

COMPASS_TEMPEST_SGW_2024: June

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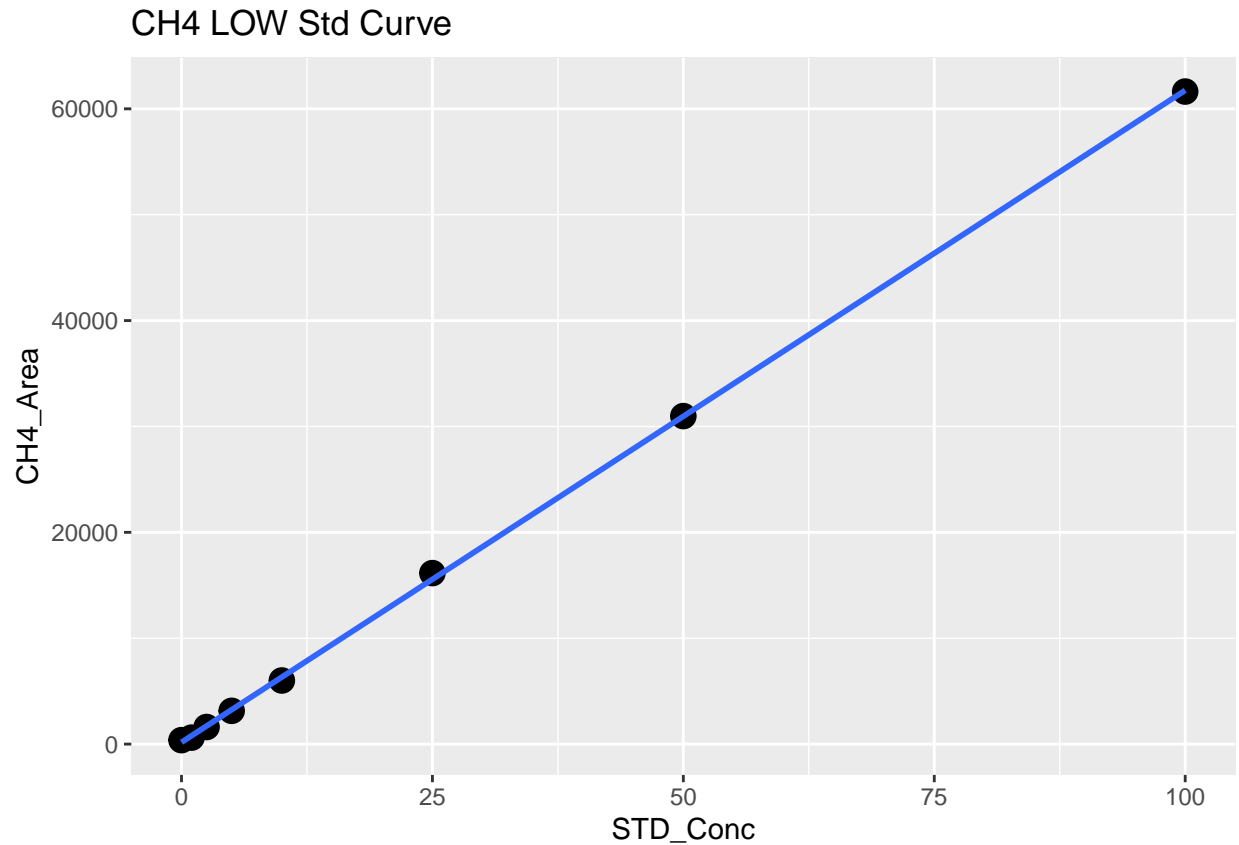
2023-01-14

