COMPASS_TEMPEST_SGW_2023: April

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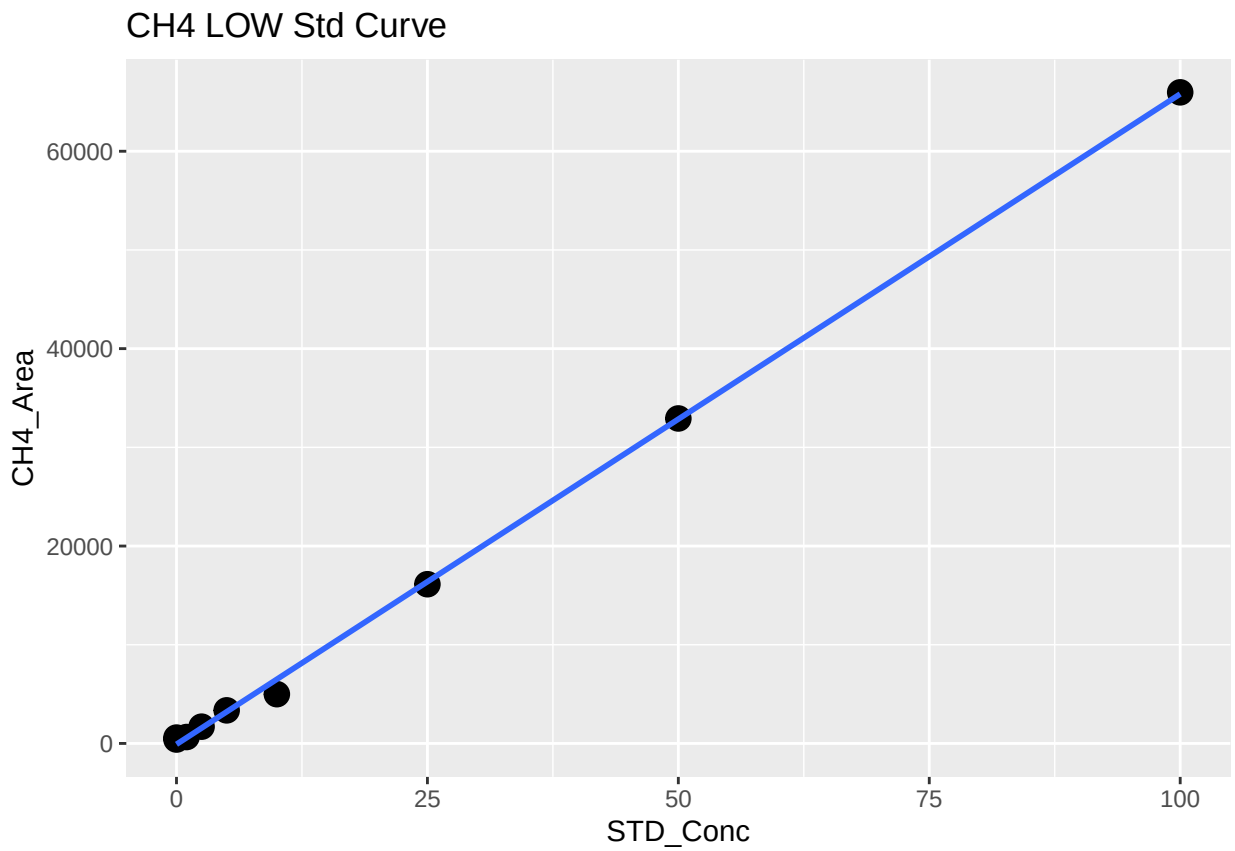
##Set Up

