

COMPASS_TEMPEST_SGW_2023: August

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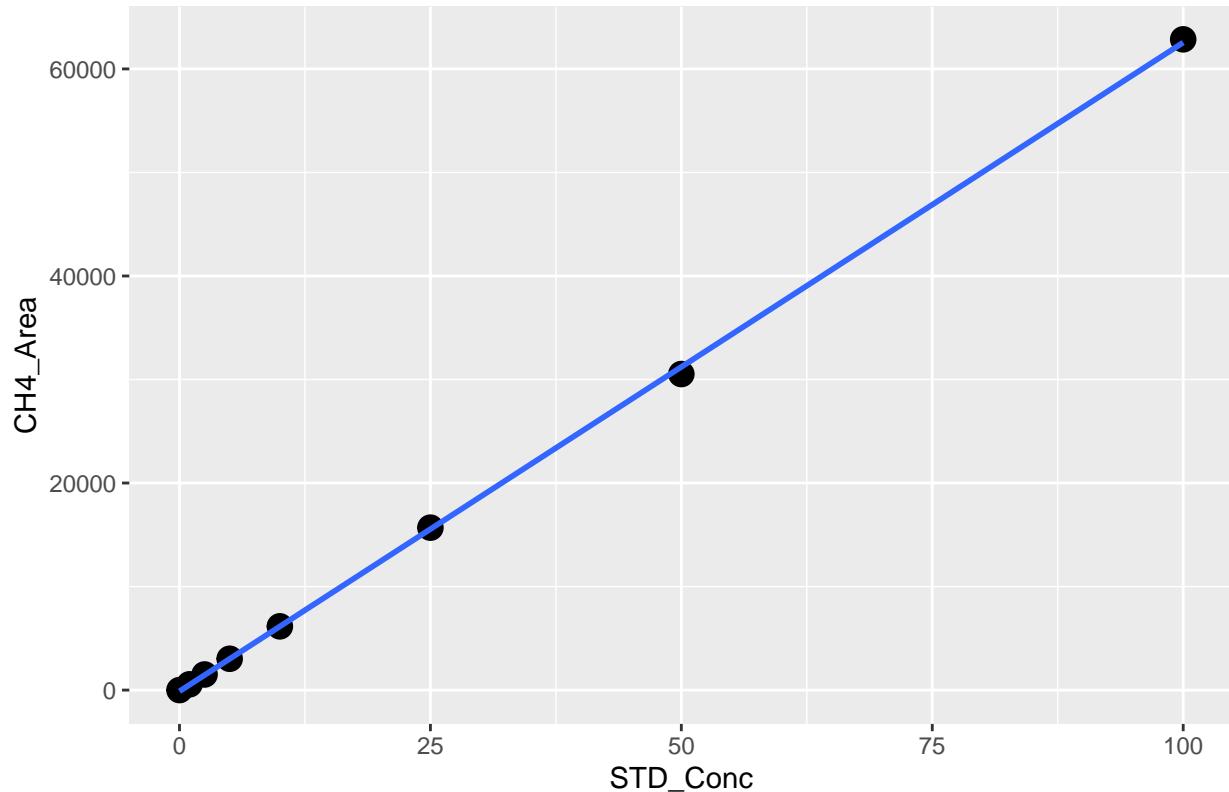
2023-01-14

```
##Set Up
```

