Predicting methane and biogas production with the biogas package

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Theory for predicting biogas production based on substrate composition and degradability is well-developed. But the calculations are tedious and seldom done. The 'biogas' package includes a single function `predBg()` to make these predictions. This document describes usage of the `predBg()` function through examples. In a final section, the methods behind the calculations are presented.

1 Getting started

To use the 'biogas' package, it must be installed on your computer. Since the package is available on CRAN (The Comprehensive R Archive Network)[1], it can be installed with the following command.

```
install.packages("biogas")
```

To use any installed package, it must be loaded. Use the next command to load the 'biogas' package.

```
library(biogas)
```

2 Methane production from defined substrates

2.1 Cellulose control in BMP test

Cellulose is often included in biochemical methane potential (BMP) experiments as a positive control–a comparison between the measured and expected quantity of CH_4 produced is used to evaluate the accuracy of the measurements. How much CH_4 should we expect from cellulose? To predict this we only need the chemical formula of cellulose.

[1] You can download the package manually and find more information on getting started with the package at https://cran.r-project.org/web/packages/biogas/index.html.

```
  predBg(form = "C6H10O5")

## [1] 413.7274
```

So if it were all converted to CH_4, we should see about 414 mL of CH_4 (dry, at 101.325 kPa and 0°C)[2] per g of cellulose. This quantity is sometimes referred to as the theoretical BMP.

Since `form` is the first argument, we can easily omit the `form =` tag and use positional matching–we'll do this in the remainder of the document.

```
  predBg("C6H10O5")

## [1] 413.7274
```

By default, the result is per 1 g of substrate, but any mass can be used using the `mass` argument[3].

You can see all the arguments and some default values using the `arg()` function.

```
  args(predBg)

## function (form = NULL, mass = 1, mol = NULL, fs = 0, fd = 1,
##     mcomp = NULL, COD = NULL, conc.sub = NULL, pH = NULL, temp = NULL,
##     mu = 0.1, shortform = NULL, value = "CH4")
## NULL
```

The only required argument is `form`, or an alternative called `mcomp`. All these arguments will be described below. In this section, we'll focus on `form` and `mass` only.

Continuing with our example, to predict CH_4 from 5.75 g of cellulose, set `mass = 5.75`.

```
  predBg("C6H10O5", mass = 5.75)

## [1] 2378.933
```

In this case we should expect about 2400 mL of CH_4. For a pure degradable compound like microcrystaline cellulose, it is reasonable to expect that 100% of the added mass is degraded by the microbial community. In other cases (e.g., when the substrate is plant biomass), we should reduce the degradability using the `fd` argument (which has a default of unity). But even for a substrate that is completely consumed by the bacteria and archaea in an anaerobic reactor (like microcrystaline cellulose) not all of the substrate is converted to CH_4. This is

[2] All volumes returned by the function are standardised to dry conditions at 0°C and 101.325 kPa (1.0 atm). They can be converted to different conditions using `stdVol()`.

[3] Alternatively, the moles or total chemical oxygen demand (COD) can be specified with the `mol` and `COD` arguments.

beacuse the microorganisms use some fraction of it to synthesize their own cell biomass. The fraction of substrate that is used for cell synthesis can be set with the `fs` argument (which has a default of zero). In our example, we might expect `fs` between 5% and 25%, so we might find it useful to compare results from the calls below.

```
  predBg("C6H10O5", mass = 5.75, fs = 0)

## [1] 2378.933

  predBg("C6H10O5", mass = 5.75, fs = 0.05)

## [1] 2259.986

  predBg("C6H10O5", mass = 5.75, fs = 0.20)

## [1] 1903.146
```

But the function is vectorized in almost all arguments, so the single call below is a better option.

```
  predBg("C6H10O5", mass = 5.75, fs = c(0, 0.05, 0.2))

## [1] 2378.933 2259.986 1903.146
```

We can conclude that CH_4 production from our 5.75 g of cellulose should be at least 1900 mL.