##Set Up

Read in first data file and assess standard curves

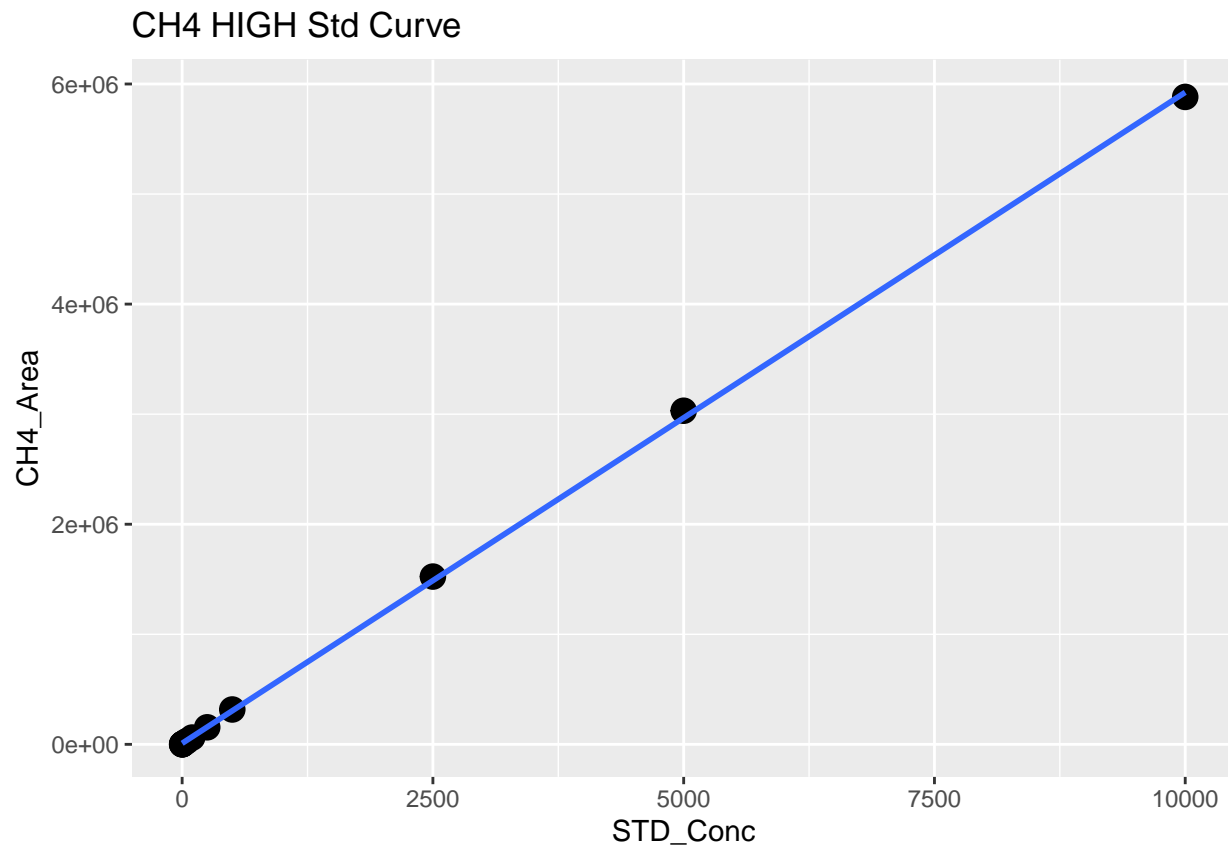
```
##      Machine   User Run_Date Sample_Type Type1 Sample_Year Sample_Month
## 1 Varian GC Wegner 20240711      Blank Blank      2024      <NA>
## 2 Varian GC Wegner 20240711    STD_CH4 STDs      2024      <NA>
## 3 Varian GC Wegner 20240711    STD_CO2 STDs      2024      <NA>
## 4 Varian GC Wegner 20240711    STD_CH4 STDs      2024      <NA>
## 5 Varian GC Wegner 20240711    STD_CH4 STDs      2024      <NA>
## 6 Varian GC Wegner 20240711    STD_CH4 STDs      2024      <NA>
##      Sample_ID Dilution_Factor STD_Conc CO2_Area CH4_Area Lab_Notes
## 1          Blank_1              1      0.0   16571    375
## 2 Blank_1_repeatforCH4          1      0.0   16571    375
## 3 Blank_1_repeatforCO2          1      0.0   16571    375
## 4          STD_1ppm_CH4          1      1.0   