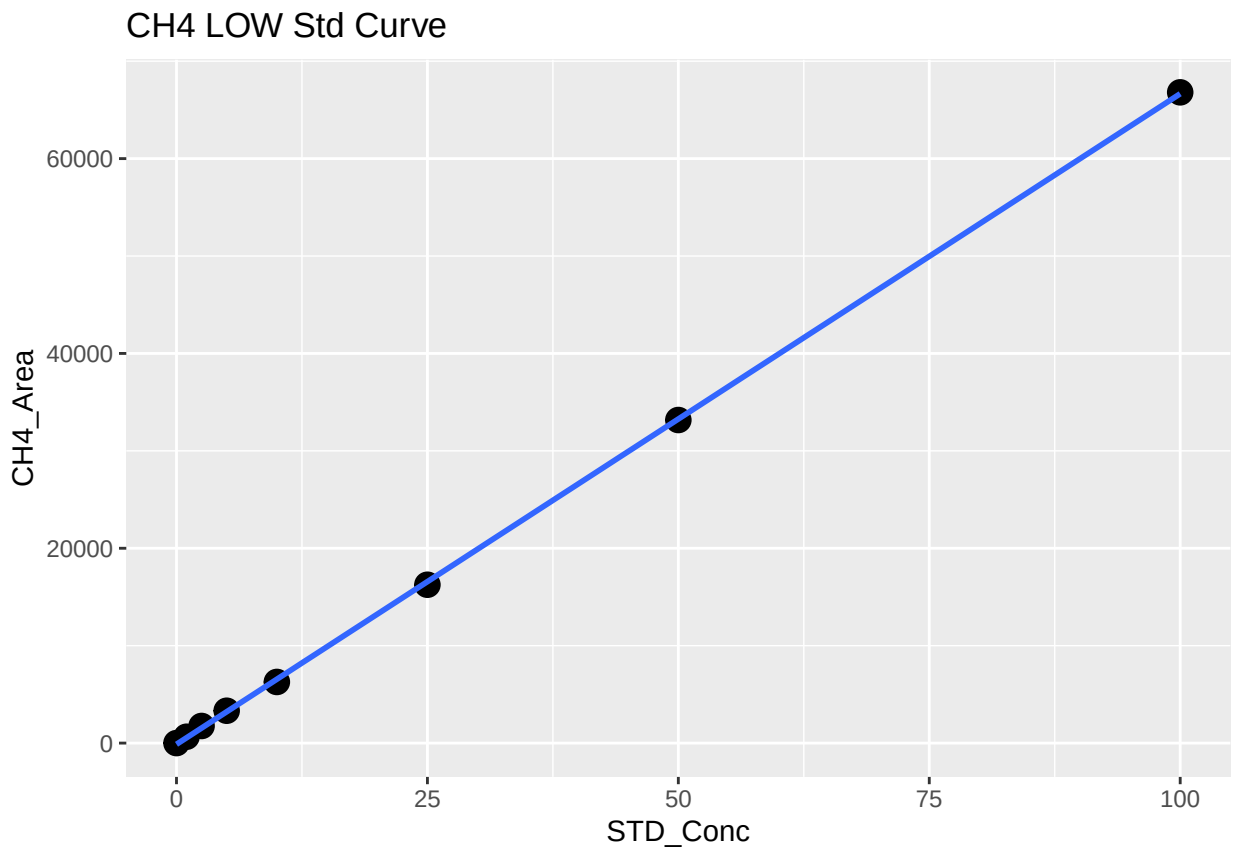
##Set Up

Read in first data file and assess standard curves

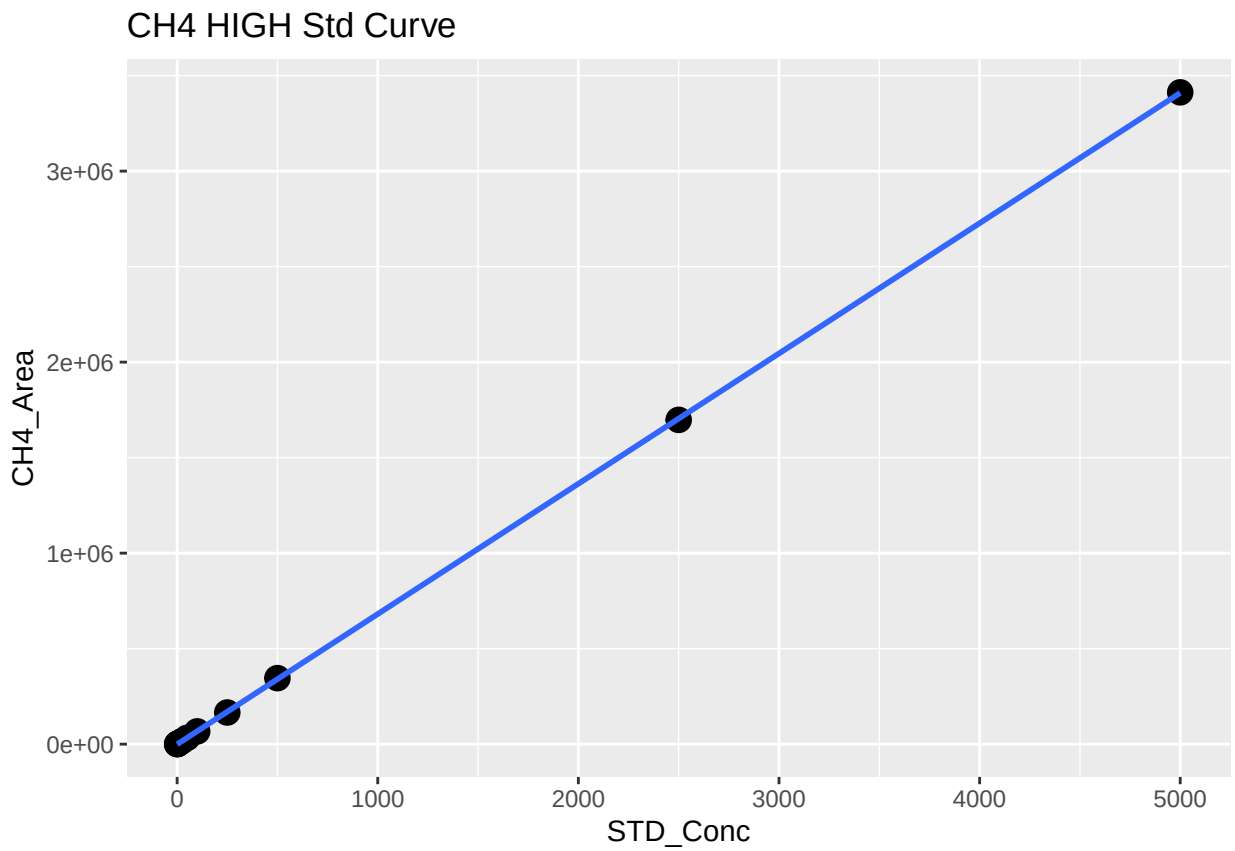
```
##     Machine   User Run_Date Sample_Type   Type1 Sample_Year Sample_Month
## 1 Varian GC Wegner 20240307       Blank   Blank        2024         <NA>
## 2 Varian GC Wegner 20240307     STD_CH4 STD_CH4        2024         <NA>
## 3 Varian GC Wegner 20240307     STD_CO2 STD_CO2        2024         <NA>
## 4 Varian GC Wegner 20240307     STD_CH4 STD_CH4        2024         <NA>
## 5 Varian GC Wegner 20240307     STD_CH4 STD_CH4        2024         <NA>
## 6 Varian GC Wegner 