relation_between_organic_acids

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2022-05-25

offline data main

```
#data = read.csv( "C:/Users/85212/Desktop/Pro-Data/main.csv" ,header=TRUE)
data = read.csv("C:/Users/85212/Desktop/Pro-Data/online.csv", header=TRUE)
#names(data) = c( 'Sample.Key',names(data)[-1] )
#data = data[-1,]
data= data[,-2]
colnames(data)[1]='EFT..Hours'
#names(data)
ac = read.csv( "C:/Users/85212/Desktop/Pro-Data/acids.csv" ,header=TRUE)
#names(ac) = c( 'Date',names(ac)[-1] )
ac = dplyr:: filter( ac , EFT < 360)
data = dplyr:: filter( data , EFT..Hours < 360)
```

Merging by Cubic Spline Interpolation

```
x = ac$EFT
y = ac$Acc.rate.acetic
x_out = data$EFT..Hours
interpolated__acc_acetic = spline(x = x ,y = y , xout = x_out )
interpolated__acc_formic = spline( x = x , y = ac$Acc.rate.formic , xout = x_out)
data1 = cbind(data,  interpolated_formic = interpolated__acc_formic$y , interpolated__acc_acetic=interpo
# data1 = dplyr:: filter( data1 , EFT..Hours < 360)
index = which( names(data1) == 'headspace.pressure')
data1 = data1[,-index]  ## remove constant headspace.pressure
names(data1)
```

```
##  [1] "EFT..Hours"
##  [2] "total.air.flow"
##  [3] "vent.flow"
##  [4] "vessel"
##  [5] "Station.3.Loop.Temperature"
##  [6] "Station.5.Loop.Temperature"
##  [7] "Level.on.the.seperator"
##  [8] "harvest.flow"
##  [9] "pH.at.stn5"
## [10] "pH.at.stn3"
## [11] "pH.at.stn1"
```

