COMPASS_Synoptic_TGW_2023: Aug & Sept

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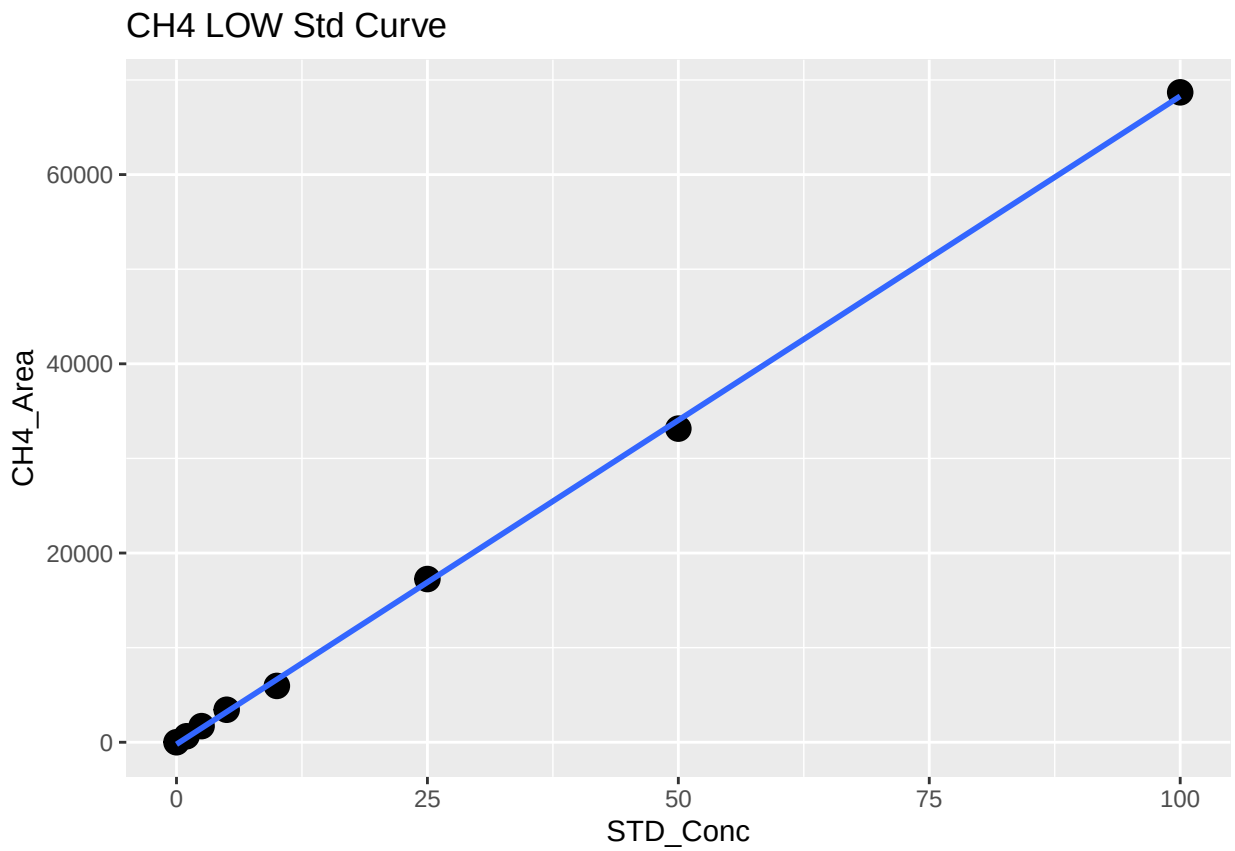
##Set Up

