COMPASS_TEMPEST_SGW_2024: May

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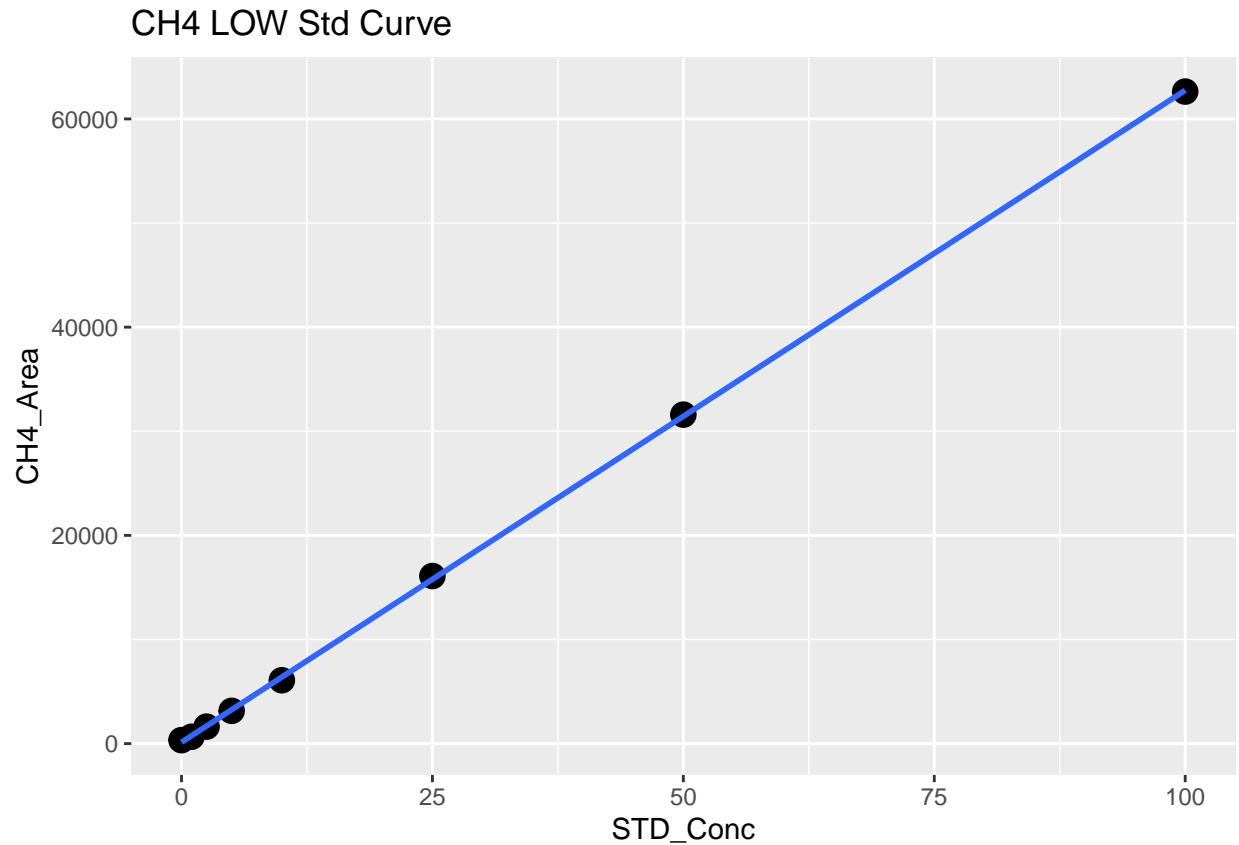
2023-01-14

##Set Up

Read in first data file and assess standard curves
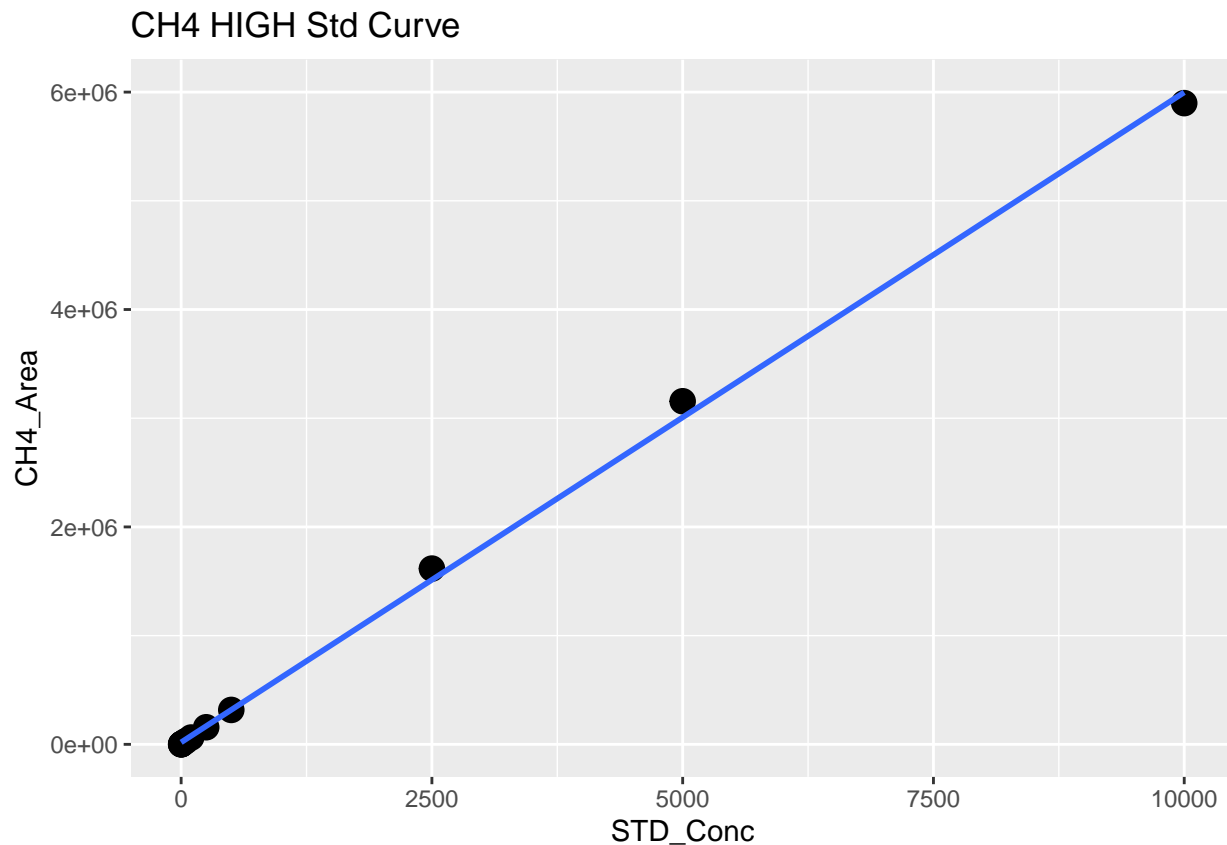
```
##      Machine    User Run_Date Sample_Type Type1 Sample_Year Sample_Month
## 1 Varian GC Wegner 20240710       Blank Blank        2024         <NA>
## 2 Varian GC Wegner 20240710     STD_CH4  STDs        2024         <NA>
## 3 Varian GC Wegner 20240710     STD_CO2  STDs        2024         <NA>
## 4 Varian GC Wegner 20240710     STD_CH4  STDs        2024         <NA>
## 5 Varian GC Wegner 20240710     STD_CH4  STDs        2024         <NA>
## 6 Varian GC Wegner 20240710     STD_CH4  STDs        2024         <NA>
##            Sample_ID Dilution_Factor STD_Conc CO2_Area CH4_Area Lab_Notes
## 1            Blank_04               1      