COMPASS_Synoptic_TGW_2022: Oct part 2 & Nov

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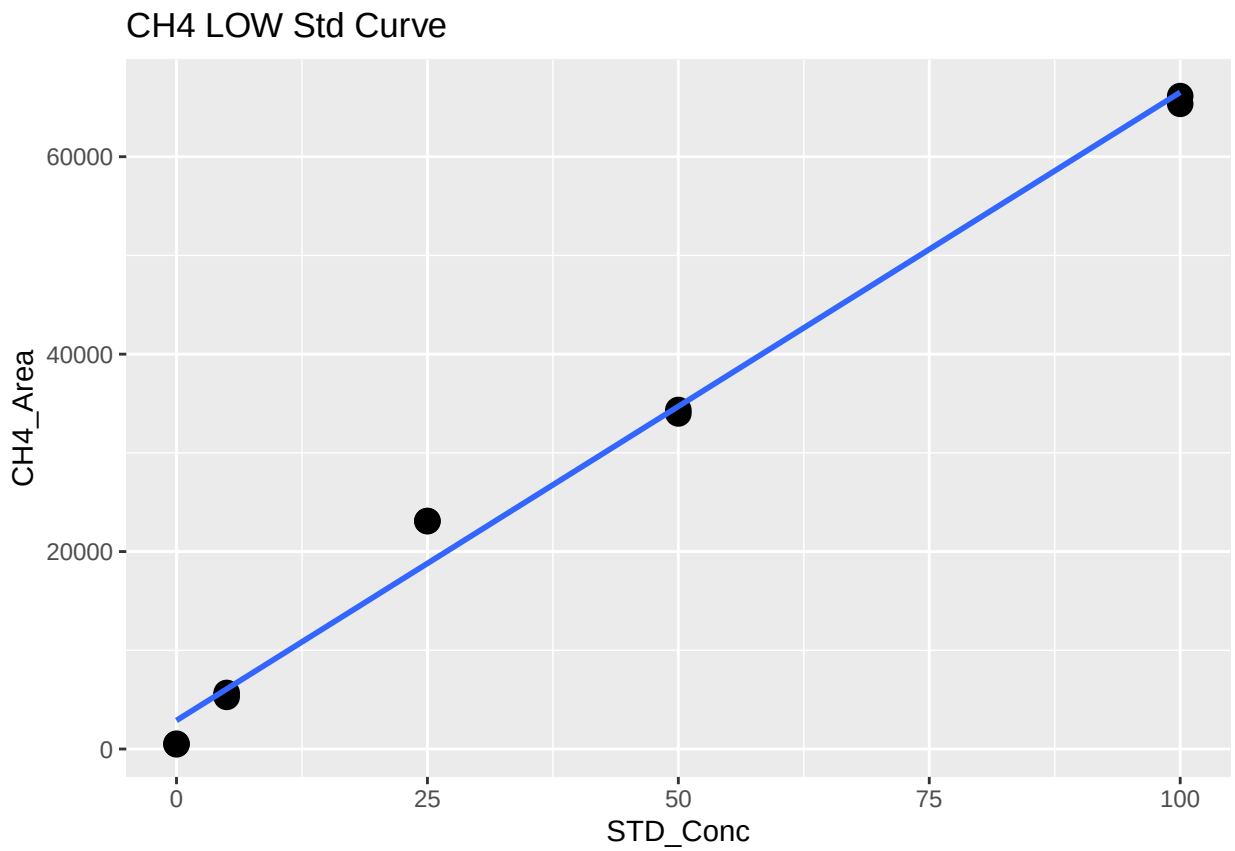
##Set Up