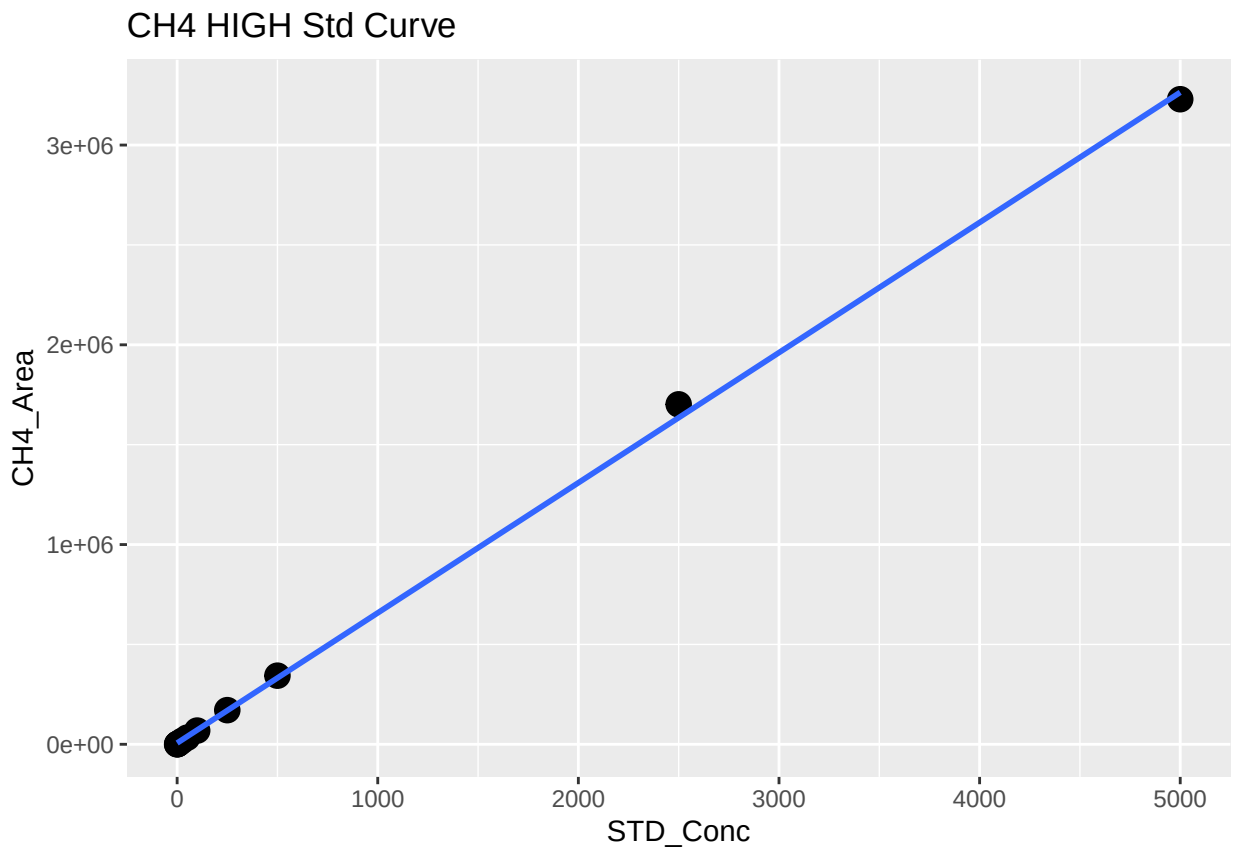
Read in first data file and assess standard curves

```
##     Machine   User Run_Date Sample_Type   Type1 Sample_Year Sample_Month
## 1 Varian GC Wegner 20240306       Blank   Blank        2024         <NA>
## 2 Varian GC Wegner 20240306     STD_CH4 STD_CH4        2024         <NA>
## 3 Varian GC Wegner 20240306     STD_CO2 STD_CO2        2024         <NA>
## 4 Varian GC Wegner 20240306     STD_CH4 STD_CH4        2024         <NA>
## 5 Varian GC Wegner 20240306     STD_CH4 STD_CH4        2024         <NA>
## 6 Varian GC Wegner 20240306     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    25966      633          NA
## 5       STD_2.5ppm_CH4               1      2.5    74737     1704          NA
## 6         STD_5ppm_CH4               1      5.0   150044     3434          NA
##   Lab.Notes
## 1
## 2
## 3
## 4
## 5
## 6
```