20240307     STD_CH4 STD_CH4        2024         <NA>
##              Sample_ID Dilution_Factor STD_Conc CO2_Area CH4_Area Field.Notes
## 1              Blank_0               1      0.0        0        0          NA
## 2 Blank_0_repeatforCH4               1      0.0        0        0          NA
## 3 Blank_0_repeatforCO2               1      0.0        0        0          NA
## 4         STD_1ppm_CH4               1      1.0    24660      652          NA
## 5       STD_2.5ppm_CH4               1      2.5    72273     1757          NA
## 6         STD_5ppm_CH4               1      5.0   145672     3321          NA
##   Lab.Notes
## 1
## 2
## 3
## 4
## 5
## 6
```

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



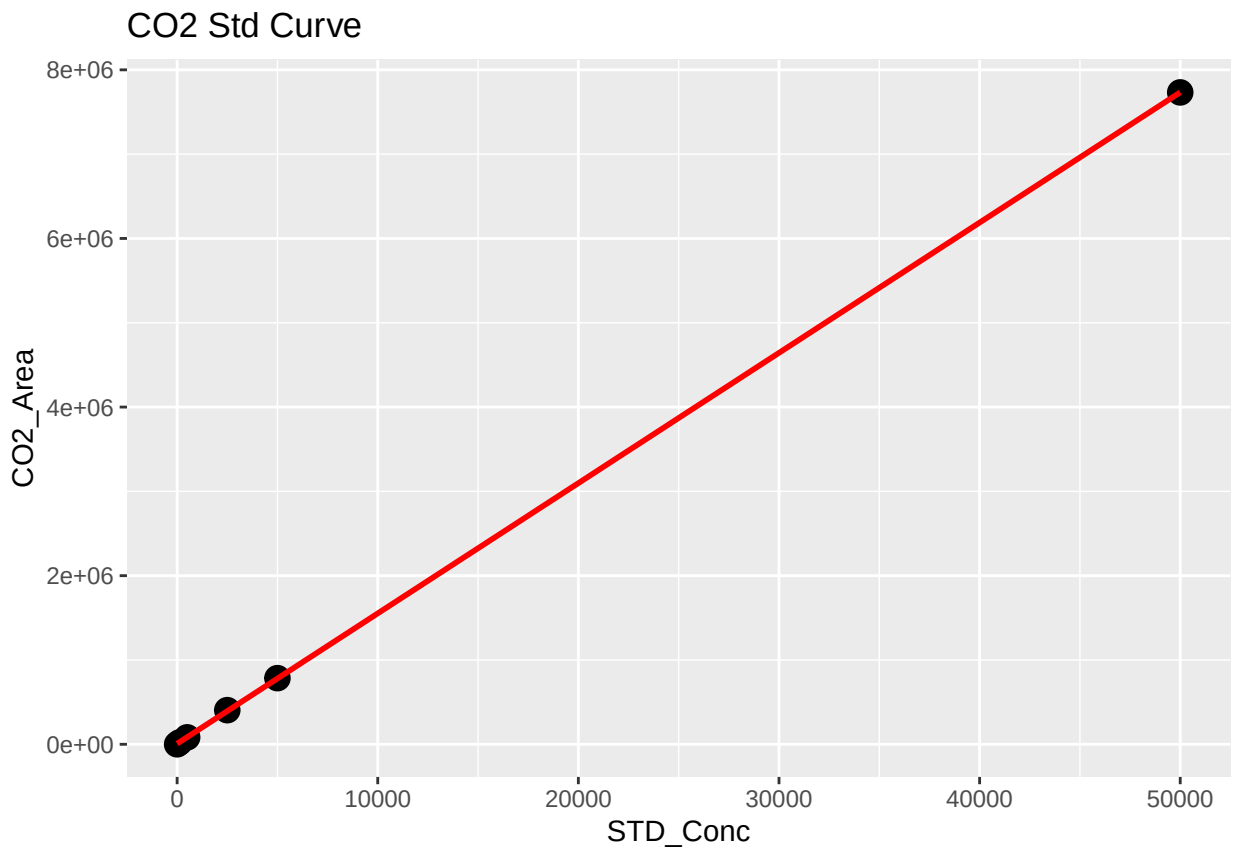

```
##
## Call:
## lm(formula = stds_ch4_low$CH4_Area ~ stds_ch4_low$STD_Conc)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -315.1 -146.1  107.0  129.4  211.4
##
## Coefficients:
##                       Estimate Std. Error t value Pr(>|t|)
## (Intercept)           -123.898     96.849  -1.279    0.248
## stds_ch4_low$STD_Conc  667.799      2.379 280.694 1.38e-13 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 220.3 on 6 degrees of freedom
## Multiple R-squared:  