28795    611
## 5          STD_2.5ppm_CH4          1      2.5   88416   1615
## 6          STD_5ppm_CH4          1      5.0  171674   3144
##      Field_Notes
## 1          NA
## 2          NA
## 3          NA
## 4          NA
## 5          NA
## 6          NA

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



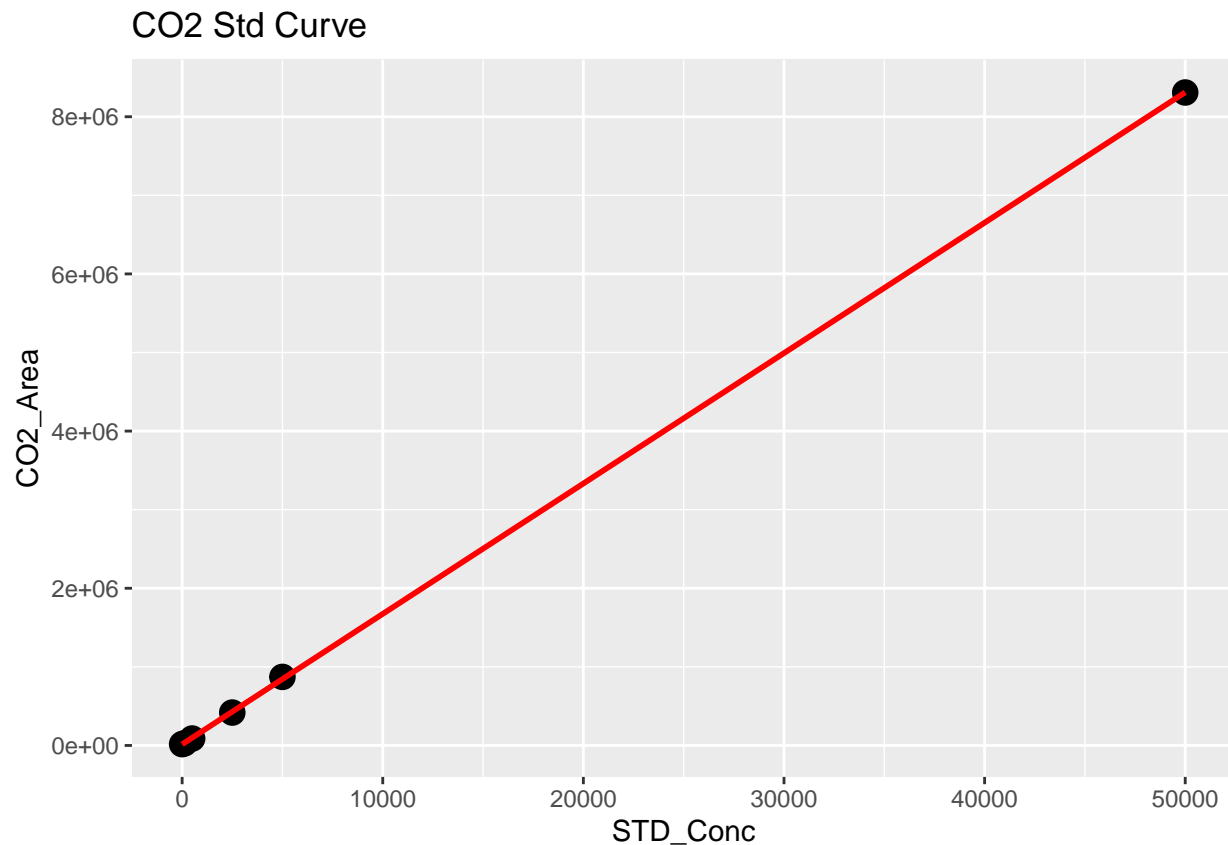
```
##
## Call:
## lm(formula = stds_ch4_low$CH4_Area ~ stds_ch4_low$STD_Conc)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -320.01 -130.61 -100.06   67.55  584.70
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)    170.488    133.175     1.28   0.248
## stds_ch4_low$STD_Conc  615.752      3.271  188.22 1.52e-12 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 303 on 6 degrees of freedom
## Multiple R-squared:  0.9998, Adjusted R-squared:  0.9998
## F-statistic: 3.543e+04 on 1 and 6 DF, p-value: 1.517e-12