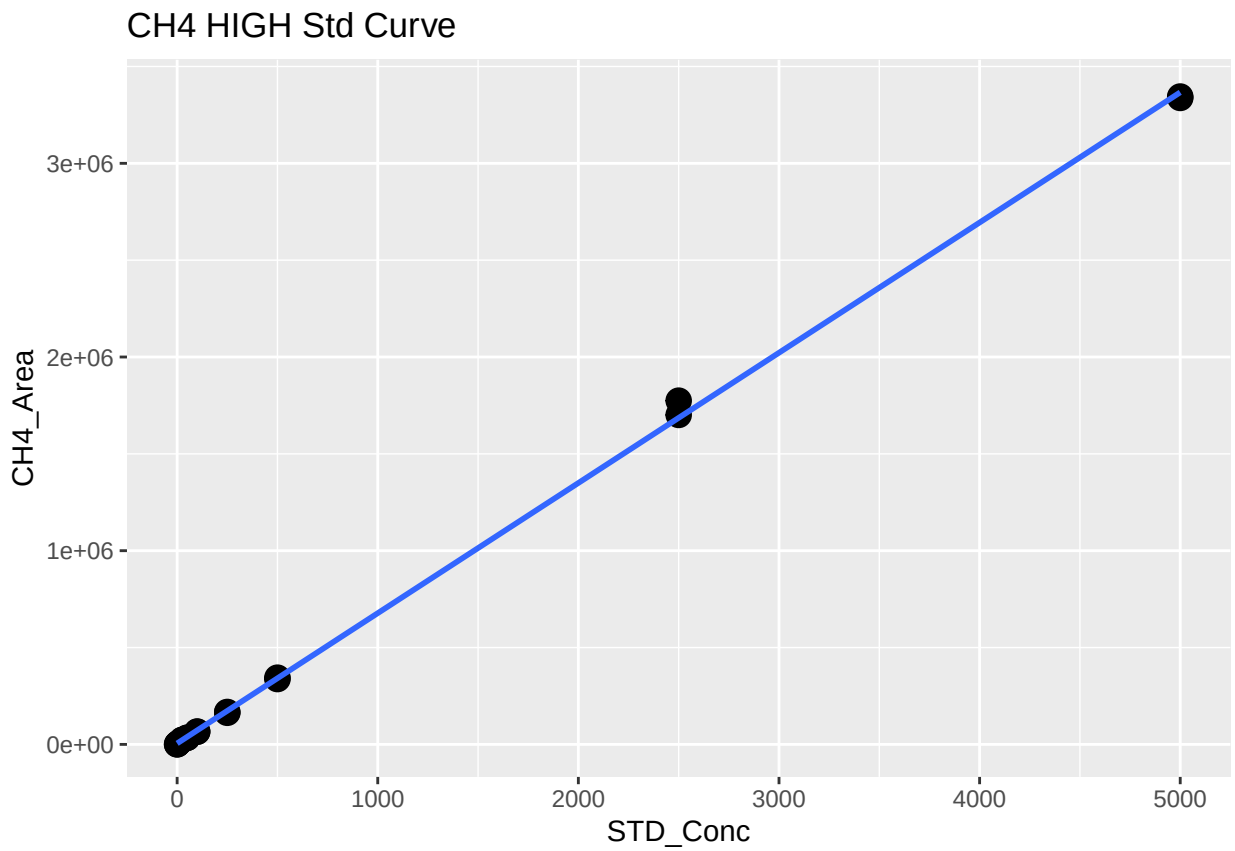
Read in first data file and assess standard curves

```
##     Machine                User Run_Date Sample_Type Type1 Sample_Year
## 1 Varian GC Stephanie J. Wilson 202212.5       Blank  TGAS        2022
## 2 Varian GC Stephanie J. Wilson 202212.5     Chk_STD  TGAS        2022
## 3 Varian GC Stephanie J. Wilson 202212.5     Chk_STD  TGAS        2022
## 4 Varian GC Stephanie J. Wilson 202212.5     Unknown  TGAS        2022
## 5 Varian GC Stephanie J. Wilson 202212.5     Unknown  TGAS        2022
## 6 Varian GC Stephanie J. Wilson 202212.5     Unknown  TGAS        2022
##   Sample_Month        Sample_ID Dilution_Factor STD_Conc CH4_Area CO2_Area
## 1         <NA>            Blank               1       NA      391    18821
## 2         <NA>   CH4 Chk 100ppm               1      100    65160       NA
## 3         <NA>   CO2 Chk 500ppm               1      500       NA    86005
## 4      October GWI_TGAS_UP_SF_1               2       NA    18193  3989643
## 5      October GWI_TGAS_UP_SF_2               2       NA    22122  6882701
## 6      October GWI_TGAS_UP_SF_3               2       NA    21739  5279576
##   Field.Notes Lab.Notes
## 1          NA        NA
## 2          NA        NA
## 3          NA        NA
## 4          NA        NA
## 5          NA        NA
## 6          NA        NA
```