2.2 Designing a methanogen activity assay

Any chemical formula–for a pure compound, a mixture, or an empirical biomass formula–can be used for the `form` argument. For example, in methanogen activity tests, media typically include acetate, formate, or propionate as substrates. Let's assume we are developing an assay and want to determine how much substrate to use. We can start by comparing theoretical CH_4 production from each substrate on mass and molar bases.

```
  predBg(c("CHOOH", "CH3COOH", "CH3CH2COOH"), mol = 1)

## [1]  5590.147 22360.588 39131.029

  predBg(c("CHOOH", "CH3COOH", "CH3CH2COOH"), mass = 1)

## [1] 121.4563 372.3538 528.2409
```

From these results we can see that CH_4 production increases with the molecular mass of the acid, on both a mass and mole basis[4]. For a particular assay,

[4] This trend is consistent with the relative degree of oxidation: the O content is the same

assume we plan on using 60 mL of medium containing formic acid:acetic acid at 1:1 (mole basis) in a 100 mL serum bottle, and need at least 5 mL of CH_4 for accurate quantification. We can specify predict CH_4 production from such a mixture using the notation for `form` shown below.

```
  predBg("(CHOOH)0.5 (CH3COOH)0.5", mass = 1)
```

```
## [1] 263.4923
```

```
  predBg("(CHOOH)0.5 (CH3COOH)0.5", mol = 1)
```

```
## [1] 13975.37
```

What concentration should we use? We should have total production much higher than our 5 mL limit, since only a fraction of substrate is consumed during an activity assay. If we assume we need a predicted maximum of at least 50 mL, the required substrate quantity using the following call.

```
  50/predBg("(CHOOH)0.5 (CH3COOH)0.5", mol = 1)
```

```
## [1] 0.003577723
```

Based on this result, we could plan on 3.6 mmol of our combined substrate. Let's double-check to make sure it would provide a maximum of 50 mL of CH_4.

```
  predBg("(CHOOH)0.5 (CH3COOH)0.5", mol = 0.0036)
```

```
## [1] 50.31132
```

A quantity of 3.6 mmol in a 60 mL solution requires a concentration of exactly 60 mmol L^{-1}, which is therefore the concentration we should select based on our results.

3 Output options

So far all our examples have used the default value of the `value` argument to specify the type of output that is returned: `"CH4"`. If we set the `value` argument to `"all"`, more details are provided. Let's illustrate this with the acetic acid/formic acid example from above.

```
  predBg("(CHOOH)0.5 (CH3COOH)0.5", mol = 0.0036, value = "all")
```

```
##                      form      mass mol.mass  moles   COD      hydro
## 1 (CHOOH)0.5 (CH3COOH)0.5 0.1909404   53.039 0.0036 0.144 -0.0162144
##        fCH4     vCH4      mCH4      mCO2
## 1 0.4166667 50.31132 0.0360945 0.1386315
```

for these three acids is 2 moles per mole acid while the quantity of C and H increases with size.

In the ouput we can see the substrate formula (`form`) and mass (`mass`, g), along with its molar mass (`mol.mass`, g mol^{-1}), and calculated oxygen demand (`COD`, g). The response variable that we are interested in (and the one we worked with above) is the predicted CH_4 volume `vCH4`, in mL. The remaining columns show hydrolytic water consumption (`hydro`, g of H_2O) (in this example, H_2O is produced, not consumed), the molar fraction of CH_4 in the reaction products (CH_4 + CO_2) (`fCH4`), and the masses of of CH_4 and CO_2 produced (`mCH4` and `mCO2`, g).