```
## [12] "CH4.in.offgas.."
## [13] "O2.in.offgas.."
## [14] "CO2.in.offgas.."
## [15] "LEL.in.offgas.."
## [16] "dissolved.oxygen.at.stn1"
## [17] "dissolved.oxygen.at.stn2"
## [18] "dissolved.oxygen.at.stn3"
## [19] "dissolved.oxygen.at.stn4"
## [20] "dissolved.oxygen.at.stn5"
## [21] "methane.flow.stn1"
## [22] "methane.flow.stn2"
## [23] "methane.flow.stn3"
## [24] "methane.flow.stn4"
## [25] "methane.flow.stn5"
## [26] "oxygen.flow.stn1"
## [27] "oxygen.flow.stn2"
## [28] "oxygen.flow.stn3"
## [29] "oxygen.flow.stn4"
## [30] "oxygen.flow.stn5"
## [31] "NH3.online.reading"
## [32] "optical.density"
## [33] "ammonia.pump.flow.1"
## [34] "ammonia.pump.flow.2"
## [35] "ammonia.pump.flow.3"
## [36] "nitrogen.flow.stn1"
## [37] "nitrogen.flow.stn2"
## [38] "Cooling.Loop.A.Broth.Return.to.Fermenter.mixer"
## [39] "Cooling.Loop.B.Broth.Return.to.Fermenter.mixer.J1117"
## [40] "Tempered.Water.Temperature.before.Temped.water.cooler"
## [41] "Tempered.Water.Temperature.after.Temped.water.cooler"
## [42] "Cooling.Water.Return.for.Temped.System"
## [43] "Cooling.loop.A.valve.opening.."
## [44] "Cooling.loop.B.valve.opening.."
## [45] "pump.outlet"
## [46] "pump.inlet"
## [47] "pressure.at.position.4"
## [48] "Pressure.at.the.end.of.the.loop"
## [49] "oxygen..pressure.to.fermentor.loop.mixture"
## [50] "methane..pressure.to.fermentor.loop.mixture"
## [51] "circulation.pump"
## [52] "End.of.the.loop.control.valve.output.."
## [53] "partial.pressure..DP."
## [54] "Nitric.acid.flow"
## [55] "phosphoric.acid.flow"
## [56] "sodium.hydroxide.flow"
## [57] "trace.elements.flow"
## [58] "ferrus.sulphate.flow"
## [59] "calcium.chloride.flow"
## [60] "magnesium.potassium.flow"
## [61] "spare.dosing.pump.flow"
## [62] "KOH.flow"
## [63] "Nitric.acid.totalier"
## [64] "phosphoric.acid.totaliser"
## [65] "sodium.hydroxide.totaliser"
```

```
## [66] "trace.elements.totaliser"
## [67] "ferrous.sulphate.totaliser"
## [68] "calcium.chloride.totaliser"
## [69] "magnesium.potassium.totalier"
## [70] "spare.dosing.pump.totaliser"
## [71] "KOH.totaliser"
## [72] "ammonia.totalier"
## [73] "Methane.totalier"
## [74] "oxygen.totaliser"
## [75] "Fermentor.fliud.to.ammonia...OD.meter.L.h"
## [76] "interpolated_formic"
## [77] "interpolated__acc_acetic"
```

Pre-process

```
data1 =  data1[complete.cases(data1) ,]
#data1$interpolated_acc_acetic[ which(data1$interpolated__acc_acetic < 0 )] = 0
remove_col = c()
for (j in 1:(ncol(data1)-2) )
{
