COMPASS_TEMPEST_SGW_2025: Well Test #3

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2025-02-11

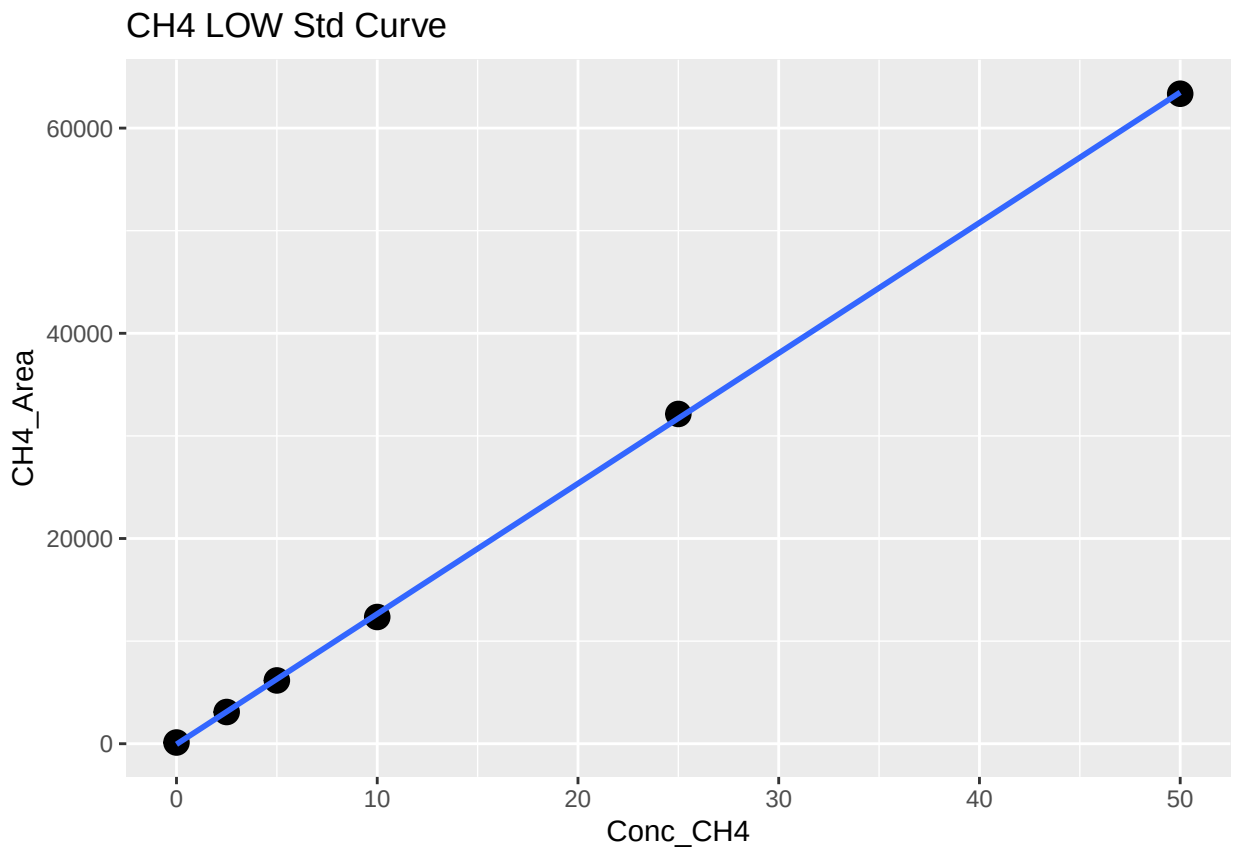
Contents

##Set Up

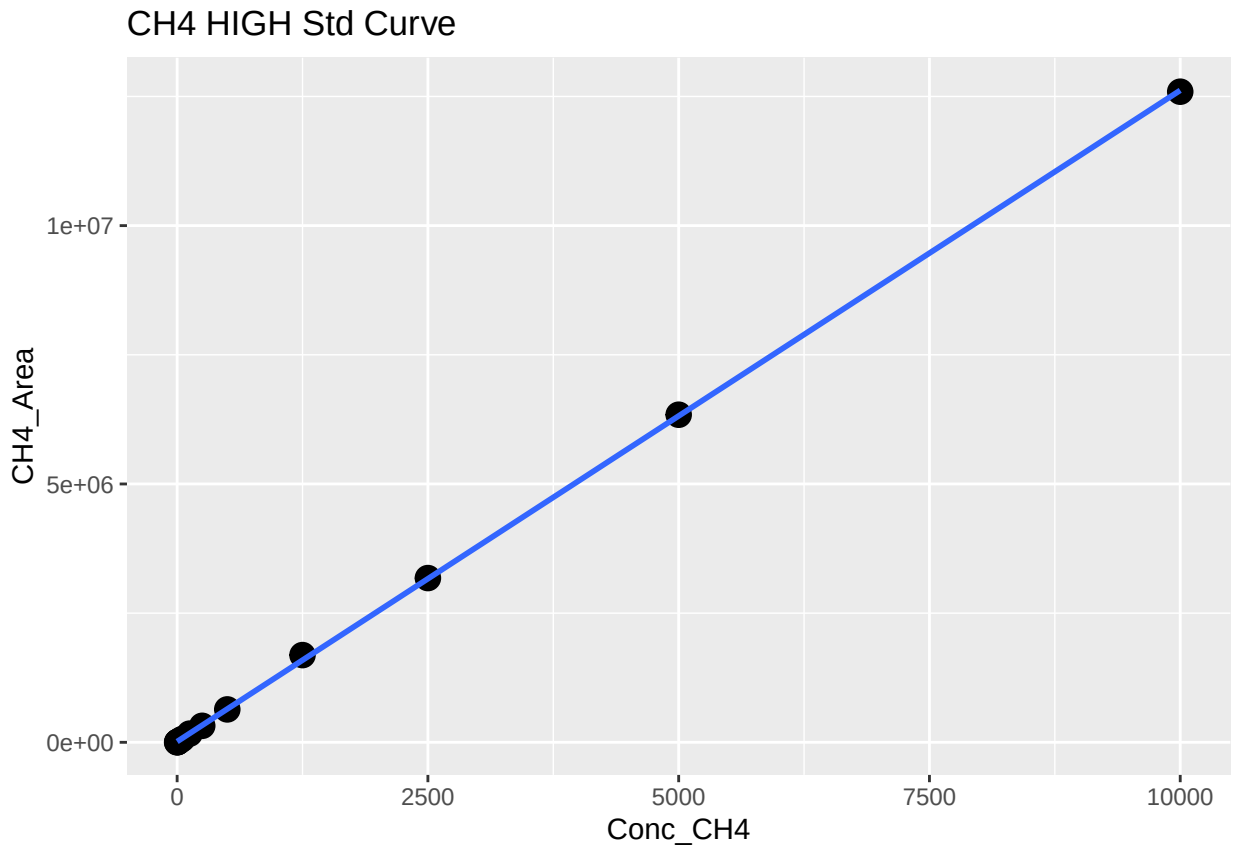
0.1 Read in first data file and assess standard curves

```
##       Machine       User Run_Date Sample_Year Sample_Month Sample_Day
## 1 Shimadzu GC B. Blakley 20251006          NA         <NA>         NA
## 2 Shimadzu GC B. Blakley 20251006          NA         <NA>         NA
## 3 Shimadzu GC B. Blakley 20251006          NA         <NA>         NA
## 4 Shimadzu GC B. Blakley 20251006          NA         <NA>         NA
## 5 Shimadzu GC B. Blakley 20251006          NA         <NA>         NA
## 6 Shimadzu GC B. Blakley 20251006          NA         <NA>         NA
##   Event_Stamp Sample_Time Time_Zone  G_W Sample_ID Sample_Type Conc_CO2
## 1        <NA>          NA      <NA> <NA>    LabAir     Lab air  unknown
## 2        <NA>          NA      <NA> <NA>    Blank1       Blank  unknown
## 3        <NA>          NA      <NA> <NA>    Blank2       Blank  unknown
## 4        <NA>          NA      <NA> <NA>      0ppm    Standard        0
## 5        <NA>          NA      <NA> <NA>    2.5ppm    Standard     0.05
## 6        <NA>          NA      <NA> <NA>      5ppm    Standard      0.1
##   Conc_CH4 Conc_N2O CO2_Area CH4_Area Dilution_Factor Minutes
## 1  unknown  unknown    51622     1840              NA      NA
## 2  unknown  unknown     3532      179              NA      NA
## 3  unknown  unknown     3213      158              NA      NA
## 4     0.00     <NA>     3171      117              NA      NA
## 5     2.50     <NA>    33055     3091              NA      NA
## 6     5.00     <NA>    63027     6168              NA      NA
```

