

COMPASS_TEMPEST_SGW_2024: August

Stephanie J. Wilson

2023-01-14

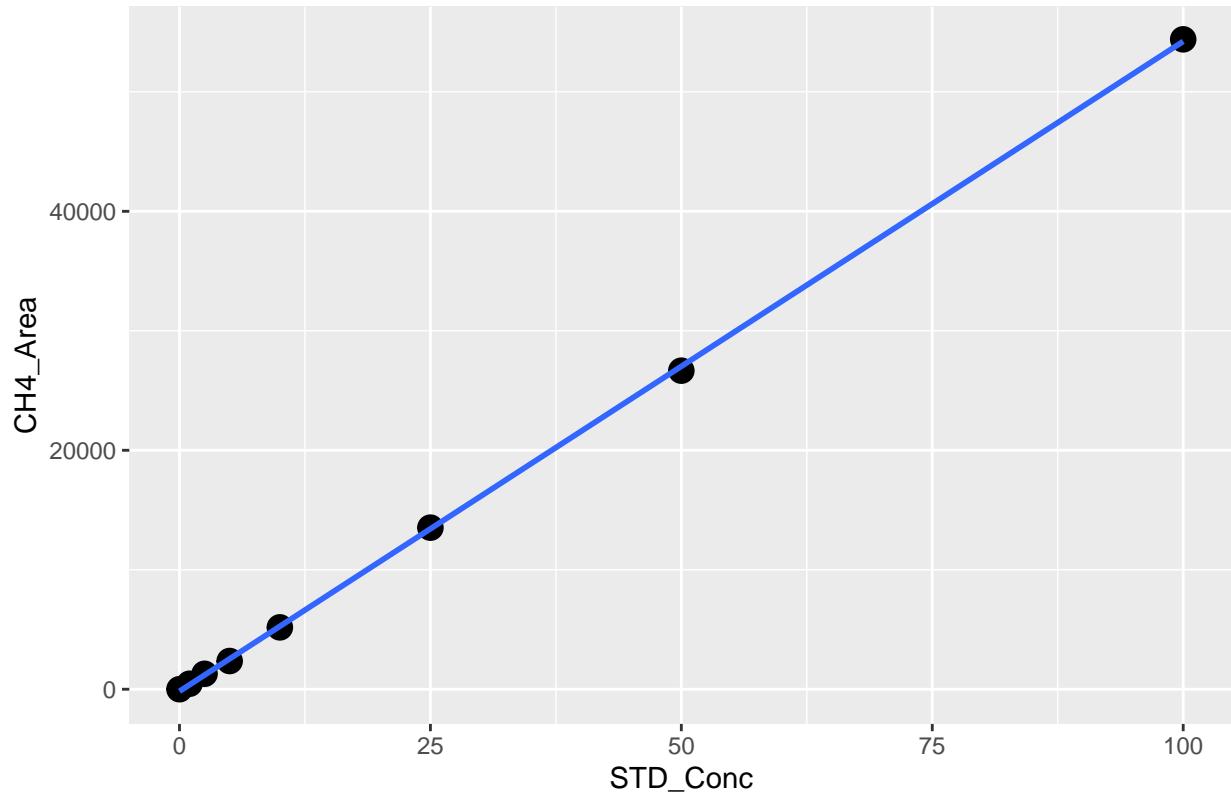
##Set Up

Read in first data file and assess standard curves

```
##      Machine   User Run_Date Sample_Type Type1 Sample_Year Sample_Month
## 1 Varian GC Wegner 20241030     Blank Blank        2024       <NA>
## 2 Varian GC Wegner 20241030    STD_CH4 STDs        2024       <NA>
## 3 Varian GC Wegner 20241030    STD_CO2 STDs        2024       <NA>
## 4 Varian GC Wegner 20241030    STD_CH4 STDs        2024       <NA>
## 5 Varian GC Wegner 20241030    STD_CH4 STDs        2024       <NA>
## 6 Varian GC Wegner 20241030    STD_CH4 