

COMPASS_TEMPEST_SGW_2024: June

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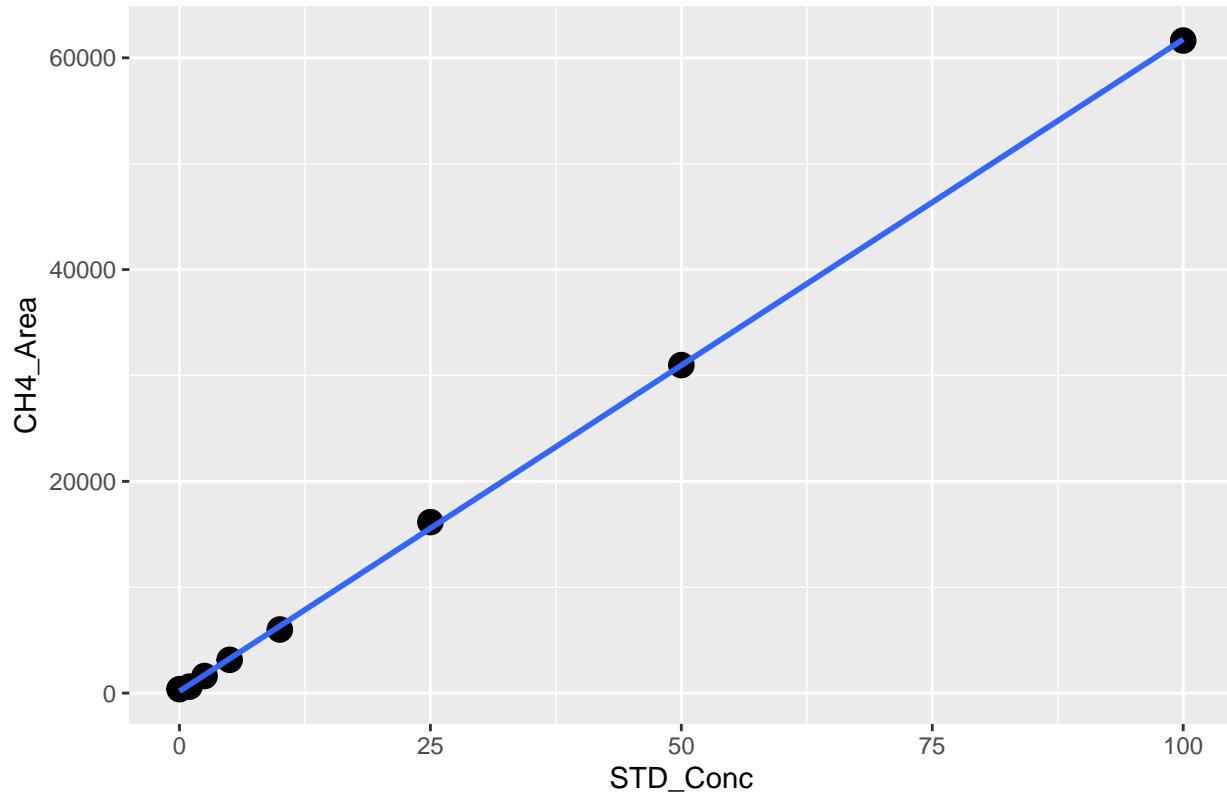
##Set Up

