Carbon Balance

This notebook contains calculations to estimate carbon balances on the reactors

Import data from web page

Read the Exp1.dat file. Drop the first two records that correspond to TecPlot header

```
In[20]:= exp1Dat = Import["http://dryas.mbl.edu/A2M/Exp1/data/Exp1.dat"][[3 ;;]]

Out[20]= {{5, 21, 2015, 19, 52, 51, 20.9, 0.02, 0.23, 0.05, 0, 0.0144, 0.1542,
  0.81972, 1, 3, 4.2, 227, 20, 20.75, 0.03, -0.0036, 7.389, 280.84,
  0.82831, 2, 15.5, 7, 229.4, 19.9, 18.21, 0.014, 0.0964, 7.325, 272.46, 0},
  ··· 1740 ···, {10., 18., 2015., 9., 58., 4., 20.48, 2.08, -0.54, 0.027,
  0.061, 0.0136, 0.1276, 150.406, ··· 8 ···, 7.024, 320.86, 150.415,
  2., 17.9, 4.6, 231.1, 29.9, 0.56, 0.263, 0.3388, 7.359, 5.04, 0}}

 large output | show less | show more | show all | set size limit...
```

The dimension of the data array is:

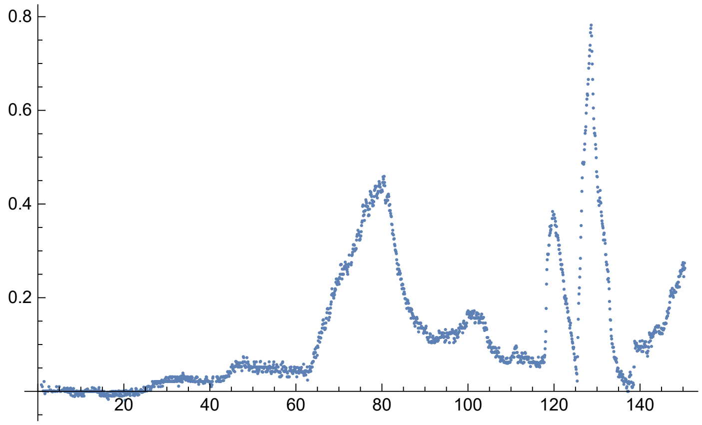
```
In[21]:= Dimensions[exp1Dat]

Out[21]= {1742, 36}
```

Digestor Carbon Balance

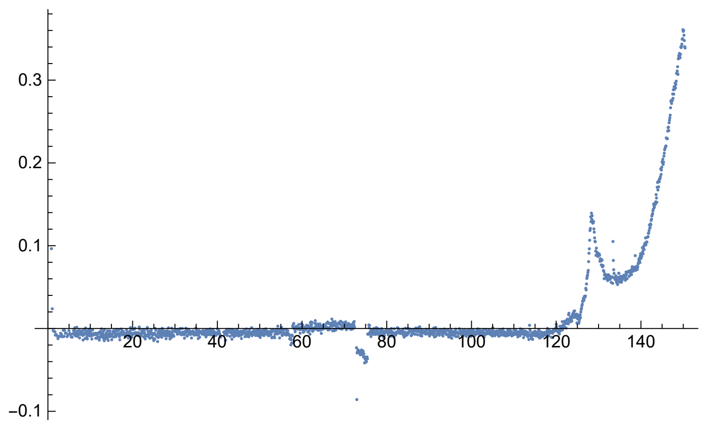
Some crude estimates of carbon export from the digestor are calculated in this section. Note, these simple calculations do not account for C exchange between the reactors when the exchange pump is on. There is a very large carbon import from the algal reactor via carbonate chemistry that needs to be accounted for.

Below are plots of CO_2, CH_4 (in %) and gas flow rate (mL/min) to digestor since this notebook was last executed.

In[22]:=
```
ListPlot[exp1Dat[[All, {25, 32}]], PlotRange → All]
```

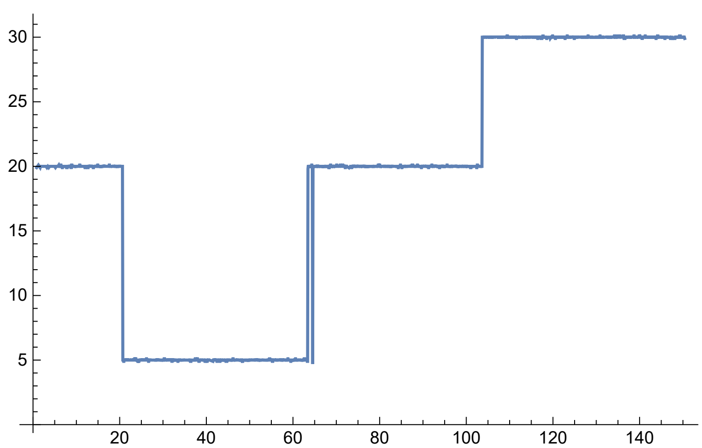
Out[22]=


In[23]:=
```
ListPlot[exp1Dat[[All, {25, 33}]], PlotRange → All]
```

Out[23]=


Gas flow rate to digestorn (in mL/min) is given here:

In[24]:=
```
ListLinePlot[exp1Dat[[All, {25, 30}]]]
```

Out[24]=


Fit interpolating polynomials to CO_2 and CH_4 data.