STDs        2024       <NA>
##                   Sample.ID Dilution_Factor STD_Conc CO2_Area CH4_Area Lab_Notes
## 1                 Blank_0            1     0.0       0         0
## 2 Blank_0_repeatforCH4           1     0.0       0         0
## 3 Blank_0_repeatforCO2          1     0.0       0         0
## 4      STD_1ppm_CH4             1     1.0    20998       459
## 5      STD_2.5ppm_CH4            1     2.5    75750      1291
## 6      STD_5ppm_CH4             1     5.0   136692      2360
##   Field_Notes
## 1
## 2
## 3
## 4
## 5
## 6

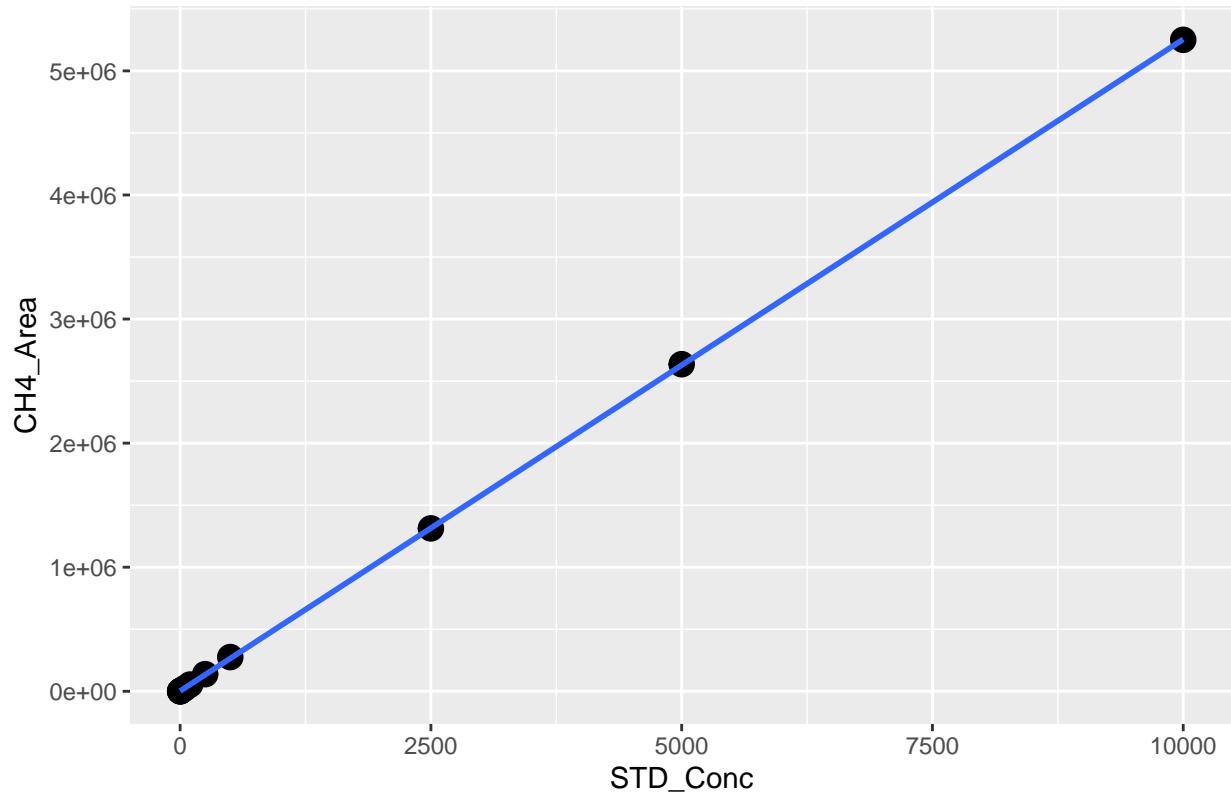
## `geom_smooth()` using formula = 'y ~ x'
```