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



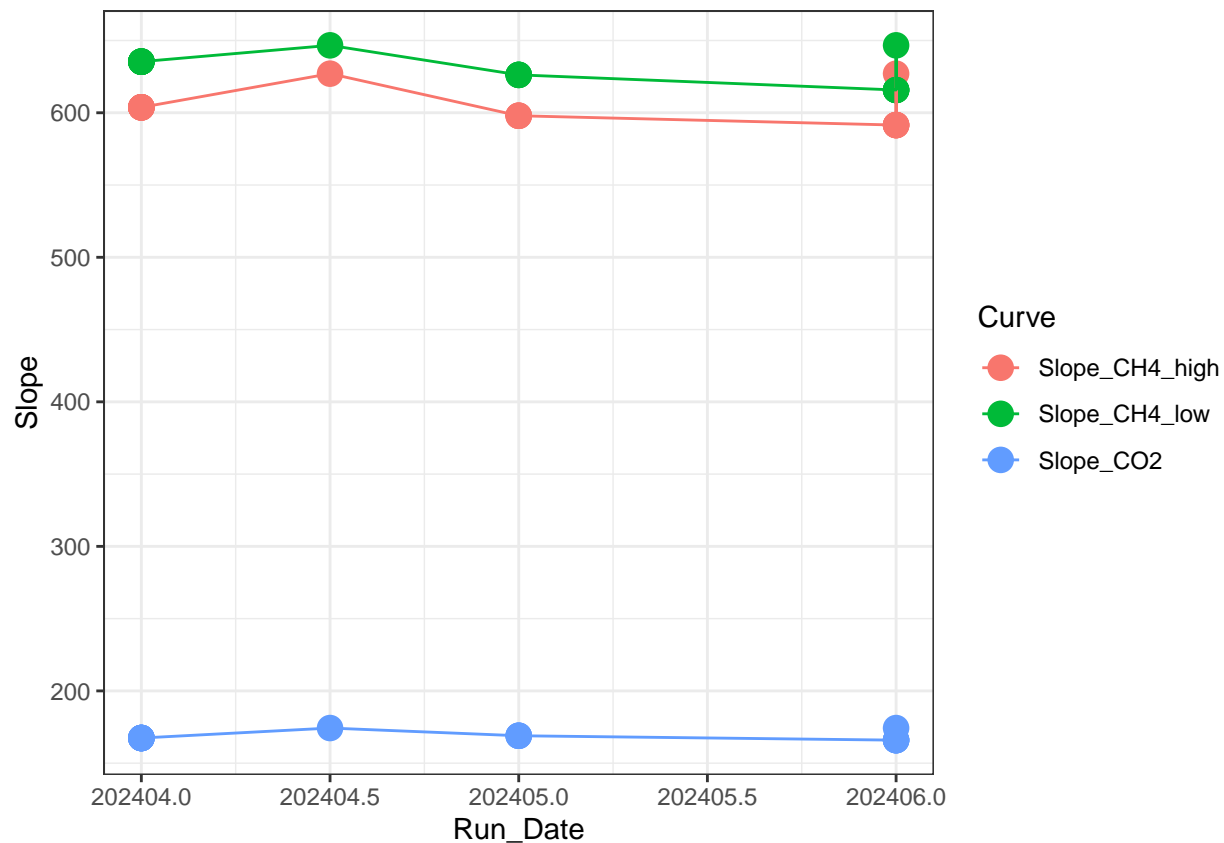
```
##
## Call:
## lm(formula = stds_ch4$CH4_Area ~ stds_ch4$STD_Conc)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -41651  -9159  -7934  -2360   64420
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)    9295.621    8319.152     1.117   0.288
## stds_ch4$STD_Conc  591.493       2.615  226.197  <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 26850 on 11 degrees of freedom
## Multiple R-squared:  0.9998, Adjusted R-squared:  0.9998
## F-statistic: 5.116e+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      6
## 1899 -7280 -9628 -10871 28024 -2144
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)   1.467e+04  7.527e+03   1.949   0.123
## stds_co2$STD_Conc 1.659e+02  3.665e-01 452.746 1.43e-10 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 16260 on 4 degrees of freedom
## Multiple R-squared:  1, Adjusted R-squared:  1
## F-statistic: 2.05e+05 on 1 and 4 DF, p-value: 1.428e-10

##   X      Curve      R2    Slope  Intercept Run_Date
## 1 1 Slope_CH4_low 0.9998964 626.2155   125.6616 202405
## 2 2 Slope_CH4_high 0.9986961 597.9392 18399.0623 202405
## 3 3      Slope_CO2 0.9999864 168.9656   9100.0798 202405
## 4 4 Slope_CH4_low 0.9998964 626.2155   125.6616 202405
## 5 5 Slope_CH4_high 0.9986961 597.9392 18399.0623 202405
## 6 6      Slope_CO2 0.9999864 168.9656   9100.0798 202405
```



