COMPASS_TEMPEST_SGW_2023: April

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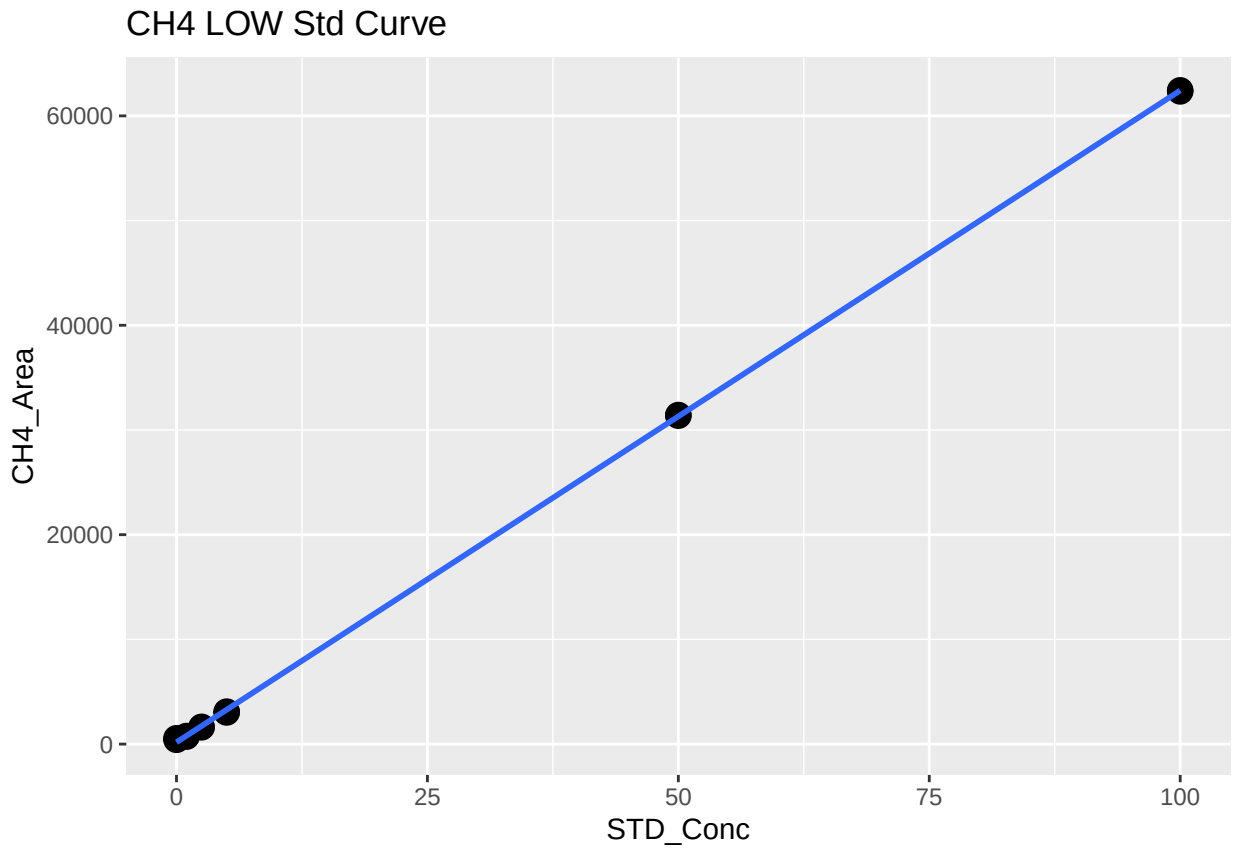
##Set Up

