COMPASS_Synoptic_TGW_2023: June & July

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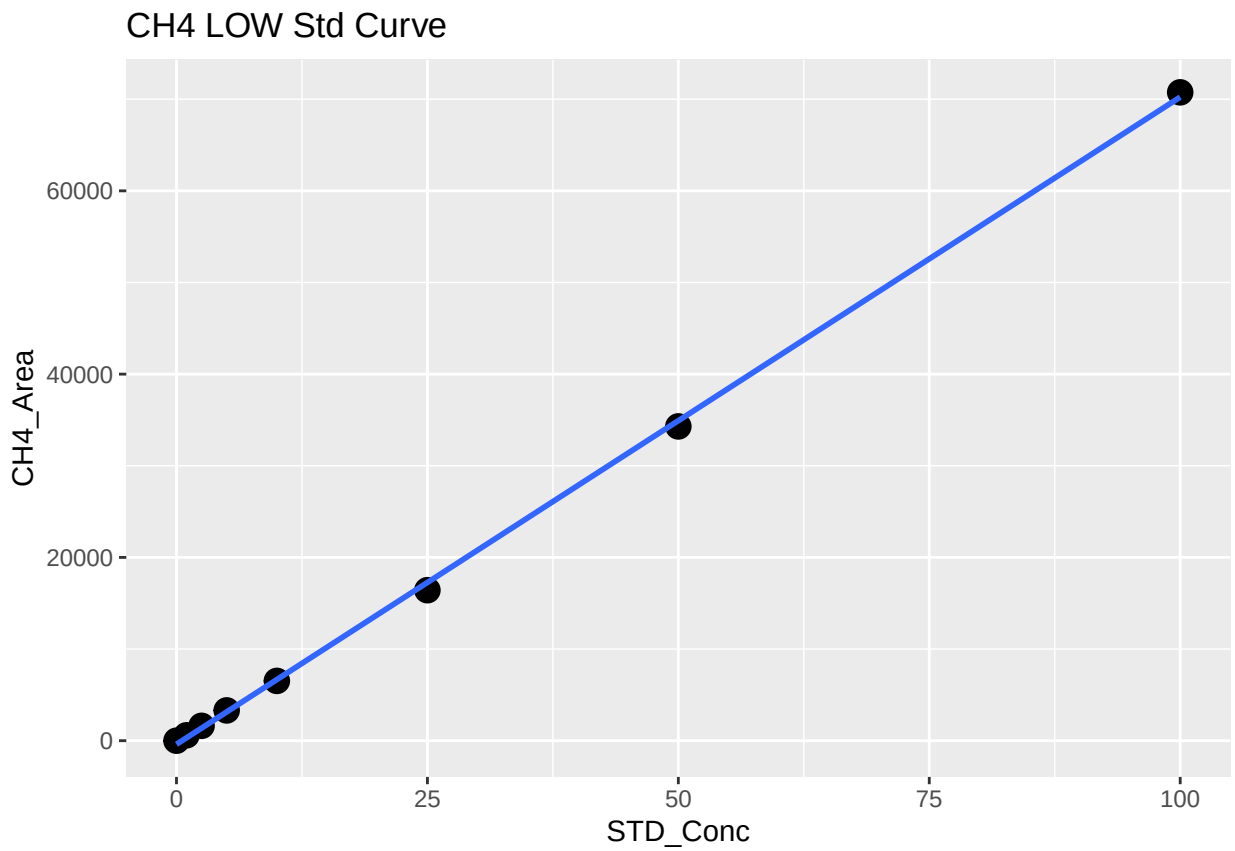
##Set Up

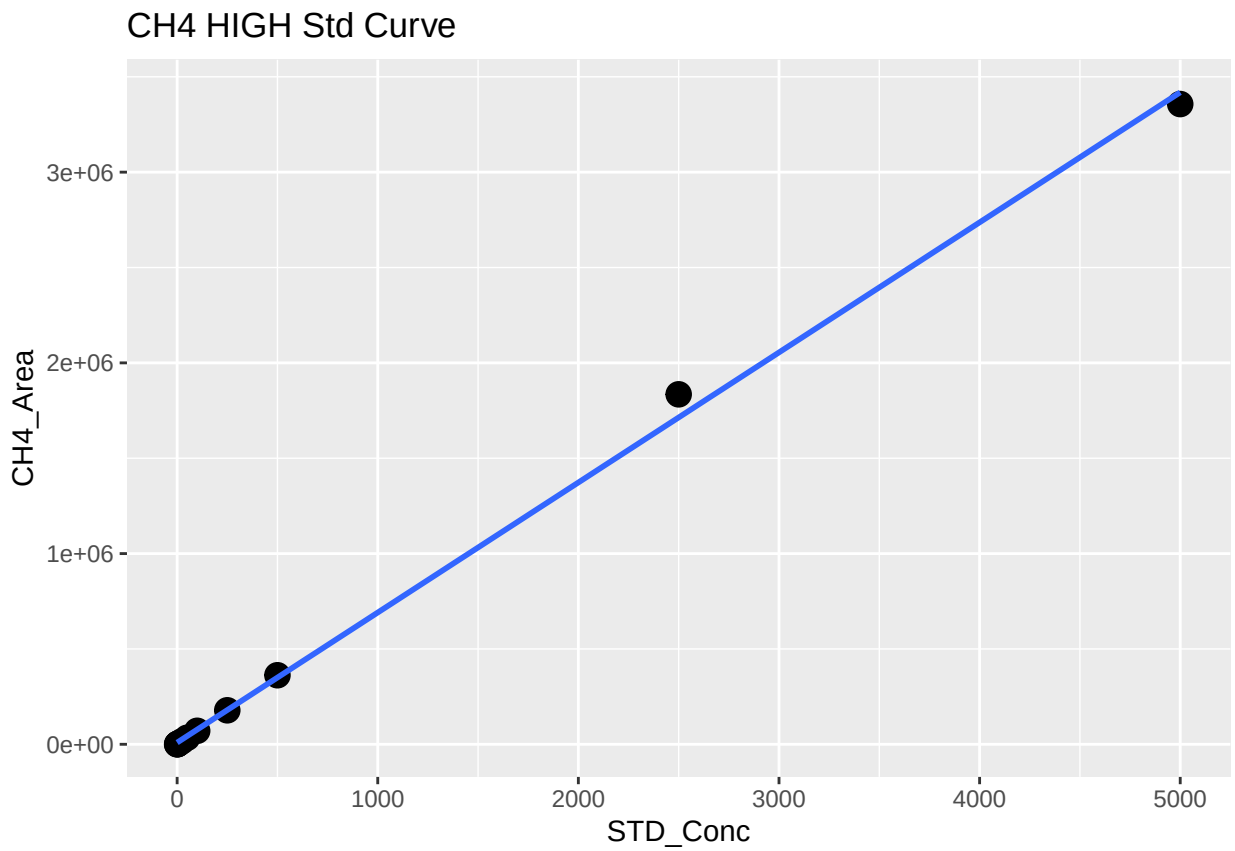
Read in first data file and assess standard curves

```
##     Machine   User Run_Date Sample_Type   Type1 Sample_Year Sample_Month
## 1 Varian GC Wegner 20230301       Blank   Blank        2023         <NA>
## 2 Varian GC Wegner 20230301     STD_CH4 STD_CH4        2023         <NA>
## 3 Varian GC Wegner 20230301     STD_CO2 STD_CO2        2023         <NA>
## 4 Varian GC Wegner 20230301     STD_CH4 STD_CH4        2023         <NA>
## 5 Varian GC Wegner 20230301     STD_CH4 STD_CH4        2023         <NA>
## 6 Varian GC Wegner 20230301     