In[25]:=
```
co2Digestor = Interpolation[exp1Dat⟦2 ;;⟧⟦All, {25, 32}⟧]
```

Out[25]= InterpolatingFunction[Domain: {{1.04, 150.}} Output: scalar]

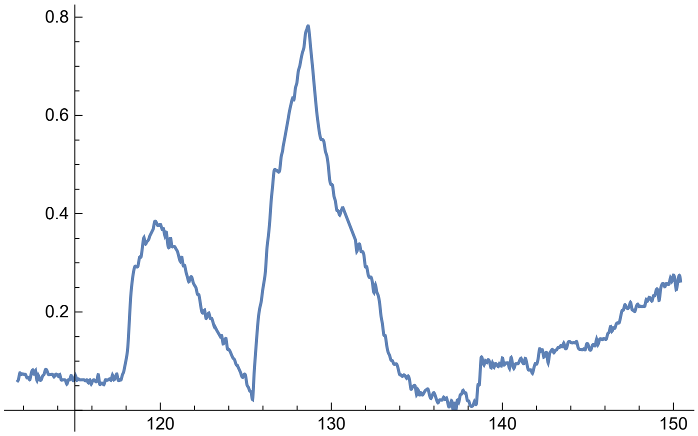
In[26]:=
```
ch4Digestor = Interpolation[exp1Dat⟦2 ;;⟧⟦All, {25, 33}⟧]
```

Out[26]= InterpolatingFunction[Domain: {{1.04, 150.}} Output: scalar]

CO_2 leaving the reactor:

In[27]:=
```
Plot[co2Digestor[t], {t, 111.67, Last[exp1Dat]⟦25⟧}]
```

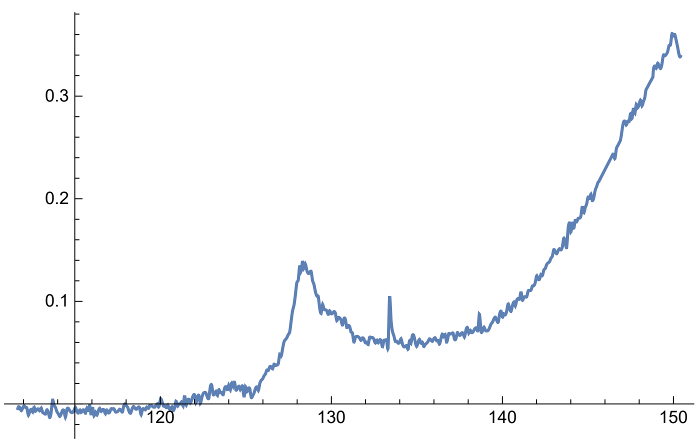
Out[27]=



Methane leaving digestor:

In[28]:=
```
Plot[ch4Digestor[t], {t, 111.67, Last[exp1Dat]⟦25⟧}]
```

Out[28]=



The number of mmols of CO_2 or CH_4 produced right after the addition of acetate and glucose is calculated from the ideal gas law (n = PV/RT) where volume is given by the flow rate (flow rate was 30 mL/min or 43.2 L/d) and the partial pressure of CO_2 or CH_4 is determined by integrating over the time interval of interest. Since flow rate was constant, it can be pulled out of the integral, but if it changes then it needs to be left in.

For CO_2, the total carbon leaving the digestor is given by

In[29]:= $$\frac{1000}{100}\left(\frac{43.2}{298\times 0.082057}\right)\left(\int_{111.67}^{\text{Last[exp1Dat][[25]]}}\text{co2Digestor}[t]\,dt\right)\text{"(mmol } CO_2\text{)"}$$

Out[29]= 133.71 (mmol CO_2)

However, this calculation does not account for the significant amounts of DIC (dissolved inorganic carbon) entering the reactor from the algal reactor via the carbonate system. Consequently, the above value is of not much meaning with regard to glucose or acetate consumed. Instead look at methane output, which is given by,

In[30]:= $$\text{ch4Totalmmol} = \frac{1000}{100}\left(\frac{43.2}{298\times 0.082057}\right)\left(\int_{111.67}^{\text{Last[exp1Dat][[25]]}}\text{ch4Digestor}[t]\,dt\right)\text{"(mmol } CH_4\text{)"}$$

Out[30]= 56.9673 (mmol CH_4)

One mM of glucose was added to the 18 L digestor, which could have produced a maximum (under aerobic conditions) of 108 mmol CO_2, while the 1 mM of acetate would produce 36 mmol, so a total of 144 mmol. But, we need to account for dilution of glucose and Ac by exchange with algal reactor for the short time they were coupled (assume no glucose or Ac are consume in the algal reactor). We also assume no labile carbon existed in the algal reactor during the exchange (a poor assumption). Based on the reactor volumes, the dilution factor would be $\frac{18}{18+4} = 0.818$, so this would mean there could have been 117.8 mmol of C.

Assuming a 50/50 ratio of CH_4 to CO_2 production, then the % consumed glucose and Ac in the digestor is crudely approximated by twice the CH_4 production, or

In[31]:= $$\left\{2\,\frac{\text{ch4Totalmmol[[1]]}}{117.8}\,100\,\text{"\% at time "},\ \text{Last[exp1Dat][[25]]}\right\}$$

Out[31]= {96.7186 % at time , 150.415}

The instantaneous CH_4 production rate (mmol/d) at the last sample point is given by:

In[32]:= $$\frac{\text{ch4Digestor[Last[exp1Dat][[25]]]}}{100}\,1000\left(\frac{60\times 24\,\text{Last[exp1Dat][[30]]}/1000}{298\times 0.082057}\right)\text{"(mmol/d)"}$$

Out[32]= 5.96548 (mmol/d)