COMPASS_TEMPEST_SGW_2023: September

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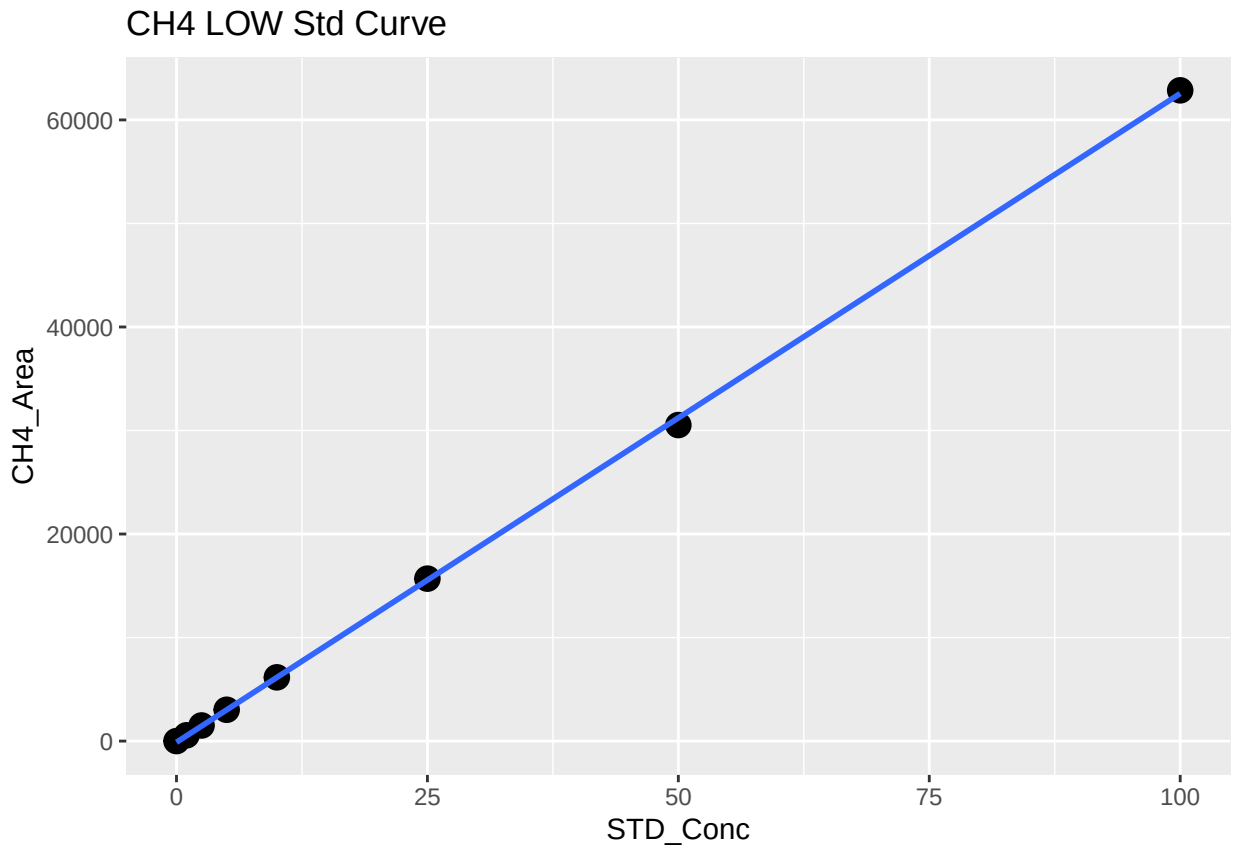
##Set Up

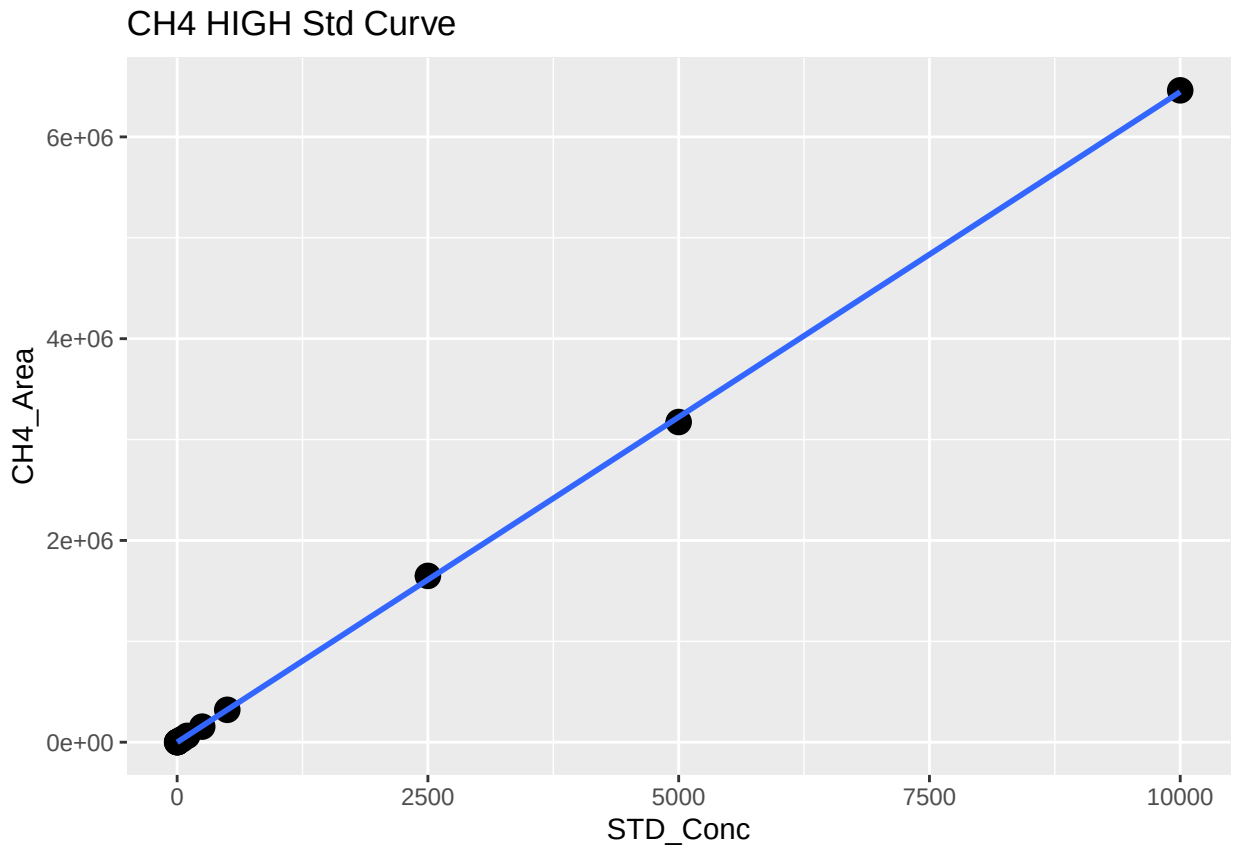
Read in first data file and assess standard curves

```
##     Machine      User Run_Date Sample_Type Type1 Sample_Year Sample_Month
## 1 Varian GC M. Wegner 20231006       Blank Blank        2023         <NA>
## 2 Varian GC