STD_CH4 STD_CH4        2023         <NA>
##              Sample_ID Dilution_Factor STD_Conc CO2_Area CH4_Area Field.Notes
## 1              Blank_0               1      0.0     2844        0          NA
## 2 Blank_0_repeatforCH4               1      0.0     2844        0          NA
## 3 Blank_0_repeatforCO2               1      0.0     2844        0          NA
## 4         STD_1ppm_CH4               1      1.0    27299      587          NA
## 5       STD_2.5ppm_CH4               1      2.5    72256     1621          NA
## 6         STD_5ppm_CH4               1      5.0   149377     3304          NA
##   Lab.Notes
## 1
## 2
## 3
## 4
## 5
## 6
```

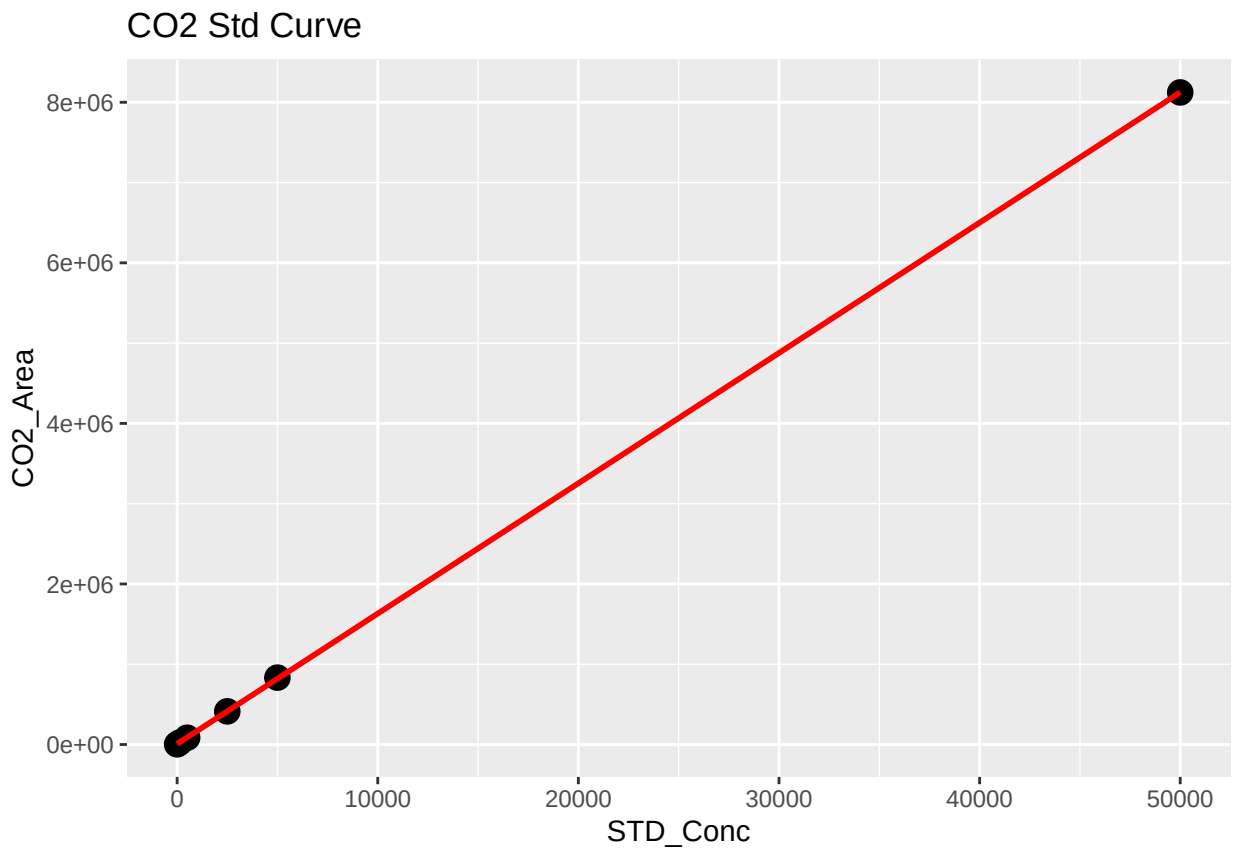
```