CH4 LOW Std Curve

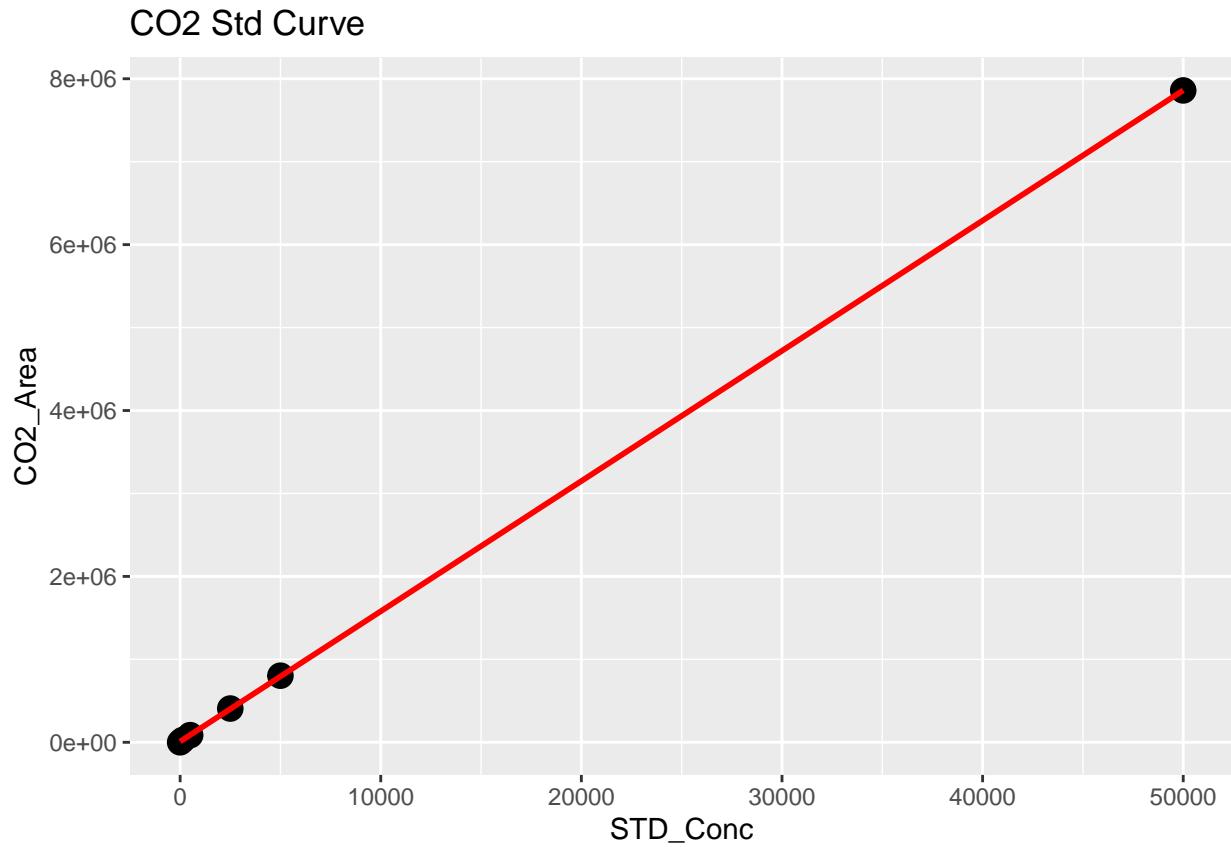


```
##  
## Call:  
## lm(formula = stds_ch4_low$CH4_Area ~ stds_ch4_low$STD_Conc)  
##  
## Residuals:  
##      Min       1Q   Median       3Q      Max  
## -362.35 -113.04    93.36   121.59   173.91  
##  
## Coefficients:  
##                               Estimate Std. Error t value Pr(>|t|)  
## (Intercept)           -173.909     91.827  -1.894   0.107  
## stds_ch4_low$STD_Conc  543.965     2.256 241.149 3.43e-13 ***  
## ---  
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1  
##  
## Residual standard error: 208.9 on 6 degrees of freedom  
## Multiple R-squared:  0.9999 , Adjusted R-squared:  0.9999  
## F-statistic: 5.815e+04 on 1 and 6 DF,  p-value: 3.431e-13  
  
## 'geom_smooth()' using formula = 'y ~ x'
```