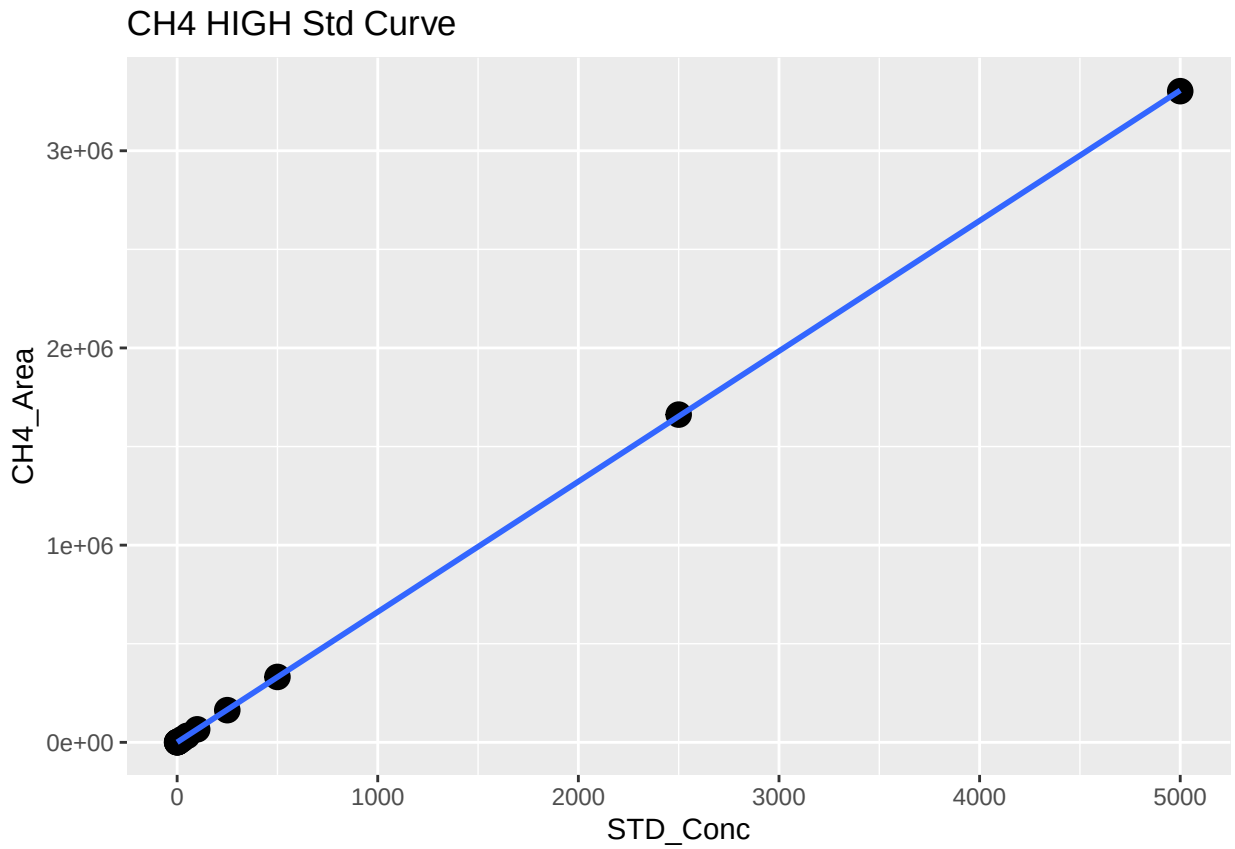
Read in first data file and assess standard curves

```
##     Machine               User Run_Date Sample_Type Type1 Sample_Year
## 1 Varian GC Stephanie J. Wilson 9/9/2023     Unknown  POND        2023
## 2 Varian GC Stephanie J. Wilson 9/9/2023     Unknown   SGW        2023
## 3 Varian GC Stephanie J. Wilson 9/9/2023     Unknown   SGW        2023
## 4 Varian GC Stephanie J. Wilson 9/9/2023     Unknown   SGW        2023
## 5 Varian GC Stephanie J. Wilson 9/9/2023     Unknown   SGW        2023
## 6 Varian GC Stephanie J. Wilson 9/9/2023     Unknown   SGW        2023
##   Sample_Month        Sample_ID Dilution_Factor STD_Conc CO2_Area CH4_Area
## 1          May     EQ_Test_Pond               1       NA  1689713  1334844
## 2          May       GWI_TR_ATM               1       NA    83562     1513
## 3          May GWI_TR_SgwA_10cm               1       NA 10402550    15862
## 4          May GWI_TR_SgwA_20cm               1       NA 14748363    60769
## 5          May GWI_TR_SgwA_45cm               1       NA  8103990    22015
## 6          May GWI_TR_SgwB_10cm               1       NA  5483393    87591
##   Lab_Notes
## 1        NA
## 2        NA
## 3        NA
## 4        NA
## 5        NA
## 6        NA
```