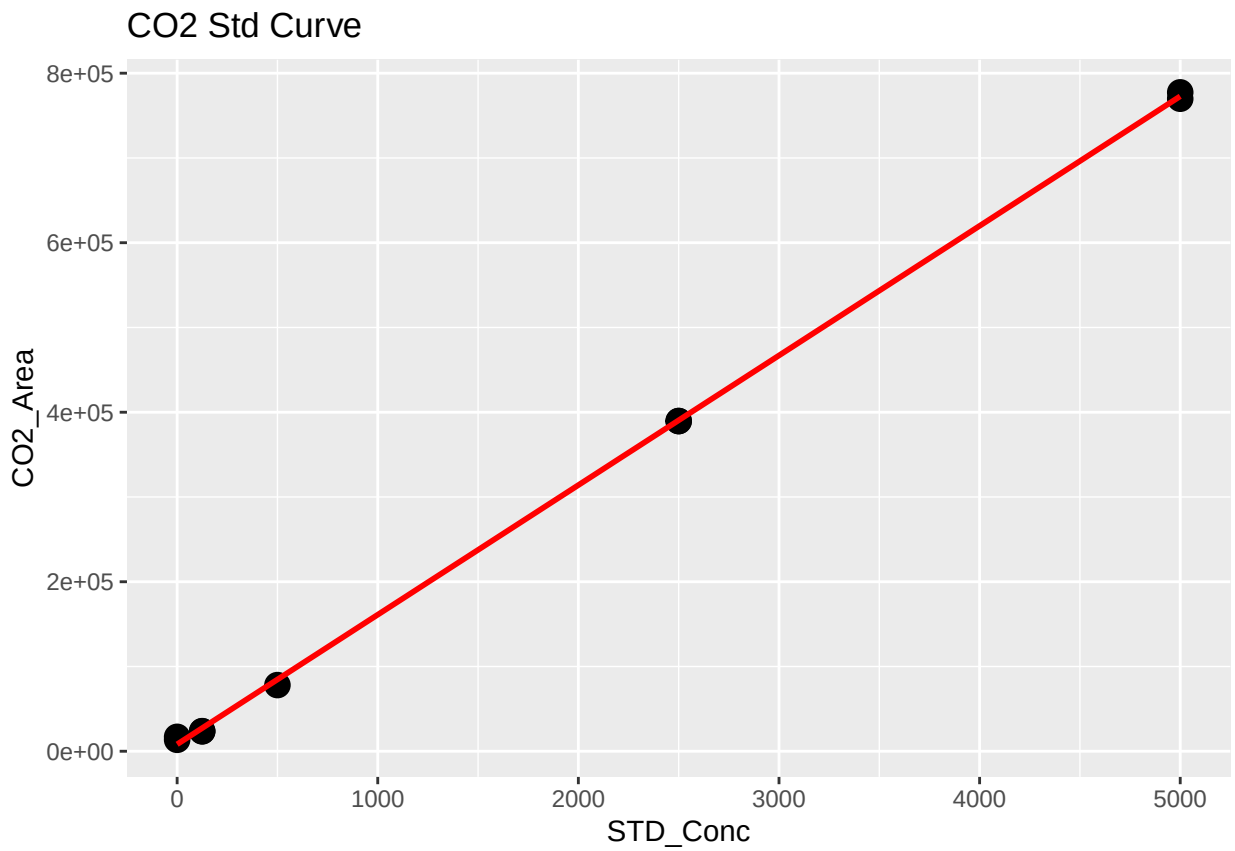
```
## `geom_smooth()` using formula = 'y ~ x'
```