Read in first data file and assess standard curves

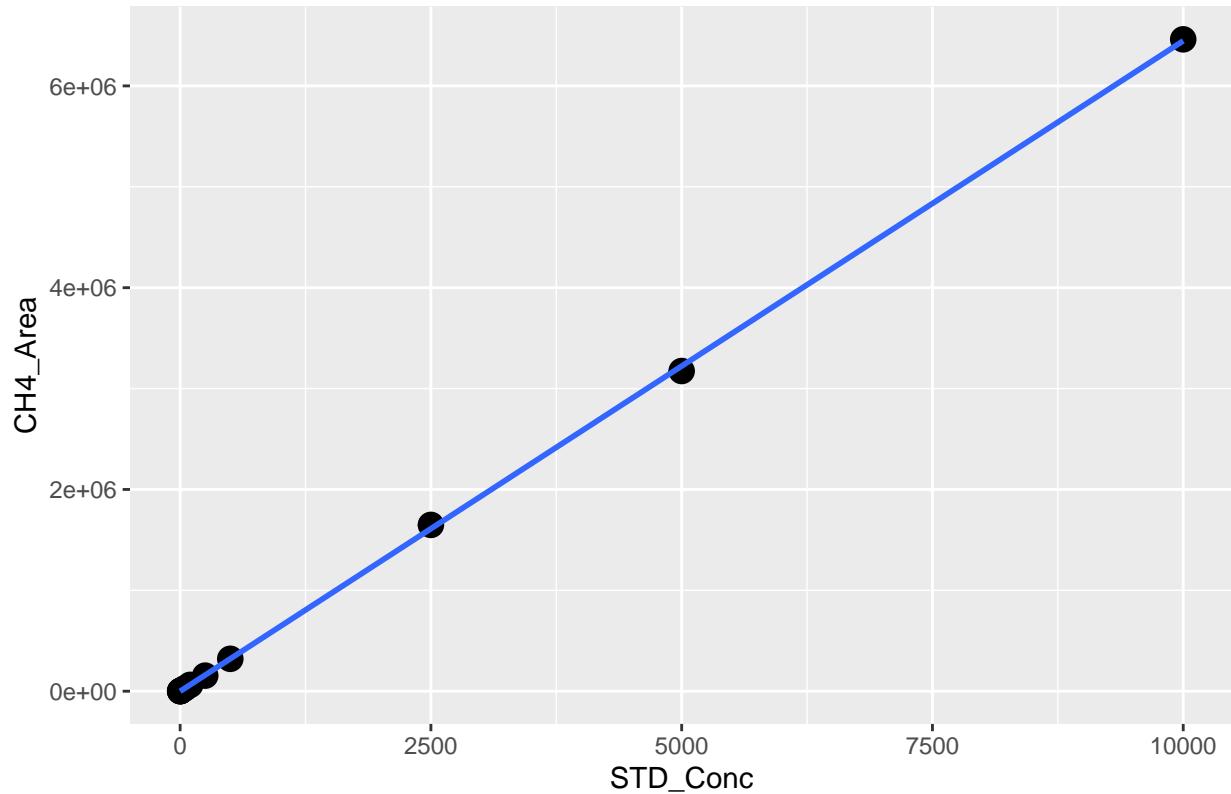
```
##      Machine      User Run_Date Sample_Type Type1 Sample_Year Sample_Month
## 1 Varian GC M. Wegner 20231005     Blank Blank        2023       <NA>
## 2 Varian GC M. Wegner 20231005 STD_CH4 STDs        2023       <NA>
## 3 Varian GC M. Wegner 20231005 STD_CO2 STDs        2023       <NA>
## 4 Varian GC M. Wegner 20231005 STD_CH4 STDs        2023       <NA>
## 5 Varian GC M. Wegner 20231005 STD_CH4 STDs        2023       <NA>
## 6 Varian GC M. Wegner 20231005 STD_CH4 STDs        2023       <NA>
##           Sample_ID Dilution_Factor STD_Conc CO2_Area CH4_Area Lab_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    24190      559       NA
## 5          STD_2.5ppm_CH4     1    2.5    70266     1508       NA
## 6          STD_5ppm_CH4      1    5.0   134586     3025       NA
## `geom_smooth()` using formula = 'y ~ x'
```