0.0    30628      333
## 2 Blank_0_repeatforCH4               1      0.0    30628      333
## 3 Blank_0_repeatforCO2               1      0.0    30628      333
## 4       STD_1ppm_CH4               1      1.0        0      659
## 5     STD_2.5ppm_CH4               1      2.5    84376     1631
## 6       STD_5ppm_CH4               1      5.0   165368     3150
##   Field_Notes
## 1          NA
## 2          NA
## 3          NA
## 4          NA
## 5          NA
## 6          NA
```

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

CH4 LOW Std Curve


```
##
## Call:
## lm(formula = stds_ch4_low$CH4_Area ~ stds_ch4_low$STD_Conc)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -302.82 -110.36  -76.54  172.26  315.95
##
## Coefficients:
##                       Estimate Std. Error t value Pr(>|t|)
## (Intercept)            125.662     98.063   1.281    0.247
## stds_ch4_low$STD_Conc  626.216      2.409 259.957 2.19e-13 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 223.1 on 6 degrees of freedom
## Multiple R-squared:  0.9999, Adjusted R-squared:  0.9999
## F-statistic: 6.758e+04 on 1 and 6 DF,  p-value: 2.187e-13


## 'geom_smooth()' using formula = 'y ~ x'
```
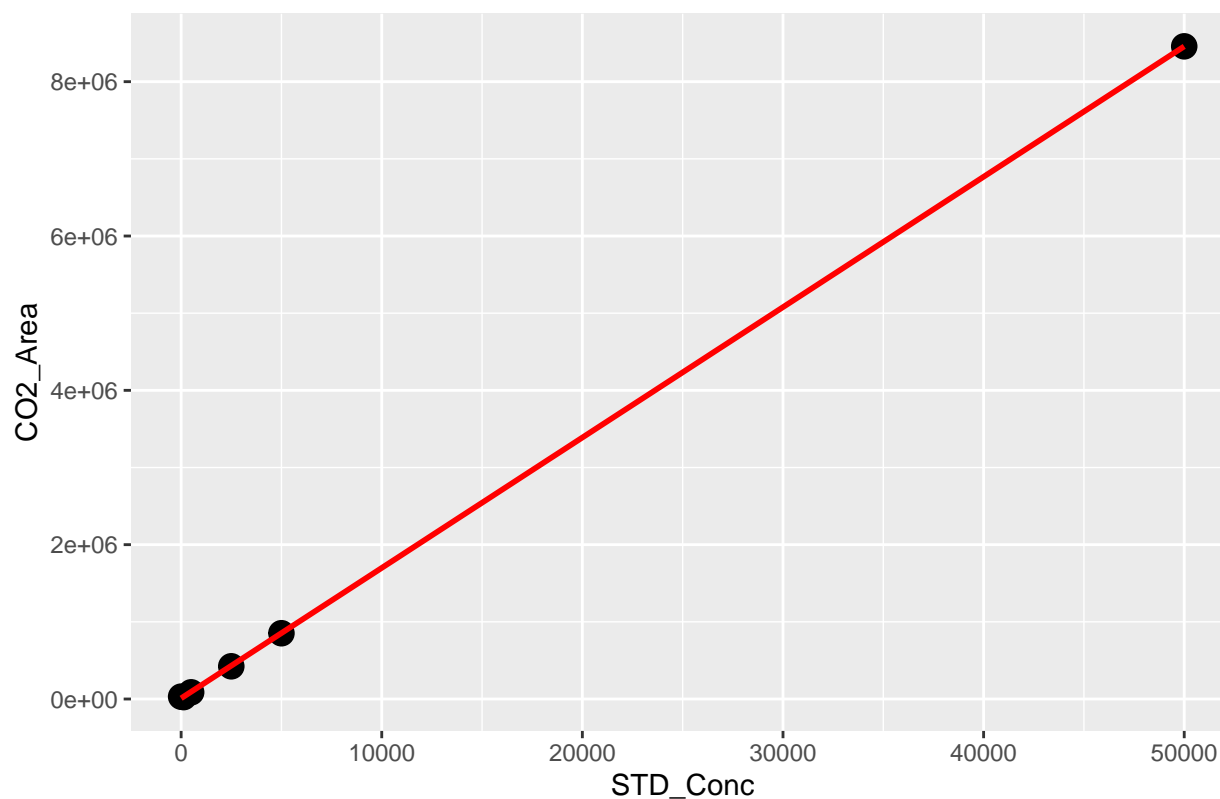
CH4 HIGH Std Curve


```
## 
## Call:
## lm(formula = stds_ch4$CH4_Area ~ stds_ch4$STD_Conc)
## 
## Residuals:
##    Min     1Q Median     3Q    Max 
## -99287 -18263 -17251 -10731 148050 
## 
## Coefficients:
##                   Estimate Std. Error t value Pr(>|t|)    
## (Intercept)      18399.062  19841.130   0.927    0.374    
## stds_ch4$STD_Conc  597.939      6.237  95.875   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## 
## Residual standard error: 64030 on 11 degrees of freedom
## Multiple R-squared:  