0.9999, Adjusted R-squared:  0.9999
## F-statistic: 7.879e+04 on 1 and 6 DF,  p-value: 1.38e-13

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



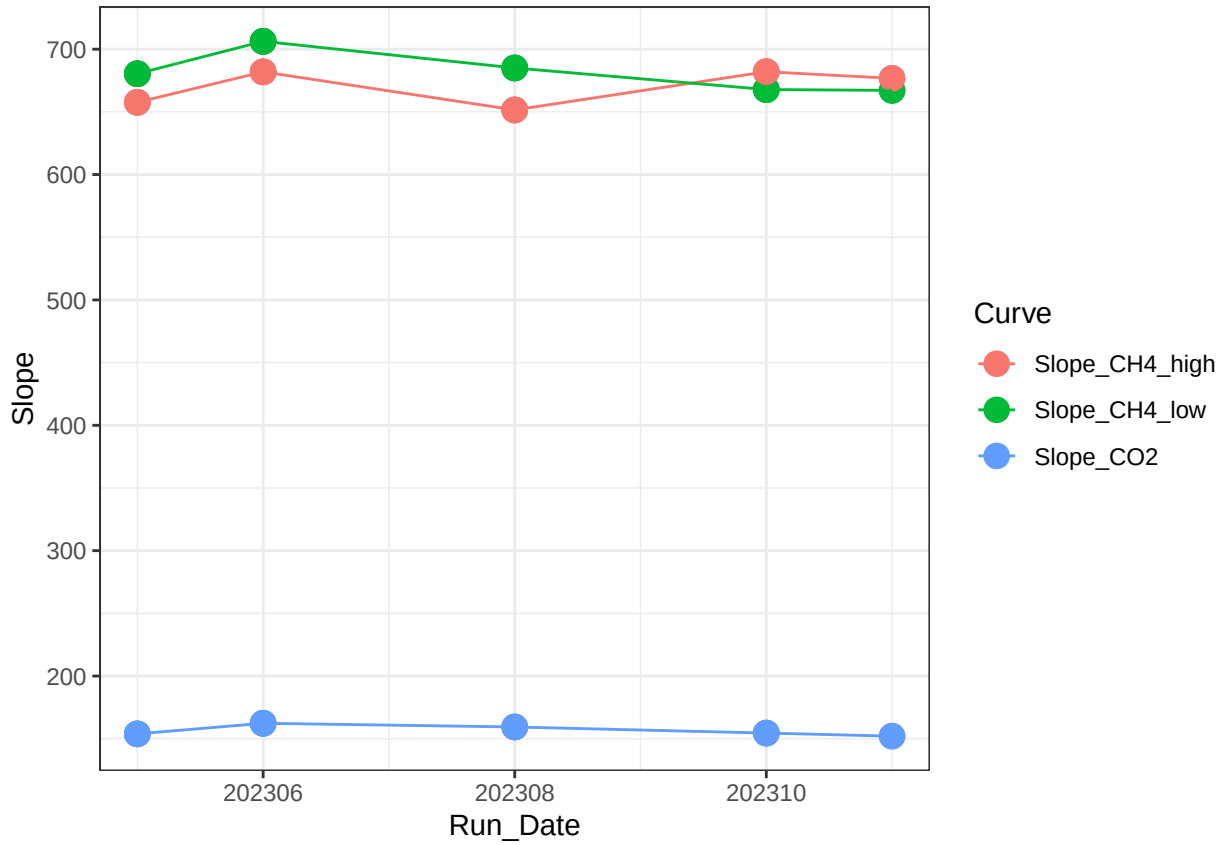

```
##
## Call:
## lm(formula = stds_ch4$CH4_Area ~ stds_ch4$STD_Conc)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -6670.7  -298.4   437.9   767.6  5367.7
##
## Coefficients:
##                   Estimate Std. Error  t value Pr(>|t|)
## (Intercept)       -754.608   1018.631   -0.741    0.476
## stds_ch4$STD_Conc  682.024      0.628 1086.097   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 3179 on 10 degrees of freedom