Read in first data file and assess standard curves

```
##      Machine   User Run_Date Sample_Type Type1 Sample_Year Sample_Month
## 1 Varian GC Wegner 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

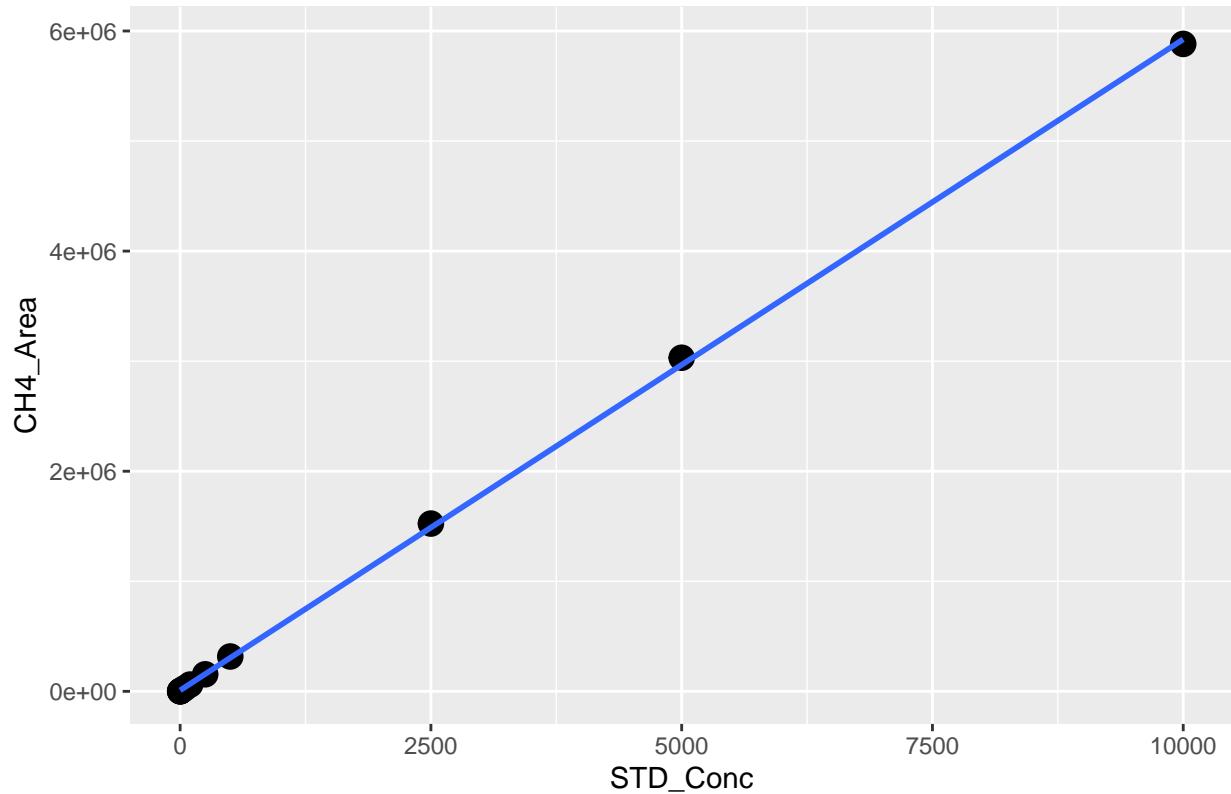
## `geom_smooth()` using formula = 'y ~ x'
```