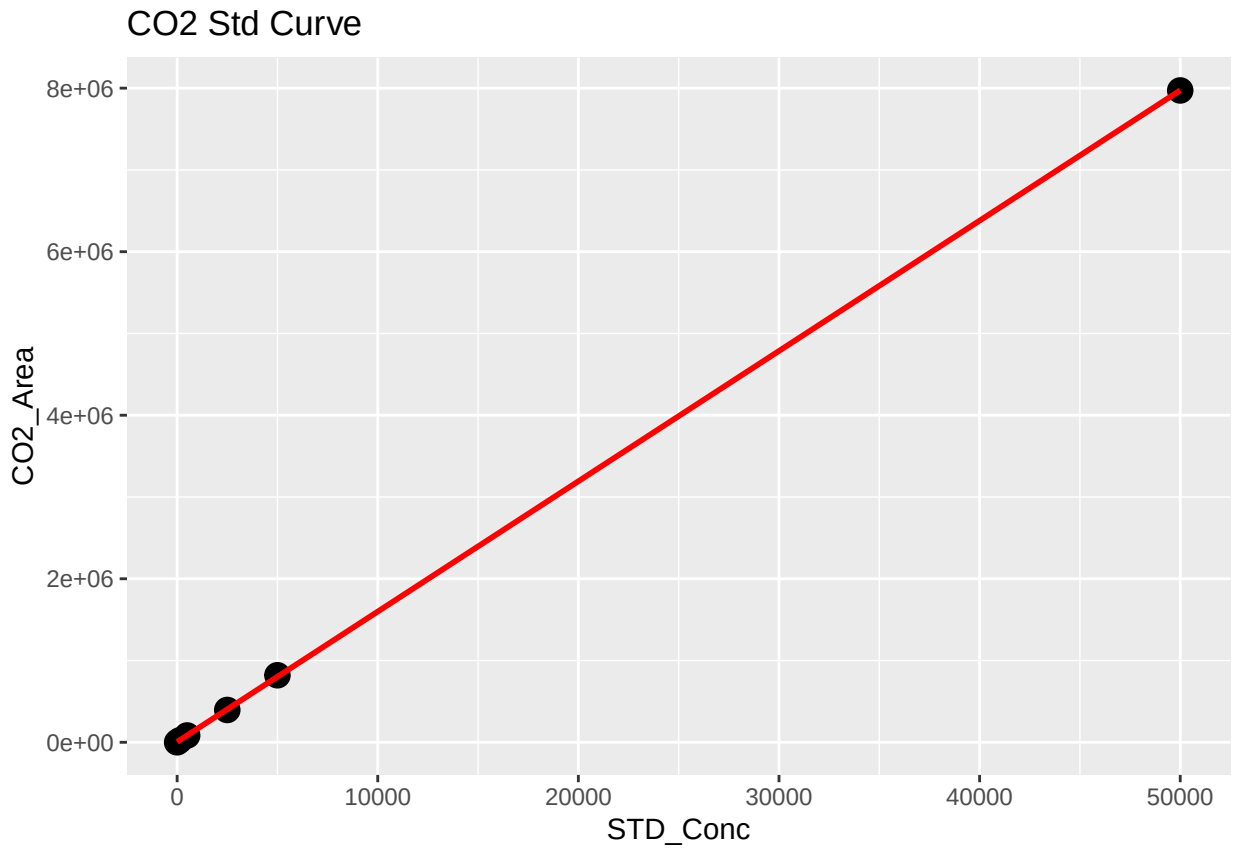
```
## `geom_smooth()` using formula = 'y ~ x'
```