CH4 LOW Std Curve



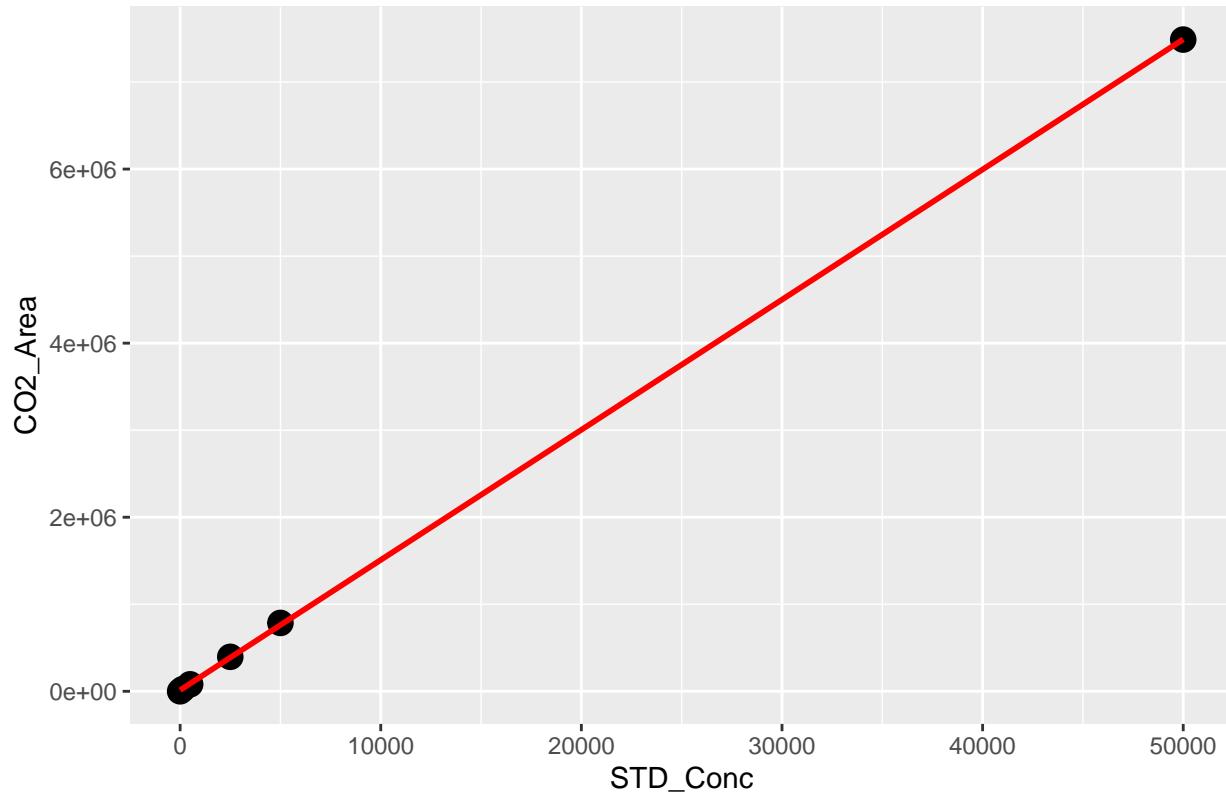
```
##  
## Call:  
## lm(formula = stds_ch4_low$CH4_Area ~ stds_ch4_low$STD_Conc)  
##  
## Residuals:  
##      Min       1Q   Median       3Q      Max  
## -689.90     8.72    54.32   123.22   306.68  
##  
## Coefficients:  
##                               Estimate Std. Error t value Pr(>|t|)  
## (Intercept)           -117.527    140.107 -0.839   0.434  
## stds_ch4_low$STD_Conc  626.688     3.442 182.085 1.85e-12 ***  
## ---  
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1  
##  
## Residual standard error: 318.7 on 6 degrees of freedom  
## Multiple R-squared:  0.9998, Adjusted R-squared:  0.9998  
## F-statistic: 3.315e+04 on 1 and 6 DF,  p-value: 1.851e-12  
  
## 'geom_smooth()' using formula = 'y ~ x'
```