## Multiple R-squared:      1,  Adjusted R-squared:      1
## F-statistic: 1.18e+06 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
## -7722.1 -4197.3 -2406.0 10925.2  4346.6  -946.4
##
## Coefficients:
##                   Estimate Std. Error t value Pr(>|t|)
## (Intercept)       7722.096   3450.512   2.238   0.0888 .
## stds_co2$STD_Conc  154.506      0.168 919.763 8.38e-12 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 7453 on 4 degrees of freedom
## Multiple R-squared:      1,  Adjusted R-squared:      1
## F-statistic: 8.46e+05 on 1 and 4 DF,  p-value: 8.384e-12

##   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)
```

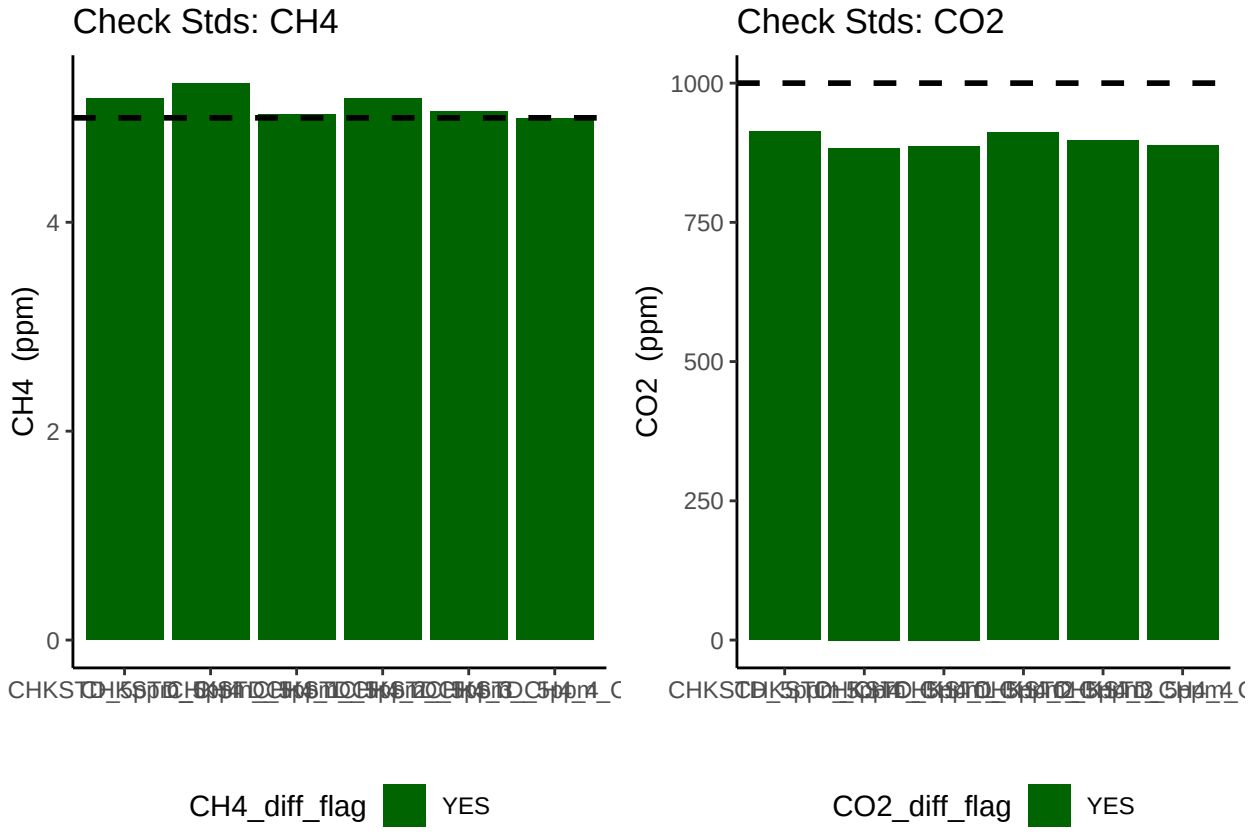
```
#head(Samples)

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

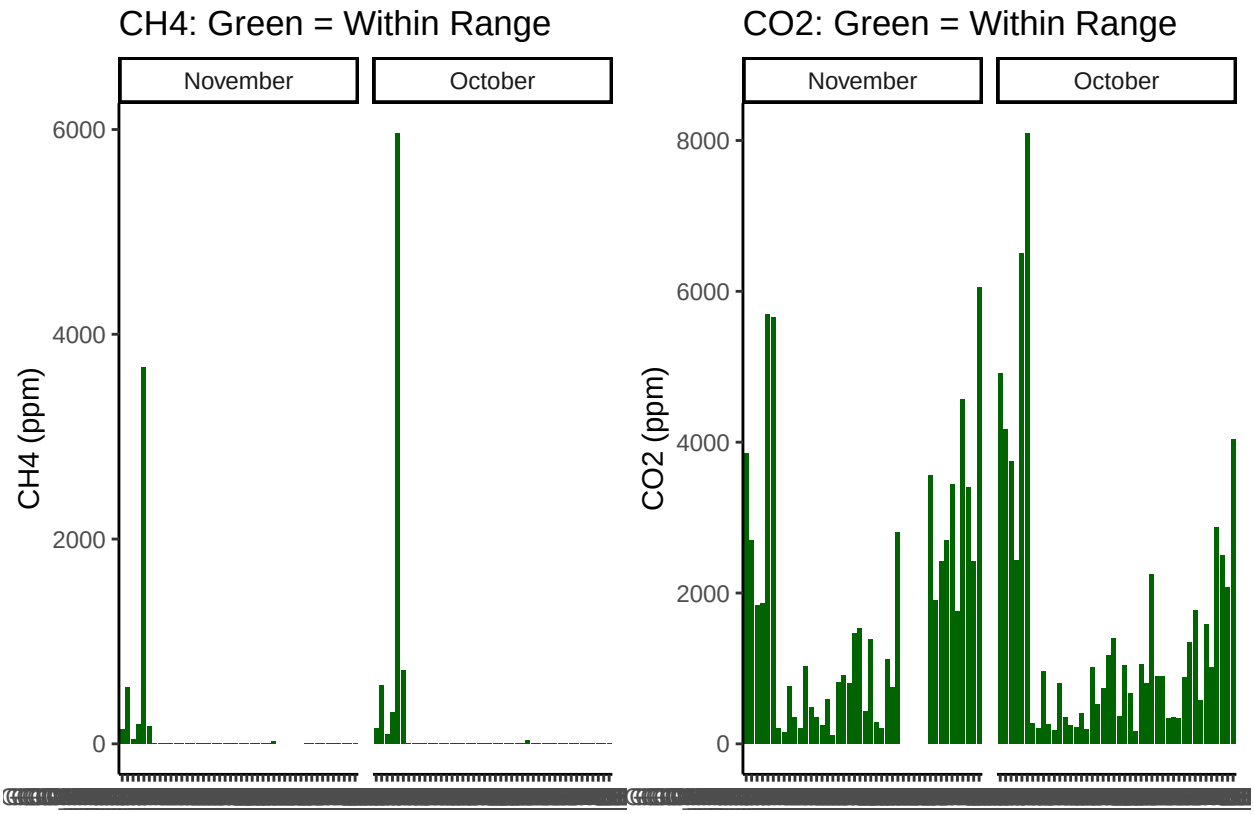
```
Samples$CO2_Conc_ppm_dilcorr <- (Samples$CO2_Conc_ppm * Samples$Dilution_Factor)

#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") +
        facet_grid(~Sample_Month)


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") +
        facet_grid(~Sample_Month)

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 20240307     Unknown   TGW        2023      October
## 2 Varian GC Wegner 20240307     Unknown   TGW        2023      October
## 3 Varian GC Wegner 20240307     Unknown   TGW        2023      October
## 4 Varian GC Wegner 20240307     Unknown   TGW        2023      October
## 5 Varian GC Wegner 20240307     Unknown   TGW        2023      