M. Wegner 20231006     STD_CH4  STDs        2023         <NA>
## 3 Varian GC M. Wegner 20231006     STD_CO2  STDs        2023         <NA>
## 4 Varian GC M. Wegner 20231006     STD_CH4  STDs        2023         <NA>
## 5 Varian GC M. Wegner 20231006     STD_CH4  STDs        2023         <NA>
## 6 Varian GC M. Wegner 20231006     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
```

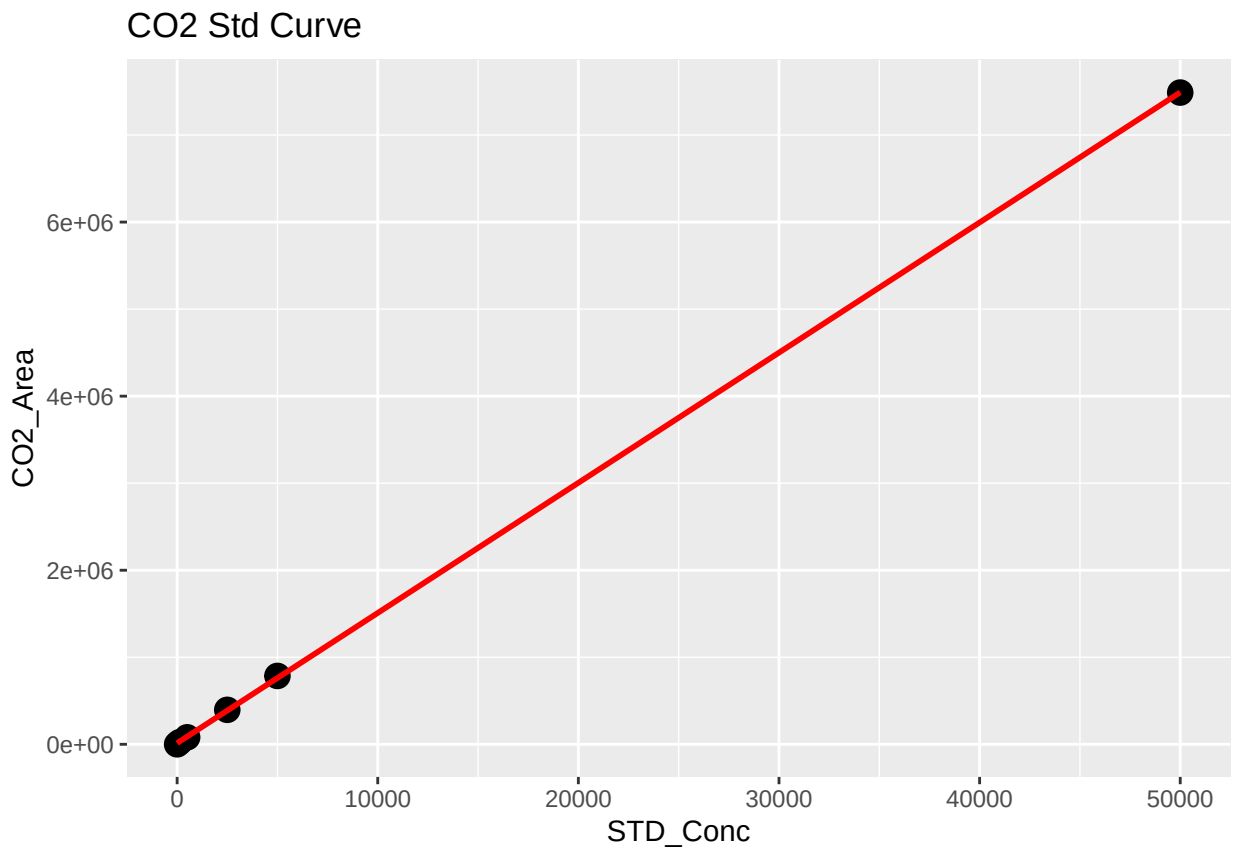
