COMPASS_Synoptic_SGW_2023: November

Stephanie J. Wilson

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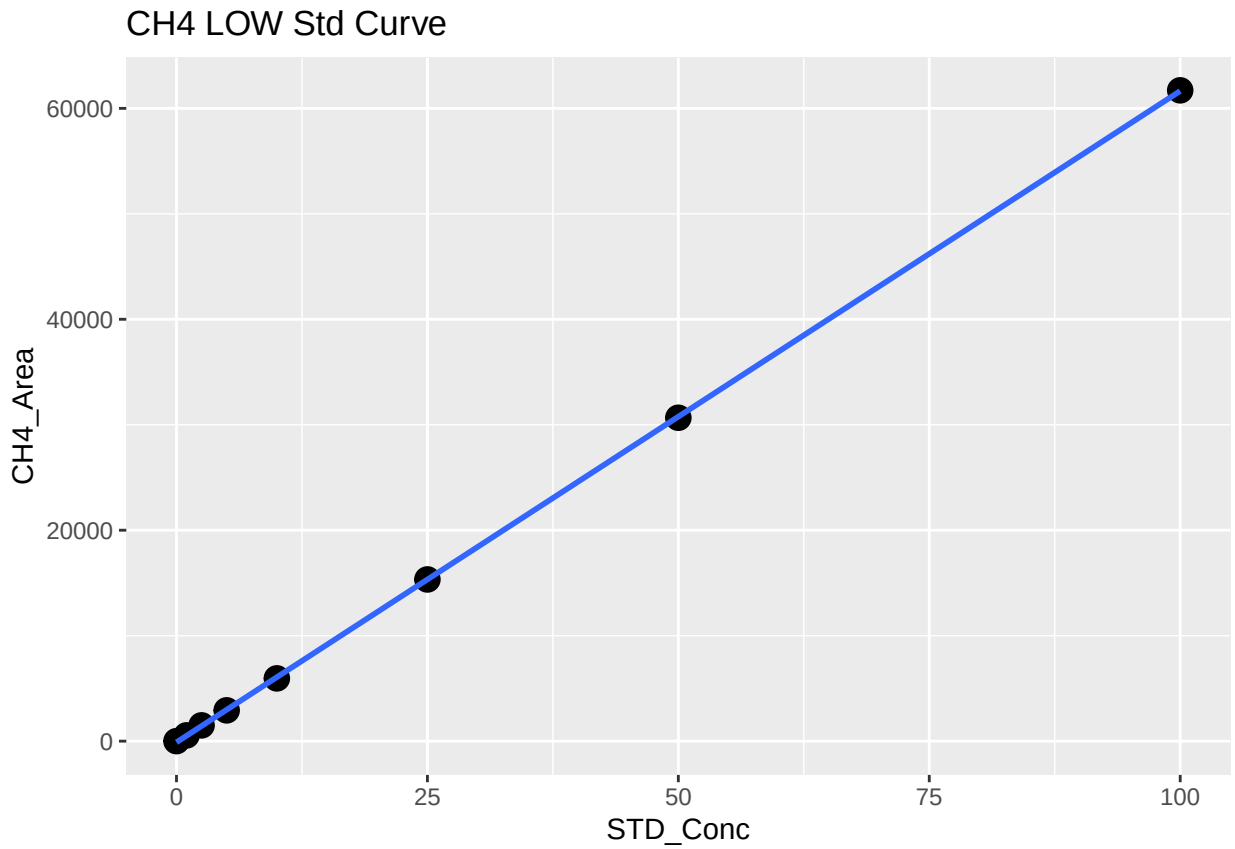
##Set Up