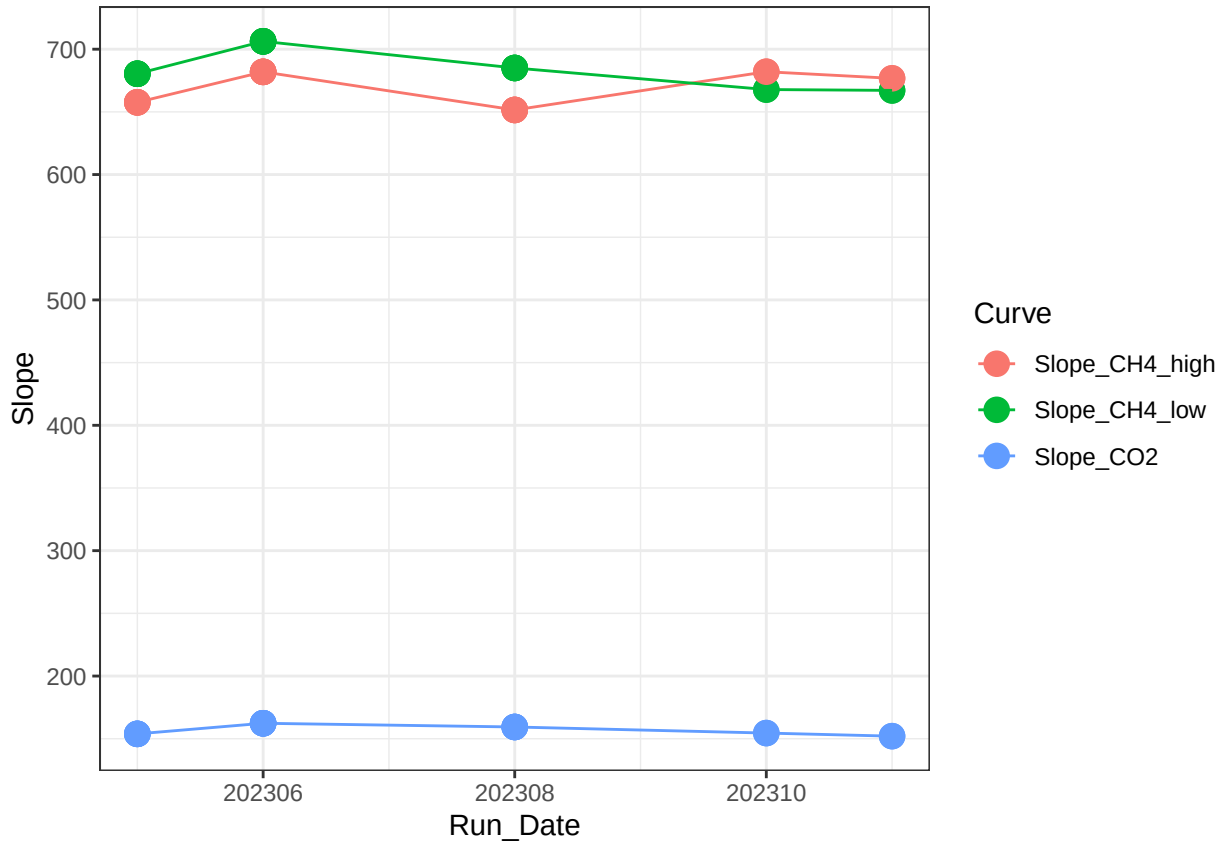

```
##
## Call:
## lm(formula = stds_ch4_low$CH4_Area ~ stds_ch4_low$STD_Conc)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -885.15  -46.06  212.47  254.57  406.96
##
## Coefficients:
##                       Estimate Std. Error t value Pr(>|t|)
## (Intercept)           -216.745    233.575  -0.928    0.389
## stds_ch4_low$STD_Conc  685.018      5.738 119.387 2.33e-11 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 531.4 on 6 degrees of freedom
## Multiple R-squared:  0.9996, Adjusted R-squared:  0.9995
## F-statistic: 1.425e+04 on 1 and 6 DF,  p-value: 2.329e-11

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




