Getting started with the biogas package

Charlotte Rennuit and Sasha D. Hafner (sasha.hafner@eng.au.dk)

December 26, 2019

1 Introduction

Anaerobic digestion is a popular technology for production of renewable energy and stabilisation of organic wastes, and research on the topic is carried out in laboratories in many countries. Transformation of raw data collected in laboratory experiments into quantities and rates of methane (CH$_4$) production requires a sequence of simple calculations. Although conceptually simple, these steps are time-consuming, and seldom described in detail in publications, so results may not be reproducible among laboratories or experiments. We developed the biogas package to address these issues. This document provides a brief introduction to the biogas package for new users. We have assumed that readers are familiar with biogas data collection and R.

2 Overview of functions

The package includes seven “low-level” functions (Table 1) and three “high-level” functions (Table 2). To go from data collected in the laboratory to biogas and methane (CH$_4$) production or biochemical methane potential (BMP), two high-level functions are needed: cumBg() and summBg(). Comparing results to theory is facilitated by the remaining high-level function: predBg(). The low-level functions support the calculations carried out by the high-level functions, and may also be useful for some simple operations (e.g., converting reported biogas volumes to different standard conditions). This document describes the use of the high-level functions.

3 An example: calculation and prediction of biochemical methane potential

Calculation of biochemical methane potential (BMP) typically requires three data frames: initial mass, biogas quantity (volume, pressure, or bottle mass loss), and biogas composition. Input data may be structured in one of three ways: “long”, “wide”, or “combined”. In a “long” format (data.struct = ’long’, the default), the measured variable (e.g., biogas volume) is in a single
Table 1: Operations done with the low-level functions in the biogas package. All functions are vectorized. See help files for more details.

<table>
<thead>
<tr>
<th>Operation</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standardise gas volume</td>
<td>stdVol()</td>
</tr>
<tr>
<td>Interpolate composition etc.</td>
<td>interp()</td>
</tr>
<tr>
<td>Calculate oxygen demand of a compound</td>
<td>calcCOD()</td>
</tr>
<tr>
<td>Calculate molar mass of a compound</td>
<td>molMass()</td>
</tr>
<tr>
<td>Calculate biogas volume from mass loss</td>
<td>mass2vol()</td>
</tr>
<tr>
<td>Calculate mass loss from biogas volume</td>
<td>vol2mass()</td>
</tr>
<tr>
<td>Convert gas volume to moles</td>
<td>vol2mol()</td>
</tr>
</tbody>
</table>

Table 2: Operations done with the high-level functions in the biogas package. The cumBg() and summBg() functions can handle data from any number of bottles. predBg() is vectorized.

<table>
<thead>
<tr>
<th>Operation</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>Calculate cumulative CH$_4$ production and rates from volume (mass), composition</td>
<td>cumBg()</td>
</tr>
<tr>
<td>Calculate biochemical methane potential, summarise cumulative production or rates</td>
<td>summBg()</td>
</tr>
<tr>
<td>Predict biogas production based on substrate composition</td>
<td>predBg()</td>
</tr>
</tbody>
</table>

column (Fig. 1). In this case columns with unique bottle IDs and time allow the biogas functions to link observations in the two data frames$^1$. Any order of observations can be used in input data frames.

<table>
<thead>
<tr>
<th>Reactor ID</th>
<th>Time</th>
<th>Response variable (volume or mass)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>1</td>
<td>$y_{1,1}$</td>
</tr>
<tr>
<td>R2</td>
<td>1</td>
<td>$y_{2,1}$</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>$R_n$</td>
<td>1</td>
<td>$y_{i,1}$</td>
</tr>
<tr>
<td>R1</td>
<td>2</td>
<td>$y_{1,2}$</td>
</tr>
<tr>
<td>R2</td>
<td>2</td>
<td>$y_{2,2}$</td>
</tr>
<tr>
<td>$R_n$</td>
<td>2</td>
<td>$y_{i,2}$</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>$R_n$</td>
<td>$t_k$</td>
<td>$y_{n,k}$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Reactor ID</th>
<th>Time</th>
<th>Response variable (Composition)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>2</td>
<td>$y_{1,2}$</td>
</tr>
<tr>
<td>R2</td>
<td>2</td>
<td>$y_{2,2}$</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>$R_n$</td>
<td>2</td>
<td>$y_{n,2}$</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>$R_n$</td>
<td>$t_k$</td>
<td>$y_{n,k}$</td>
</tr>
</tbody>
</table>

Figure 1: General structure of time-dependent data frames for the dat (left) and comp (right) arguments to the cumBg() function.

