

Data processing for manometric BMP measurements

Nanna Løjborg and Sasha D. Hafner

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1 Introduction

Manometric methods are commonly used for measuring biogas and methane production in order to determine methane potential and anaerobic biodegradability of a given substrate. In manometric methods, bottle headspace pressure is measured under constant temperature conditions from different techniques such as using pressure manometers or transducers, manometer assisted syringes, or low flow pressure [1]. The measured pressure is converted to biogas and methane (if composition is provided) volume data using manometric calculation methods. Manometric methods require accumulation of biogas within the bottle headspace. Headspace pressure is usually measured with a portable manometer, which evaluates the pressure relative to atmospheric pressure.

Determination of CH_4 volume from manometric measurements requires data processing. The `calcBgMan()` function was developed to process manometric data. A newly developed biogas package (available for the R environment since 2015) address issues with time-consuming calculations and lack of reproducibility among laboratories for obtaining BMP [2]. The biogas package consists of ten functions including `cumBg()`, which are used for processing volumetric, manometric, gravimetric, and gas density measurements. The resulting biogas and methane production and production rates can be further used to calculate BMP using the `summBg()` function. This document describes how to process manometric biogas measurements using the `calcBgMan()` function. We assumed that readers are familiar with biogas data collection and R.

2 Overview of the Function

`calcBgMan()` is a "high-level" function within the biogas package. The purpose of `calcBgMan()` is to convert pressure data collected in the laboratory to cumulative biogas and CH_4 production and production rates. Typically, these values will then be used for calculation of BMP, e.g. using the `summBg()` function. `calcBgMan()` can handle data from multiple bottles and accepts three different data structures. For simple operations (e.g. interpolation and standardization

of biogas volume) `calcBgMan()` is supported by calls to external "low-level" functions (refer to Section 5, Table 1).

Two manometric methods are commonly used to calculate methane production from pressure and composition measurements. Method 1 is based on normalized CH_4 concentrations, whereas method 2 accounts for the actual CH_4 in the bottle headspace. Both methods are available through `calcBgMan()` and results are expected to be virtually identical. The examples below describe cumulative biogas calculation on two different datasets. The "long" structured dataset is evaluated using manometric method 1, whereas the "longcombo" dataset is evaluated using manometric method 2, as true methane concentrations are provided.

2.1 Function Arguments

The arguments for the `calcBgMan()` function are:

```
## function (dat, comp = NULL, temp = NULL,
##         interval = TRUE, data.struct = "longcombo",
##         id.name = "id", time.name = "time",
##         pres.name = "pres", comp.name = "xCH4",
##         temp.init = NULL, pres.init = NULL, pres.resid = NULL,
##         rh.resid = NULL, rh.resid.init = 1,
##         headspace = NULL, vol.hs.name = "vol.hs",
##         absolute = TRUE, pres.amb = NULL,
##         cmethod = "removed", imethod = "linear",
##         extrap = FALSE, addt0 = TRUE, showt0 = TRUE,
##         dry = FALSE, empty.name = NULL,
##         std.message = !quiet, check = TRUE,
##         temp.std = getOption("temp.std", as.numeric(NA)),
##         pres.std = getOption("pres.std", as.numeric(NA)),
##         unit.temp = getOption("unit.temp", "C"),
##         unit.pres = getOption("unit.pres", "atm"),
##         quiet = FALSE)
## NULL
```

Most of the arguments have default values, but to calculate CH_4 production we must provide values for at least `dat` (data frame with pressure measurements), `comp` (data frame with gas composition), and `temp` (biogas temperature)¹ along with the names of a few columns in the input data frames. If the `comp` argument (or, for the "longcombo" format, the `comp.name` argument) is not provided, `calcBgMan()` will return results for biogas only and not CH_4 .

¹. 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`. The same default values apply for temperature and pressure for presentation of biogas and methane, but these can be changed in the function call with the `temp.std` and `pres.std` arguments.