In contrast to the default output (`value = "CH4"`), which is a vector, here output is a data frame. This difference isn't really apparent unless we get multiple sets of results. To illustrate, let's modify the previous call by adding four `fs` values. This addition will result in multiple rows in the output, as well as some additional columns.

```
  predBg("(CHOOH)0.5 (CH3COOH)0.5", mol = 0.0036, fs = c(0, 0.01, 0.05, 0.1),
         value = "all")

##                      form      mass mol.mass  moles   COD   fs   fe fd
## 1 (CHOOH)0.5 (CH3COOH)0.5 0.1909404   53.039 0.0036 0.144 0.00 1.00  1
## 2 (CHOOH)0.5 (CH3COOH)0.5 0.1909404   53.039 0.0036 0.144 0.01 0.99  1
## 3 (CHOOH)0.5 (CH3COOH)0.5 0.1909404   53.039 0.0036 0.144 0.05 0.95  1
## 4 (CHOOH)0.5 (CH3COOH)0.5 0.1909404   53.039 0.0036 0.144 0.10 0.90  1
##         hydro      fCH4     vCH4       mCH4      mCO2       m.bio
## 1 -0.01621440 0.4166667 50.31132 0.03609450 0.1386315 0.000000000
## 2 -0.01686298 0.4159664 49.80821 0.03573356 0.1376413 0.001018017
## 3 -0.01945728 0.4130435 47.79576 0.03428978 0.1336804 0.005090085
## 4 -0.02270016 0.4090909 45.28019 0.03248505 0.1287292 0.010180170
##         N.req
## 1 0.000000000
## 2 0.000126063
## 3 0.000630315
## 4 0.001260630
```

Since `fs` is given, substrate partitioning parameters `fs` and `fe` (as well as degradability `fd`). Substrate partitioning parameters `fs` and `fe` are the fraction of substrate used for cell synthesis and energy production, and always sum to unity. With these parameters, biomass production (`m.bio`, g) and the reduced N requirement (NH_4^+) for biomass production (`N.req`, g) can be calculate and are returned.

Now we have enough information to answer a second question: how much N is required in our medium? To get the most useful anser, let's switch our call a bit to use concentrations and not total masses. The only needed change is in `mol`, which we will switch from the total substrate quantity to the concentration (60 mmol L^{-1}).

```
  predBg("(CHOOH)0.5 (CH3COOH)0.5", mol = 0.06, fs = c(0, 0.05, 0.08, 0.1, 0.15),
         value = "all")
```

```
##                      form    mass mol.mass moles COD   fs   fe fd
## 1 (CHOOH)0.5 (CH3COOH)0.5 3.18234   53.039  0.06 2.4 0.00 1.00  1
## 2 (CHOOH)0.5 (CH3COOH)0.5 3.18234   53.039  0.06 2.4 0.05 0.95  1
## 3 (CHOOH)0.5 (CH3COOH)0.5 3.18234   53.039  0.06 2.4 0.08 0.92  1
## 4 (CHOOH)0.5 (CH3COOH)0.5 3.18234   53.039  0.06 2.4 0.10 0.90  1
## 5 (CHOOH)0.5 (CH3COOH)0.5 3.18234   53.039  0.06 2.4 0.15 0.85  1
##        hydro      fCH4     vCH4      mCH4     mCO2      m.bio      N.req
## 1 -0.2702400 0.4166667 838.5220 0.6015750 2.310525 0.00000000 0.00000000
## 2 -0.3242880 0.4130435 796.5959 0.5714963 2.228006 0.08483475 0.01050525
## 3 -0.3567168 0.4107143 771.4403 0.5534490 2.178495 0.13573560 0.01680840
## 4 -0.3783360 0.4090909 754.6698 0.5414175 2.145487 0.16966950 0.02101050
## 5 -0.4323840 0.4047619 712.7437 0.5113388 2.062969 0.25450425 0.03151575
```

For methanogens, `fs` should not exceed 0.08[4], but to provide a safety factor, we could use the N need from the case where `fs = 0.15`. So we can conclude that we need at least 31 mg L^{-1} of NH_4^+ in our medium.

4 Unknown composition: using COD

If the composition of a substrate is not known, it is still possible to predict CH_4 production based on a measured chemical oxygen demand (COD). For example, assume we have a waste stream with a COD of 2600 mg L^{-1}. What is the maximum volume of CH_4 that could be produced?

```
  predBg(COD = 2.6)
```

```
## [1] 908.3989
```

We should expect no more than 908 mL CH_4, and probably much less, depending on the degradability of our substrate. For example, perhaps we have data indicating that the organic matter in the waste stream is 60% degradable, and we assume that `fs` is 0.10.

```
  predBg(COD = 2.6, fd = 0.6, fs = 0.1)
```

```
## [1] 490.5354
```