Read in first data file and assess standard curves

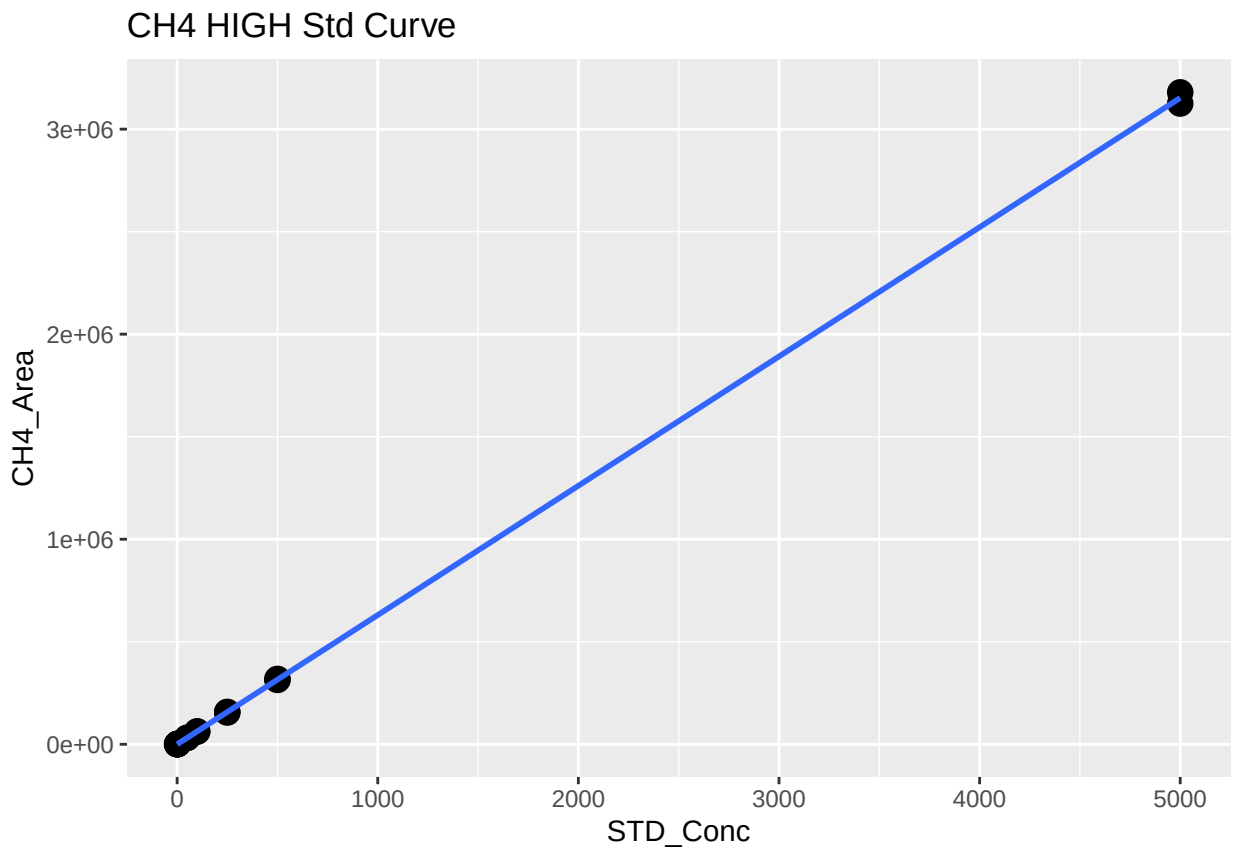
```
##     Machine                User Run_Date Sample_Type Type1 Sample_Year
## 1 Varian GC Stephanie J. Wilson 202212.5       Blank  STDs        2023
## 2 Varian GC Stephanie J. Wilson 202212.5       Blank  STDs        2023
## 3 Varian GC Stephanie J. Wilson 202212.5       Blank  STDs        2023
## 4 Varian GC Stephanie J. Wilson 202212.5     Unknown   SGW        2023
## 5 Varian GC Stephanie J. Wilson 202212.5     Unknown   SGW        2023
## 6 Varian GC Stephanie J. Wilson 202212.5     Unknown   SGW        2023
##   Sample_Month        Sample_ID Dilution_Factor STD_Conc CO2_Area CH4_Area
## 1         <NA>          Blank_3               1       NA    16988      743
## 2         <NA>          Blank_4               1       NA    17548      691
## 3         <NA>          Blank_5               1       NA    27120      638
## 4        April MSM_UP_SgwA_10cm               1       NA  1632065     2714
## 5        April MSM_UP_SgwA_20cm               1       NA  5696277    38659
## 6        April MSM_UP_SgwA_45cm               1       NA  8700674    90922
##   Lab_Notes
## 1
## 2
## 3
## 4
## 5
## 6
```