Read in first data file and assess standard curves

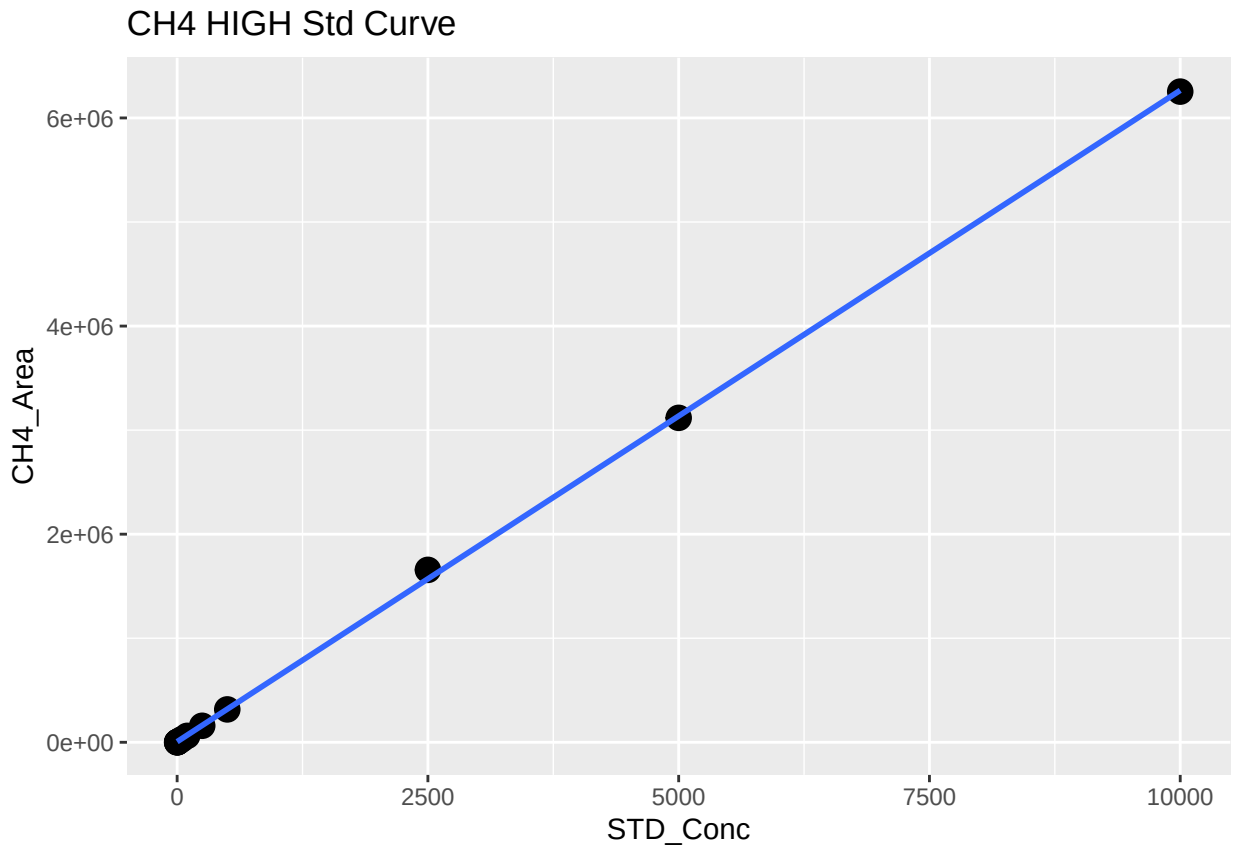
```
##     Machine   User   Run_Date Sample_Type Type1 Sample_Year Sample_Month
## 1 Varian GC Wegner 11/28/2023     STD_CH4  STDs        2023         <NA>
## 2 Varian GC Wegner 11/28/2023     STD_CH4  STDs        2023         <NA>
## 3 Varian GC Wegner 11/28/2023     STD_CH4  STDs        2023         <NA>
## 4 Varian GC Wegner 11/28/2023     STD_CH4  STDs        2023         <NA>
## 5 Varian GC Wegner 11/28/2023     STD_CH4  STDs        2023         <NA>
## 6 Varian GC Wegner 11/28/2023     STD_CH4  STDs        2023         <NA>
##   Sample_ID Dilution_Factor STD_Conc CO2_Area CH4_Area Lab_Notes
## 1       CH4               1      0.0        0        0        NA
## 2       CH4               1      1.0    19812      545        NA
## 3       CH4               1      2.5    65112     1497        NA
## 4       CH4               1      5.0   130478     2919        NA
## 5       CH4               1     10.0   266905     5951        NA
## 6       CH4               1     25.0        0    15332        NA
```