  if (  mean(data1[,j]) < 0.01 | min(data1[,j])  == mean(data1[,j])  )
  remove_col = c(remove_col , j)
  else
  {
    wrong_row = which(data1[,j] < 0 )
    data1[wrong_row , j] = 0
  }

}
data1 = data1[,-remove_col]
#summary(data1)
```

Correlation

Since the P-value of cor.test is high, we should accept null hypothesis and conclude that they are independent

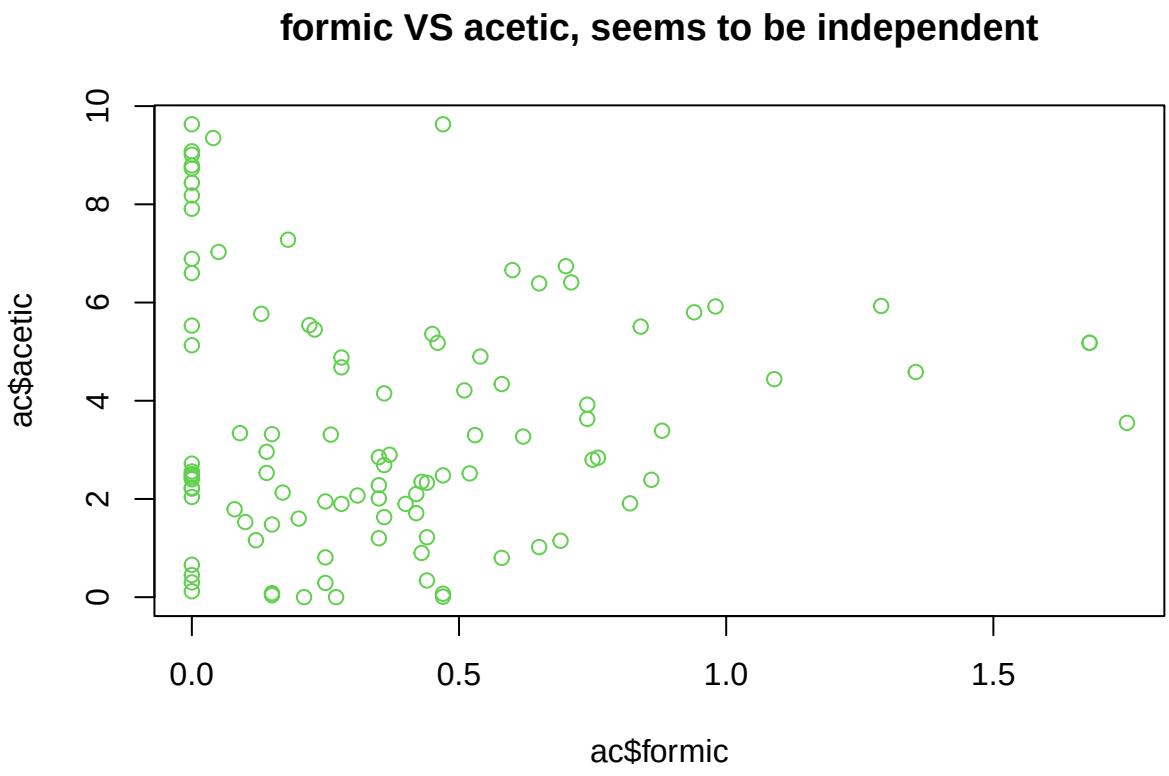
```
cor.test( ac$formic , ac$acetic )
```

```
##
##  Pearson's product-moment correlation
##
## data:  ac$formic and ac$acetic
## t = 0.22691, df = 102, p-value = 0.8209
## alternative hypothesis: true correlation is not equal to 0
## 95 percent confidence interval:
##  -0.1708652  0.2141241
## sample estimates:
##        cor
## 0.02246218
```

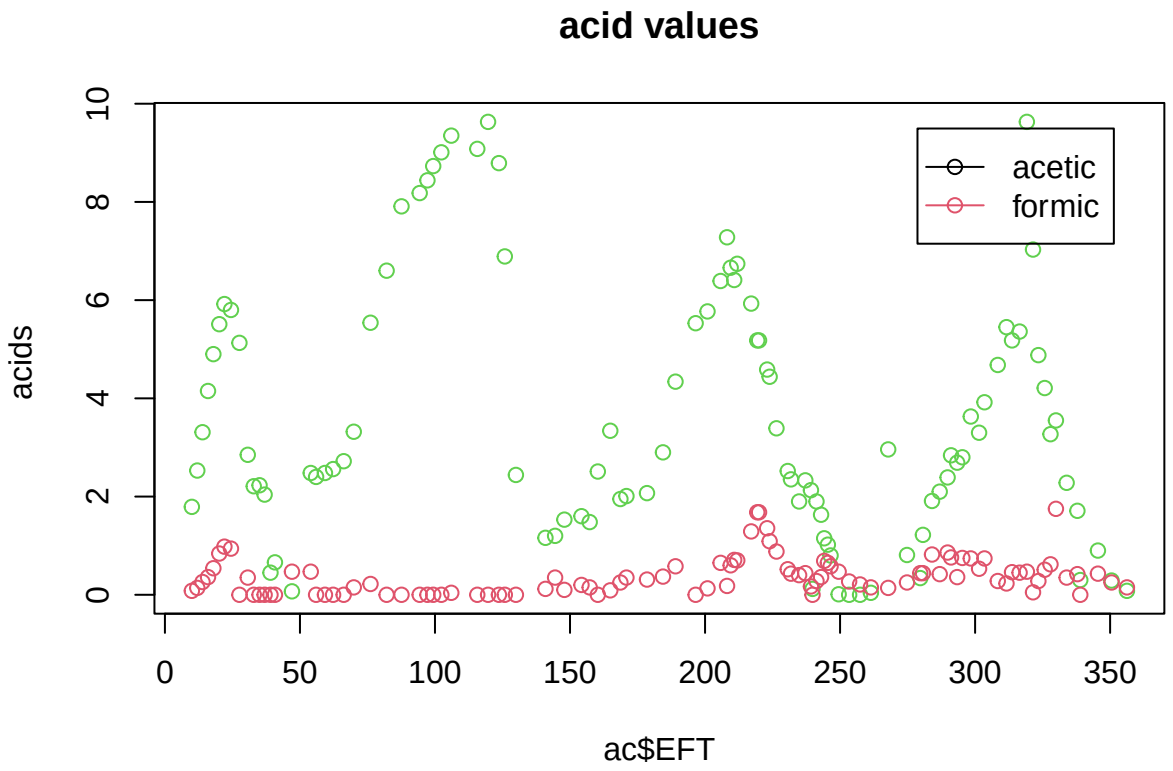
```r
summary(  lm(ac$formic~ac$acetic ) )
```

```
##
## Call:
## lm(formula = ac$formic ~ ac$acetic)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.39749 -0.34319 -0.07676  0.15497  1.37297
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 0.365081   0.065376   5.584 1.95e-07 ***
## ac$acetic   0.003366   0.014833   0.227    0.821
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.3869 on 102 degrees of freedom
## Multiple R-squared:  0.0005045,  Adjusted R-squared:  -0.009294
## F-statistic: 0.05149 on 1 and 102 DF,  p-value: 0.8209
```

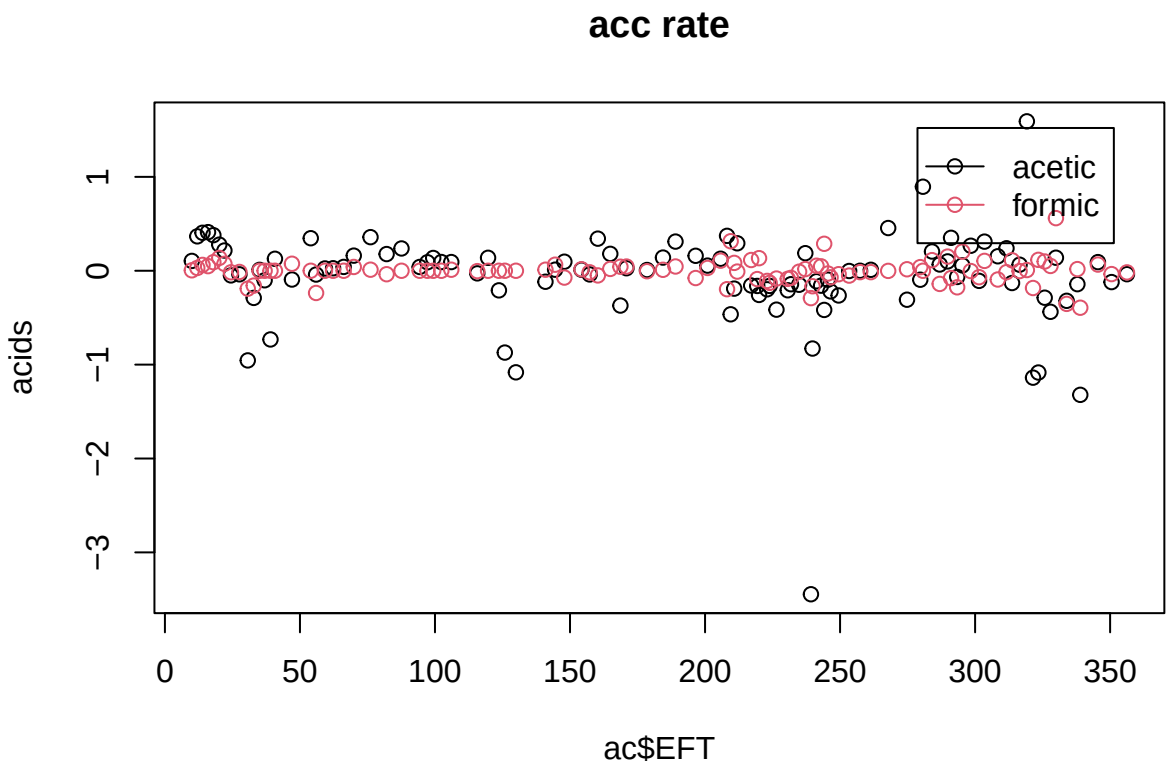
```r
plot( ac$formic , ac$acetic , col = 3 , main = 'formic VS acetic, seems to be independent')
```



```
plot( ac$EFT , ac$acetic, main = 'acid values' , col = 3 , ylab = 'acids '  )
points( ac$EFT , ac$formic , col = 2 )
legend("topright", inset=.05, c('acetic','formic'),lty=c(1, 1), pch=c(1, 1), col=c(1, 2))
```




```
plot( ac$EFT , ac$Acc.rate.acetic, col = 1 , ylab = 'acids' , main = 'acc rate')
points( ac$EFT , ac$Acc.rate.formic , col = 2 )
legend("topright", inset=.05, c('acetic','formic'),lty=c(1, 1), pch=c(1, 1), col=c(1, 2))
```



Regresssion on accumulate rate since the model for values of acetic acid may be overfitting. Inspired by methods in finance(stocks analysis), normally it's easier to predict the values than rate. However, the rate contains more information. ### Following results show that the stepwise selection of regression can't predict the trend(of accumulation rate) well. Initially, this was meant to detect mediation effect if the correlation is significant. But it's not. So we can just ignore this step. (Notice that, the formic accid is excluded in the final model, which means that: no relationship is detected)