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)
```

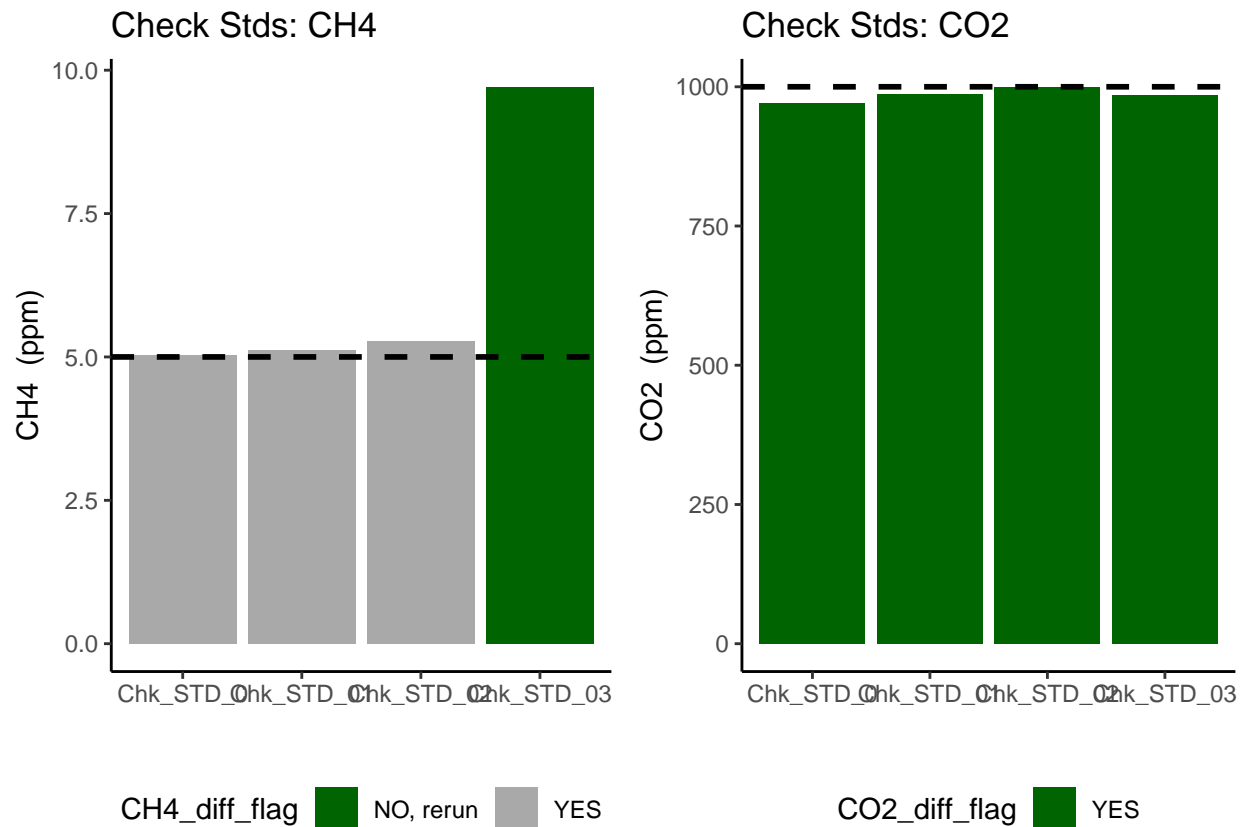
```
#head(Samples)

#####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)