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



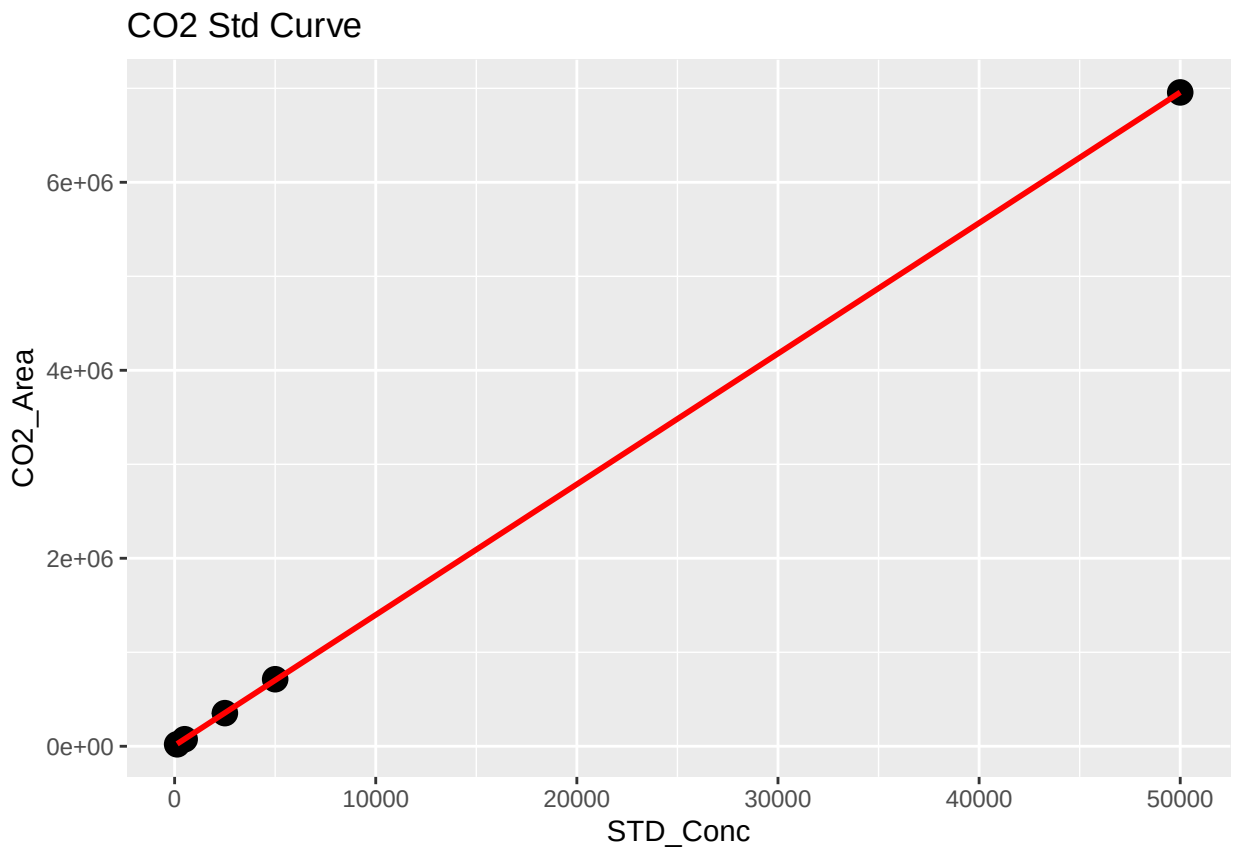

```
##
## Call:
## lm(formula = stds_ch4_low$CH4_Area ~ stds_ch4_low$STD_Conc)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -114.49  -70.19   20.36   63.33  110.02
##
## Coefficients:
##                         Estimate Std. Error t value Pr(>|t|)
## (Intercept)           -110.0215    39.7533  -2.768   0.0325 *
## stds_ch4_low$STD_Conc  617.5513     0.9765 632.385 1.06e-15 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 90.44 on 6 degrees of freedom
## Multiple R-squared:      1,  Adjusted R-squared:      1
## F-statistic: 3.999e+05 on 1 and 6 DF,  p-value: 1.055e-15

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



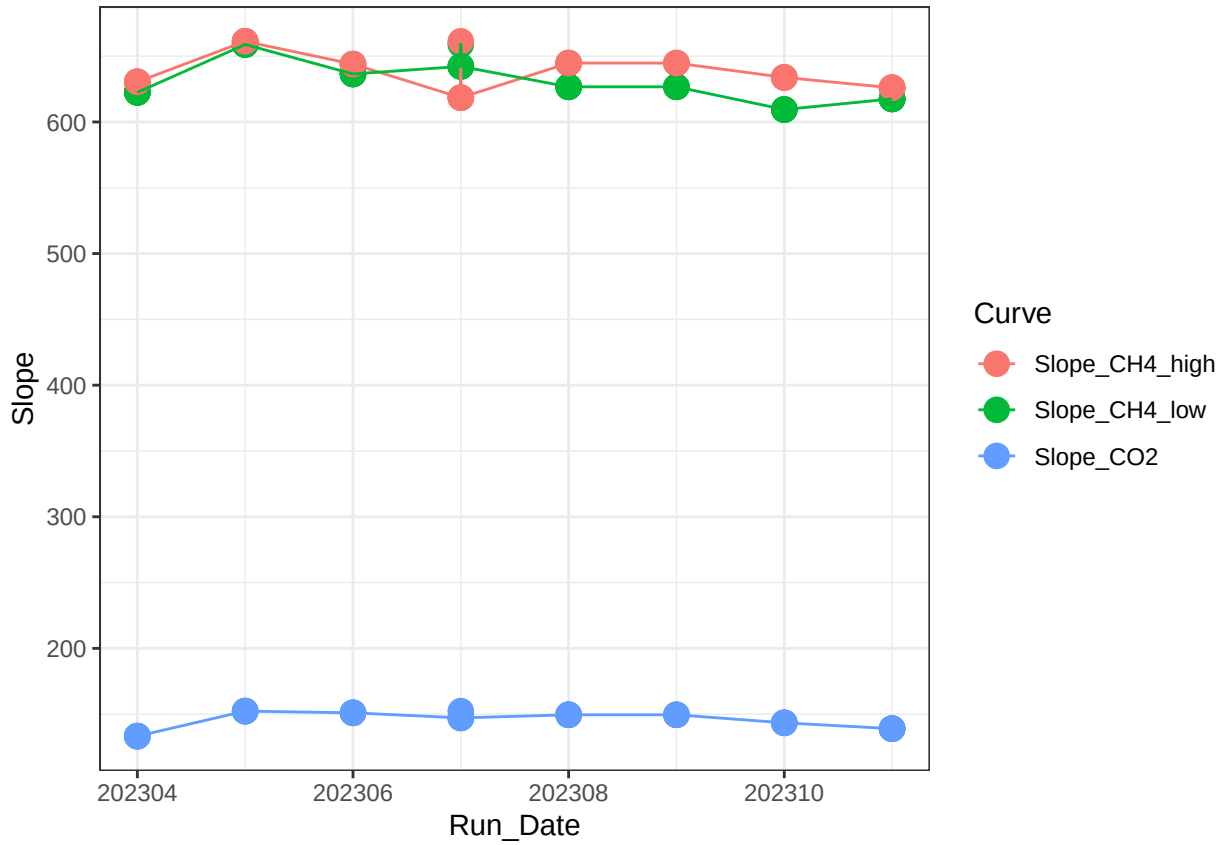