## `geom_smooth()` using formula = 'y ~ x'
```



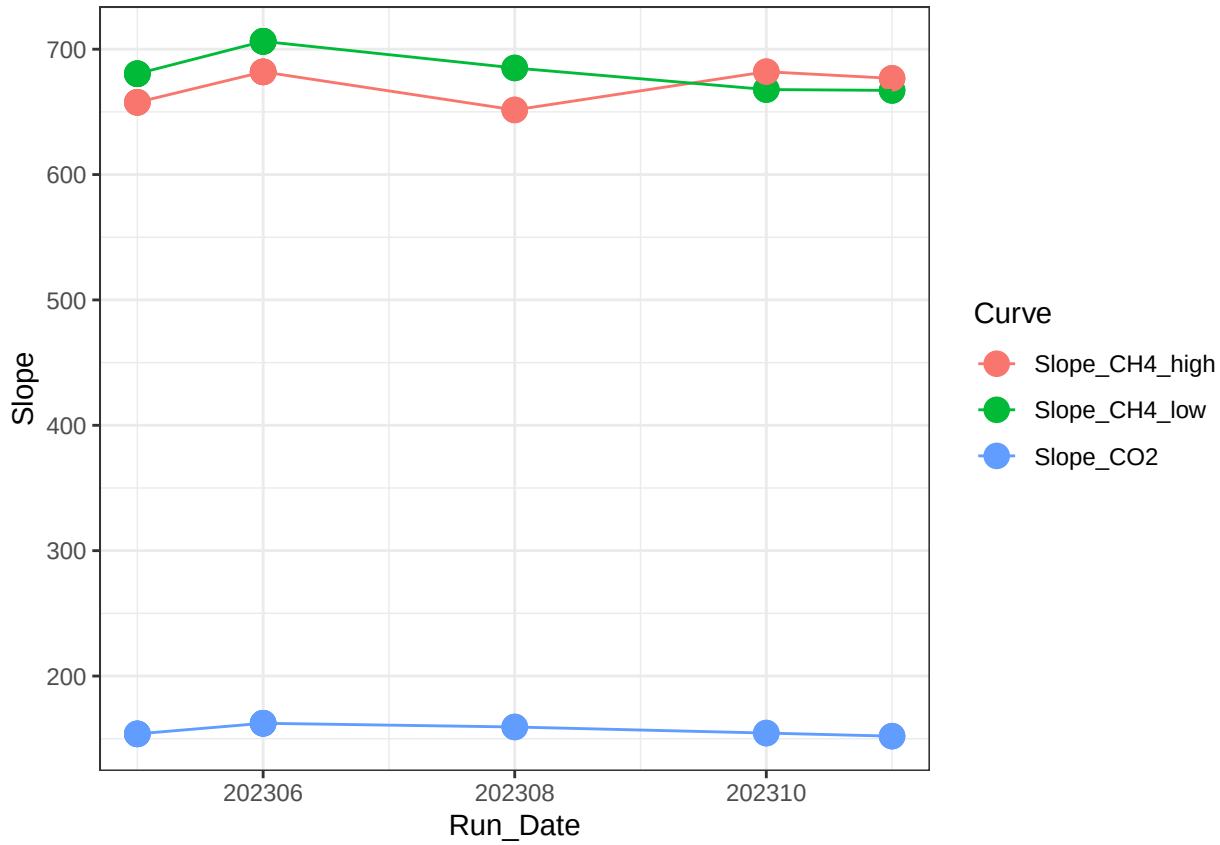

```
##
## Call:
## lm(formula = stds_ch4_low$CH4_Area ~ stds_ch4_low$STD_Conc)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -840.3 -263.6  209.0  305.5  518.8
##
## Coefficients:
##                       Estimate Std. Error t value Pr(>|t|)
## (Intercept)           -394.95     234.50  -1.684    0.143
## stds_ch4_low$STD_Conc   706.25       5.76 122.605 1.99e-11 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 533.5 on 6 degrees of freedom
## Multiple R-squared:  0.9996, Adjusted R-squared:  0.9995
## F-statistic: 1.503e+04 on 1 and 6 DF,  p-value: 1.985e-11

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




```