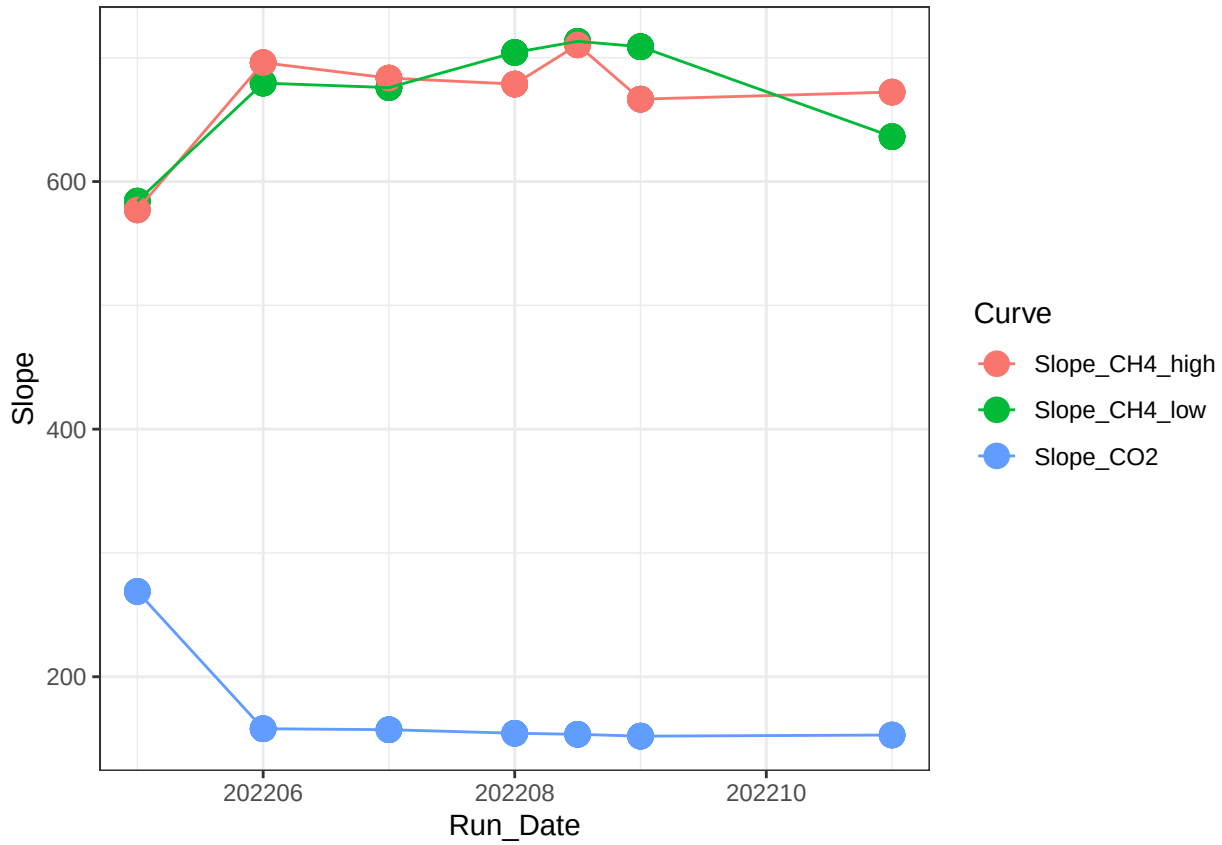

```
##
## Call:
## lm(formula = stds_ch4_low$CH4_Area ~ stds_ch4_low$STD_Conc)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -2416.3 -1073.6  -554.3  -367.8  4298.4
##
## Coefficients:
##                       Estimate Std. Error t value Pr(>|t|)
## (Intercept)            2893.27    1122.74   2.577   0.0328 *
## stds_ch4_low$STD_Conc   636.29      21.89  29.064 2.13e-09 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2529 on 8 degrees of freedom
## Multiple R-squared:  0.9906, Adjusted R-squared:  0.9894
## F-statistic: 844.7 on 1 and 8 DF,  p-value: 2.126e-09

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