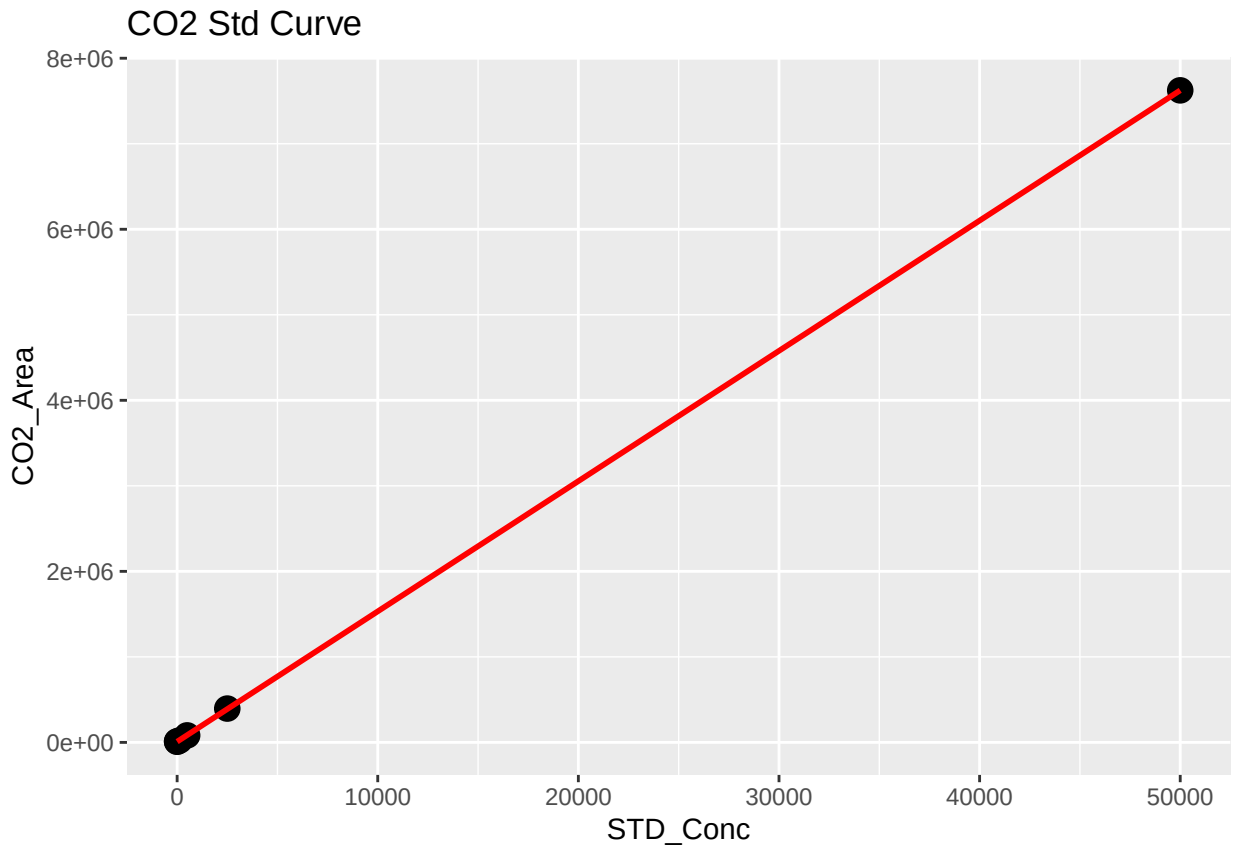
```
## `geom_smooth()` using formula = 'y ~ x'
```




```
##
## Call:
## lm(formula = stds_ch4_low$CH4_Area ~ stds_ch4_low$STD_Conc)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -1509.28    69.36   138.35   168.15   681.56
##
## Coefficients:
##                       Estimate Std. Error t value Pr(>|t|)
## (Intercept)            -87.565    