CH4 HIGH Std Curve



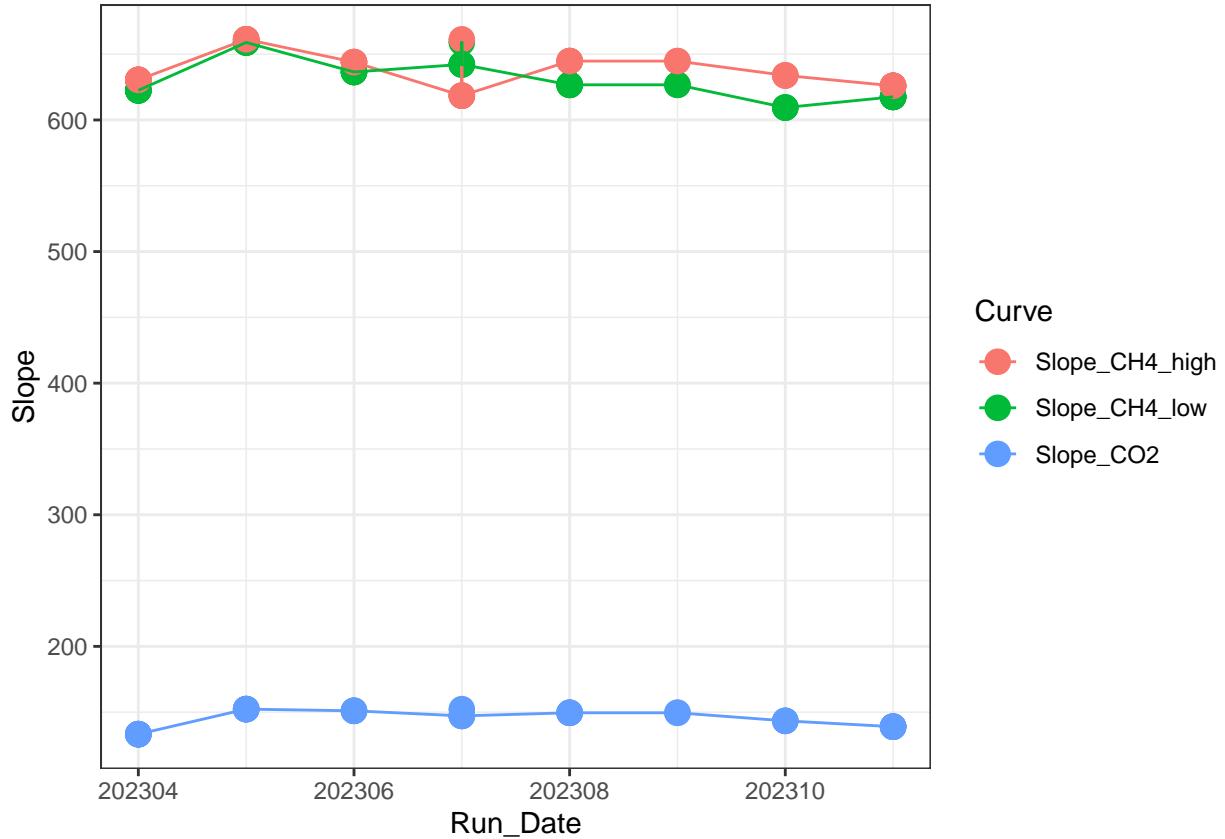
```
##  
## Call:  
## lm(formula = stds_ch4$CH4_Area ~ stds_ch4$STD_Conc)  
##  
## Residuals:  
##      Min       1Q   Median       3Q      Max  
## -48924    -758     567    771  37619  
##  
## Coefficients:  
##                 Estimate Std. Error t value Pr(>|t|)  
## (Intercept)     -856.851   5968.126  -0.144   0.888  
## stds_ch4$STD_Conc  644.724      1.876 343.679 <2e-16 ***  
## ---  
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1  
##  
## Residual standard error: 19260 on 11 degrees of freedom  
## Multiple R-squared:  0.9999 , Adjusted R-squared:  0.9999  
## F-statistic: 1.181e+05 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 
## -13719  -8062  -8127   8463  24185  -2740 
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)    
## (Intercept) 1.372e+04 7.259e+03  1.89   0.132    
## stds_co2$STD_Conc 1.495e+02 3.534e-01 423.15 1.87e-10 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 15680 on 4 degrees of freedom
## Multiple R-squared:      1, Adjusted R-squared:      1
## F-statistic: 1.791e+05 on 1 and 4 DF,  p-value: 1.871e-10

##      X          Curve        R2      Slope    Intercept Run_Date
## 1 1 Slope_CH4_low 0.9997982 642.2013 -176.61917 202307
## 2 2 Slope_CH4_high 0.9995317 618.4551 11202.40792 202307
## 3 3 Slope_CO2 0.9999842 147.1737 10330.39781 202307
## 4 4 Slope_CH4_low 0.9990979 658.8841 -87.56451 202307
## 5 5 Slope_CH4_high 0.9999901 661.2523 176.62351 202307
## 6 6 Slope_CO2 0.9999978 152.3154 8787.66721 202307
```



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, "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)/Slope_CH4_high$Slope, (Samples$CH4_Area-Slope_CH4_low$Intercept)/Slope_CH4_low$Slope)

#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)