##
## Call:
## lm(formula = stds_ch4$CH4_Area ~ stds_ch4$STD_Conc)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -61479  -9176  -9065  -5162 121261
##
## Coefficients:
##                    Estimate Std. Error t value Pr(>|t|)
## (Intercept)        9023.428  14061.392   0.642    0.535
## stds_ch4$STD_Conc   681.911      8.668  78.666 2.69e-15 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 43890 on 10 degrees of freedom
## Multiple R-squared:  0.9984, Adjusted R-squared:  0.9982
## F-statistic:  6188 on 1 and 10 DF,  p-value: 2.692e-15

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




```
##
## Call:
## lm(formula = stds_co2$CO2_Area ~ stds_co2$STD_Conc)
##
## Residuals:
##       1       2       3       4       5       6
## -4881.4 -3366.5 -3846.6  -493.3 13906.9 -1319.1
##
## Coefficients:
##                     Estimate Std. Error t value Pr(>|t|)
## (Intercept)       7725.4277  3625.8651   2.131      0.1
## stds_co2$STD_Conc  162.3283     0.1765 919.597 8.39e-12 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 7832 on 4 degrees of freedom
## Multiple R-squared:      1,  Adjusted R-squared:      1
## F-statistic: 8.457e+05 on 1 and 4 DF,  p-value: 8.39e-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
```



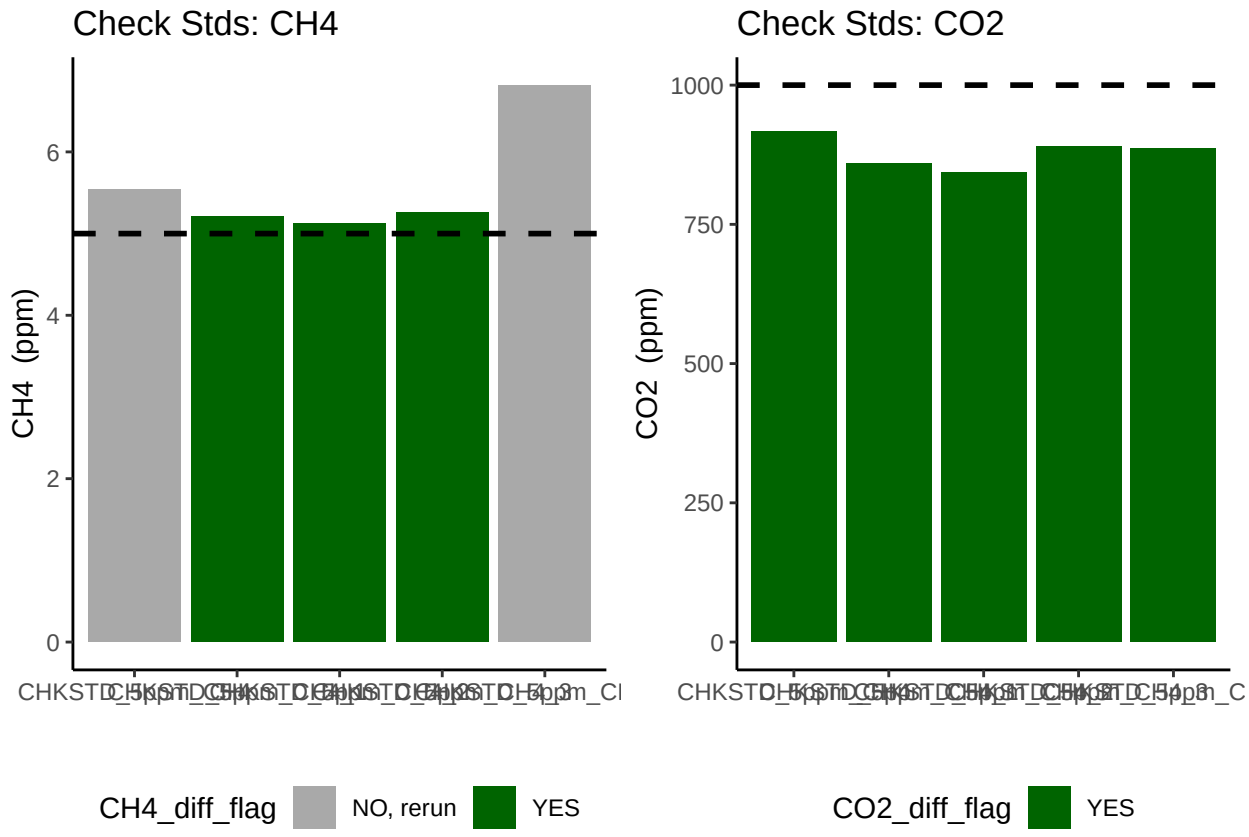
Now calculate the CH4 & CO2 concentrations in ppm

```
#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)
```

```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.