5 Complex substrates

Most real substrates are more complex than a single chemical compound such as cellulose or acetic acid. For example, both animal manure and wastewater sludge

are mixtures of many types of compounds. Composition of biomass substrates are sometimes described based on macromolecular characterization, as in [3] The `mcomp` argument[5] is designed for this approach. The approach is based on default empirical formulas for macromolecular groups, such as carbohydrates and proteins. The `mcomp` argument is given as a named numeric vector, where values are relative or absolute mass-based concentrations within the substrate. For example, for cattle manure sample 2 in [3], we could use reported relative concentrations: carbohydrate, 682 mg g^{-1}; protein 158 mg g^{-1}; lipids, 54 mg g^{-1}; organic acids, 31 mg g^{-1}; and lignin, 75 mg g^{-1} (all g per g organic matter) as shown below.

```
  predBg(mcomp = c(carbohydrate = 0.682, protein = 0.158, lipid = 0.054,
                   VFA = 0.031, lignin = 0.075),
         mass = 1, fd = 0.4, fs = 0.1)

## [1] 173.0555
```

The `predBg()` function uses a single representative composition for each group and the relative masses provided to calculate an overall empirical formula. The empirical formula of the substrate, calculated using the provided macromolecular composition, can be seen by setting `value = "all"`.

```
  predBg(mcomp = c(carbohydrate = 0.682, protein = 0.158, lipid = 0.054,
                   VFA = 0.031, lignin = 0.075),
         mass = 1, fd = 0.4, fs = 0.1, value = "all")

##                       form mass mol.mass       moles      COD  fs  fe  fd
## 1 C29.2624H46.9901O18.9492N    1 716.0016 0.001396645 1.375877 0.1 0.9 0.4
##        hydro      fCH4     vCH4     mCH4      mCO2     m.bio        N.req
## 1 0.07374917 0.5290814 173.0555 0.124154 0.3031636 0.0389074 -0.003007143
```

To see which formulas are used for each macromolecular group, use `shortform = FALSE`. The ouput now shows an alternative expression for the empirical formula.

```
  predBg(mcomp = c(carbohydrate = 0.682, protein = 0.158, lipid = 0.054,
                   VFA = 0.031, lignin = 0.075),
         mass = 1, fd = 0.4, fs = 0.1, shortform = FALSE, value = "all")

##                                                                  form mass
## 1 (C6H10O5)68.97(C5H7O2N)22.9(C57H104O6)1(C2H4O2)8.464(C10H13O3)6.786    1
##   mol.mass        moles      COD  fs  fe  fd      hydro      fCH4     vCH4
## 1 16396.42 6.098894e-05 1.375878 0.1 0.9 0.4 0.07374893 0.5290818 173.0556
##        mCH4      mCO2      m.bio       N.req
## 1 0.1241541 0.3031632 0.03890743 -0.00300715
```

[5] Short for "macromolecular composition" or "mass composition".

This approach is only needed if an empirical formula is not available for a substrate. If the elemental composition of a substrate has been determined, an empirical chemical formula can be calculated, and this formula can be used with `predBg()`. For example, we could take the empirical formula calculated above, $C_{29.2587}H_{46.984}O_{18.9464}N_1$, round it for simplicity to $C_{29.3}H_{47}O_{18.9}N$ and use it as the `form` argument.

```
  predBg("C29.2H47O18.9N", mass = 1, fd = 0.4, fs = 0.1, shortform = FALSE, value = "all")
```

```
##             form mass mol.mass       moles      COD  fs  fe  fd      hydro
## 1 C29.2H47O18.9N    1  714.475 0.001399629 1.377235 0.1 0.9 0.4 0.07352903
##        fCH4     vCH4      mCH4      mCO2     m.bio        N.req
## 1 0.5296651 173.2263 0.1242765 0.3027526 0.0389458 -0.003019109
```

This results are slightly different than the result from above, but only because we rounded our formula.