CH4 LOW Std Curve



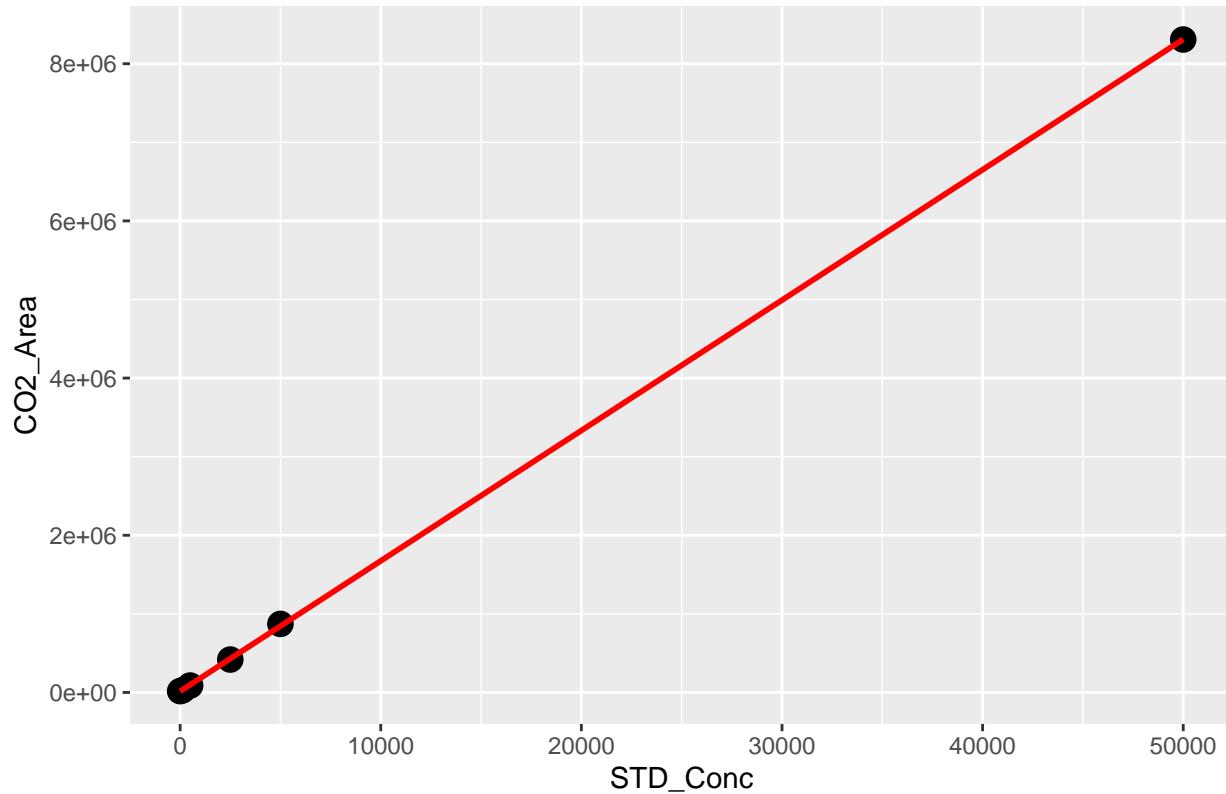
```
##  
## Call:  
## lm(formula = stds_ch4_low$CH4_Area ~ stds_ch4_low$STD_Conc)  
##  
## Residuals:  
##      Min       1Q   Median       3Q      Max  
## -320.01 -130.61 -100.06    67.55  584.70  
##  
## Coefficients:  
##                               Estimate Std. Error t value Pr(>|t|)  
## (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'
```

CH4 HIGH Std Curve



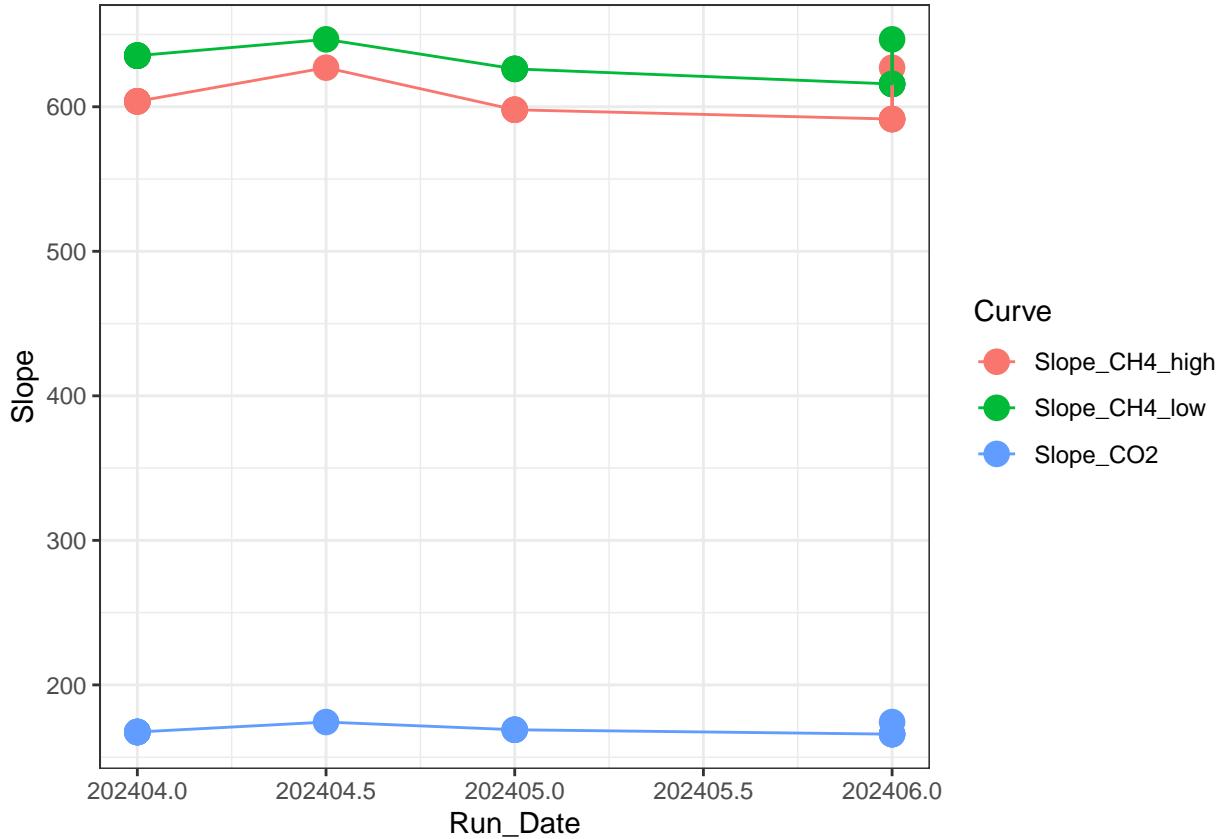
```
##  
## Call:  
## lm(formula = stds_ch4$CH4_Area ~ stds_ch4$STD_Conc)  
##  
## Residuals:  
##      Min       1Q   Median       3Q      Max  
## -41651  -9159  -7934  -2360  64420  
##  
## Coefficients:  
##                 Estimate Std. Error t value Pr(>|t|)  
## (Intercept)  9295.621   8319.152   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'
```