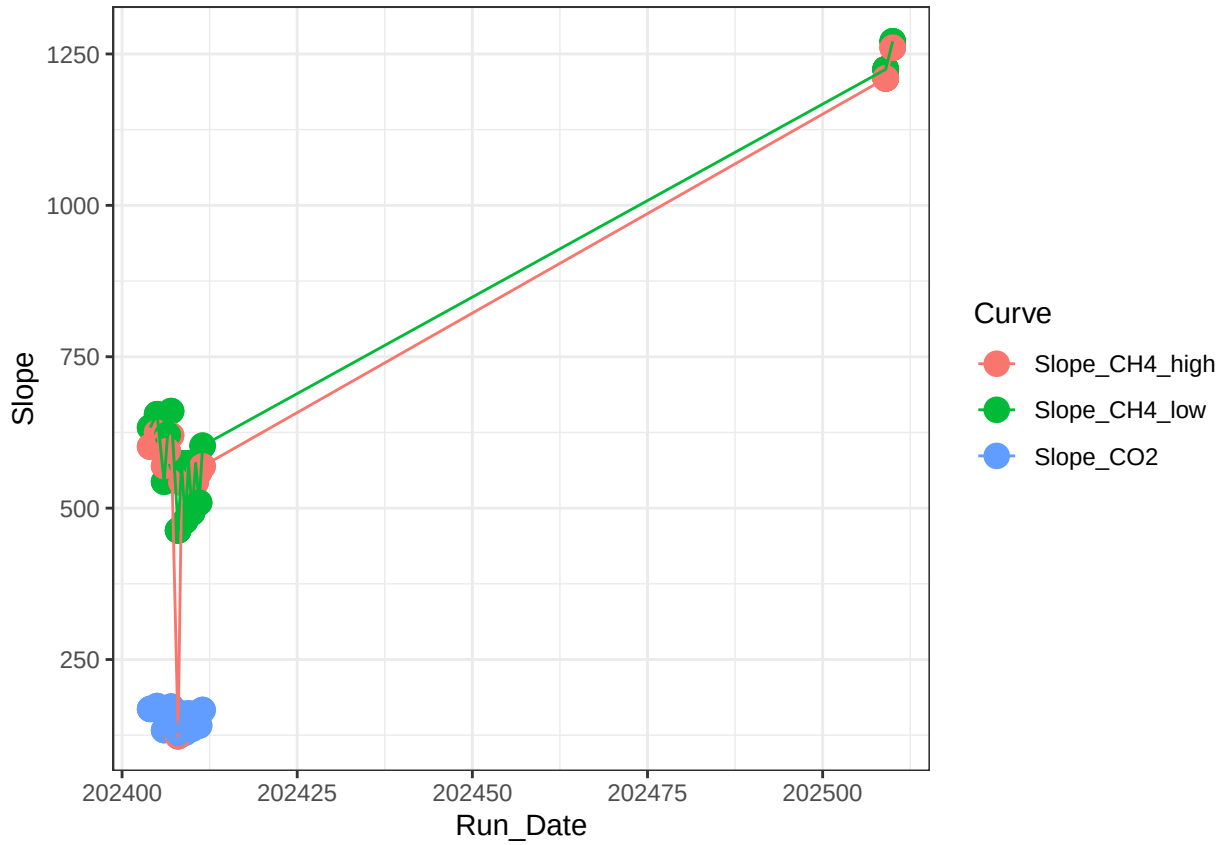
```
## `geom_smooth()` using formula = 'y ~ x'
```




```
##
## Call:
## lm(formula = stds_ch4_low$CH4_Area ~ stds_ch4_low$Conc_CH4)
##
## Residuals:
##       1       2       3       4       5       6
##  173.76  -29.34 -129.43 -301.62  423.80 -137.16
##
## Coefficients:
##                       Estimate Std. Error t value Pr(>|t|)
## (Intercept)            -56.760    158.106  -0.359    0.738
## stds_ch4_low$Conc_CH4 1270.838      6.787 187.252 4.88e-09 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 290.3 on 4 degrees of freedom
## Multiple R-squared:  0.9999, Adjusted R-squared:  0.9999
## F-statistic: 3.506e+04 on 1 and 4 DF,  p-value: 4.879e-09

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