```
## `geom_smooth()` using formula = 'y ~ x'
```



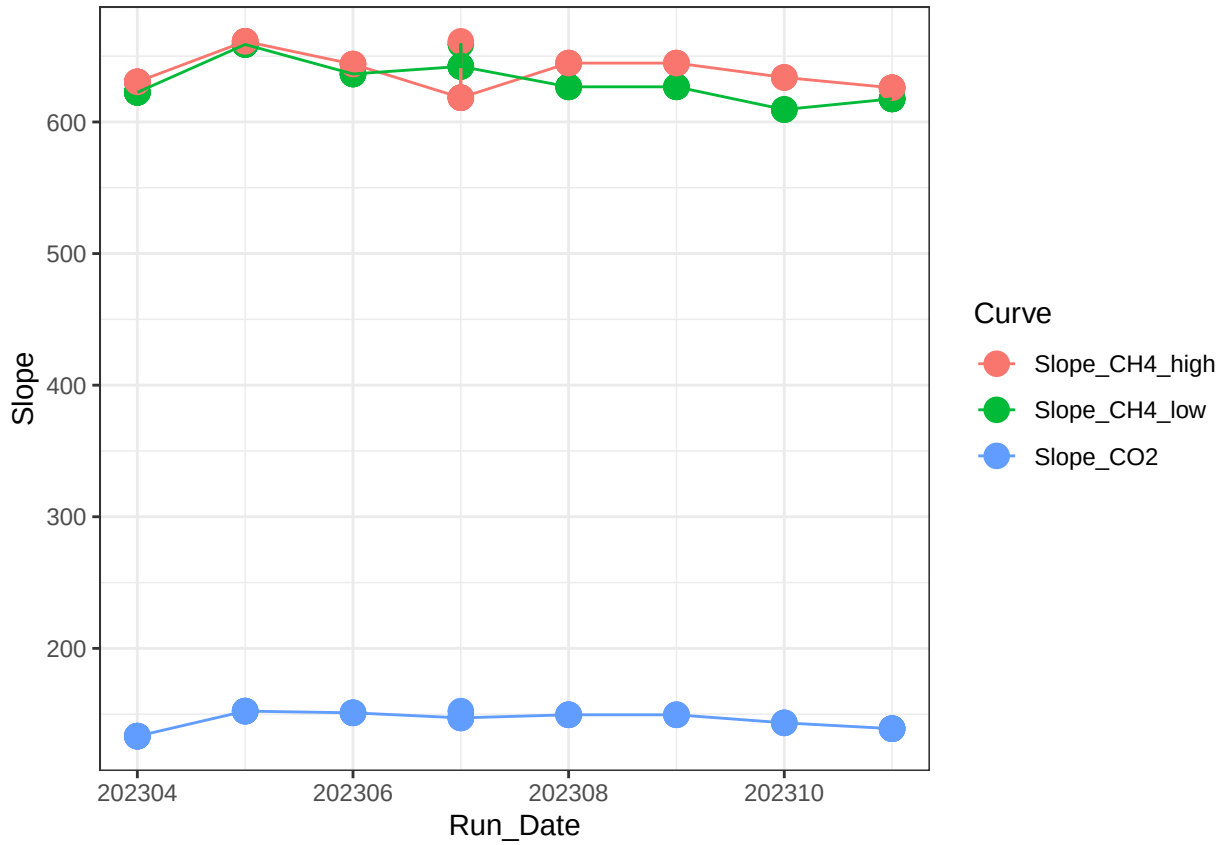

```
##
## Call:
## lm(formula = stds_ch4_low$CH4_Area ~ stds_ch4_low$STD_Conc)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -689.90    8.72   54.32  123.22  306.68
##
## Coefficients:
##                       Estimate Std. Error t value Pr(>|t|)
## (Intercept)           -117.527    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'
```