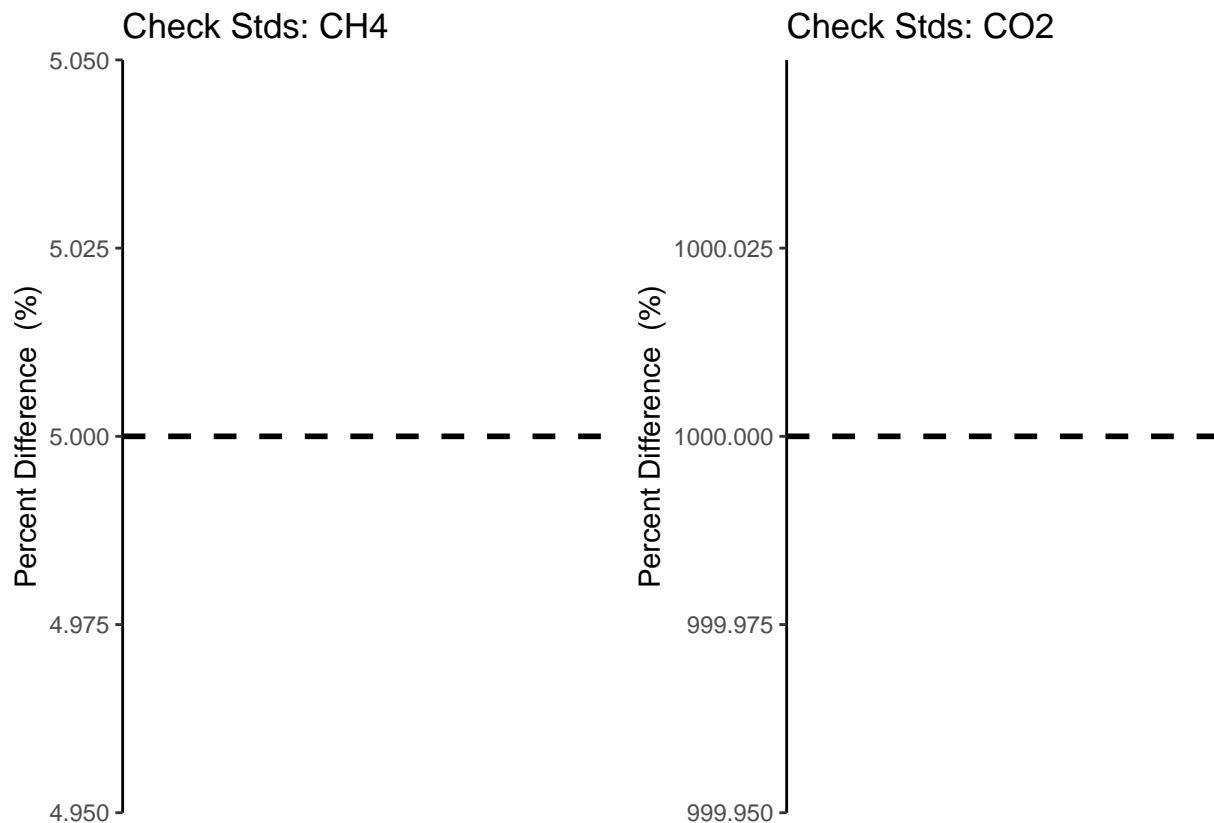
```

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)

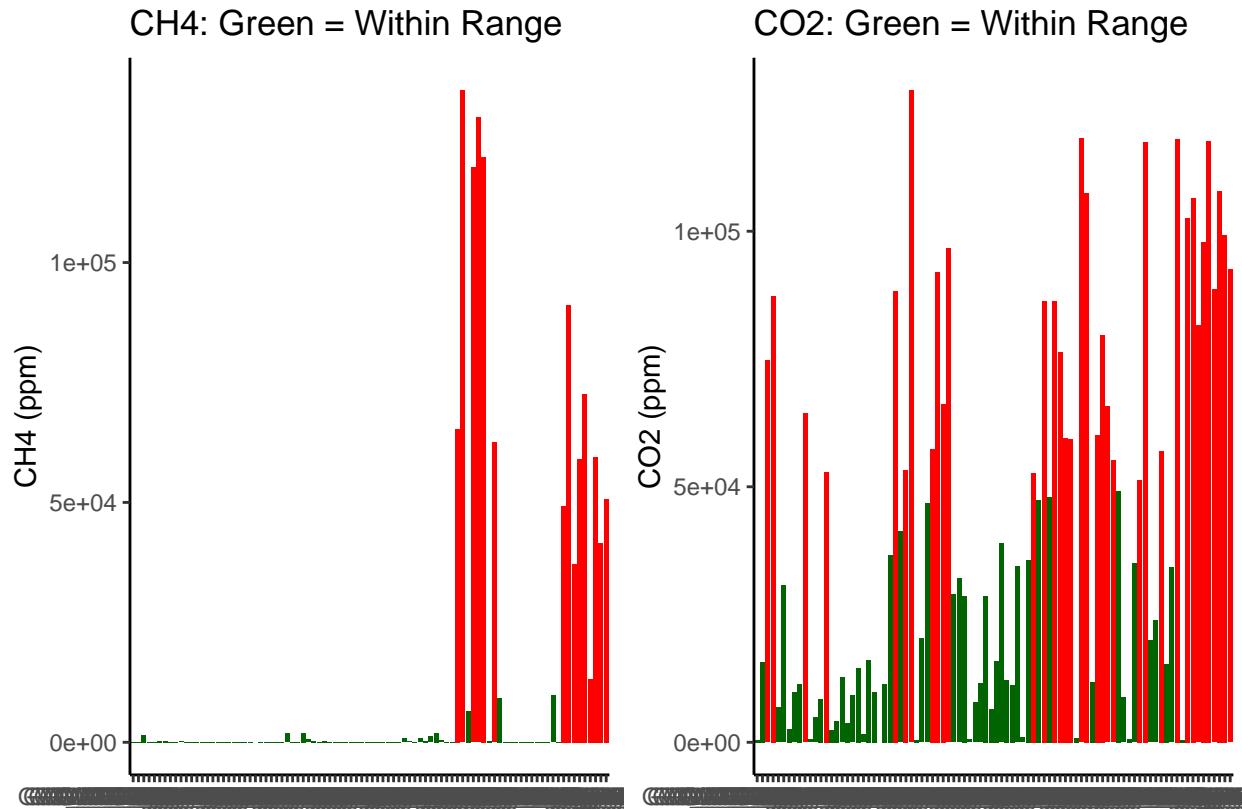
#quick first look at the samples
ch4_samples <- ggplot(data = Samples, aes(x = Sample_ID, y = CH4_Conc_ppm, fill=CH4_Flag)) +
  geom_bar(stat = 'identity') +
  scale_fill_manual(values=c("red","darkgreen"))+
  #scale_fill_gradient2(low='red', mid='white', high='blue', space='Lab') +
  theme_classic() + 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 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()').