$^1$ But observations need not be for the same times. Interpolation by interp takes care of this. Note that the time columns can be date/time objects as well as numeric or integer.
The third data frame on initial conditions is used by the `summBg()` function. It should contain at least a bottle ID column and a description of the bottle contents. If the contribution of an inoculum is to be subtrated (as in the BMP test), the mass of inoculum added should be included here. Any measurements to be used to normalise biogas or CH\(_4\) production are included here, using a “wide” format (Fig. 2). Note that there is no time column in this data frame—these values are independent of time.

With the “wide” data structure (`data.struct = 'wide'`) the biogas quantity data frame contains a separate column for each bottle. And in the “combined” option (`data.struct = 'longcombo'`) a single data frame contains both biogas quantity and composition in a “long” structure.

<table>
<thead>
<tr>
<th>Reactor ID</th>
<th>Description</th>
<th>Substrate VS mass</th>
<th>Inoculum total mass</th>
<th>...</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>Substrate A</td>
<td>10.2</td>
<td>302</td>
<td>...</td>
</tr>
<tr>
<td>R2</td>
<td>Substrate A</td>
<td>9.85</td>
<td>301</td>
<td>...</td>
</tr>
<tr>
<td>R3</td>
<td>Substrate A</td>
<td>10.3</td>
<td>298</td>
<td>...</td>
</tr>
<tr>
<td>R4</td>
<td>Substrate B</td>
<td>8.5</td>
<td>300</td>
<td>...</td>
</tr>
<tr>
<td>R6</td>
<td>Inoculum only</td>
<td></td>
<td>502</td>
<td>...</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>R_n</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

Figure 2: General structure of initial conditions data frame for the `setup` argument to the `summBg()` function.
In this example, we will use the example data sets included with the package: `vol` for biogas volumes, `comp` for composition, and `setup` for grouping and substrate and inoculum masses. These data are from a BMP test that was carried out on two different substrates A and B, and cellulose (included as a “control”). The experiment included 12 batch bottles:

- 3 bottles with substrate A and inoculum
- 3 bottles with substrate B and inoculum
- 3 bottles with cellulose and inoculum
- 3 bottles with inoculum only

Reactors consisted of 500 mL or 1.0 L glass bottles, and were sealed with a butyl rubber septum and a screw cap. Initial substrate and inoculum masses were determined. A typical volumetric method was used to measure biogas production: accumulated biogas was measured and removed intermittently using syringes, and composition was measured for some of these samples.

```r
library(biogas)
data("vol")
dim(vol)
## [1] 288 4
head(vol)
## id date.time days vol
## 1 2_1 2014-06-07 07:00:00 1.98 393
## 2 2_1 2014-06-08 07:00:00 2.98 260
## 3 2_1 2014-06-09 07:00:00 3.98 245
## 4 2_1 2014-06-10 07:00:00 4.98 225
## 5 2_1 2014-06-11 07:00:00 5.98 200
## 6 2_1 2014-06-12 08:00:00 7.02 175
summary(vol)
## id date.time days
## 2_1 : 24 Min. :2014-06-07 07:00:00 Min. : 1.98
## 2_2 : 24 1st Qu.:2014-06-13 20:00:00 1st Qu.: 8.52
## 2_3 : 24 Median :2014-06-28 06:00:00 Median : 22.94
## 2_5 : 24 3rd Qu.:2014-07-25 22:45:00 3rd Qu.: 50.63
## 2_6 : 24 Max. :2014-12-19 04:30:00 Max. :196.92
## (Other):144
```
## vol

Min. : 98.0  
1st Qu.: 171.5  
Median : 225.0  
Mean : 271.7  
3rd Qu.: 300.0  
Max.: 840.0  