268.637  -0.326    0.754
## stds_ch4_low$STD_Conc  658.884      6.999  94.134 4.02e-12 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 667.6 on 7 degrees of freedom
## Multiple R-squared:  0.9992, Adjusted R-squared:  0.9991
## F-statistic:  8861 on 1 and 7 DF,  p-value: 4.022e-12

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

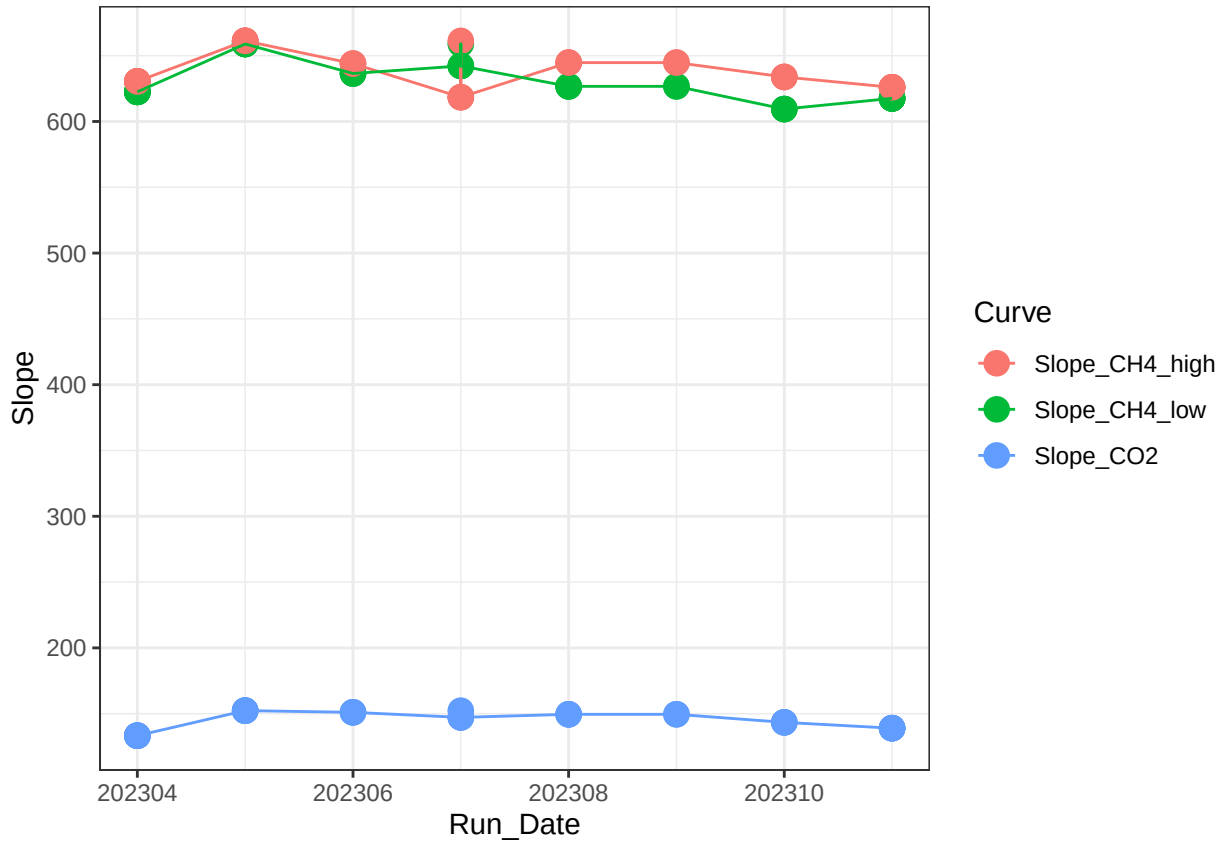