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



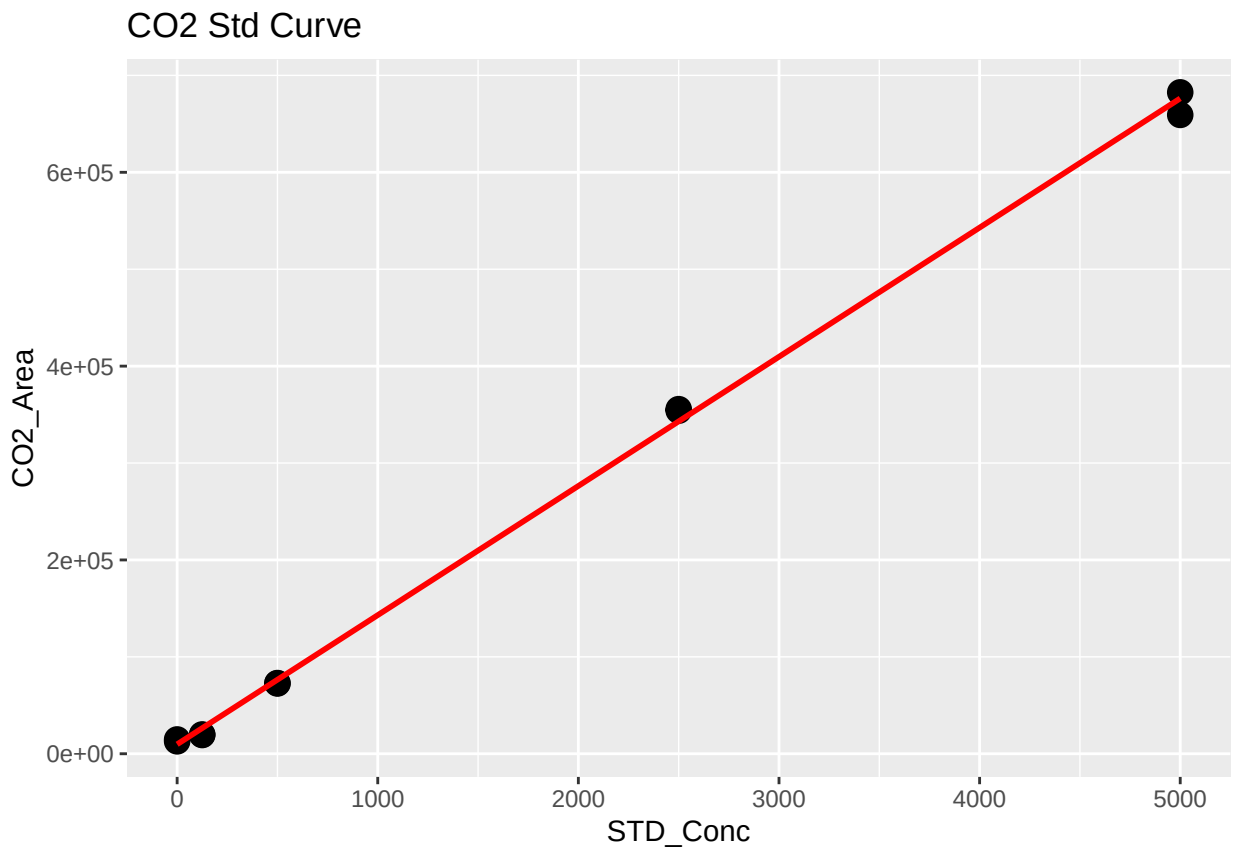

```
##
## Call:
## lm(formula = stds_ch4_low$CH4_Area ~ stds_ch4_low$STD_Conc)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -263.47  -95.04  -51.82   83.71  388.06
##
## Coefficients:
##                       Estimate Std. Error t value Pr(>|t|)
## (Intercept)            170.936     67.803   2.521   0.0303 *
## stds_ch4_low$STD_Conc  622.507      1.484 419.597   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 191.7 on 10 degrees of freedom
## Multiple R-squared:  0.9999, Adjusted R-squared:  0.9999
## F-statistic: 1.761e+05 on 1 and 10 DF,  p-value: < 2.2e-16

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



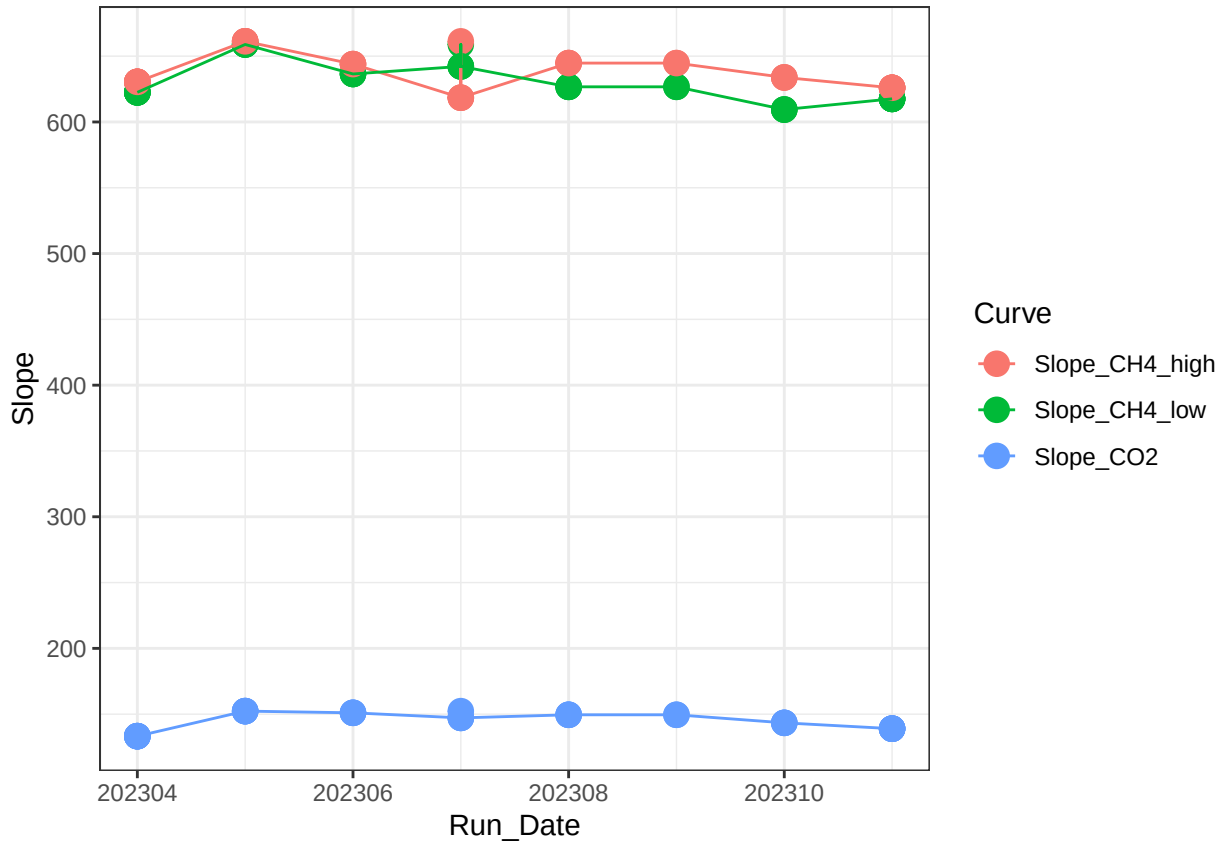