---

```r
data("comp")
dim(comp)
## [1] 132  4
head(comp)
## id date.time days xCH4
## 516 2_1 2014-06-12 08:00:00 7.02 0.7104731
## 519 2_1 2014-06-19 08:00:00 14.02 0.7024937
## 522 2_1 2014-06-26 05:00:00 20.90 0.6659919
## 524 2_1 2014-07-03 04:00:00 27.85 0.6789466
## 525 2_1 2014-07-10 03:00:00 34.81 0.6951429
## 528 2_1 2014-07-24 04:00:00 48.85 0.6693053
```

```r
summary(comp)
## id date.time days
## 2_1 :11 Min. :2014-06-12 08:00:00 Min. : 7.02
## 2_2 :11 1st Qu.:2014-06-26 05:00:00 1st Qu.: 20.90
## 2_3 :11 Median :2014-07-24 04:00:00 Median : 48.85
## 2_4 :11 Mean :2014-07-31 07:47:43 Mean : 56.01
## 2_5 :11 3rd Qu.:2014-08-28 04:00:00 3rd Qu.: 83.85
## 2_6 :11 Max. :2014-10-13 07:00:00 Max. :129.98
## (Other):66

## xCH4
## Min. : 0.5647
## 1st Qu.: 0.6393
## Median : 0.6598
## Mean : 0.6587
## 3rd Qu.: 0.6786
## Max. : 0.7115
```
3.1 Cumulative production

The first step in processing these data is to calculate cumulative production of biogas and CH$_4$ and production rates. We can do this with the `cumBg()` function, using `vol` and `comp` data frames as input. The arguments for the function are:

```r
args(cumBg)

## function (dat, dat.type = "vol", comp = NULL, temp = NULL, pres = NULL,
##         interval = TRUE, data.struct = "long", id.name = "id", time.name = "time",
##         dat.name = dat.type, comp.name = "xCH4", pres.resid = NULL,
##         temp.init = NULL, pres.init = NULL, rh.resid = NULL, rh.resid.init = 1,
##         headspace = NULL, vol.hs.name = "vol.hs", headcomp = "N2",
```
Most of the arguments have default values, but to calculate CH$_4$ production we must provide values for at least `dat` (we will use `vol`), `comp` (we will use `comp`), `temp` (biogas temperature), and `pres` (biogas pressure)$^2$, along with the names of a few columns in our input data frames. We need to specify the name of the time column in `vol` and `comp` using the `time.name` argument. This name must be the same in both data frames. Similarly, there is an `id.name` argument for the bottle ID column (used to match up volume and composition data), but we can use the default value ("id") here because it matches the column name in `vol` and `comp`. And, the `comp.name` argument is used to indicate which column within the `comp` data frame contains the CH$_4$ content (as mole fraction in dry biogas, normalised so the sum of mole fractions of CH$_4$ and CO$_2$ sum to unity). We can use the default ("xCH4") because it matches the name in `comp`. Lastly, the name of the column that contains the response variable in the `dat` data frame (`vol` here) can be specified with the `dat.name` argument. Here too we can use the default ("vol" for volumetric measurements or "mass" for gravimetric). By default (cmethod = "removed") the function calculates volumes following [2] as the product of standardised volume of biogas removed and normalised CH$_4$ content.

```r
cum.prod <- cumBg(vol, comp = comp, time.name = "days", temp = 35, pres = 1, 
                  extrap = TRUE)
```

Note the message about standard temperature and pressure–it is important to make sure these values are correct, therefore users are reminded by a message$^3$. The output looks like this:

---

$^2$ By default, temperature is in °C and pressure in atm, but these can be changed in the function call with the `temp.unit` and `pres.unit` arguments, or globally with `options`.

$^3$ Remember that standard conditions can be set in the function call with `temp.std` and `pres.std`, or globally with `options()`.
head(cum.prod)
## id date.time days vol xCH4 temperature pressure vBg
## 1 2_1 <NA> 0.00 NA NA NA NA 0.0000
## 2 2_1 2014-06-07 07:00:00 1.98 393 0.7104731 35 1 328.9470
## 3 2_1 2014-06-08 07:00:00 2.98 260 0.7104731 35 1 217.6240
## 4 2_1 2014-06-09 07:00:00 3.98 245 0.7104731 35 1 205.0687
## 5 2_1 2014-06-10 07:00:00 4.98 225 0.7104731 35 1 188.3284
## 6 2_1 2014-06-11 07:00:00 5.98 200 0.7104731 35 1 167.4031

dim(cum.prod)
## [1] 300 13

The data frame that is returned has all the original columns in vol, plus others. In these columns, v stands for (standardised) volume, cv (standardised) cumulative volume, rv stands for (standardised) volume production rate, and Bg and CH4 for biogas and methane. So cvCH4 contains standardised cumulative CH4 production. It is probably easier to understand the data in the output graphically. Here we’ll use the qplot function from the ggplot2 package to plot it.