```
##
## Call:
## lm(formula = stds_ch4$CH4_Area ~ stds_ch4$STD_Conc)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -34495  -6299  -5920  -1627  66839
##
## Coefficients:
##                   Estimate Std. Error t value Pr(>|t|)
## (Intercept)       6294.027   7889.680   0.798    0.444
## stds_ch4$STD_Conc  651.543      4.864 133.958   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 24630 on 10 degrees of freedom
## Multiple R-squared:  0.9994, Adjusted R-squared:  0.9994
## F-statistic: 1.794e+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
## -5197 -1784 -1449 -8110 17905 -1366
##
## Coefficients:
##                     Estimate Std. Error t value Pr(>|t|)
## (Intercept)       5197.2408  4746.9719   1.095    0.335
## stds_co2$STD_Conc  159.3629     0.2311 689.581 2.65e-11 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 10250 on 4 degrees of freedom
## Multiple R-squared:      1,  Adjusted R-squared:      1
## F-statistic: 4.755e+05 on 1 and 4 DF,  p-value: 2.653e-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
```



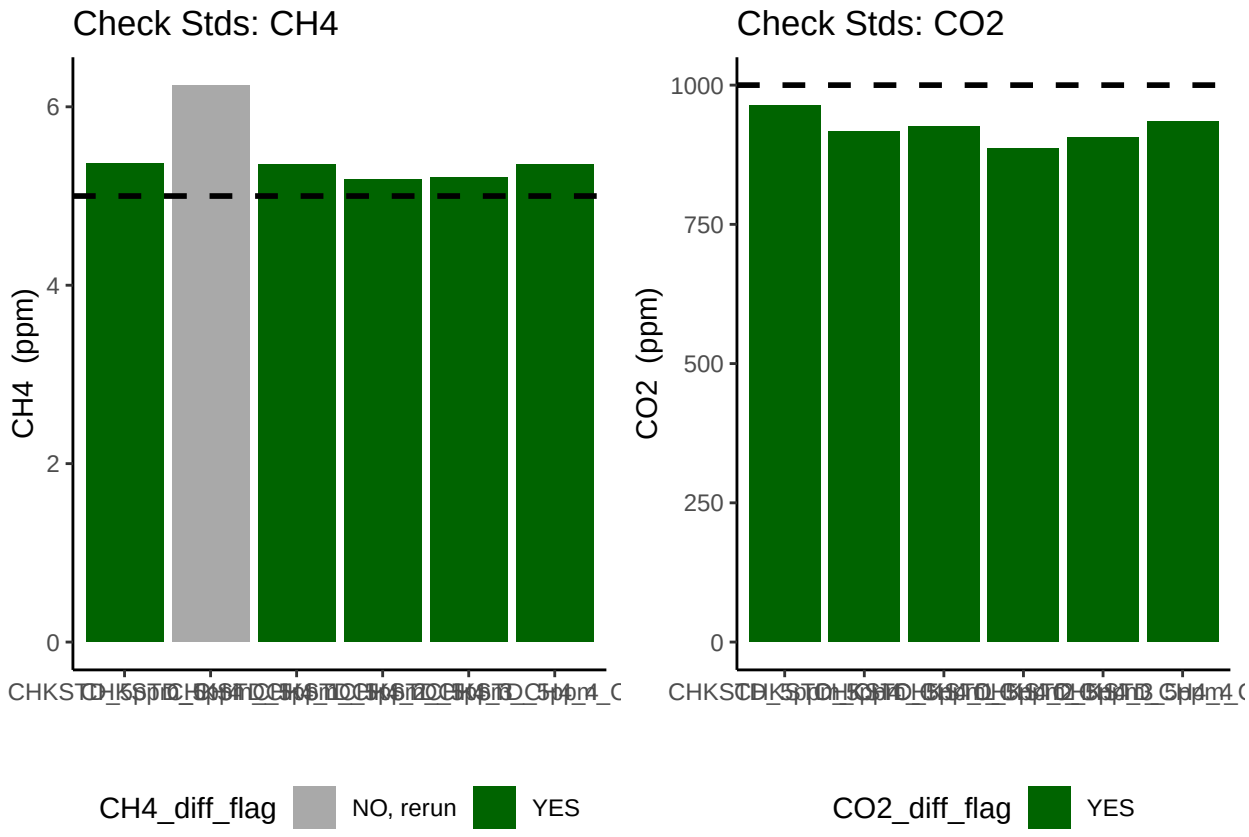
Now calculate the CH4 & CO2 concentrations in ppm