CH4 HIGH Std Curve

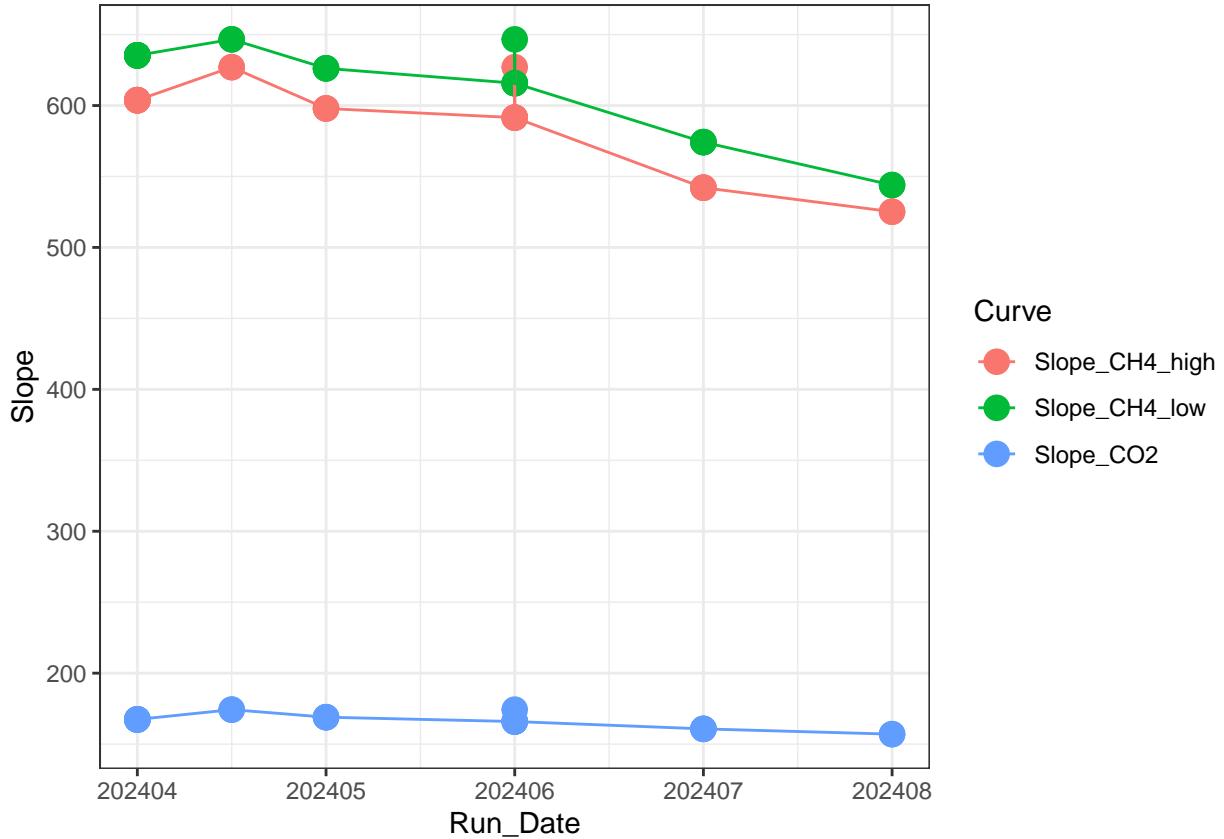


```
##  
## Call:  
## lm(formula = stds_ch4$CH4_Area ~ stds_ch4$STD_Conc)  
##  
## Residuals:  
##      Min       1Q   Median       3Q      Max  
## -3896.3 -2424.4 -2358.2 - 482.9 10776.0  
##  
## Coefficients:  
##                               Estimate Std. Error t value Pr(>|t|)  
## (Intercept)           2358.1742  1489.6850   1.583   0.142  
## stds_ch4$STD_Conc  525.1876     0.4683 1121.596 <2e-16 ***  
## ---  
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1  
##  
## Residual standard error: 4807 on 11 degrees of freedom  
## Multiple R-squared:      