library(ggplot2)

qplot(x = days, y = cvCH4, data = cum.prod, xlab = "Time (d)", ylab = "Cumulative methane production (mL)", geom = "line")
3.2 Other data structures

As of biogas version 1.5.0, the "long" data structures described above is not the only option. In addition, "wide" and combined "long" structures are possible. We can compare the three possible approaches using the same dataset.

Let’s load data on biogas production from three bottles with wastewater sludge.

```r
data("s3voll")
data("s3compl")
data("s3volw")
data("s3compw")
data("s3lcombo")
```

The "long" structure described above looks like this:

```r
s3voll
## id time.d vol.ml cvol.ml
## 1 D 0.9438 103 103
## 2 E 0.9451 106 106
## 3 F 0.9472 107 107
## 4 D 2.9060 192 295
## 5 E 2.9090 181 287
## 6 F 2.9100 203 310
## 7 D 5.8860 141 436
```
### s3compl

<table>
<thead>
<tr>
<th>id</th>
<th>time.d</th>
<th>xCH4</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.906</td>
<td>0.6983</td>
</tr>
<tr>
<td>2</td>
<td>2.909</td>
<td>0.6817</td>
</tr>
<tr>
<td>3</td>
<td>2.910</td>
<td>0.6869</td>
</tr>
<tr>
<td>4</td>
<td>10.000</td>
<td>0.6646</td>
</tr>
<tr>
<td>5</td>
<td>10.000</td>
<td>0.6644</td>
</tr>
<tr>
<td>6</td>
<td>10.010</td>
<td>0.6632</td>
</tr>
<tr>
<td>7</td>
<td>23.100</td>
<td>0.6946</td>
</tr>
<tr>
<td>8</td>
<td>23.100</td>
<td>0.6871</td>
</tr>
<tr>
<td>9</td>
<td>23.100</td>
<td>0.6829</td>
</tr>
<tr>
<td>10</td>
<td>34.010</td>
<td>0.6626</td>
</tr>
<tr>
<td>11</td>
<td>34.010</td>
<td>0.6556</td>
</tr>
<tr>
<td>12</td>
<td>34.010</td>
<td>0.6527</td>
</tr>
<tr>
<td>13</td>
<td>57.840</td>
<td>0.6651</td>
</tr>
<tr>
<td>14</td>
<td>57.840</td>
<td>0.6600</td>
</tr>
</tbody>
</table>

The "wide" format contains (mostly) the same data, but there are separate columns for each bottle.

### s3volw

<table>
<thead>
<tr>
<th>time.d</th>
<th>D</th>
<th>E</th>
<th>F</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.9438</td>
<td>103</td>
<td>106</td>
<td>107</td>
</tr>
<tr>
<td>2.9060</td>
<td>192</td>
<td>181</td>
<td>203</td>
</tr>
<tr>
<td>34.0100</td>
<td>109</td>
<td>110</td>
<td>112</td>
</tr>
<tr>
<td>5.8860</td>
<td>141</td>
<td>133</td>
<td>140</td>
</tr>
<tr>
<td>10.0000</td>
<td>112</td>
<td>111</td>
<td>110</td>
</tr>
<tr>
<td>23.1000</td>
<td>200</td>
<td>190</td>
<td>200</td>
</tr>
<tr>
<td>57.8400</td>
<td>146</td>
<td>136</td>
<td>138</td>
</tr>
</tbody>
</table>
Note the missing composition value in `s3compw`. With the "long" structure, a row was simply omitted. Both approaches will result in the same output though. With the "wide" approach all bottles must be measured at the same times.