The `mcomp` argument can also be used for mixtures of pure chemicals. For example, crude glycerol is a waste product from biodiesel production, and is often added to anaerobic digesters. It isn't uncommon for glycerol to make up $> 65\%$ of the waste. We'll mix it with manure here, assuming a glycerol:manure VS ratio of 0.25:1.

```
  predBg(mcomp = c(carbohydrate = 0.682, protein = 0.158, lipid = 0.054,
                   VFA = 0.031, lignin = 0.075,
                   C3H8O3 = 0.25),
         mass = 1, fd = 0.4, fs = 0.1)
```

```
## Warning in predBg(mcomp = c(carbohydrate = 0.682, protein = 0.158,
lipid = 0.054, :  Sum of mcomp != 1.0 so dividing all elements by the
sum for calculation of formula.
```

```
## [1] 169.0375
```

Alternatively, since we now have an approximate empirical formula for this manure, we could use the following approach, which makes it easier to keep track of masses of the components of our mixture.

```
  predBg(mcomp = c(C29.2H47O18.9N = 0.8, C3H8O3 = 0.2), mass = 1, fd = 0.4, fs = 0.1)
```

```
## [1] 169.1733
```

We can see that predicted CH_4 production per g of (mixed) substrate increases substantially when crude glycerol is added. Any chemical formula can be used in this way through the `mcomp` argument. But one limitation at the present is that a single degradability parameter `fd` applies to the complete mixture.

Both `form` and `mcomp` can be used to specify mixed substrates. There are two differences between them: `mcomp` can be used with both macromolecular

groups (e.g., `carbohydrate`) and chemical formulas, and quantities are mass-based, while `form` can only accept chemical formulas, and quantities are mole-based. An example may clarify these differences. Assume we are working with a mixture of waste paper (primarily cellulose) and waste vegetable oil at a 5:1 ratio (dry mass basis). The easiest approach here is to use `mcomp`[6].

```
  predBg(mcomp = c(C6H10O5 = 5, C54H100O7 = 1), mass = 1)

## Warning in predBg(mcomp = c(C6H10O5 = 5, C54H100O7 = 1), mass =
1):  Sum of mcomp != 1.0 so dividing all elements by the sum for calculation
of formula.

## [1] 508.1105
```

To use `form` in this case, we need to translate this mass ratio to a mole ratio, which requires an additional step (where errors could be introduced). In this case the calculation is shown below.

```
  1/5*molMass("C6H10O5")/molMass("C54H100O7")

## [1] 0.03764832
```

```
  predBg("(C6H10O5)1 (C54H100O7)0.037648")

## [1] 508.1053
```

6 Total biogas production and composition

Predicting total biogas production is complicated by the behavior of CO_2 after it is produced. Unlike CH_4, which is only sparingly soluble in water, a significant fraction of CO_2 produced remains in solution, and therefore does not contribute to biogas volume or affect its composition. Let's continue with the paper and vegetable oil example from the last section[7].

```
  predBg(mcomp = c(C6H10O5 = 5/6, C54H100O7 = 1/6), mass = 1, value = "all")

##                form mass mol.mass      moles      COD    hydro     fCH4
## 1 C1.52618H2.61516O    1  36.9655 0.02705225 1.454303 0.181493 0.550384
##       vCH4      mCH4      mCO2
## 1 508.1105 0.3645301 0.8169628
```

The `fCH4` value is $\approx 55\%$ in our example, which is not the same as the CH_4 fraction in biogas. The difference is caused by a significant fraction of the CO_2

[6] To avoid the resulting warning, be sure that the sum of the `mcomp` vector is unity.
[7] But change our masses to avoid a warning.

remaining in solution as CO_2(aq), H_2CO_3, HCO_3^-, and CO_3^{-2}. The `predBg()` function can also predict this partitioning of inorganic carbon between biogas and solution, if values are provided for three additional arguments: `conc.sub`, which is substrate concentration in g per kg H_2O; `pH`, which is the pH of the final solution; and `temp`, which is the system temperature in °C. Here, we'll assume the pH is well-buffered at pH 7.5, and our total substrate concentration is 50 g kg^{-1}. We will also assume that degradability is high (`fd = 0.8`) and substrate used for cell synthesis is typical (`fs = 0.1`).

```
predBg(mcomp = c(C6H10O5 = 5/6, C54H100O7 = 1/6), mass = 1,
       fd = 0.8, fs = 0.1, conc.sub = 50, pH = 7.5, temp = 35,
       value = "all")
```