0.9988, Adjusted R-squared:  0.9987 
## F-statistic:  9192 on 1 and 11 DF,  p-value: < 2.2e-16


## 'geom_smooth()' using formula = 'y ~ x'
```
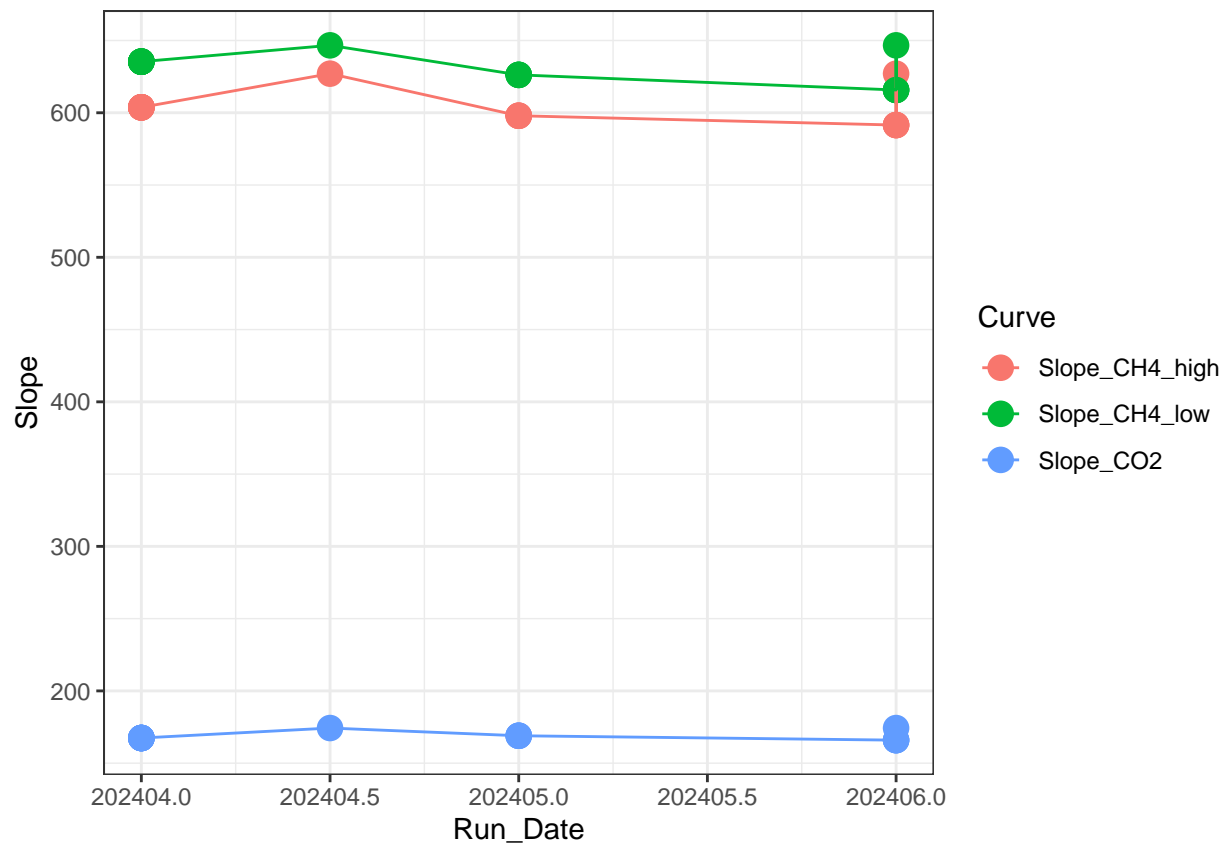
CO2 Std Curve


```
## 
## Call:
## lm(formula = stds_co2$CO2_Area ~ stds_co2$STD_Conc)
## 
## Residuals:
##       1       2       3       4       5       6
## 21527.9 -5836.8 -6986.9 -7744.0 -1591.0   630.8
## 
## Coefficients:
##                    Estimate Std. Error t value Pr(>|t|)
## (Intercept)       9100.0798  5713.6961   1.593    0.186
## stds_co2$STD_Conc  168.9656     0.2782 607.429 4.41e-11 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## 
## Residual standard error: 12340 on 4 degrees of freedom
## Multiple R-squared:      1,  Adjusted R-squared:      1
## F-statistic: 3.69e+05 on 1 and 4 DF,  p-value: 4.407e-11


##   X          Curve        R2     Slope   Intercept Run_Date