```
##
## Call:
## lm(formula = stds_ch4$CH4_Area ~ stds_ch4$Conc_CH4)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -26492 -14481 -13793  -3862  97920
##
## Coefficients:
##                   Estimate Std. Error t value Pr(>|t|)
## (Intercept)       14421.35   10591.97   1.362    0.201
## stds_ch4$Conc_CH4  1260.39       3.31 380.818   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 33630 on 11 degrees of freedom
## Multiple R-squared:  0.9999, Adjusted R-squared:  0.9999
## F-statistic: 1.45e+05 on 1 and 11 DF,  p-value: < 2.2e-16

##   X          Curve        R2    Slope  Intercept Run_Date
## 1 1  Slope_CH4_low 0.9996407 633.0314  -320.6965   202404
## 2 2 Slope_CH4_high 0.9993443 601.5512 14817.1191   202404
## 3 3      Slope_CO2 0.9999907 168.3200 10075.2183   202404
## 4 4  Slope_CH4_low 0.9996407 633.0314  -320.6965   202404
## 5 5 Slope_CH4_high 0.9993443 601.5512 14817.1191   202404
## 6 6      Slope_CO2 0.9999907 168.3200 10075.2183   202404
```

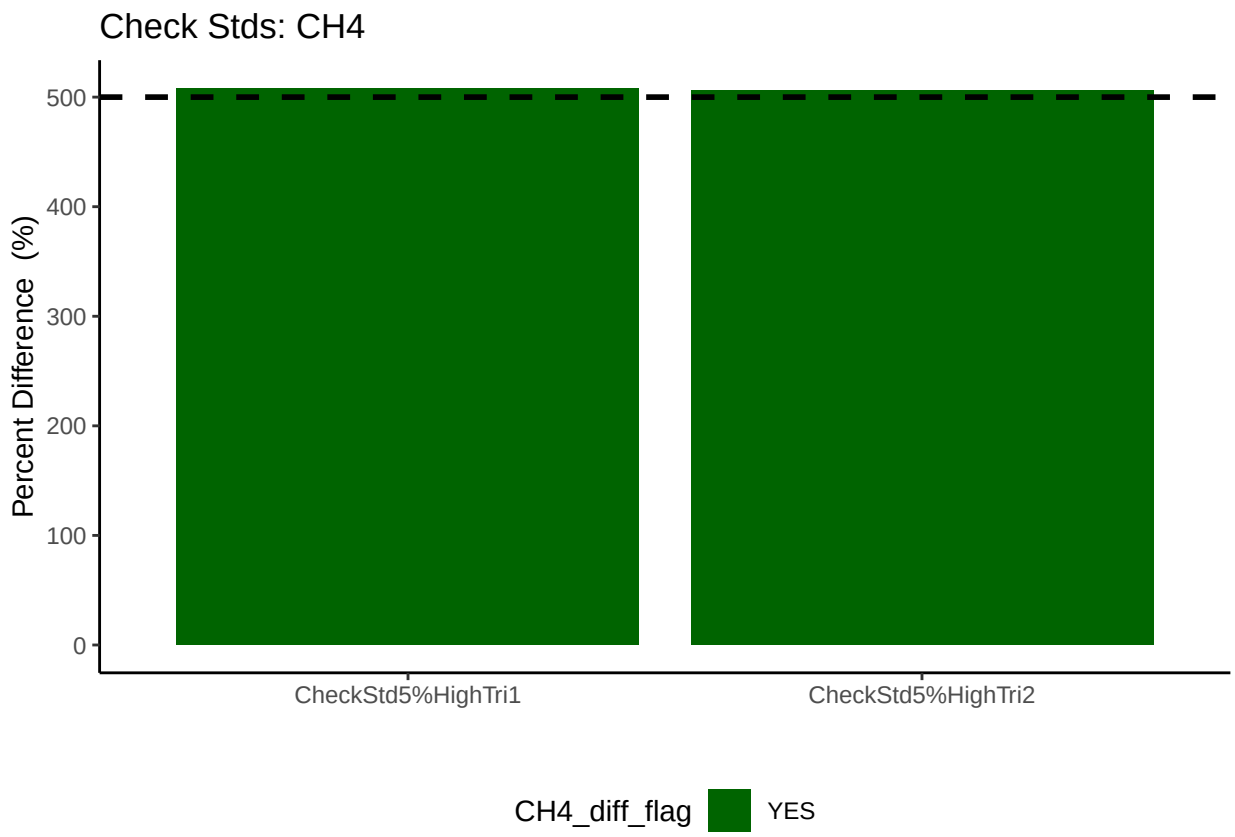


0.2 Now calculate the CH4 & CO2 concentrations in ppm