```
##
## 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'
```




```
##
## 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
```



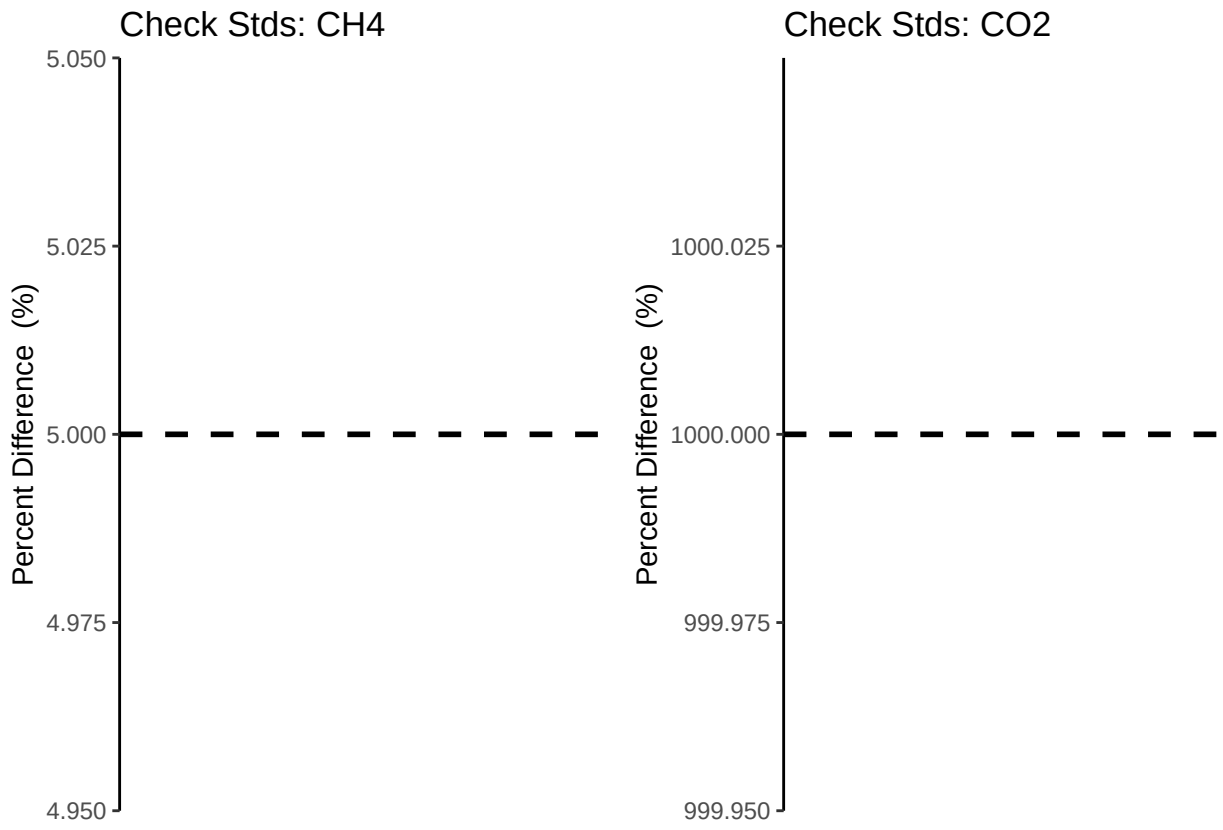
Now calculate the CH4 & CO2 concentrations in ppm

```
#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)/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.