```
##
## Call:
## lm(formula = stds_ch4$CH4_Area ~ stds_ch4$STD_Conc)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -28938  -6190  -4585     69  88709
##
## Coefficients:
##                   Estimate Std. Error t value Pr(>|t|)
## (Intercept)       5220.127   6726.336   0.776    0.449
## stds_ch4$STD_Conc  672.248      3.591 187.200   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 24710 on 16 degrees of freedom
## Multiple R-squared:  0.9995, Adjusted R-squared:  0.9995
## F-statistic: 3.504e+04 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
## -6593.6 -3598.0  -961.4  4658.3  8811.9
##
## Coefficients:
##                     Estimate Std. Error t value Pr(>|t|)
## (Intercept)       8210.1166  2428.5240   3.381   0.0117 *
## stds_co2$STD_Conc  152.9109     0.9195 166.299  7.5e-14 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 5457 on 7 degrees of freedom
## Multiple R-squared:  0.9997, Adjusted R-squared:  0.9997
## F-statistic: 2.766e+04 on 1 and 7 DF,  p-value: 7.502e-14

##   X          Curve        R2    Slope  Intercept Run_Date
## 1 1  Slope_CH4_low 0.9989050 584.1700   292.6667   202205
## 2 2 Slope_CH4_high 0.9988404 577.1458 -1829.3469   202205
## 3 3      Slope_CO2 0.8941001 268.8803 82323.2843   202205
## 4 4  Slope_CH4_low 0.9989050 584.1700   292.6667   202205
## 5 5 Slope_CH4_high 0.9988404 577.1458 -1829.3469   202205
## 6 6      Slope_CO2 0.8941001 268.8803 82323.2843   202205
```



Now calculate the CH4 & CO2 concentrations in ppm

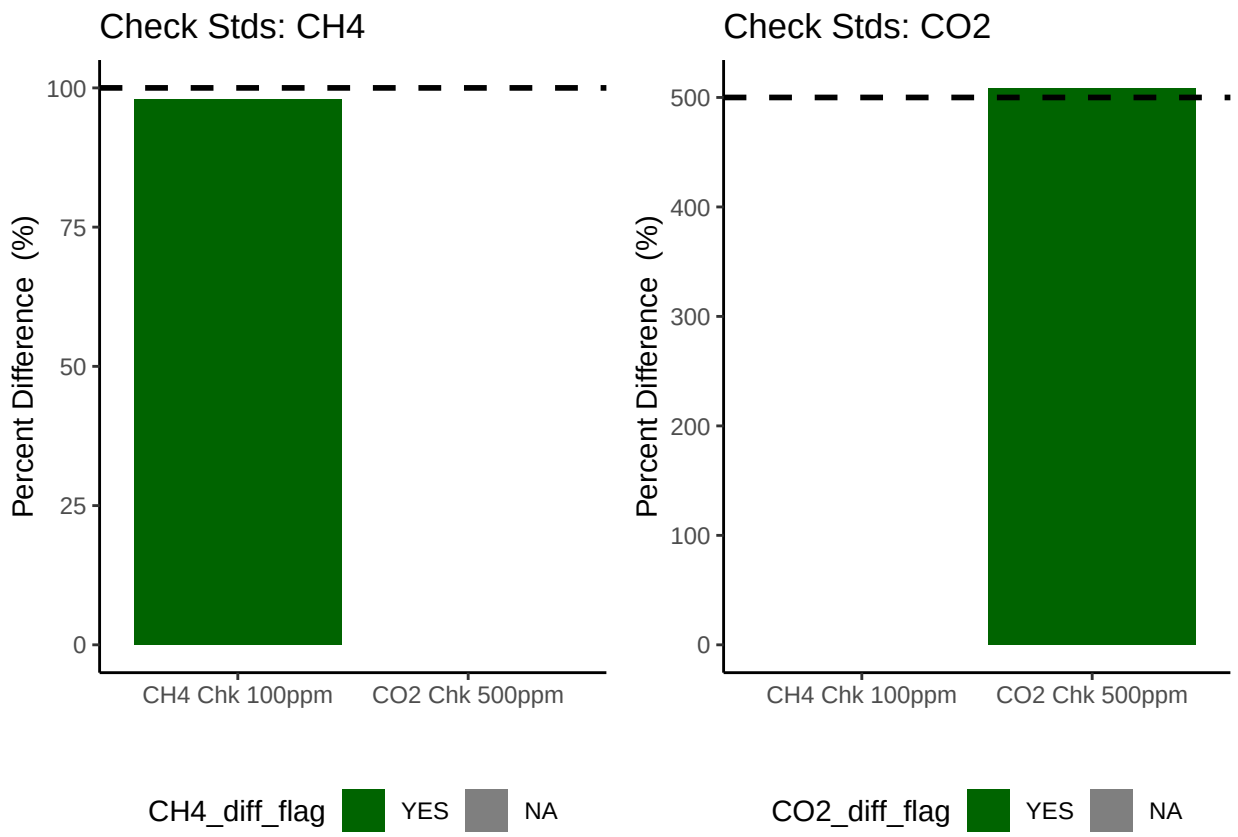
```
#head(raw)