```
#head(raw)

#pull out methane standards
Samples <-  raw %>%
  filter(!str_detect(Sample_Type, "Standard")) %>%
  filter(!str_detect(Sample_Type, "STD_CO2")) %>%
  filter(!str_detect(Sample_Type, "Blank")) %>%
  filter(!str_detect(Sample_Type, "Lab air")) %>%
   filter(!str_detect(Sample_Type, "ChkStd")) %>%
   filter(!str_detect(Sample_ID, "Shakey")) %>%
  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)
```

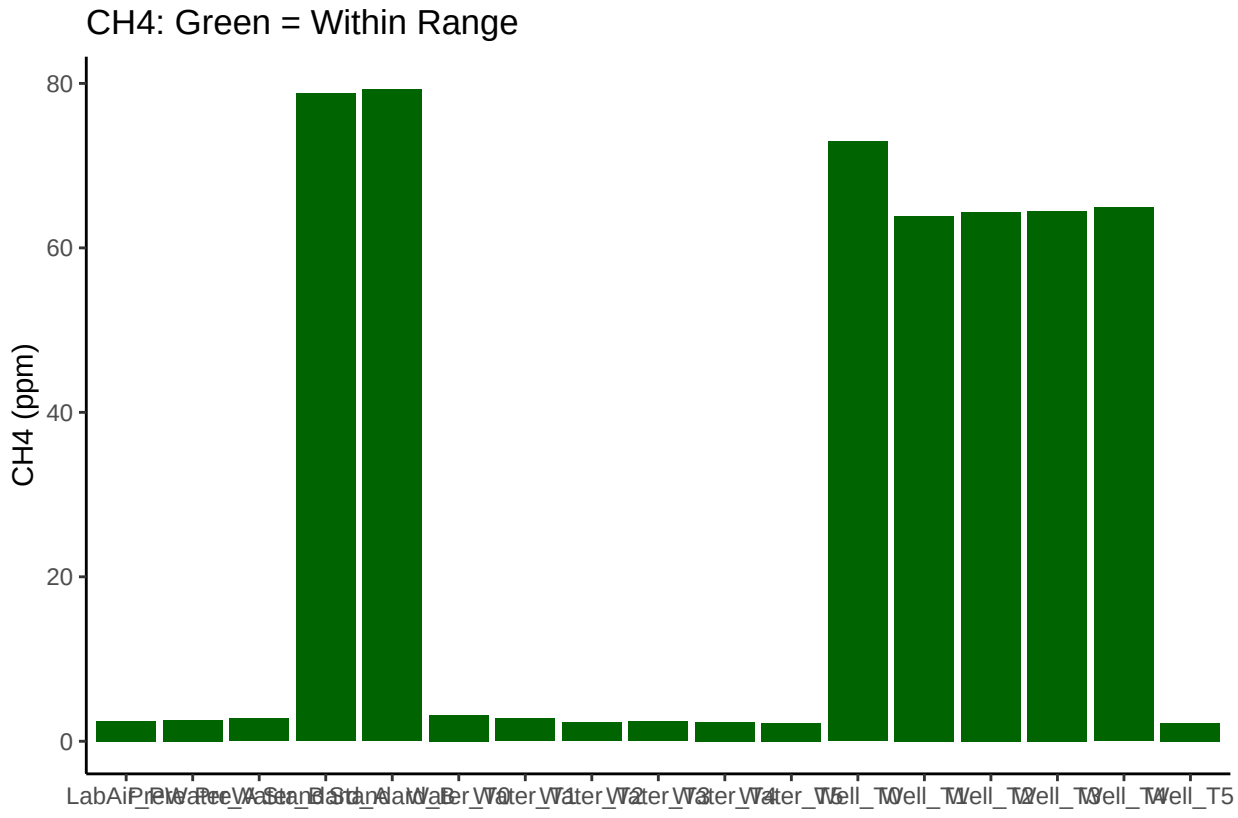
0.3 Check the Check Standards



0.4 Dilution correct samples