```
##
## Call:
## lm(formula = stds_ch4$CH4_Area ~ stds_ch4$STD_Conc)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -17758  -6526  -6102  -5891  86227
##
## Coefficients:
##                   Estimate Std. Error t value Pr(>|t|)
## (Intercept)       5891.337   8477.033   0.695    0.501
## stds_ch4$STD_Conc  625.944      2.665 234.913   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 27360 on 11 degrees of freedom
## Multiple R-squared:  0.9998, Adjusted R-squared:  0.9998
## F-statistic: 5.518e+04 on 1 and 11 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
## -4255 -2474 -2785 10376  -863
##
## Coefficients:
##                     Estimate Std. Error t value Pr(>|t|)
## (Intercept)       7748.1692  3572.9453   2.169    0.119
## stds_co2$STD_Conc  138.9870     0.1588 875.292 3.29e-09 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 6841 on 3 degrees of freedom
## Multiple R-squared:      1,  Adjusted R-squared:      1
## F-statistic: 7.661e+05 on 1 and 3 DF,  p-value: 3.289e-09

##   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)/Slo

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

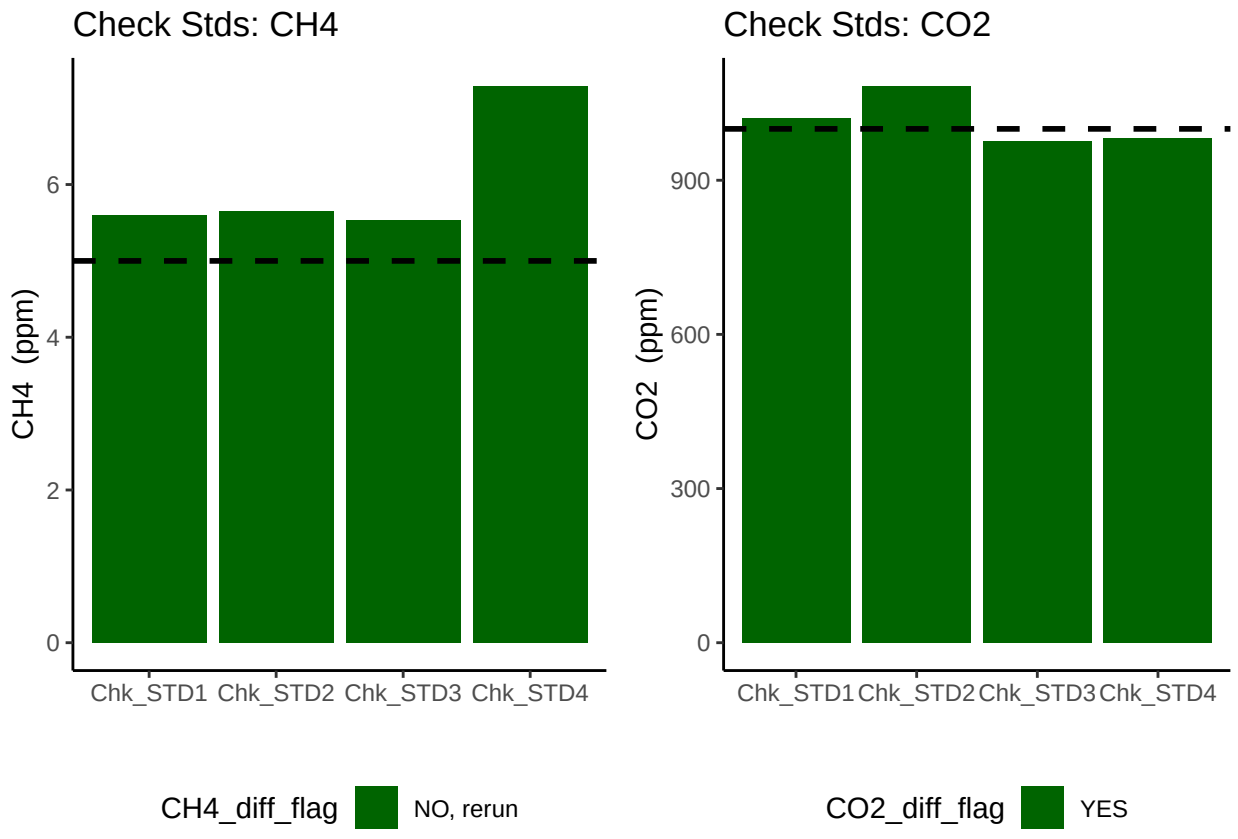
```r
#head(Samples)

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

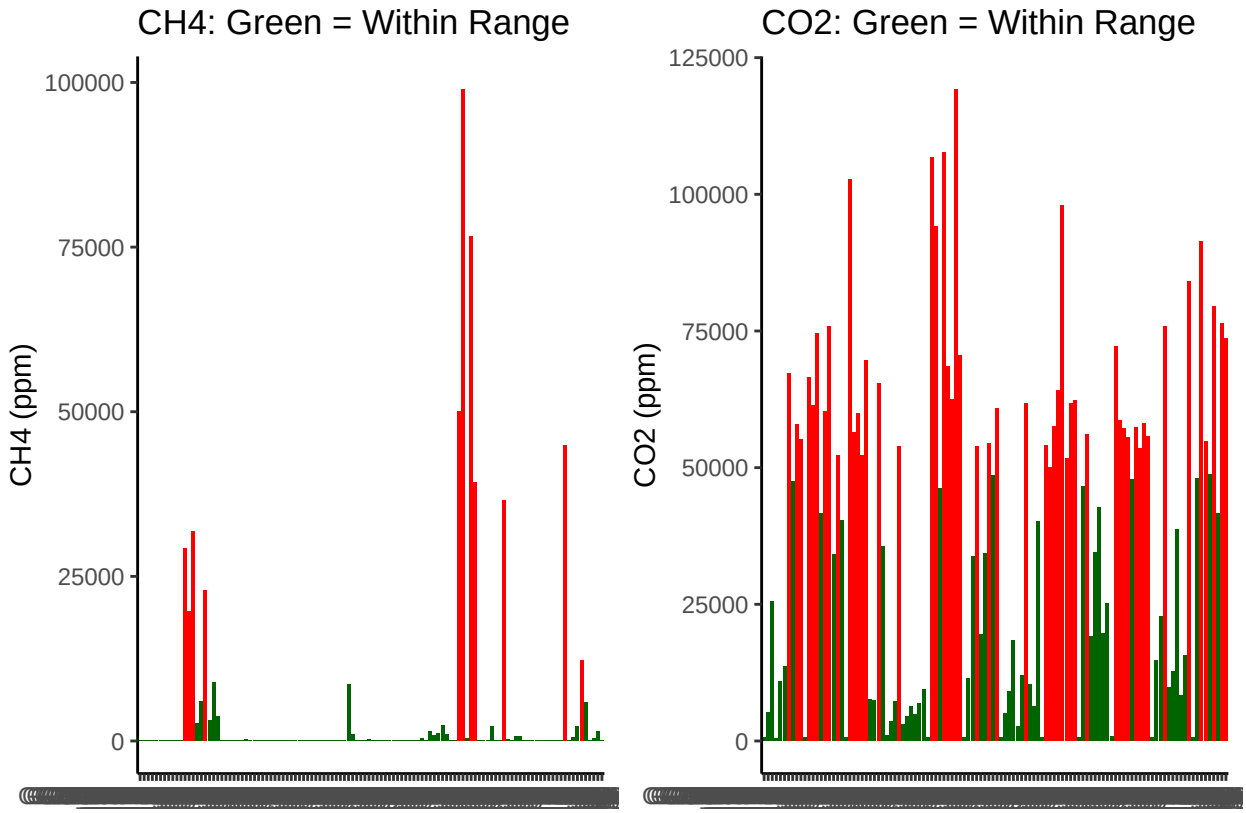
```
Samples$CO2_Conc_ppm_dilcorr <- (Samples$CO2_Conc_ppm * Samples$Dilution_Factor)