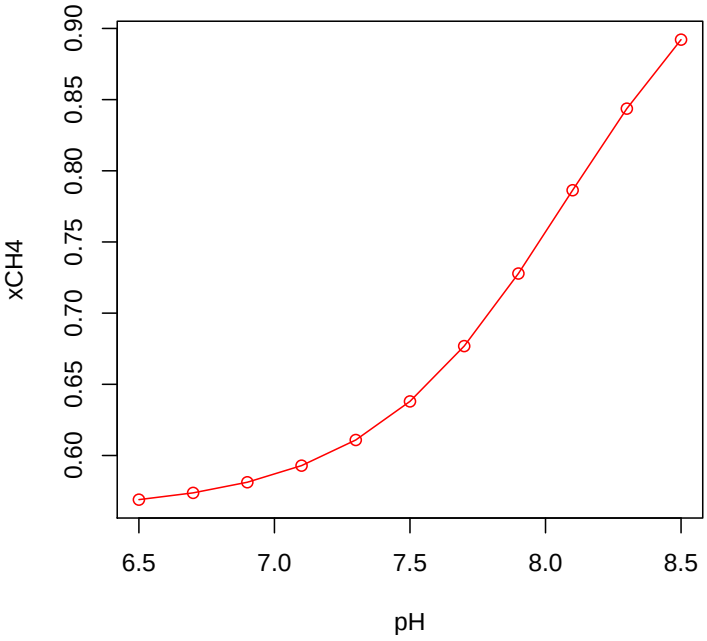
```
##                form mass mol.mass      moles      COD  fs  fe  fd conc.sub
## 1 C1.52618H2.61516O    1  36.9655 0.02705225 1.454303 0.1 0.9 0.8       50
##   temp  pH      hydro      fCH4      xCH4     vCH4     vCO2      vBg
## 1   35 7.5 0.09279292 0.5566161 0.6380063 365.8395 206.6652 572.5047
##        mCH4      mCO2    mCO2Bg  mCO2.sol      cTIC      m.bio      N.req
## 1 0.2624617 0.5735654 0.4085402 0.1650252 0.1874861 0.08225028 0.01018521
```

Only after specifying values for these additional arguments will `predBg` return a column with biogas composition: `xCH4` gives the mole fraction of CH_4 in dry biogas. In this example, we can see that at 62% `xCH4` is substantially higher than based on stoichiometry alone (`fCH4`). The difference between the two is, as explained above, TIC in solution. Additional new columns in this output give data for the volume of CO_2 in biogas (`vCO2`, mL), the total volume of (dry, standardized) biogas (`vBg`, mL), the mass of CO_2 in biogas and in solution (`mCO2Bg` and `mCO2.sol`, g), and the total inorganic carbon concentration in solution (`cTIC`, mol kg^{-1}). In fact, nearly one-third of all the CO_2 produced ends up in the solution in this example–it may be higher in other cases.

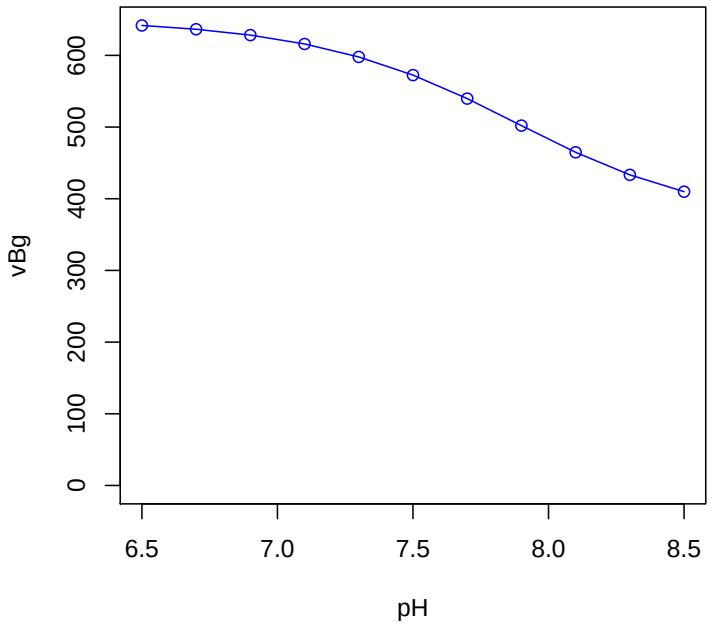
How might pH affect biogas composition? Let's look at a range of values.

```
bg1 <- predBg(mcomp = c(C6H10O5 = 5/6, C54H100O7 = 1/6), mass = 1,
              fd = 0.8, fs = 0.1, conc.sub = 50, pH = c(6.5 + 0:10*0.2),
              temp = 35, value = "all")
```

```
plot(xCH4 ~ pH, data = bg1, type = 'o', col = "red")
```