```r
#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)
```

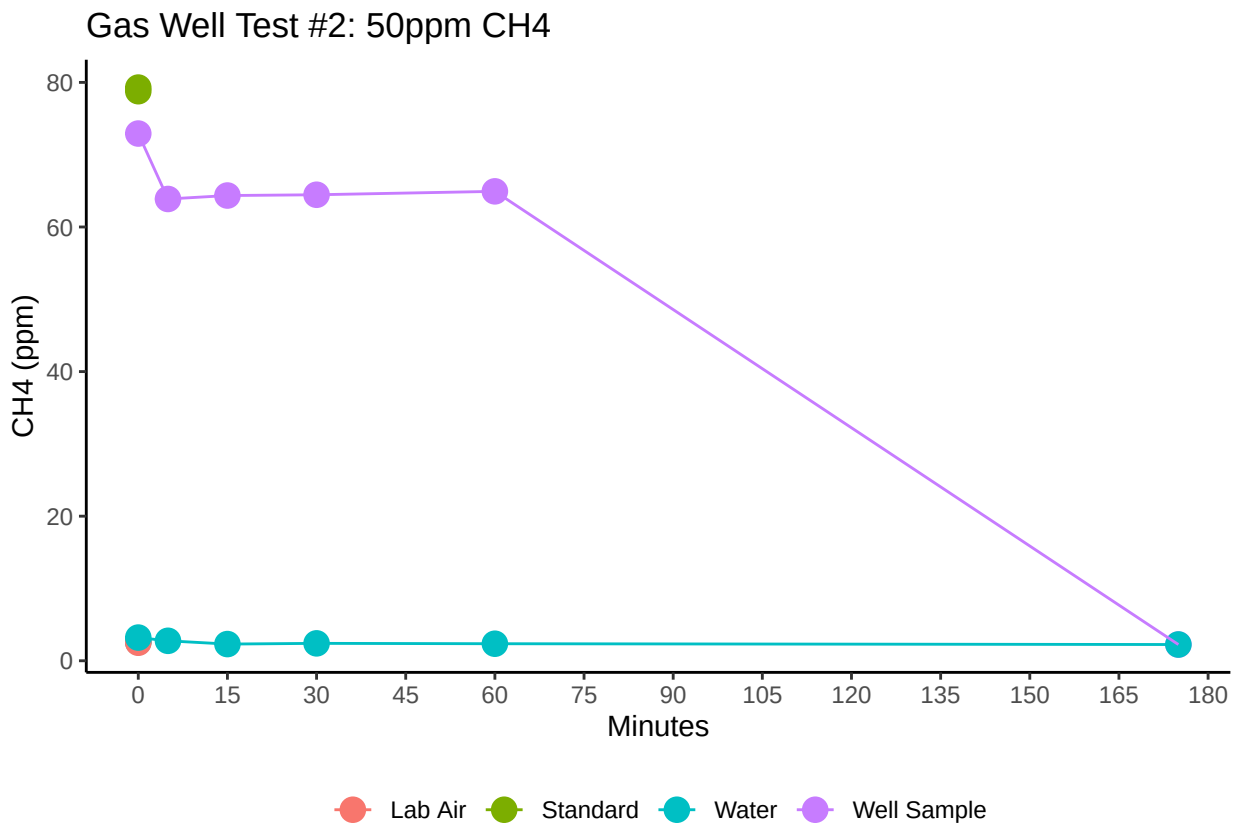
```r
#quick first look at the samples
ch4_samples <-  ggplot(data = Samples, aes(x = Sample_ID, y = CH4_Conc_ppm, fill=CH4_Flag)) +
       geom_bar(stat = 'identity') +
        scale_fill_manual(values=c("darkgreen","red"))+
        #scale_fill_gradient2(low='red', mid='white', high='blue', space='Lab')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