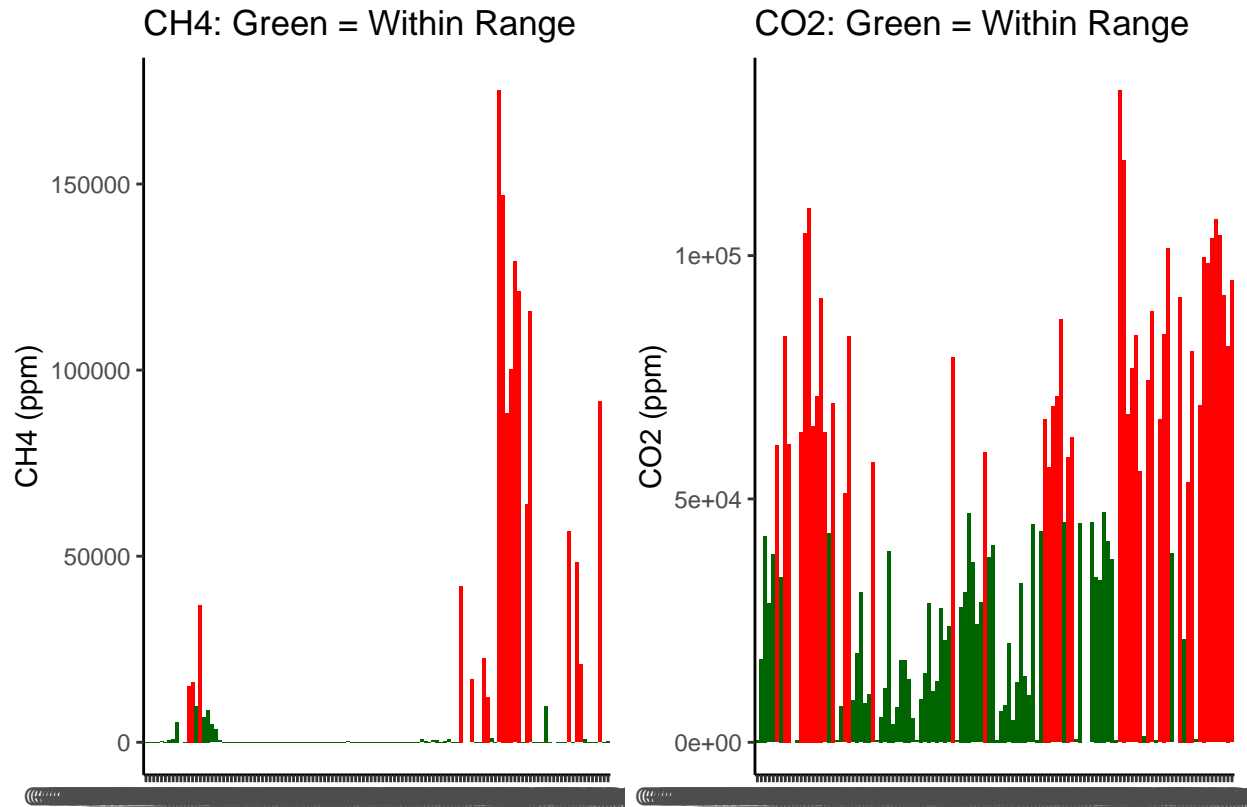
#quick first look at the samples
ch4_samples <- ggplot(data = Samples, aes(x = Sample_ID, y = CH4_Conc_ppm, fill=CH4_Flag)) +
  geom_bar(stat = 'identity') +
  scale_fill_manual(values=c("red", "darkgreen"))+
  #scale_fill_gradient2(low='red', mid='white', high='blue', space='Lab') +
  theme_classic() + 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 4 rows containing missing values or values outside the scale range
## ('geom_bar()').
## Removed 4 rows 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(1:3,6:9,18:21)]
#head(Samples1)

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

## Warning in rbind(c("GCW", "TR", "SgwA", "10cm"), c("GCW", "TR", "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  GCW   TR      SgwA  10cm     10
## 2  GCW   TR      SgwA  20cm     20
## 3  GCW   TR      SgwA  45cm     45
```



```
## 4 GCW TR SgwB 10cm 10
## 5 GCW TR SgwB 20cm 20
## 6 GCW TR 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 GCW TR SgwA 10cm 10 Varian GC Wegner 20240711 2024
## 2 GCW TR SgwA 20cm 20 Varian GC Wegner 20240711 2024
## 3 GCW TR SgwA 45cm 45 Varian GC Wegner 20240711 2024
## 4 GCW TR SgwB 10cm 10 Varian GC Wegner 20240711 2024
## 5 GCW TR SgwB 20cm 20 Varian GC Wegner 20240711 2024
## 6 GCW TR SgwB 45cm 45 Varian GC Wegner 20240711 2024
## Sample_Month Sample_ID Dilution_Factor CH4_Flag CO2_Flag
## 1 June GCW_TR_SgwA_10cm 1 Within Range Within Range
## 2 June GCW_TR_SgwA_20cm 1 Within Range Within Range
## 3 June GCW_TR_SgwA_45cm 1 Within Range Within Range
## 4 June GCW_TR_SgwB_10cm 1 Within Range Within Range
## 5 June GCW_TR_SgwB_20cm 1 Within Range Needs Dilution
## 6 June GCW_TR_SgwB_45cm 1 Within Range Within Range
## CH4_Conc_ppm_dilcorr CO2_Conc_ppm_dilcorr
## 1 1.45921 17089.48
## 2 145.60350 42409.19
## 3 37.36163 28491.53
## 4 164.33070 38543.84
## 5 107.20138 61011.57
## 6 581.00209 33915.11
```

```
write.csv(alldat, "Processed Data/COMPASS_CBSYN_SGW_202406_Processed.csv")
```

```
#end
```