```
##
## Call:
## lm(formula = stds_ch4$CH4_Area ~ stds_ch4$STD_Conc)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -27348.0   -467.9     16.6    225.7  27236.0
##
## Coefficients:
##                   Estimate Std. Error t value Pr(>|t|)
## (Intercept)        -28.370   2490.433  -0.011    0.991
## stds_ch4$STD_Conc  630.460      1.485 424.655   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 9723 on 16 degrees of freedom
## Multiple R-squared:  0.9999, Adjusted R-squared:  0.9999
## F-statistic: 1.803e+05 on 1 and 16 DF,  p-value: < 2.2e-16

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




```
##
## Call:
## lm(formula = stds_co2$CO2_Area ~ stds_co2$STD_Conc)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -17027.7  -5848.8   -213.5   5969.3  12610.8
##
## Coefficients:
##                   Estimate Std. Error t value Pr(>|t|)
## (Intercept)       9757.829   4053.664   2.407   0.0427 *
## stds_co2$STD_Conc  133.295      1.615  82.555 5.17e-13 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 9771 on 8 degrees of freedom
## Multiple R-squared:  0.9988, Adjusted R-squared:  0.9987
## F-statistic:  6815 on 1 and 8 DF,  p-value: 5.169e-13

##   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)
```

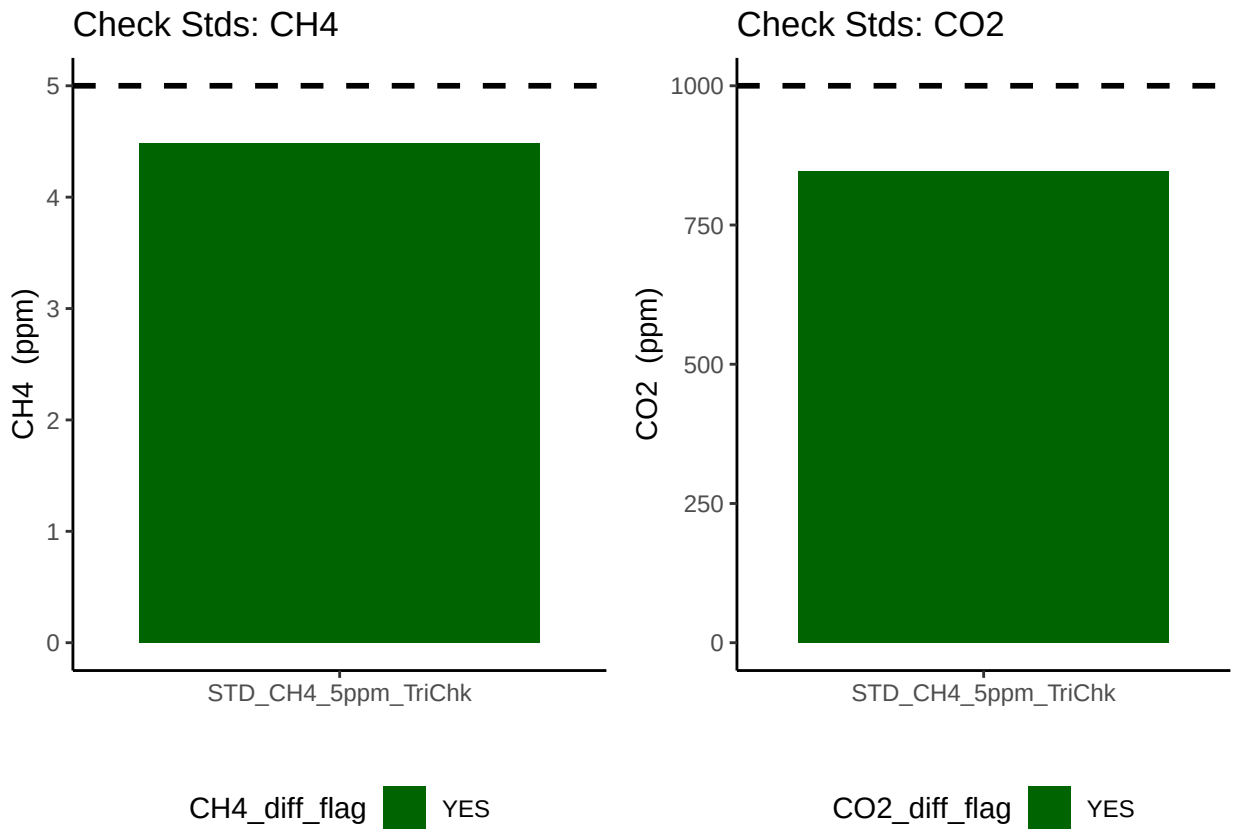
```r
#head(Samples)

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

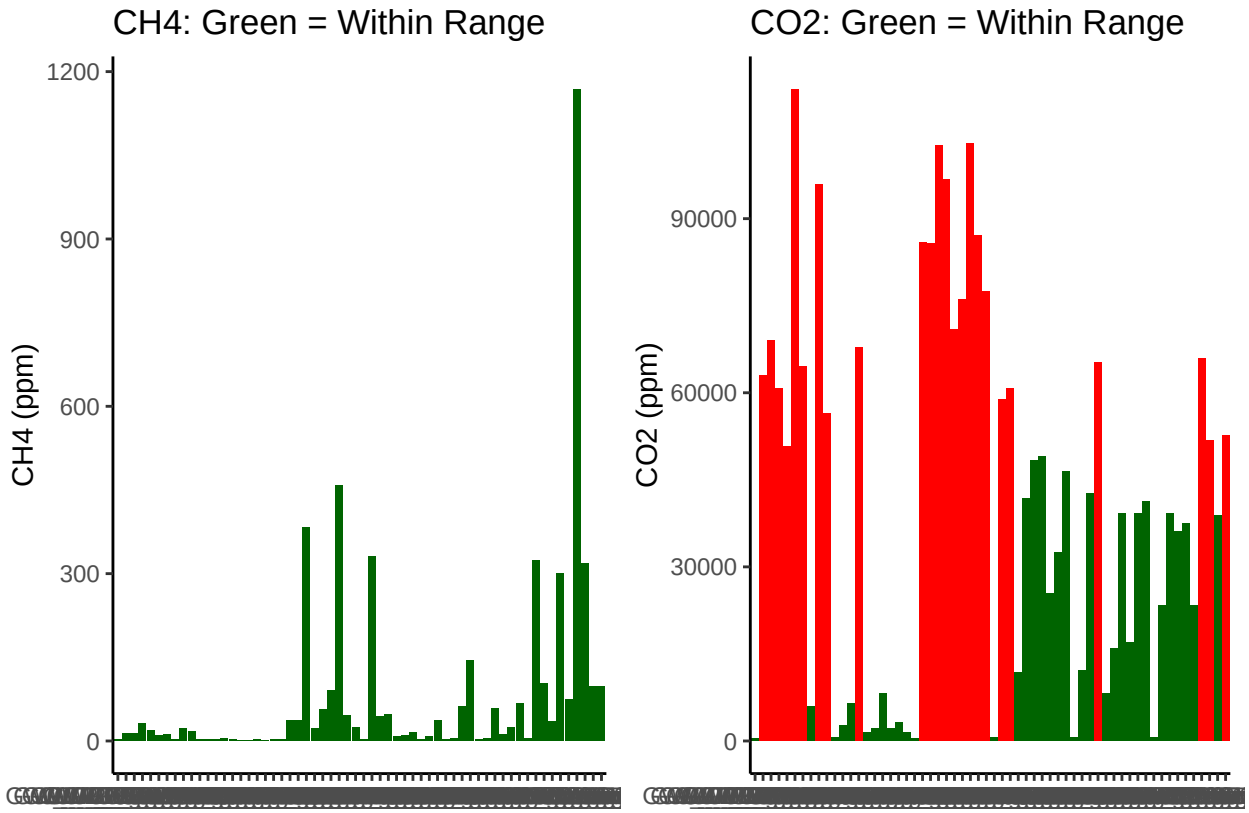
```r
Samples$CO2_Conc_ppm_dilcorr <- (Samples$CO2_Conc_ppm * Samples$Dilution_Factor)