Finally, in the combined approach both volume and composition are in the same "long" data frame.

```r
cpl <- cumBg(s3lcombo, comp = s3compl, temp = 25, pres = 1, id.name = 'id', time.name = 'time.d',
```

dat.name = 'vol.ml', comp.name = 'xCH4',
extrap = TRUE)

## Biogas composition is interpolated.
## Working with volume data, applying volumetric method.
## Using a standard pressure of 1 atm and standard temperature of 0
## C for standardizing volume.

cpw <- cumBg(s3volw, comp = s3compw, temp = 25, pres = 1,
time.name = 'time.d',
data.struct = 'wide',
dat.name = 'D', comp.name = 'D',
extrap = TRUE)

## Biogas composition is interpolated.
## Working with volume data, applying volumetric method.
## Using a standard pressure of 1 atm and standard temperature of 0
## C for standardizing volume.

cpc <- cumBg(s3lcombo, temp = 25, pres = 1,
id.name = 'id', time.name = 'time.d',
data.struct = 'longcombo',
dat.name = 'vol.ml', comp.name = 'xCH4',
extrap = TRUE)

## Biogas composition is interpolated.
## Working with volume data, applying volumetric method.
## Using a standard pressure of 1 atm and standard temperature of 0
## C for standardizing volume.

Output is nearly identical here. The small differences result from the use of
unique times for each bottle in the long formats.

head(cpl)

## id  time.d vol.ml  xCH4  temperature  pressure  vBg  vCH4
## 1    D    0.0000     NA      NA       NA      NA     0.00000     0.00000
## 2    D    0.9438    103.6983000  25       1  91.40334  63.82696
## 3    D    2.9060    192.6983000  25       1  170.38293 118.97840
## 4    D    5.8860    141.6841435  25       1  125.12497  85.60344
## 5    D  10.0000    112.6646000  25       1  99.39004  66.05462
## 6    D   23.1000    200.6946000  25       1 177.48222 123.27915
## cvBg  cvCH4  rvBg  rvCH4
## 1    0.00000     0.00000  NA      NA
## 2  91.40334  63.82696  96.84609  67.627628
## 3 261.78628 182.80536  86.83260  60.635206
## 4 386.91124 268.40879  41.98824  28.725985

12
3.3 Calculating BMP from cumulative production

To calculate BMP we need to subtract the contribution of the inoculum to CH₄ production for each bottle, normalise by substrate volatile solids (VS), and calculate means and standard deviations. This is done by the `summBg()` function using the results from `cumBg()`, along with the `setup` data frame. The arguments for `summBg()` are:
This is a flexible function, and is useful for more than just calculating BMP. For example, to simply determine the mean cumulative CH$_4$ production for each substrate at 30 d, we could use:

```
summBg(cum.prod, setup = setup, time.name = "days", descrip.name = "descrip", when = 30)
```

Response variable (volume) is `cum.prod$cvCH4`. Inoculum contribution not subtracted. No normalization by substrate mass.

<table>
<thead>
<tr>
<th>descrip</th>
<th>days</th>
<th>mean</th>
<th>se</th>
<th>sd</th>
<th>n</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>30</td>
<td>1608.362</td>
<td>22.06860</td>
<td>38.22393</td>
<td>3</td>
</tr>
<tr>
<td>B</td>
<td>30</td>
<td>2078.248</td>
<td>26.48733</td>
<td>45.87740</td>
<td>3</td>
</tr>
<tr>
<td>cellu</td>
<td>30</td>
<td>3686.127</td>
<td>33.35392</td>
<td>57.77069</td>
<td>3</td>
</tr>
<tr>
<td>inoc</td>
<td>30</td>
<td>1575.326</td>
<td>19.18801</td>
<td>33.23460</td>
<td>3</td>
</tr>
</tbody>
</table>

Here, the response variable was `cvCH4` (cumulative CH$_4$ production, the default—but `vol.name` could be used to specify any column). The argument `descrip.name` is the name of the column in `setup` that gives a description of the bottle. Here it is used for grouping bottles. We could have used the default value in this call.

To calculate BMP, we need to provide information on where inoculum and substrate VS masses can be found. To subtract the inoculum contribution, we need to provide a value for the `inoc.name` argument, which should be the value in the `setup$descrip.name` column that indicates that the bottle contained inoculum only. In our `setup` data frame, the value is "inoc". Inoculum mass is given in the `minoc` column, and we need to provide this information using the `inoc.m.name` argument (although here also, we could use the default value).