```

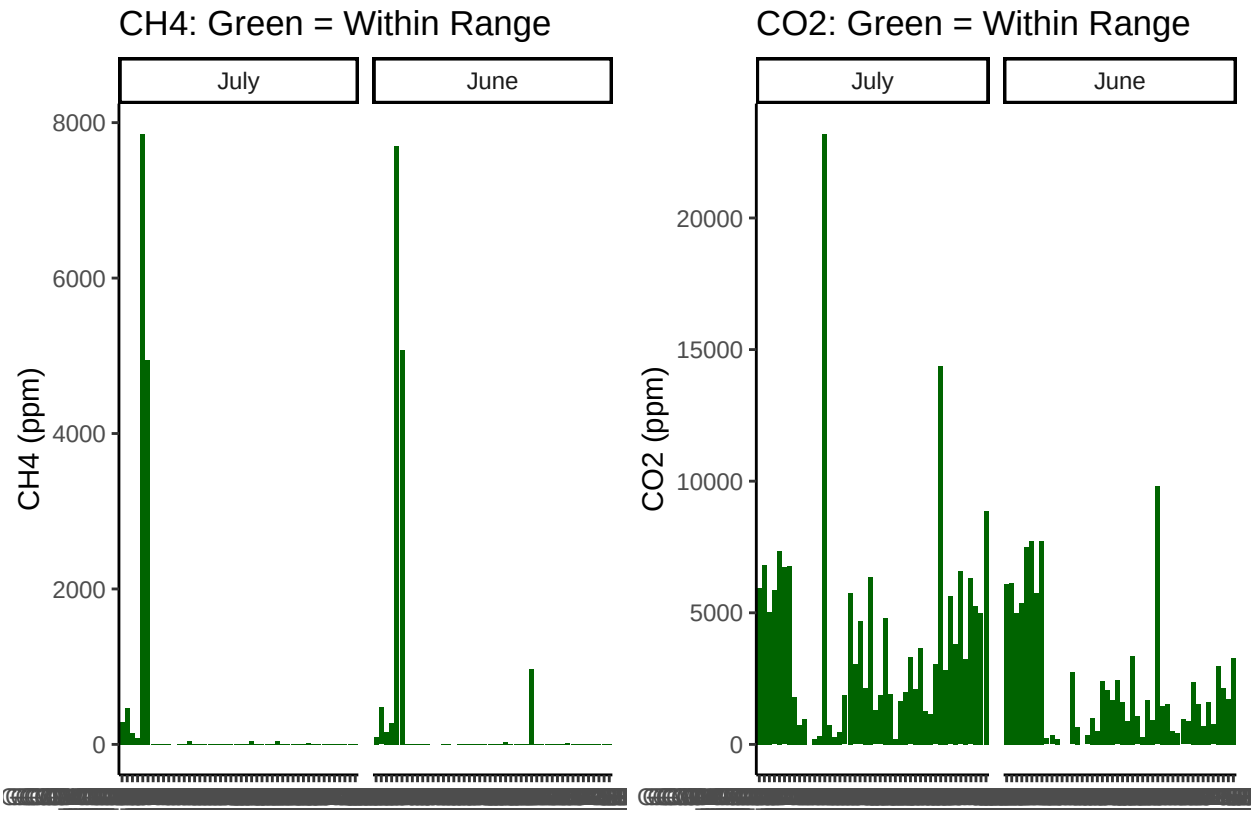


Dilution correct samples

```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") +
        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 20230301     Unknown   TGW        2023         June
## 2 Varian GC Wegner 20230301     Unknown   TGW        2023         June
## 3 Varian GC Wegner 20230301     Unknown   TGW        2023         June
## 4 Varian GC Wegner 20230301     Unknown   TGW        2023         June
## 5 Varian GC Wegner 20230301     Unknown   TGW        2023         June
## 6 Varian GC Wegner 20230301     Unknown   TGW        2023         June
##         Sample_ID Dilution_Factor STD_Conc CO2_Area CH4_Area Field.Notes
## 1 GCW_TGW_TR_SF_1              12       NA   995839    74179          NA
## 2 GCW_TGW_TR_SF_2              12       NA  1002126   332049          NA
## 3 GCW_TGW_TR_SF_3              12       NA   819981   115222          NA
## 4 GCW_TGW_TR_SF_4              12       NA   878772   198883          NA
## 5 GCW_TGW_TR_SF_5              12       NA  1223752  5258787          NA
## 6 GCW_TGW_TR_SF_6              12       NA  1261107  3472444          NA
##              Lab.Notes CH4_Curve CH4_Conc_ppm CO2_Conc_ppm     CH4_Flag
## 1 10mL N2 added in lab      High     95.54849     6087.129 Within Range
## 2 10mL N2 added in lab      High    473.70632     6125.860 Within Range
## 3 10mL N2 added in lab      High    155.73670     5003.782 Within Range
## 4 10mL N2 added in lab      High    278.42279     5365.955 Within Range
```

```
## 5 10mL N2 added in lab      High   7698.60475     7491.154 Within Range
## 6 10mL N2 added in lab      High   5078.99179     7721.274 Within Range
##       CO2_Flag CH4_Conc_ppm_dilcorr CO2_Conc_ppm_dilcorr
## 1 Within Range             1146.582             73045.55