```
##
## Call:
## lm(formula = stds_ch4$CH4_Area ~ stds_ch4$STD_Conc)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -4265.2  -576.9  -189.9   219.4  8634.6
##
## Coefficients:
##                    Estimate Std. Error  t value Pr(>|t|)
## (Intercept)        176.6235   933.7756    0.189    0.853
## stds_ch4$STD_Conc 661.2523     0.5992 1103.646   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 3060 on 11 degrees of freedom
## Multiple R-squared:      1,  Adjusted R-squared:      1
## F-statistic: 1.218e+06 on 1 and 11 DF,  p-value: < 2.2e-16

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

## Warning: Removed 2 rows containing non-finite outside the scale range
## (`stat_smooth()`).

## Warning: Removed 2 rows containing missing values or values outside the scale range
## (`geom_point()`).
```




```
##
## Call:
## lm(formula = stds_co2$CO2_Area ~ stds_co2$STD_Conc)
##
## Residuals:
##       1       2       3       4       5       7
## -1238.7  3474.3 -5029.1 -2876.4  5924.7  -254.9
##
## Coefficients:
##                    Estimate Std. Error  t value Pr(>|t|)
## (Intercept)       8787.6672  2055.0680    4.276   0.0129 *
## stds_co2$STD_Conc  152.3154     0.1005 1514.877 1.14e-12 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 4537 on 4 degrees of freedom
##   (2 observations deleted due to missingness)
## Multiple R-squared:      1,  Adjusted R-squared:      1
## F-statistic: 2.295e+06 on 1 and 4 DF,  p-value: 1.139e-12