The last step is normalisation of cumulative CH$_4$ production, based on substrate VS mass. This mass must be stored in the `setup` data frame and the name of column is given using the `norm.name` argument. Here, it is "mvs.sub". We will evaluate CH$_4$ production at at time selection by the function when relative methane production drops below 1% of cumulative (after subtracting inoculum production) per day for at least 3 days (`when` argument).
BMP <- `summBg`(cum.prod, setup = setup, time.name = "days", inoc.name = "inoc", 
inoc.m.name = "minoc", norm.name = "mvs.sub", when = "1p3d")

## Response variable (volume) is cum.prod$cvCH4.
## Inoculum contribution subtracted based on setup$minoc.
## Response normalized by setup$mvs.sub.

BMP

Note the messages–because any response variable could be used and subtraction of an inoculum contribution and normalisation are optional, it is important to check these messages and be sure that `summBg()` did what you think it did. Additionally, it is good practice to view and save results from individual bottles, and check the apparent contribution of the inoculum to each bottle’s biogas production. This additional information can be returned by setting `show.obs` = TRUE.

### 3.4 Predicting methane production

The function `predBg()` provides a flexible approach for predicting methane potential, and in our example can be used to quickly check our experimental values. Predictions can be based on an empirical chemical formula, chemical oxygen demand (COD), or macromolecule composition.

Our BMP test included cellulose as a control. Using its chemical formula (C\(_{6}\)H\(_{10}\)O\(_{5}\)), we can calculate theoretical methane potential to compare to our measurements\(^4\).

`predBg("C6H10O5")`

## [1] 413.7274

So we see that theoretical methane potential of cellulose is 414 mL g\(^{-1}\). Comparing expected cellulose BMP to measurements is an important way to check BMP experiments. How does this compare to our measurements?

BMP

\(^4\) In this case, the calculation is based on Eq. (13.5) in Rittmann and McCarty [3]. When the input is COD, it is based on the COD of CH\(_4\), as described in [3].
The measured value is a bit lower, which is reasonable. It is common to assume that 5 – 10% of substrate is used to produce microbial biomass, and so not converted to biogas. We can incorporate this assumption into our prediction using the fs argument, which is the fraction of substrate electrons used for cell synthesis.

```r
predBg("C6H10O5", fs = 0.1)
## [1] 372.3547
```

Measured and predicted values are close after making this correction.

We don’t have empirical formulas for substrates A and B, but we can predict theoretical potential by using the COD. Initial COD masses are in the setup data frame, and from these we can calculate COD:VS ratios for substrates A and B of 1.439 and 1.561 g g\(^{-1}\). Cellulose has a calculated oxygen demand (COD\(^\prime\))\(^5\) of 1.184 g g\(^{-1}\). Predicted CH\(_4\) production per g VS is therefore:

```r
predBg(COD = c(A = 1.439, B = 1.561, cellu = 1.184))
## [1] 502.7638 545.3887 413.6709
```

Measured BMP was substantially lower for substrates A and B, indicating very low degradability. In fact, we could use `predBg()` to estimate effective degradability (ignoring synthesis of microbial biomass).

```r
BMP$mean/predBg(COD = c(A = 1.439, B = 1.561, cellu = 1.184))
## [1] 0.2976613 0.2365155 0.9012315
```

We see that substrates A and B had low degradability, while degradability of cellulose was high. Both substrates A and B were digestate from digesters, i.e., they had already been anaerobically digested once before these measurements, and so we should expect low degradability.

## 4 Continuing with the biogas package

The three functions demonstrated in this document can be used in other ways not described here. For example, `cumBg()` can be used with measurements of bottle mass over time to determine biogas production[1], `summBg()` can return results for multiple times, and `predBg()` function can predict microbial nitrogen requirements and biogas composition. More details can be found in the help files for these functions, or, for `predBg`, in the `predBg` vignette. The low-level functions are straight-forward to use, and details can also be found in the help files.

\(^5\) Oxygen demand can be calculated with the `calcCOD` function.
To receive updates on the biogas package, you can subscribe to a mailing list by sending an e-mail to either of us. And please send us a message if you find a bug or have a suggestion for improving an existing function or adding a new one.

References