```
summary(slr)
```

```
##
## Call:
## lm(formula = interpolated__acc_acetic ~ EFT..Hours + total.air.flow +
##     vent.flow + Station.5.Loop.Temperature + pH.at.stn3 + pH.at.stn1 +
##     O2.in.offgas.. + dissolved.oxygen.at.stn1 + dissolved.oxygen.at.stn2 +
##     dissolved.oxygen.at.stn3 + dissolved.oxygen.at.stn4 + dissolved.oxygen.at.stn5 +
##     methane.flow.stn1 + methane.flow.stn3 + methane.flow.stn5 +
##     oxygen.flow.stn1 + oxygen.flow.stn2 + oxygen.flow.stn3 +
##     oxygen.flow.stn4 + NH3.online.reading + ammonia.pump.flow.1 +
##     ammonia.pump.flow.2 + Cooling.Loop.A.Broth.Return.to.Fermenter.mixer +
##     Cooling.Loop.B.Broth.Return.to.Fermenter.mixer.J1117 + Tempered.Water.Temperature.after.Temped.wa
##     Cooling.loop.A.valve.opening.. + Cooling.loop.B.valve.opening.. +
##     pump.outlet + pump.inlet + pressure.at.position.4 + Pressure.at.the.end.of.the.loop +
##     oxygen..pressure.to.fermentor.loop.mixture + partial.pressure..DP. +
##     trace.elements.flow + ferrus.sulphate.flow + calcium.chloride.flow +
##     magnesium.potassium.flow + phosphoric.acid.totaliser + trace.elements.totaliser +
##     ferrous.sulphate.totaliser + magnesium.potassium.totalier +
```

```
##     spare.dosing.pump.totaliser + ammonia.totalier + Methane.totalier +
##     oxygen.totaliser + Fermentor.fliud.to.ammonia...OD.meter.L.h,
##     data = data1)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -3.9273 -0.2270  0.0221  0.2678  5.6920
##
## Coefficients:
##                                                    Estimate Std. Error
## (Intercept)                                      103.533420  14.579875
## EFT..Hours                                         0.070527   0.005888
## total.air.flow                                     0.009709   0.001212
## vent.flow                                          0.015494   0.001128
## Station.5.Loop.Temperature                        -0.575070   0.132558
## pH.at.stn3                                         2.387778   0.635015
## pH.at.stn1                                         2.820844   0.593158
## O2.in.offgas..                                    -0.325135   0.185652
## dissolved.oxygen.at.stn1                          -0.123678   0.045232
## dissolved.oxygen.at.stn2                           0.213885   0.033690
## dissolved.oxygen.at.stn3                          -0.029462   0.014988
## dissolved.oxygen.at.stn4                          -0.032908   0.012522
## dissolved.oxygen.at.stn5                           0.014169   0.006035
## methane.flow.stn1                                  0.840237   0.165658
## methane.flow.stn3                                  0.999000   0.135501
## methane.flow.stn5                                 -0.346483   0.139564
## oxygen.flow.stn1                                  -0.810310   0.136480
## oxygen.flow.stn2                                  -0.374861   0.096352
## oxygen.flow.stn3                                  -0.869762   0.158058
## oxygen.flow.stn4                                  -0.321002   0.094638
## NH3.online.reading                                 0.004569   0.002063
## ammonia.pump.flow.1                                1.431489   0.363589
## ammonia.pump.flow.2                                0.737853   0.390003
## Cooling.Loop.A.Broth.Return.to.Fermenter.mixer     0.456802   0.184537
## Cooling.Loop.B.Broth.Return.to.Fermenter.mixer.J1117 -0.345375   0.186386
## Tempered.Water.Temperature.after.Temped.water.cooler -0.005502   0.002550
## Cooling.loop.A.valve.opening..                    -0.005277   0.002838
## Cooling.loop.B.valve.opening..                     0.004829   0.001660
## pump.outlet                                       -3.226273   0.746656
## pump.inlet                                        -0.788399   0.281599
## pressure.at.position.4                           -40.841864   4.573506
## Pressure.at.the.end.of.the.loop                   -0.708086   0.357850
## oxygen..pressure.to.fermentor.loop.mixture        -0.723675   0.476787
## partial.pressure..DP.                             -1.357064   0.577670
## trace.elements.flow                               -3.354935   0.217738
## ferrus.sulphate.flow                               2.735348   0.167410
## calcium.chloride.flow                             -1.088488   0.200069
## magnesium.potassium.flow                          -0.141235   0.078745
## phosphoric.acid.totaliser                         -0.053855   0.018944
## trace.elements.totaliser                           0.043710   0.014296
## ferrous.sulphate.totaliser                         0.073381   0.012006
## magnesium.potassium.totalier                       0.033833   0.005928
## spare.dosing.pump.totaliser                       -0.103463   0.005632
## ammonia.totalier                                  -1.207151   0.364652
```