#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")


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

```
#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   TR      SgwA  10cm     10
## 5  MSM   TR      SgwA  20cm     20
## 6  MSM   TR      SgwA  45cm     45
```

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

```
##   Site Zone Replicate Depth Depth1   Machine                User Run_Date
## 1  MSM   UP      SgwA  10cm     10 Varian GC Stephanie J. Wilson 202212.5
## 2  MSM   UP      SgwA  20cm     20 Varian GC Stephanie J. Wilson 202212.5
## 3  MSM   UP      SgwA  45cm     45 Varian GC Stephanie J. Wilson 202212.5
## 4  MSM   TR      SgwA  10cm     10 Varian GC Stephanie J. Wilson 202212.5
## 5  MSM   TR      SgwA  20cm     20 Varian GC Stephanie J. Wilson 202212.5
## 6  MSM   TR      SgwA  45cm     45 Varian GC Stephanie J. Wilson 202212.5
##   Sample_Year Sample_Month        Sample_ID Dilution_Factor     CH4_Flag
## 1        2023        April MSM_UP_SgwA_10cm               1 Within Range
## 2        2023        April MSM_UP_SgwA_20cm               1 Within Range
## 3        2023        April MSM_UP_SgwA_45cm               1 Within Range
## 4        2023        April MSM_TR_SgwA_10cm               1 Within Range
## 5        2023        April MSM_TR_SgwA_20cm               1 Within Range
## 6        2023        April MSM_TR_SgwA_45cm               1 Within Range
##         CO2_Flag CH4_Conc_ppm_dilcorr CO2_Conc_ppm_dilcorr
## 1   Within Range             4.085196             12170.84
## 2   Within Range            61.827506             42661.30
```

```
## 3 Needs Dilution          144.260317             65200.83
## 4 Needs Dilution          331.141304             58873.57
## 5 Needs Dilution           43.986746             60713.39
## 6   Within Range           47.205987             11845.67
```

```
write.csv(alldat, "Processed Data/COMPASS_CBSYN_SGW_202304_Processed.csv")
```

#end