##   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
```



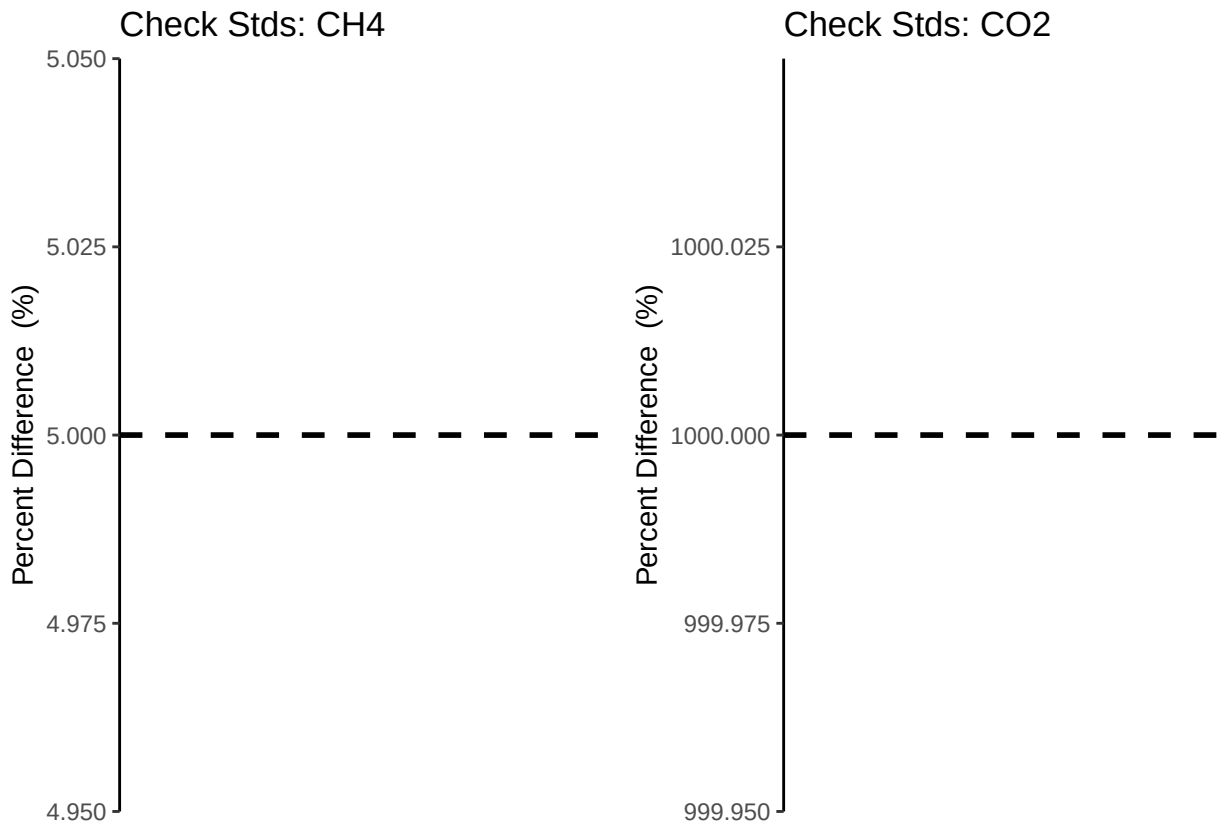
Now calculate the CH4 & CO2 concentrations in ppm

```
#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
```

```r
#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)
```

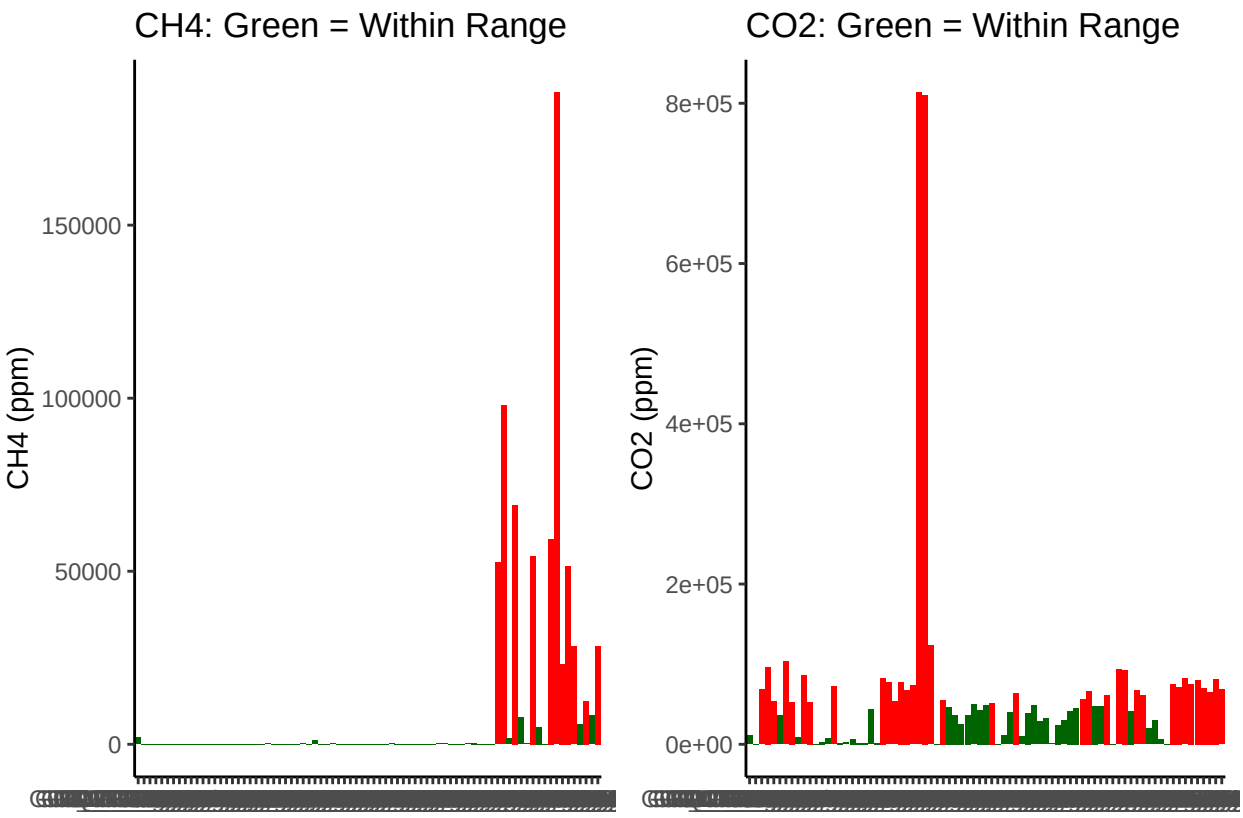
Check the Check Standards