xCH4
0.60
0.65
0.70
0.75
0.80
0.85
0.90
6.5
7.0
7.5
8.0
8.5
pH

```
plot(vBg ~ pH, data = bg1, type = 'o', ylim = c(0, max(bg1$vBg)), col = "blue")
```



Clearly, pH alone could have a major effect on biogas quality and volume!

Predicting production and quality of biogas when the starting solution contains inorganic carbon is more complicated. The method assumes that all CO_2 in the system is accounted by the empirical formula (`form`). This may not be the case–for example if a bicarbonate (HCO_3^-) salt is included as a buffer in our BMP test with cellulose, or for our manure example, there is certainly significant TIC in raw manure. Here we need to be careful, and understand where our empirical formula came from. Does it include all C, or just the amount in the organic fraction? Does it include the O in TIC? Additional TIC could easily be added in with the `predBg()` function, but it is necessary to first determine the mole or mass ratio of substrate:TIC to correctly specify the resulting mixture using `form` or `mcomp`.

7 Calculation methods

How are the calculations presented above carried out? Stoichiometry of a complete biomethanation reaction is determined based on [4].

$$\mathrm{C_nH_aO_bN_c} + (2\,\mathrm{n} + \mathrm{c} - \mathrm{b} - \frac{9\,\mathrm{df_s}}{20} - \frac{9\,\mathrm{f_e}}{4})\mathrm{H_2O} \longrightarrow$$

$$\frac{\mathrm{df_e}}{8}\mathrm{CH_4} + (\mathrm{n} - \mathrm{c} - \frac{\mathrm{df_s}}{5} - \frac{\mathrm{df_e}}{8})\mathrm{CO_2} + \frac{\mathrm{df_s}}{20}\mathrm{C_5H_7O_2N}$$

$$+ (\mathrm{c} - \frac{\mathrm{df_s}}{20})\mathrm{NH_4^+} + (\mathrm{c} - \frac{\mathrm{df_s}}{20})\mathrm{HCO_3^-}$$

Here, f_s and f_e are the fraction of substrate electrons going to cell synthesis and energy production, respectively, the formula $\mathrm{C_5H_7O_2N}$ is an empirical formula for cell biomass[8], and $d = 4n + a - 2b - 3c$. In addition to providing estimates of $\mathrm{CH_4}$ production, this approach allows `predBg()` to return production of $\mathrm{CO_2}$[9], consumption or production of ammonia, and production of cell biomass. Predicted $\mathrm{CH_4}$ is always expressed in mL ($\mathrm{cm^3}$) at standard conditions of 101.325 kPa (1.0 atm) and 0°C (273.15 K).