CO2 Std Curve



```
##
## 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_low, (Samples$CH4_Area-Slope_CH4_low$Intercept)/Slope_CH4_high)

#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)

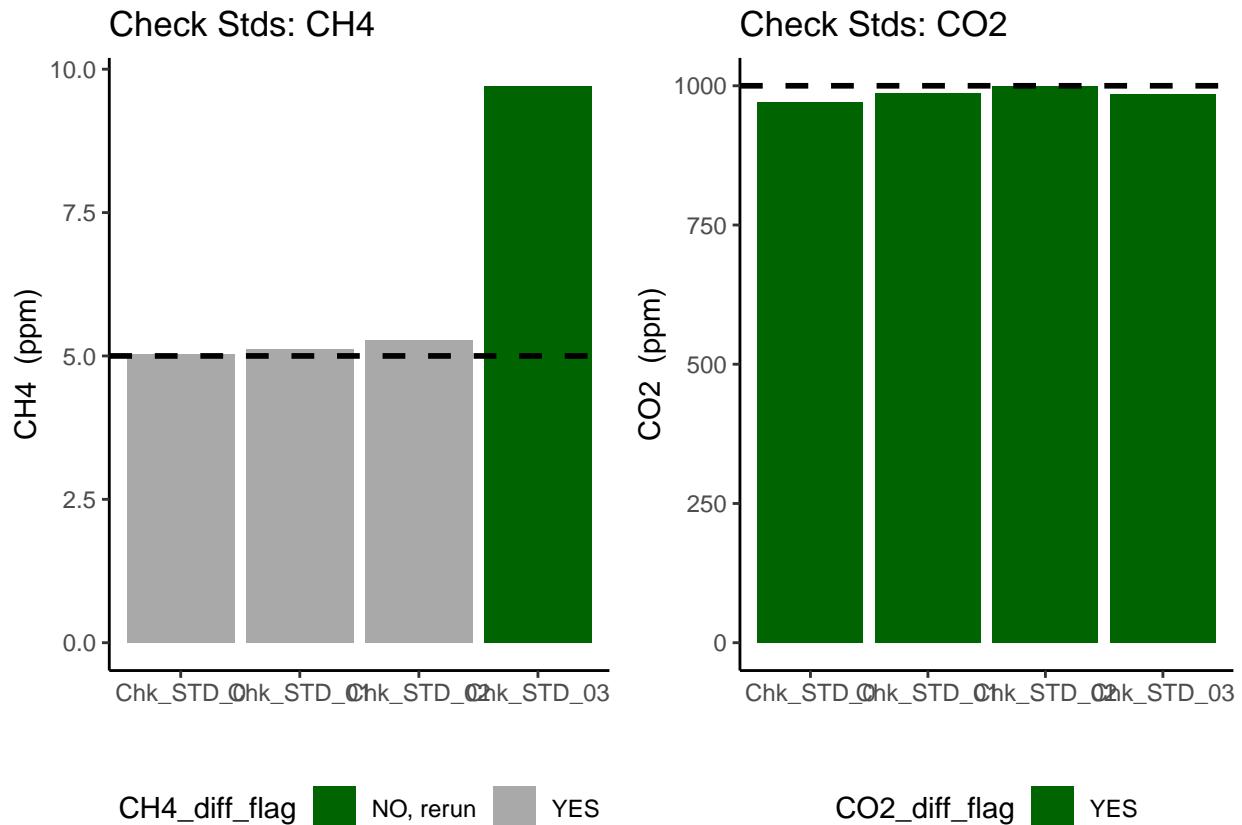
```