#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)
```



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

Write out processed data & slopes

```
#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 Wegner 11/28/2023        2023
## 2  MSM   UP      SgwA  20cm     20 Varian GC Wegner 11/28/2023        2023
## 3  MSM   UP      SgwA  45cm     45 Varian GC Wegner 11/28/2023        2023
## 4  MSM   UP      SgwB  10cm     10 Varian GC Wegner 11/28/2023        2023
## 5  MSM   UP      SgwB  20cm     20 Varian GC Wegner 11/28/2023        2023
## 6  MSM   UP      SgwB  45cm     45 Varian GC Wegner 11/28/2023        2023
##   Sample_Month        Sample_ID Dilution_Factor     CH4_Flag       CO2_Flag
## 1     November MSM_UP_sgwA_10cm               1 Within Range   Within Range
## 2     November MSM_UP_SgwA_20cm               1 Within Range   Within Range
## 3     November MSM_UP_SgwA_45cm               1 Within Range   Within Range
## 4     November MSM_UP_SgwB_10cm               1 Within Range   Within Range
## 5     November MSM_UP_SgwB_20cm               1 Within Range   Within Range
## 6     November MSM_UP_SgwB_45cm               1 Within Range Needs Dilution
##   CH4_Conc_ppm_dilcorr CO2_Conc_ppm_dilcorr
## 1             3.611071             4963.773
## 2             3.376273             9050.759
## 3             3.054032            18396.468
## 4             3.141474             2628.489
## 5             2.961732            11943.246
## 6             2.454892            61812.695
```

```
write.csv(alldat, "Processed Data/COMPASS_CBSYN_SGW_202311_Processed.csv")
```

#end