By default `interval = TRUE` and `data.struct` is set as `‘‘longcombo’’`. `‘‘wide’’` and `‘‘long’’` structured data will be restructured to `‘‘longcombo’’` internally by `cumBgDataPrep()`, when specified by the `data.struct` argument (refer to Section 2.2). When data are cumulative, the `interval` argument should be set to `FALSE`.

Similarly, there is an `id.name` argument for the bottle identification code (ID) column (default is `‘‘id’’`). For `data.struct = ‘‘wide’’`, there is no ID column. Instead data for each bottle, have individual columns and column names, which are used as ID codes. Here, the name of the column containing the response variables (`pres.name`), is set as the name of the first column with response variables. All following columns are assumed to have measurement data.

Furthermore, we need to specify the name of the time column containing time data using the `time.name` argument (default is `‘‘time’’`). If separate data frames are used for `dat` and `comp`, the name must match. Time data may be POSIXct objects, but then `t0` will not be added to rows by the `calcBgMan()` function. In addition, the `addt0` argument is used to add row with “time zero” (`time.name = 0`) for each bottle in order to calculate production rates for the first observation (default is `TRUE`). `showt0` determines if the “time zero” should be returned in the output (default is `TRUE` if `time.name` is numeric and contains 0 and otherwise `FALSE`). The use of `t0` output is for plotting.

The `comp.name` argument is used to indicate which column within the `comp` data frame contains CH₄ concentrations. Default is `‘‘xCH4’’`. `comp` may also just be a single value instead of a data frame or column. When providing a single value for `comp`, this value is applied to all observations and the `comp.name` argument is not needed. The definition of `xCH4` depends on the `cmethod` argument. By default (`cmethod = ‘‘removed’’`) the function calculates volumes following [3] as the product of standardized volume of biogas removed and normalized CH₄ content (as mole fraction in dry biogas, normalized so the sum of mole fractions of CH₄ and CO₂ sum to unity). If results should be based on the sum of methane removed and methane remaining in the bottle headspace, `cmethod` should be set to `‘‘total’’`. When `cmethod = ‘‘total’’`, CH₄ concentration is expressed relative to all biogas components except water (CH₄, CO₂, N₂, H₂S, etc.) instead of CH₄ and CO₂ only.

If any CH₄ measurements are missing, `‘‘xCH4’’` is interpolated by the external “low-level” function `interp()`. Here, the `imethod` argument can be used to define interpolation method (default is `‘‘linear’’`), which is passed to `interp()`. Similar, an `extrap` argument is passed to `interp()` (default is `FALSE`). The `extrap` argument is used to indicate if composition data (`comp.name`) should be extrapolation (e.g. in the case of missing initial composition values). Extrapolation is constant (the value of the nearest observation is taken). In general, extrapolation and extensive interpolation should be avoided.

Initial headspace temperature and pressure are required to determine initial gas volume in the bottles and can be set using the `temp.init` and `pres.init`, respectively. Default values are `NULL`. Similarly, post venting headspace pressure is required for manometric calculation methods and can be set using the

`pres.resid` argument.

These are used to correct for apparent biogas production due simply to a change in headspace temperature or pressure between bottle sealing and the first measurements (frequently bottles are filled, flushed, and sealed at room temperature). Alternatively, this effect can be corrected by measuring pressure after the bottle temperature is increased to incubator temperature. In this case, the composition should be set to zero for this first measurement interval.

Initial and post venting headspace pressure can be absolute or gauge, depending on the `absolute` argument. If only a single pressure value is provided, this will be used for all observations. By default, pressure is absolute (`absolute = TRUE`). When `absolute = FALSE`, gauge pressure measurements are converted to absolute using the `pres.amb` argument, representing the absolute ambient pressure. `pres.amb` can only be set as a single value and is 101.325 kPa (1.0 atm) by default.