## 1 1  Slope_CH4_low 0.9998964 626.2155    125.6616   202405
## 2 2 Slope_CH4_high 0.9986961 597.9392 18399.0623   202405
## 3 3      Slope_CO2 0.9999864 168.9656   9100.0798   202405
## 4 4  Slope_CH4_low 0.9998964 626.2155    125.6616   202405
## 5 5 Slope_CH4_high 0.9986961 597.9392 18399.0623   202405
## 6 6      Slope_CO2 0.9999864 168.9656   9100.0798   202405
```

Now calculate the CH4 & CO2 concentrations in ppm

```r
#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, "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)/Slop

#Calculate CO2 concentrations in ppm
Samples$CO2_Conc_ppm <- ((Samples$CO2_Area-Slope_CO2$Intercept)/Slope_CO2$Slope)
```
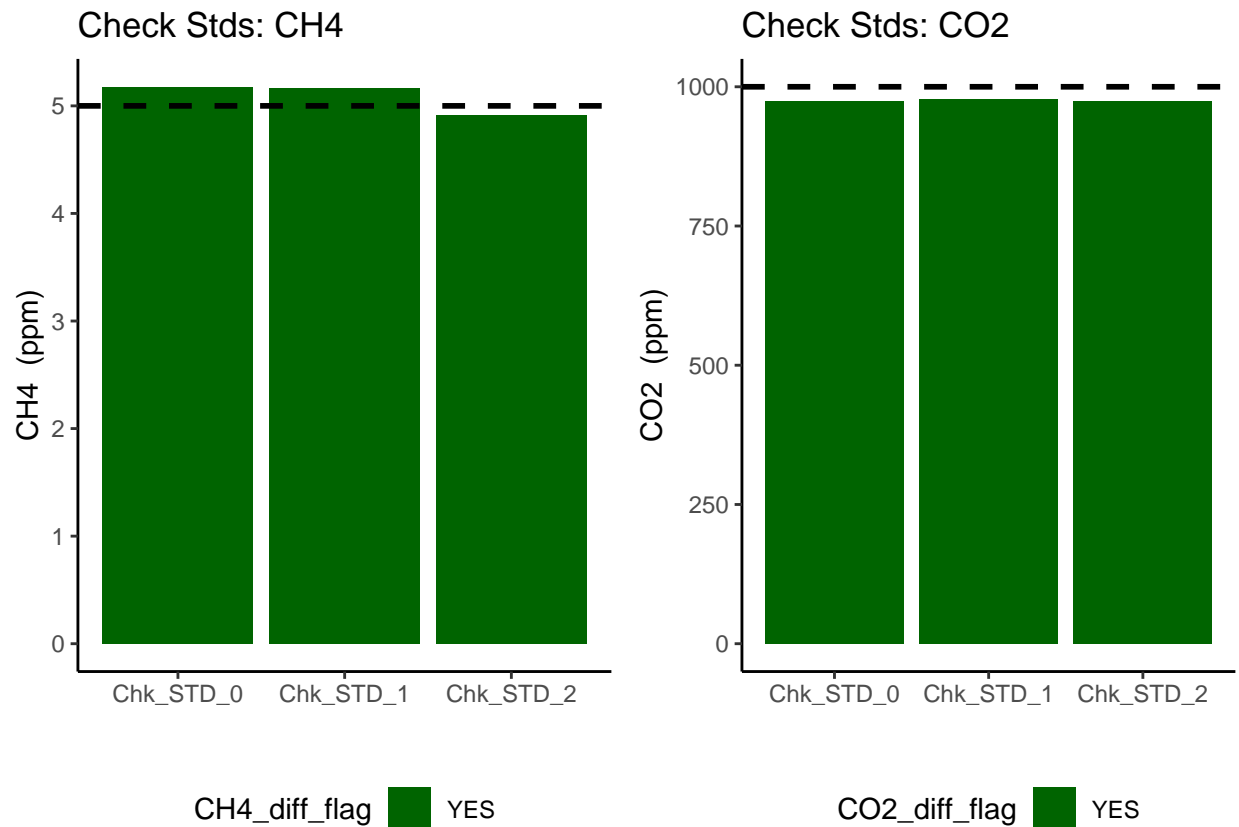
```
#head(Samples)


##########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("red","darkgreen"))+
       #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)