#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, "CHK_STD")) %>%
  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

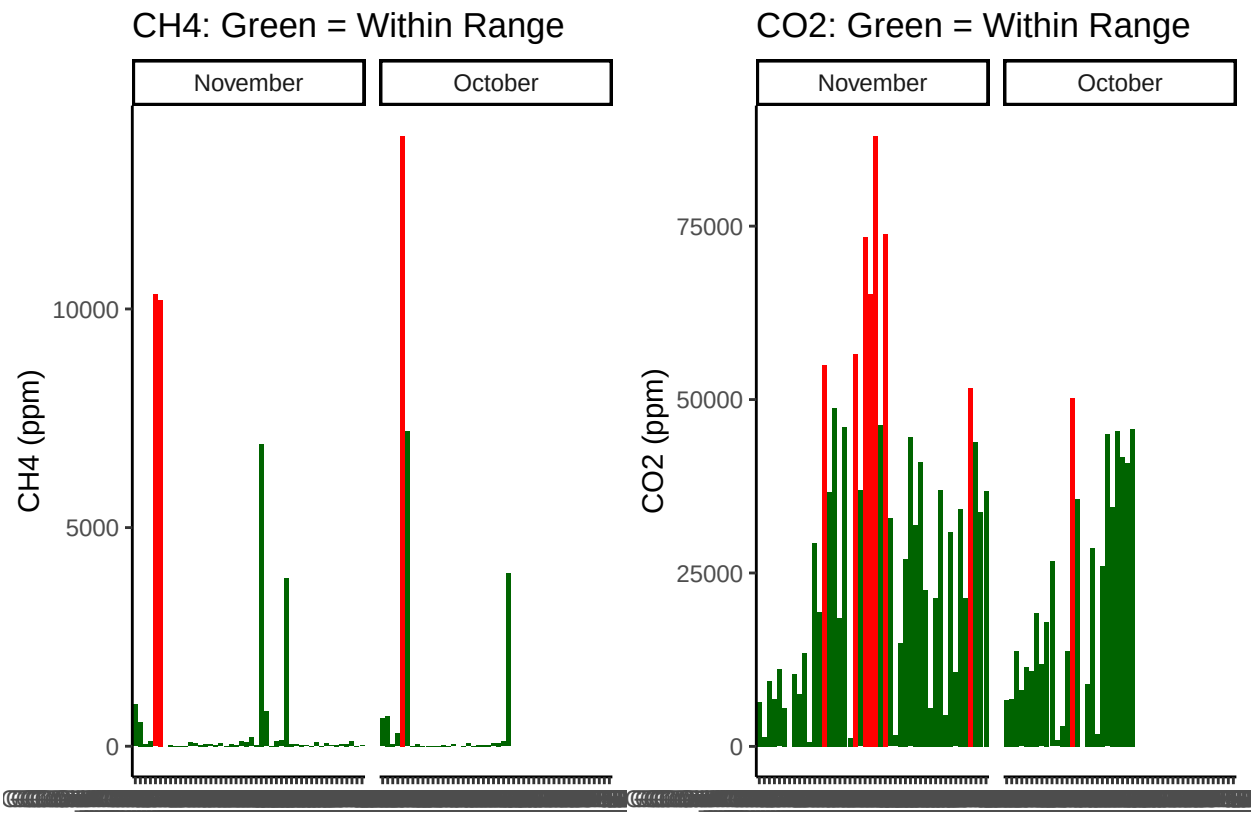
```
## Warning: Using 'size' aesthetic for lines was deprecated in ggplot2 3.4.0.
## i Please use 'linewidth' instead.
## This warning is displayed once every 8 hours.
## Call 'lifecycle::last_lifecycle_warnings()' to see where this warning was
## generated.
```

```
## Warning: Removed 1 row containing missing values or values outside the scale range
## ('geom_bar()').
## Removed 1 row containing missing values or values outside the scale range
## ('geom_bar()').
```