1, Adjusted R-squared:      1  
## F-statistic: 1.258e+06 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 
## -9303 -1839 -1652  5150  8755 -1112 
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)    
## (Intercept) 9302.5277  3249.5530   2.863   0.0458 *  
## stds_co2$STD_Conc 157.0205     0.1582 992.539 6.18e-12 *** 
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 7019 on 4 degrees of freedom
## Multiple R-squared:      1, Adjusted R-squared:      1 
## F-statistic: 9.851e+05 on 1 and 4 DF,  p-value: 6.182e-12

##      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)

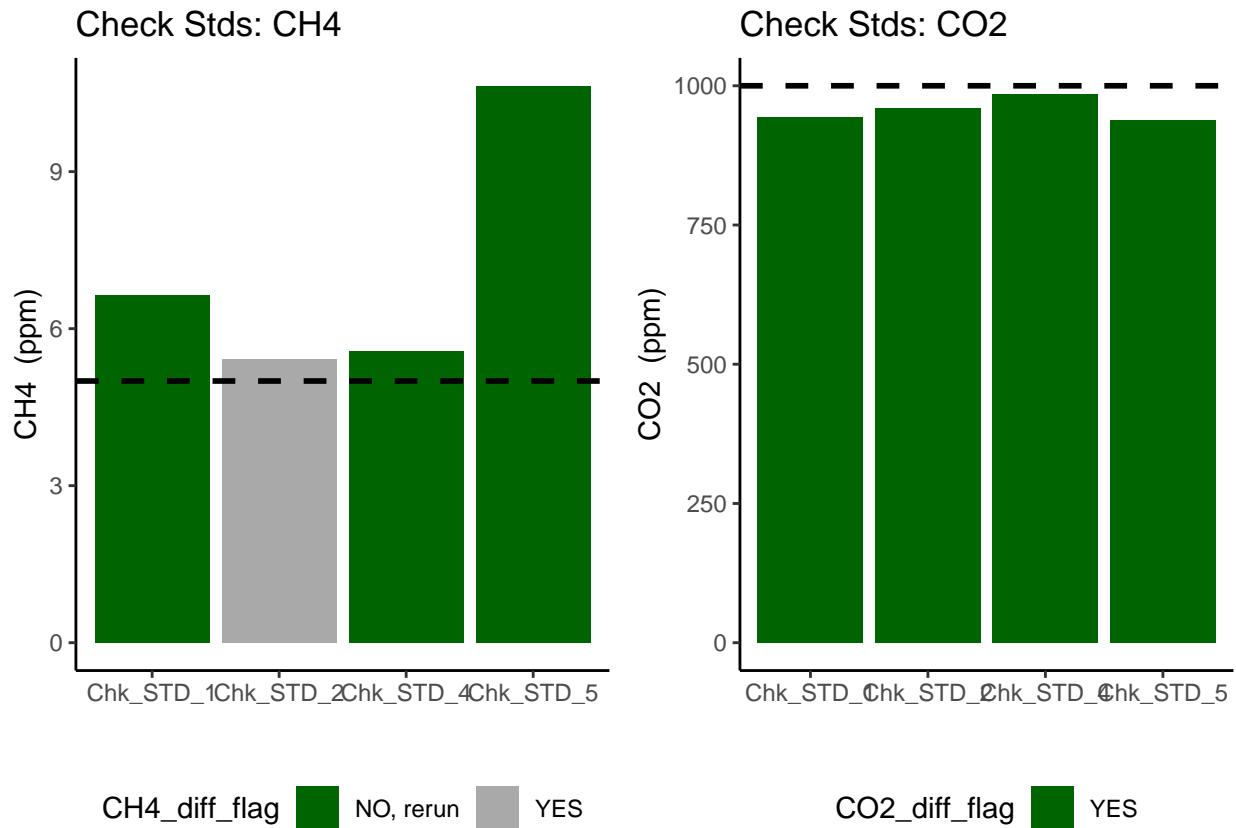
```