October
## 6 Varian GC Wegner 20240307     Unknown   TGW        2023      October
##         Sample_ID Dilution_Factor STD_Conc CO2_Area CH4_Area Field.Notes
## 1 GCW_TGW_TR_SF_1              12       NA   767202   100036          NA
## 2 GCW_TGW_TR_SF_2              12       NA   652121   388760          NA
## 3 GCW_TGW_TR_SF_3              12       NA   586460    60512          NA
## 4 GCW_TGW_TR_SF_4              12       NA   382973   206881          NA
## 5 GCW_TGW_TR_SF_5              12       NA  1012246  4064068          NA
## 6 GCW_TGW_TR_SF_6              12       NA  1257973   489927          NA
##              Lab.Notes CH4_Curve CH4_Conc_ppm CO2_Conc_ppm     CH4_Flag
## 1 10mL N2 added in lab      High    147.78168     4915.541 Within Range
## 2 10mL N2 added in lab      High    571.11592     4170.708 Within Range
## 3 10mL N2 added in lab       Low     90.79957     3745.734 Within Range
## 4 10mL N2 added in lab      High    304.44045     2428.716 Within Range
## 5 10mL N2 added in lab      High   5959.94314     6501.526 Within Range
## 6 10mL N2 added in lab      High    719.44947     8091.932 Within Range
##       CO2_Flag CH4_Conc_ppm_dilcorr CO2_Conc_ppm_dilcorr
## 1 Within Range             1773.380             58986.49
## 2 Within Range             6853.391             50048.50
## 3 Within Range             1089.595             44948.81
## 4 Within Range             3653.285             29144.59
## 5 Within Range            71519.318             78018.31
## 6 Within Range             8633.394             97103.18
```