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") +
        facet_grid(~Sample_Month)


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") +
        facet_grid(~Sample_Month)

ggarrange(ch4_samples, co2_samples, nrow=1, ncol=2)
```



Write out processed data & slopes

```
#check results
head(Samples)
```

```
##     Machine                User Run_Date Sample_Type Type1 Sample_Year
## 1 Varian GC Stephanie J. Wilson 202212.5     Unknown  TGAS        2022
## 2 Varian GC Stephanie J. Wilson 202212.5     Unknown  TGAS        2022
## 3 Varian GC Stephanie J. Wilson 202212.5     Unknown  TGAS        2022
## 4 Varian GC Stephanie J. Wilson 202212.5     Unknown  TGAS        2022
## 5 Varian GC Stephanie J. Wilson 202212.5     Unknown  TGAS        2022
## 6 Varian GC Stephanie J. Wilson 202212.5     Unknown  TGAS        2022
##   Sample_Month        Sample_ID Dilution_Factor STD_Conc CH4_Area CO2_Area
## 1      October GWI_TGAS_UP_SF_1               2       NA    18193  3989643
## 2      October GWI_TGAS_UP_SF_2               2       NA    22122  6882701
## 3      October GWI_TGAS_UP_SF_3               2       NA    21739  5279576
## 4      October GWI_TGAS_UP_SF_4               2       NA    45319  6962757
## 5      October GWI_TGAS_UP_SF_5               2       NA    52221  6386926
## 6      October GWI_TGAS_UP_SF_6               2       NA    80365  6263992
##   Field.Notes Lab.Notes CH4_Curve CH4_Conc_ppm CO2_Conc_ppm     CH4_Flag
## 1          NA        NA       Low     24.04512     26037.60 Within Range
## 2          NA        NA       Low     30.21995     44957.49 Within Range
## 3          NA        NA       Low     29.61803     34473.44 Within Range
## 4          NA        NA       Low     66.67646     45481.04 Within Range
```