```
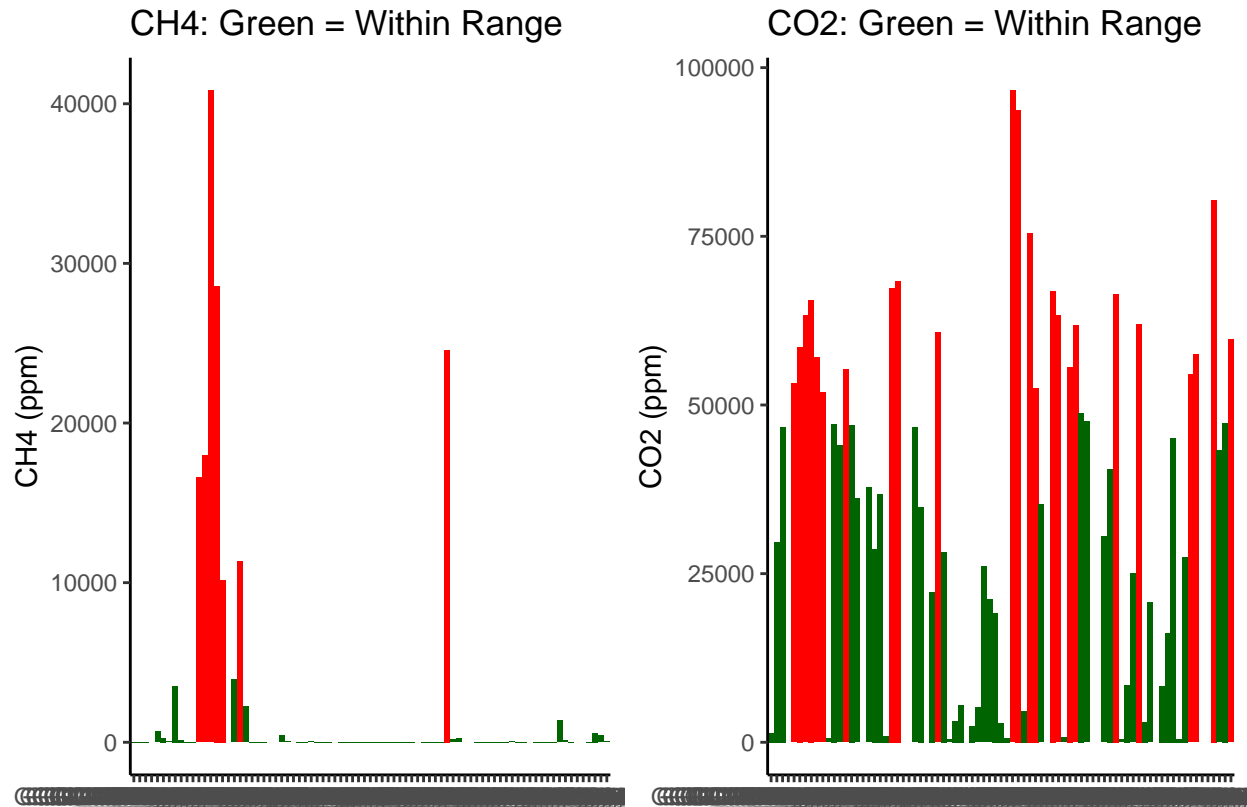
```
## Warning: Removed 12 rows containing missing values or values outside the scale range
## ('geom_bar()').
## Removed 12 rows containing missing values or values outside the scale range
## ('geom_bar()').
```

CH4: Green = Within Range

CO2: Green = Within Range

If samples are water calculate gas in water - only need if there is water

Write out processed data & slopes

```r
#pull out what we need
Samples1 <- Samples[ ,c(1:3,6:9,18:21)]
#head(Samples1)

IDs <- data.frame(do.call('rbind', strsplit(as.character(Samples1$Sample_ID),'_',fixed=TRUE)))
```

```
## Warning in rbind(c("GCW", "TR", "SgwA", "10cm"), c("GCW", "TR", "SgwA", :
## number of columns of result is not a multiple of vector length (arg 10)
```

```r
colnames(IDs) <- c("Site" , "Zone", "Replicate", "Depth")
IDs$Depth1 <- ifelse(IDs$Depth == '10cm', '10',
              ifelse(IDs$Depth == '20cm', '20',
                     ifelse(IDs$Depth == '45cm', '45', '0')))
head(IDs)
```

```
##   Site Zone Replicate Depth Depth1
## 1  GCW   TR      SgwA  10cm     10
## 2  GCW   TR      SgwA  20cm     20
## 3  GCW   TR      SgwA  45cm     45
```

```
## 4  GCW   TR       SgwB  10cm      10
## 5  GCW   TR       SgwB  20cm      20
## 6  GCW   TR       SgwB  45cm      45
```

```r
#rejoin them to the dataframe
alldat <- cbind(IDs, Samples1)
head(alldat)
```

```