```
#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)
```

```
#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.
```

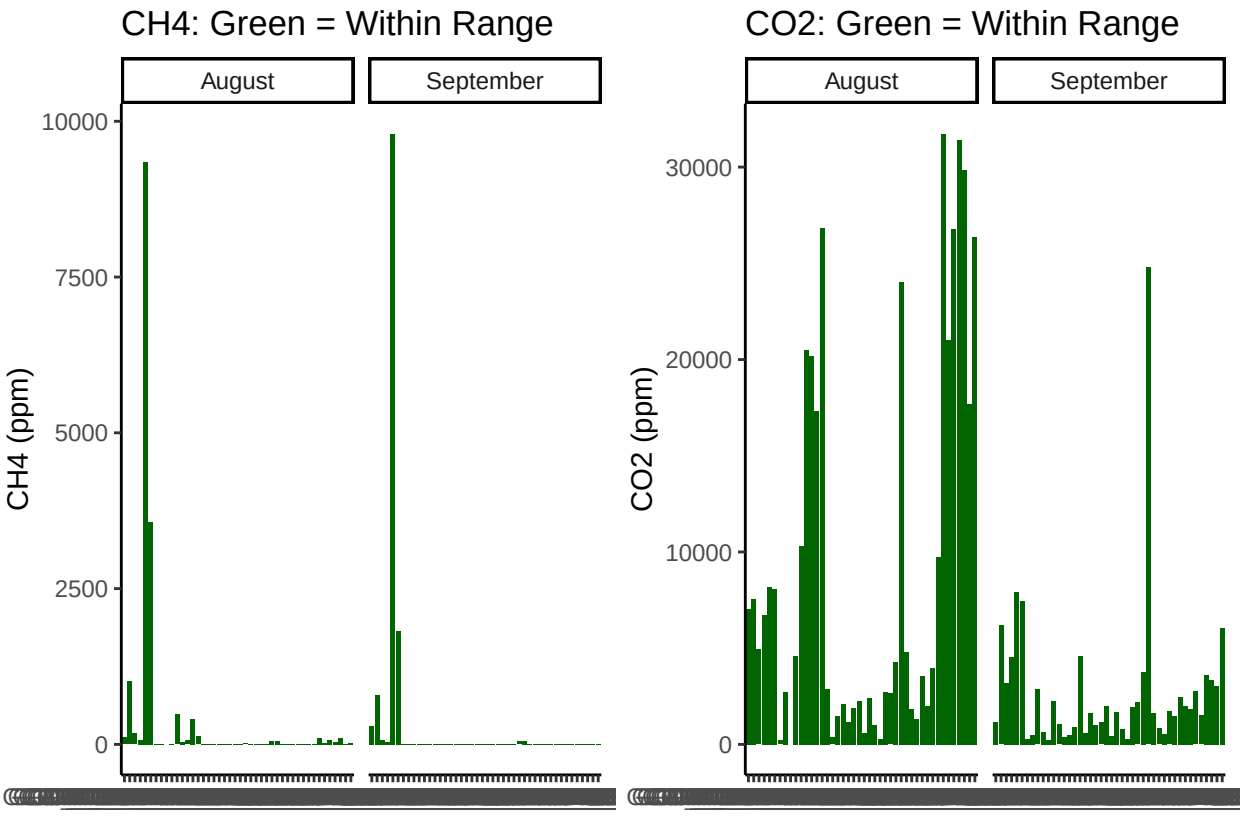


Dilution correct samples

```
#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") +
        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)
```