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)

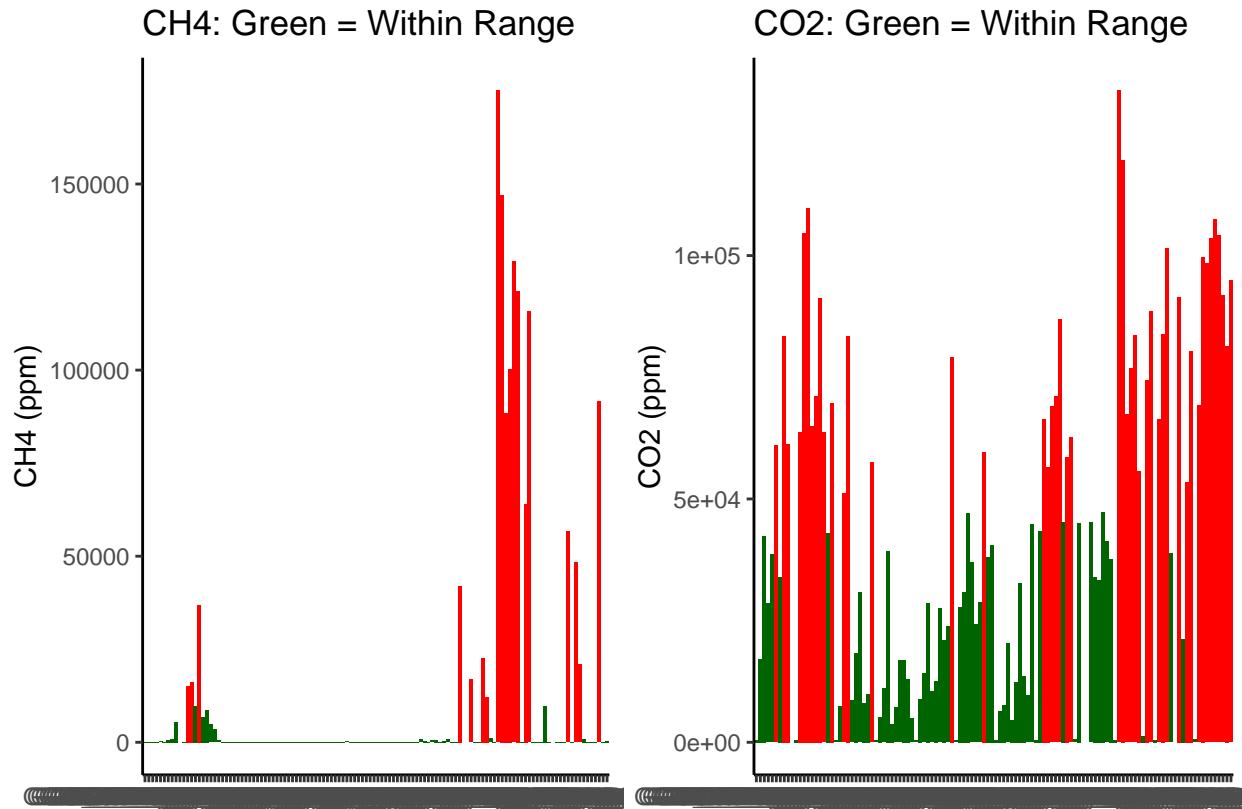
#quick first look at the samples
ch4_samples <- ggplot(data = Samples, aes(x = Sample_ID, y = CH4_Conc_ppm, fill=CH4_Flag)) +
  geom_bar(stat = 'identity') +
  scale_fill_manual(values=c("red","darkgreen"))+
  #scale_fill_gradient2(low='red', mid='white', high='blue', space='Lab') +
  theme_classic() + 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
```