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)

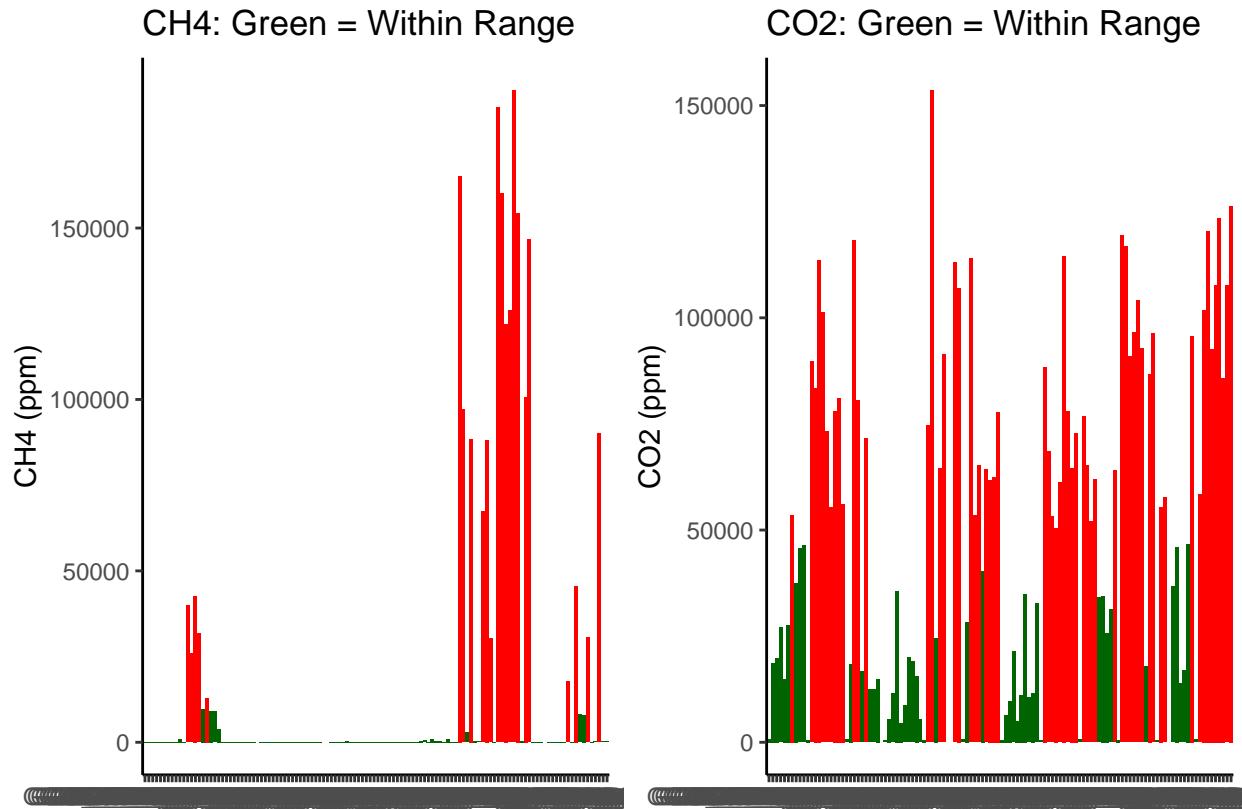
#quick first look at the samples
ch4_samples <- ggplot(data = Samples, aes(x = Sample_ID, y = CH4_Conc_ppm, fill=CH4_Flag)) +
  geom_bar(stat = 'identity') +
  scale_fill_manual(values=c("red","darkgreen"))+
  #scale_fill_gradient2(low='red', mid='white', high='blue', space='Lab') +
  theme_classic() + 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 20241030      2024
## 2 GCW TR     SgwA 20cm    20 Varian GC Wegner 20241030      2024
## 3 GCW TR     SgwA 45cm    45 Varian GC Wegner 20241030      2024
## 4 GCW TR     SgwB 10cm    10 Varian GC Wegner 20241030      2024
## 5 GCW TR     SgwB 20cm    20 Varian GC Wegner 20241030      2024
## 6 GCW TR     SgwB 45cm    45 Varian GC Wegner 20241030      2024
##   Sample_Month       Sample_ID Dilution_Factor CH4_Flag CO2_Flag
## 1 August GCW_TR_SgwA_10cm           1 Within Range Within Range
## 2 August GCW_TR_SgwA_20cm           1 Within Range Within Range
## 3 August GCW_TR_SgwA_45cm           1 Within Range Within Range
## 4 August GCW_TR_SgwB_10cm           1 Within Range Within Range
## 5 August GCW_TR_SgwB_20cm           1 Within Range Within Range
## 6 August GCW_TR_SgwB_45cm           1 Within Range Needs Dilution
##   CH4_Conc_ppm_dilcorr CO2_Conc_ppm_dilcorr
## 1             1.909881          18738.83
## 2             6.003892          19835.89
## 3             1.731560          27055.70
## 4             5.461578          14974.14
## 5             6.301705          27618.19
## 6             9.901200          53531.84

write.csv(alldat, "Processed Data/COMPASS_CBSYN_SGW_202408_Processed.csv")

```

```
#end
```