```
## 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)
```



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("EQ", "Test", "Pond"), c("GWI", "TR", "ATM"), c("GWI", :
## number of columns of result is not a multiple of vector length (arg 1)
```

```
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   EQ Test      Pond    EQ      0
## 2  GWI   TR       ATM   GWI      0
## 3  GWI   TR      SgwA  10cm     10
## 4  GWI   TR      SgwA  20cm     20
## 5  GWI   TR      SgwA  45cm     45
## 6  GWI   TR      SgwB  10cm     10
```

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

```
##   Site Zone Replicate Depth Depth1   Machine                User Run_Date
## 1   EQ Test      Pond    EQ      0 Varian GC Stephanie J. Wilson 9/9/2023
## 2  GWI   TR       ATM   GWI      0 Varian GC Stephanie J. Wilson 9/9/2023
## 3  GWI   TR      SgwA  10cm     10 Varian GC Stephanie J. Wilson 9/9/2023
## 4  GWI   TR      SgwA  20cm     20 Varian GC Stephanie J. Wilson 9/9/2023
## 5  GWI   TR      SgwA  45cm     45 Varian GC Stephanie J. Wilson 9/9/2023
## 6  GWI   TR      SgwB  10cm     10 Varian GC Stephanie J. Wilson 9/9/2023
##   Sample_Year Sample_Month        Sample_ID Dilution_Factor     CH4_Flag
## 1        2023          May     EQ_Test_Pond               1 Within Range
## 2        2023          May       GWI_TR_ATM               1 Within Range
## 3        2023          May GWI_TR_SgwA_10cm               1 Within Range
## 4        2023          May GWI_TR_SgwA_20cm               1 Within Range
## 5        2023          May GWI_TR_SgwA_45cm               1 Within Range
## 6        2023          May GWI_TR_SgwB_10cm               1 Within Range
##         CO2_Flag CH4_Conc_ppm_dilcorr CO2_Conc_ppm_dilcorr
## 1   Within Range          2018.393513           11035.8167
## 2   Within Range             2.429205             490.9176
## 3 Needs Dilution            24.206934           68238.4006
## 4 Needs Dilution            92.363074           96770.0640
## 5 Needs Dilution            33.545449           53147.6132
## 6   Within Range           132.195192           35942.5490
```

```
write.csv(alldat, "Processed Data/COMPASS_CBSYN_SGW_202305_Processed.csv")
```

#end