```
## Warning: Removed 1 row containing missing values or values outside the scale range
## (`geom_bar()`).
## Removed 1 row containing missing values or values outside the scale range
## (`geom_bar()`).
```



Write out processed data & slopes

```
#check results
head(Samples)
```

```
##     Machine   User Run_Date Sample_Type Type1 Sample_Year Sample_Month
## 1 Varian GC Wegner 20240306     Unknown   TGW        2023       August
## 2 Varian GC Wegner 20240306     Unknown   TGW        2023       August
## 3 Varian GC Wegner 20240306     Unknown   TGW        2023       August
## 4 Varian GC Wegner 20240306     Unknown   TGW        2023       August
## 5 Varian GC Wegner 20240306     Unknown   TGW        2023       August
## 6 Varian GC Wegner 20240306     Unknown   TGW        2023       August
##         Sample_ID Dilution_Factor STD_Conc CO2_Area CH4_Area Field.Notes
## 1 GCW_TGW_TR_SF_1              12       NA  1125846    78774          NA
## 2 GCW_TGW_TR_SF_2              12       NA  1207027   663101          NA
## 3 GCW_TGW_TR_SF_3              12       NA   790227   120943          NA
## 4 GCW_TGW_TR_SF_4              12       NA  1078093    44642          NA
## 5 GCW_TGW_TR_SF_5              12       NA  1311256  6097194          NA
## 6 GCW_TGW_TR_SF_6              12       NA  1292180  2333457          NA
##               Lab.Notes CH4_Curve CH4_Conc_ppm CO2_Conc_ppm     CH4_Flag
## 1 10mL N2 added in lab       High    111.24351     7032.055 Within Range
## 2 10mL N2 added in lab       High   1008.07863     7541.464 Within Range
## 3 10mL N2 added in lab       High    175.96521     4926.050 Within Range
## 4 10mL N2 added in lab        Low     65.48551     6732.405 Within Range
```

```
## 5 10mL N2 added in lab       High   9348.41793     8195.500 Within Range
## 6 10mL N2 added in lab       High   3571.76971     8075.798 Within Range
##       CO2_Flag CH4_Conc_ppm_dilcorr CO2_Conc_ppm_dilcorr
## 1 Within Range            1334.9221             84384.66
## 2 Within Range           12096.9435             90497.57
## 3 Within Range            2111.5826             59112.60
## 4 Within Range             785.8261             80788.86
## 5 Within Range          112181.0151             98346.00
## 6 Within Range           42861.2366             96909.58
```

```
#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 20240306   TGW        2023       August GCW_TGW_TR_SF_1
## 2 Varian GC Wegner 20240306   TGW        2023       August GCW_TGW_TR_SF_2
## 3 Varian GC Wegner 20240306   TGW        2023       August GCW_TGW_TR_SF_3
## 4 Varian GC Wegner 20240306   TGW        2023       August GCW_TGW_TR_SF_4
## 5 Varian GC Wegner 20240306   TGW        2023       August GCW_TGW_TR_SF_5
## 6 Varian GC Wegner 20240306   TGW        2023       August GCW_TGW_TR_SF_6
##   Dilution_Factor Field.Notes     CH4_Flag     CO2_Flag CH4_Conc_ppm_dilcorr
## 1              12          NA Within Range Within Range            1334.9221
## 2              12          NA Within Range Within Range           12096.9435
## 3              12          NA Within Range Within Range            2111.5826
## 4              12          NA Within Range Within Range             785.8261
## 5              12          NA Within Range Within Range          112181.0151
## 6              12          NA Within Range Within Range           42861.2366
##   CO2_Conc_ppm_dilcorr
## 1             84384.66
## 2             90497.57
## 3             59112.60
## 4             80788.86
## 5             98346.00
## 6             96909.58
```

```
Samples1 <- Samples1 %>%
  separate(Sample_ID, into = c("Site", "Gas_Sample", "Zone", "Tree_Code", "Replicate"), sep = "_", remo
  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_202308-09_Processed.csv")
```

#end