```
#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 20240307   TGW        2023      October GCW_TGW_TR_SF_1
## 2 Varian GC Wegner 20240307   TGW        2023      October GCW_TGW_TR_SF_2
## 3 Varian GC Wegner 20240307   TGW        2023      October GCW_TGW_TR_SF_3
## 4 Varian GC Wegner 20240307   TGW        2023      October GCW_TGW_TR_SF_4
## 5 Varian GC Wegner 20240307   TGW        2023      October GCW_TGW_TR_SF_5
## 6 Varian GC Wegner 20240307   TGW        2023      October GCW_TGW_TR_SF_6
##   Dilution_Factor Field.Notes     CH4_Flag     CO2_Flag CH4_Conc_ppm_dilcorr
## 1              12          NA Within Range Within Range             1773.380
## 2              12          NA Within Range Within Range             6853.391
## 3              12          NA Within Range Within Range             1089.595
## 4              12          NA Within Range Within Range             3653.285
## 5              12          NA Within Range Within Range            71519.318
## 6              12          NA Within Range Within Range             8633.394
```

```
##   CO2_Conc_ppm_dilcorr
## 1             58986.49
## 2             50048.50
## 3             44948.81
## 4             29144.59
## 5             78018.31
## 6             97103.18
```

```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(Samples1, "Processed Data/COMPASS_Synoptic_TGW_202310-11_Processed.csv")
```

#end