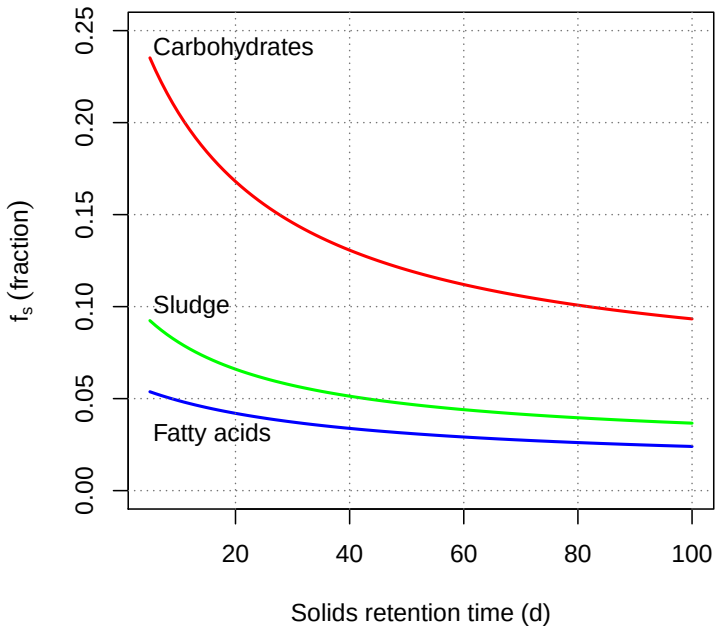
For these estimates to approach observed values, it is necessary to include and accurately set f_s. How should a f_s value be selected? Based on [4], f_s is related to the intrinsic value f_s^0, the solids retention time θ_x, the rate of microbial biomass decay b ($\mathrm{d^{-1}}$), and the degradabiilty of microbial biomass f_{bd} (fraction).

$$f_s = f_s^0 \left(\frac{1 + (1 - f_{bd})\, b\theta_x}{1 + b\theta_x} \right) \tag{1}$$

Values of f_s^0 are given in [4]. For acetate fermenting methanogens, $f_s^0 = 0.05$, and for hydrogen oxidizing methanogens, $f_s^0 = 0.08$. But most calculations should be based on an overall value for the entire microbial community, which includes fermentative bacteria as well. Table 13.2 in [4] gives estimates for f_s^0 and b for various types of wastes: f_s^0 ranges from 0.06 for lipids to 0.28 for carbohydrates, and b ranges from 0.02 $\mathrm{d^{-1}}$ for proteins to 0.05 for most other types of substrates. Calculated values of f_s are shown for three types of substrates below, assuming $f_{bd} = 0.8$ [4].

[8] Presently it is not possible to use a different formula.

[9] More accurately, total inorganic carbon (TIC), which includes both $\mathrm{CO_2}$ and $\mathrm{HCO_3^-}$ from the above reaction.



To determine "theororetical BMP", f_s should be set to zero ($f_e = 1$), which is the default.

Complex substrates are not completely degraded during anaerobic digestion, and the amount of the "degradable" (perhaps "degraded" is more accurate) fraction can be specified with the f_d argument. For complex substrates, the degradability of different components within a single substrate will differ, e.g., cellulose is much more degradable than lignin. But the current approach used for `predBg()` assumes that all components have the same degradability f_d.

The `predBg()` function can also calculate CH_4 production from COD. In this case, CH_4 volume is calculated based on the oxidation of CH_4 with O_2[10] [4]:

$$\frac{1}{8}\,CH_4 + \frac{1}{4}\,O_2 \longrightarrow \frac{1}{8}\,CO_2 + \frac{1}{4}\,H_2O$$

which gives a ratio of CH_4 to O_2 of $\frac{1}{8} : \frac{1}{4} = 1 : 2$. Based on conservation of COD, potential CH_4 production of a substrate with COD c is therefore:

$$V_{CH_4} = v_{CH_4} c/(M_{O_2}/2) \tag{2}$$

where v_{CH_4} = molar volume of CH_4 (22361 mL g^{-1}, defined at 1 atm and 0°C [2]) and M_{O_2} is the molar mass of O_2 (32.0 g mol^{-1}). If f_e and f_d are available, they reduce the fraction of COD converted.

[10] This reaction is based on a single electron equivalent.

$$V_{CH_4} = f_d f_e v_{CH_4} c/(M_{O_2}/2) \quad (3)$$

The approach used to calculate CO_2 partitioning is based on equilibrium speciation as described in [1] and should be accurate for continuous reactors with stable operation at least. Predictions for batch reactors are more difficult and results will probably be less accurate.

References

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