```
## 5          NA        NA       Low     77.52367     41715.24 Within Range
## 6          NA        NA      High    111.78146     40911.28 Within Range
##       CO2_Flag CH4_Conc_ppm_dilcorr CO2_Conc_ppm_dilcorr
## 1 Within Range             48.09024             52075.19
## 2 Within Range             60.43991             89914.98
## 3 Within Range             59.23606             68946.89
## 4 Within Range            133.35292             90962.07
## 5 Within Range            155.04734             83430.48
## 6 Within Range            223.56292             81822.57
```

```
#pull out what we need
Samples1 <- Samples[ ,c(1:3,5:9,13, 18:21)]
head(Samples1)
```

```
##     Machine                User Run_Date Type1 Sample_Year Sample_Month
## 1 Varian GC Stephanie J. Wilson 202212.5  TGAS        2022      October
## 2 Varian GC Stephanie J. Wilson 202212.5  TGAS        2022      October
## 3 Varian GC Stephanie J. Wilson 202212.5  TGAS        2022      October
## 4 Varian GC Stephanie J. Wilson 202212.5  TGAS        2022      October
## 5 Varian GC Stephanie J. Wilson 202212.5  TGAS        2022      October
## 6 Varian GC Stephanie J. Wilson 202212.5  TGAS        2022      October
##          Sample_ID Dilution_Factor Field.Notes     CH4_Flag     CO2_Flag
## 1 GWI_TGAS_UP_SF_1               2          NA Within Range Within Range
## 2 GWI_TGAS_UP_SF_2               2          NA Within Range Within Range
## 3 GWI_TGAS_UP_SF_3               2          NA Within Range Within Range
## 4 GWI_TGAS_UP_SF_4               2          NA Within Range Within Range
## 5 GWI_TGAS_UP_SF_5               2          NA Within Range Within Range
## 6 GWI_TGAS_UP_SF_6               2          NA Within Range Within Range
##   CH4_Conc_ppm_dilcorr CO2_Conc_ppm_dilcorr
## 1             48.09024             52075.19
## 2             60.43991             89914.98
## 3             59.23606             68946.89
## 4            133.35292             90962.07
## 5            155.04734             83430.48
## 6            223.56292             81822.57
```

```
Samples1 <- Samples1 %>%
  separate(Sample_ID, into = c("Site", "Gas_Sample", "Zone", "Tree_Code", "Replicate"), sep = "_", remo
  mutate(Tree_Info = case_when(
    Tree_Code == "DS" ~ "Dead Standing",
    Tree_Code == "SF" ~ "Sapflow Monitoring",
    TRUE ~ "Other"  # Optional: handles any values that aren't DS or SF
  )) %>%
  mutate(Status = case_when(
    Tree_Code == "DS" ~ "Dead Standing",
    Tree_Code == "SF" ~ "Living",
    TRUE ~ "Other"
  )) %>%
  mutate(Project = "COMPASS: Synoptic",
         Region = "CB") %>%
  rename( Year = Sample_Year,
          Month = Sample_Month,
          CH4_ppm = CH4_Conc_ppm_dilcorr ,
```

```
          CO2_ppm = CO2_Conc_ppm_dilcorr )  %>%
  mutate(CH4_Flag = case_when(
    CH4_Flag == "Needs_Dilution" ~ "Over Std Curve Range",
    TRUE ~ "Within Std Curve Range"
  )) %>%
  mutate(CO2_Flag = case_when(
    CO2_Flag == "Needs_Dilution" ~ "Over Std Curve Range",
    TRUE ~ "Within Std Curve Range"
  ))

final <- Samples1 %>%
  select( "Project", "Region" , "Year","Month" ,"Site", "Zone", "Gas_Sample",
          "Sample_ID", "Tree_Code", "Replicate", "Status", "Tree_Info",
          "CH4_ppm", "CH4_Flag", "CO2_ppm", "CO2_Flag")

write.csv(Samples1, "Processed Data/COMPASS_Synoptic_TGW_202210-11_Processed.csv")
```

#end