```
## Methane.totalier                                          -0.206652   0.073352
## oxygen.totaliser                                           0.357663   0.099016
## Fermentor.fliud.to.ammonia...OD.meter.L.h                  0.010610   0.001816
##                                                          t value Pr(>|t|)
## (Intercept)                                                7.101 1.68e-12 ***
## EFT..Hours                                                11.979  < 2e-16 ***
## total.air.flow                                             8.013 1.84e-15 ***
## vent.flow                                                 13.731  < 2e-16 ***
## Station.5.Loop.Temperature                                -4.338 1.50e-05 ***
## pH.at.stn3                                                 3.760 0.000174 ***
## pH.at.stn1                                                 4.756 2.11e-06 ***
## O2.in.offgas..                                            -1.751 0.080036 .
## dissolved.oxygen.at.stn1                                  -2.734 0.006304 **
## dissolved.oxygen.at.stn2                                   6.349 2.65e-10 ***
## dissolved.oxygen.at.stn3                                  -1.966 0.049456 *
## dissolved.oxygen.at.stn4                                  -2.628 0.008650 **
## dissolved.oxygen.at.stn5                                   2.348 0.018975 *
## methane.flow.stn1                                          5.072 4.28e-07 ***
## methane.flow.stn3                                          7.373 2.39e-13 ***
## methane.flow.stn5                                         -2.483 0.013120 *
## oxygen.flow.stn1                                          -5.937 3.38e-09 ***
## oxygen.flow.stn2                                          -3.891 0.000103 ***
## oxygen.flow.stn3                                          -5.503 4.19e-08 ***
## oxygen.flow.stn4                                          -3.392 0.000707 ***
## NH3.online.reading                                         2.214 0.026918 *
## ammonia.pump.flow.1                                        3.937 8.51e-05 ***
## ammonia.pump.flow.2                                        1.892 0.058639 .
## Cooling.Loop.A.Broth.Return.to.Fermenter.mixer             2.475 0.013387 *
## Cooling.Loop.B.Broth.Return.to.Fermenter.mixer.J1117      -1.853 0.064020 .
## Tempered.Water.Temperature.after.Temped.water.cooler      -2.157 0.031083 *
## Cooling.loop.A.valve.opening..                            -1.859 0.063111 .
## Cooling.loop.B.valve.opening..                             2.908 0.003672 **
## pump.outlet                                               -4.321 1.63e-05 ***
## pump.inlet                                                -2.800 0.005161 **
## pressure.at.position.4                                    -8.930  < 2e-16 ***
## Pressure.at.the.end.of.the.loop                           -1.979 0.047977 *
## oxygen..pressure.to.fermentor.loop.mixture                -1.518 0.129211
## partial.pressure..DP.                                     -2.349 0.018905 *
## trace.elements.flow                                      -15.408  < 2e-16 ***
## ferrus.sulphate.flow                                      16.339  < 2e-16 ***
## calcium.chloride.flow                                     -5.441 5.93e-08 ***
## magnesium.potassium.flow                                  -1.794 0.073023 .
## phosphoric.acid.totaliser                                 -2.843 0.004514 **
## trace.elements.totaliser                                   3.058 0.002259 **
## ferrous.sulphate.totaliser                                 6.112 1.17e-09 ***
## magnesium.potassium.totalier                               5.708 1.31e-08 ***
## spare.dosing.pump.totaliser                              -18.371  < 2e-16 ***
## ammonia.totalier                                          -3.310 0.000947 ***
## Methane.totalier                                          -2.817 0.004889 **
## oxygen.totaliser                                           3.612 0.000311 ***
## Fermentor.fliud.to.ammonia...OD.meter.L.h                  5.842 5.96e-09 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
```

```
## Residual standard error: 0.5364 on 2112 degrees of freedom
## Multiple R-squared:  0.6986, Adjusted R-squared:  0.6921
## F-statistic: 106.4 on 46 and 2112 DF,  p-value: < 2.2e-16
```