##    Site Zone Replicate Depth Depth1    Machine    User Run_Date Sample_Year
## 1  GCW   TR       SgwA  10cm     10 Varian GC Wegner 20240710        2024
## 2  GCW   TR       SgwA  20cm     20 Varian GC Wegner 20240710        2024
## 3  GCW   TR       SgwA  45cm     45 Varian GC Wegner 20240710        2024
## 4  GCW   TR       SgwB  10cm     10 Varian GC Wegner 20240710        2024
## 5  GCW   TR       SgwB  20cm     20 Varian GC Wegner 20240710        2024
## 6  GCW   TR       SgwB  45cm     45 Varian GC Wegner 20240710        2024
##   Sample_Month          Sample_ID Dilution_Factor    CH4_Flag        CO2_Flag
## 1          May GCW_TR_SgwA_10cm               1 Within Range    Within Range
## 2          May GCW_TR_SgwA_20cm               1 Within Range    Within Range
## 3          May GCW_TR_SgwA_45cm               1         <NA>            <NA>
## 4          May GCW_TR_SgwB_10cm               1 Within Range Needs Dilution
## 5          May GCW_TR_SgwB_20cm               1 Within Range Needs Dilution
## 6          May GCW_TR_SgwB_45cm               1 Within Range Needs Dilution
##   CH4_Conc_ppm_dilcorr CO2_Conc_ppm_dilcorr
## 1             7.387773             29686.16
## 2             4.248279             46770.62
## 3                   NA                   NA
## 4           679.553965             53204.00
## 5           252.468719             58552.20
## 6            36.058413             63256.96
```

```r
write.csv(alldat, "Processed Data/COMPASS_CBSYN_SGW_202405_Processed.csv")
```

#end
```