```



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

Write out processed data & slopes

```
#check results
#head(Samples)

#pull out what we need
Samples1 <- Samples[,c(1:3,6:9,17:20)]
#head(Samples1)

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

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

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 MSM UP SgwA 10cm 10
## 2 MSM UP SgwA 20cm 20
## 3 MSM UP SgwA 45cm 45
## 4 MSM UP SgwB 10cm 10
## 5 MSM UP SgwB 20cm 20
## 6 MSM UP SgwB 45cm 45

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

##   Site Zone Replicate Depth Depth1 Machine      User Run_Date Sample_Year
## 1  MSM   UP       SgwA  10cm     10 Varian GC M. Wegner 20231005    2023
## 2  MSM   UP       SgwA  20cm     20 Varian GC M. Wegner 20231005    2023
## 3  MSM   UP       SgwA  45cm     45 Varian GC M. Wegner 20231005    2023
## 4  MSM   UP       SgwB  10cm     10 Varian GC M. Wegner 20231005    2023
## 5  MSM   UP       SgwB  20cm     20 Varian GC M. Wegner 20231005    2023
## 6  MSM   UP       SgwB  45cm     45 Varian GC M. Wegner 20231005    2023
##   Sample_Month      Sample_ID Dilution_Factor      CH4_Flag      CO2_Flag
## 1        August MSM_UP_SgwA_10cm           1 Within Range Within Range
## 2        August MSM_UP_SgwA_20cm           1 Within Range Within Range
## 3        August MSM_UP_SgwA_45cm           1 Within Range Within Range
## 4        August MSM_UP_SgwB_10cm           1 Within Range Within Range
## 5        August MSM_UP_SgwB_20cm           1 Within Range Within Range
## 6        August MSM_UP_SgwB_45cm           1 Within Range Within Range
##   CH4_Conc_ppm_dilcorr CO2_Conc_ppm_dilcorr
## 1            2.638515          7749.420
## 2            2.470968          11485.379
## 3            2.522030          28637.215
## 4            2.447032          6503.672
## 5            2.306612          15927.283
## 6            2.028962          38867.855

write.csv(alldat, "Processed Data/COMPASS_CBSYN_SGW_202308_Processed.csv")

```

#end