print(ch4_samples)
```



0.5 If samples are water calculate gas in water

0.6 Write out processed data & slopes

```
#check results
#head(Samples)

#pull out what we need
#Samples1 <- Samples[ ,c(1:3,6:17,21:24)]
#head(Samples1)

final_data <- Samples %>%
  #select(Project, Plot, grid, sample_name, Vial_ID, date, ) %>%
  mutate(
    Project = "COMPASS",   # new column with same value on every row
    Experiment = "TEMPEST: Gas Well Test #2")#,
    #Run_notes = run_notes     # new column with notes about the run
  #)

final_data$Minutes <- as.numeric(final_data$Minutes)

#plot the data thru time so we can see the equilibration
final <-  ggplot(data = final_data, aes(x = Minutes, y = CH4_Conc_ppm_dilcorr, color=Event_Stamp)) +
        geom_point(size=4) +
        geom_line() +
        scale_x_continuous(breaks = seq(0, 180, by = 15))+
        theme_classic() + labs(x= "Minutes", y="CH4 (ppm)", title="Gas Well Test #2: 50ppm CH4") +
        theme(legend.position = "bottom", legend.title=element_blank())
final
```




```
#this needs altered to match the tempest metadata and clean up
final_data <- final_data %>%
  rename(
    CH4_ppm = CH4_Conc_ppm_dilcorr ,
    CH4_uM = CH4_Conc_umol,
    # add more rename pairs as needed
  ) %>%
  select(
    Project, Experiment, Sample_Year, Sample_Month, Sample_Day, Sample_Time,
    Sample_ID, Event_Stamp, Minutes,
    CH4_ppm, CH4_uM, CH4_Flag #, tdn_mgL, tdn_uM, tdn_flag, Analysis_runtime,
    #Run_notes
    # list columns in the order you want them
  )

head(final_data)
```

```
##   Project                Experiment Sample_Year Sample_Month Sample_Day
## 1 COMPASS TEMPEST: Gas Well Test #2        2025      October          2
## 2 COMPASS TEMPEST: Gas Well Test #2        2025      October          2
## 3 COMPASS TEMPEST: Gas Well Test #2        2025      October          2
## 4 COMPASS TEMPEST: Gas Well Test #2        2025      October          2
## 5 COMPASS TEMPEST: Gas Well Test #2        2025      October          2
## 6 COMPASS TEMPEST: Gas Well Test #2        2025      October          2
##   Sample_Time  Sample_ID Event_Stamp Minutes   CH4_ppm      CH4_uM     CH4_Flag
## 1         945 Standard_B    Standard       0 79.283158 0.064810387 Within Range
```

```
## 2         945 Standard_A    Standard       0 78.780139 0.064399191 Within Range
## 3         945 PreWater_B       Water       0  2.751538 0.112462860 Within Range
## 4         945 PreWater_A       Water       0  2.572128 0.105129919 Within Range
## 5         945 LabAir_Pre     Lab Air       0  2.495014 0.002039561 Within Range
## 6        1000    Well_T0 Well Sample       0 72.926393 0.059614019 Within Range
```

```r
write.csv(final_data, "Processed Data/TMP_GasWellTest_2_GHG_Processed.csv")
```

#end