## 2 Within Range             5684.476             73510.31
## 3 Within Range             1868.840             60045.38
## 4 Within Range             3341.073             64391.46
## 5 Within Range            92383.257             89893.85
## 6 Within Range            60947.901             92655.29
```

```
#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 20230301   TGW        2023         June GCW_TGW_TR_SF_1
## 2 Varian GC Wegner 20230301   TGW        2023         June GCW_TGW_TR_SF_2
## 3 Varian GC Wegner 20230301   TGW        2023         June GCW_TGW_TR_SF_3
## 4 Varian GC Wegner 20230301   TGW        2023         June GCW_TGW_TR_SF_4
## 5 Varian GC Wegner 20230301   TGW        2023         June GCW_TGW_TR_SF_5
## 6 Varian GC Wegner 20230301   TGW        2023         June GCW_TGW_TR_SF_6
##   Dilution_Factor Field.Notes     CH4_Flag     CO2_Flag CH4_Conc_ppm_dilcorr
## 1              12          NA Within Range Within Range             1146.582
## 2              12          NA Within Range Within Range             5684.476
## 3              12          NA Within Range Within Range             1868.840
## 4              12          NA Within Range Within Range             3341.073
## 5              12          NA Within Range Within Range            92383.257
## 6              12          NA Within Range Within Range            60947.901
##   CO2_Conc_ppm_dilcorr
## 1             73045.55
## 2             73510.31
## 3             60045.38
## 4             64391.46
## 5             89893.85
## 6             92655.29
```

```
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"
  ))
```

```
## Warning: Expected 5 pieces. Additional pieces discarded in 2 rows [73, 74].
```

```
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_202306-07_Processed.csv")
```

#end