```

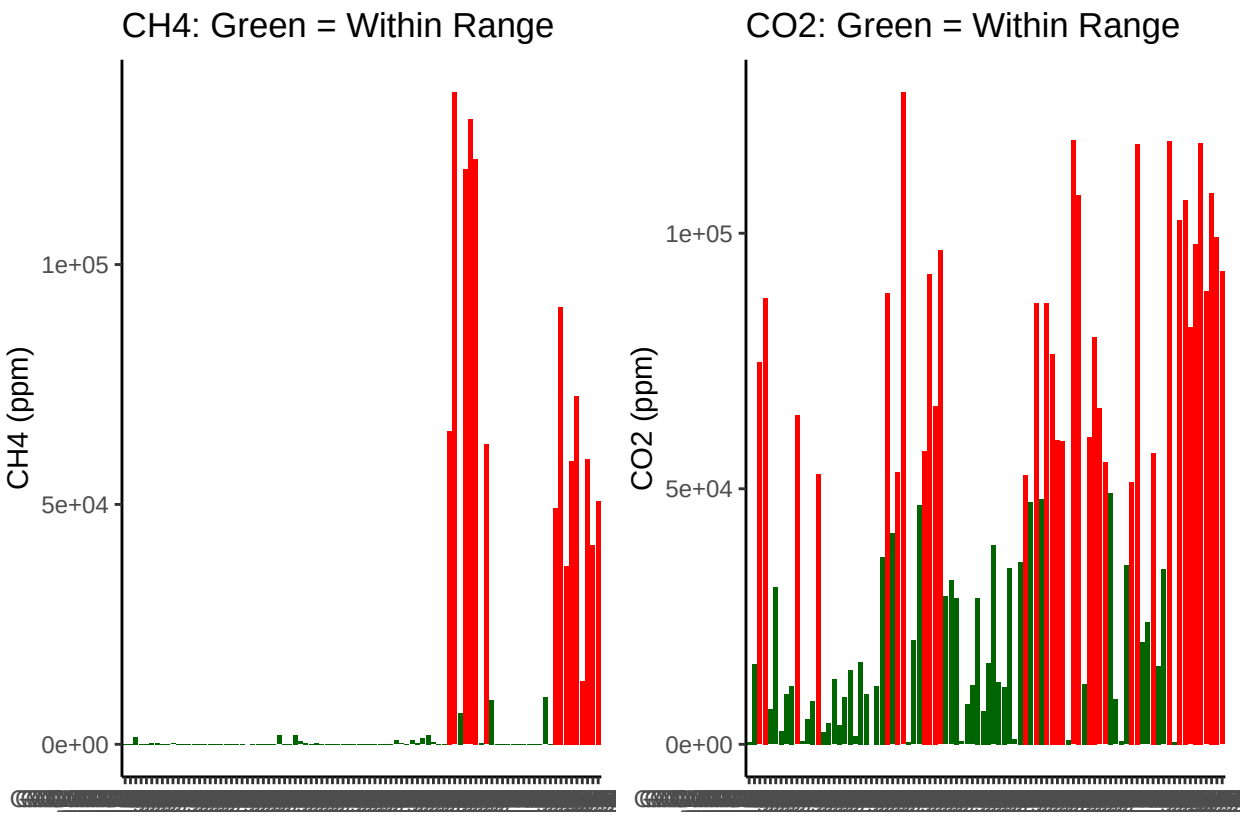


Dilution correct samples

```
#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("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

```
#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 20231006        2023
## 2  MSM   UP      SgwA  20cm     20 Varian GC M. Wegner 20231006        2023
## 3  MSM   UP      SgwA  45cm     45 Varian GC M. Wegner 20231006        2023
## 4  MSM   UP      SgwB  10cm     10 Varian GC M. Wegner 20231006        2023
## 5  MSM   UP      SgwB  20cm     20 Varian GC M. Wegner 20231006        2023
## 6  MSM   UP      SgwB  45cm     45 Varian GC M. Wegner 20231006        2023
##   Sample_Month        Sample_ID Dilution_Factor     CH4_Flag     CO2_Flag
## 1    September MSM_UP_SgwA_10cm               1 Within Range Within Range
## 2    September MSM_UP_SgwA_20cm               1 Within Range Within Range
## 3    September MSM_UP_SgwA_45cm               1 Within Range Within Range
## 4    September MSM_UP_SgwB_10cm               1 Within Range Within Range
## 5    September MSM_UP_SgwB_20cm               1 Within Range Within Range
## 6    September 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_202309_Processed.csv")
```

#end