Additionally, a data frame containing headspace volumes is required if `cmethod = "total"` and should contain at least a headspace volume column (`vol.hs.name`) and a bottle identification column, with the same column name as in `dat` and `comp` data frames. The headspace volume column can be set using the `vol.hs.name` argument (default is `"vol.hs"`). Initial relative humidity of gas in the headspace is set to 1 by default using the `rh.resid.init` argument. If values are provided for relative humidity of gas in the headspace after experiment was initiated, these can be defined by using the `rh.resid` argument.

2.2 Data Structures

Input data may be structured in one of three ways: `"long"`, `"wide"`, or `"longcombo"`. Default is `"longcombo"`, where the composition column is in the `dat` data frame and no separate composition data frame is required. In the following examples all three data structures will be addressed. For more details about each of the three data structure refer to `biogas.quick.start` vignette.

3 Examples: Calculation of Cumulative Production of Biogas and CH₄ and Production Rates from Manometric Measurements

Calculation of cumulative biogas and CH₄ production and production rates, typically requires two data frames: Biogas volume measurements and biogas composition (CH₄ fraction)

3.1 ‘‘longcombo’’ Data Structure

In this example, we will use ‘‘longcombo’’ example datasets included in the biogas package: `sludgeTwoBiogas` for both biogas volumes and composition and `sludgeTwoSetup` for grouping and headspace volumes. In this experiment both manometric and gravimetric methods were used, which is where the ‘‘Two’’ comes from. Substrate and inoculum masses provided from `sludgeTwoSetup` are not interesting before calculation of BMP using `summBg()` (refer to Section 4).

These data are from an experiment carried out with seven different ratios of sludge + inoculum to headspace. The substrate was primary wastewater sludge. The experiment included 24 batch bottles, all with inoculum and one without substrate (blank):

- Three bottles with inoculum only (Blank50)
- Three bottles with wastewater sludge 25 (WWS25)
- Three bottles with wastewater sludge 25b (WWS25b)
- Three bottles with wastewater sludge 40 (WWS40)
- Three bottles with wastewater sludge 50 (WWS50)
- Three bottles with wastewater sludge 50b (WWS50b)
- Three bottles with wastewater sludge 60 (WWS60)
- Three bottles with wastewater sludge 75 (WWS75)

More details can be found in the helpfiles for these data.

```
data("sludgeTwoBiogas")  
  
dim(sludgeTwoBiogas)  
## [1] 324 8  
  
head(sludgeTwoBiogas)
```

```
##   id   time.d pres mass.init mass.final  xCH4  xCO2  xCH4n
## 1  1 0.0000000   0  187.4168  187.4168 0.0000 0.0000 0.0000000
## 2  1 0.6270833 368  187.4149  187.3814 0.1010 0.1004 0.5014896
## 3  1 1.6027778 286  187.3823  187.3568 0.2253 0.1610 0.5832255
## 4  1 1.9972222 134  187.3538  187.3447 0.2485 0.1800 0.5799300
## 5  1 2.7152778 142  187.3406  187.3287 0.3246 0.2062 0.6115298
## 6  1 3.6180556 168  187.3295  187.3150 0.3674 0.2222 0.6231343
```

```
summary(sludgeTwoBiogas)
```

```
##           id           time.d           pres
## Min.      : 1.0   Min.      : 0.000   Min.      :  0.0
## 1st Qu.:  8.0   1st Qu.:  2.715   1st Qu.: 181.0
## Median :12.5   Median :  8.637   Median : 358.0
## Mean     :12.0   Mean     :18.113   Mean     : 565.4
## 3rd Qu.:17.0   3rd Qu.:24.029   3rd Qu.: 753.0
## Max.     :21.0   Max.     :83.662   Max.     :3785.0
##  mass.init   mass.final   xCH4
## Min.       :144.7   Min.       :144.7   Min.       :0.0000
## 1st Qu.:163.6   1st Qu.:163.6   1st Qu.:0.5479
## Median :183.5   Median :183.5   Median :0.6201
## Mean      :184.3   Mean      :184.2   Mean      :0.5460
## 3rd Qu.:200.0   3rd Qu.:199.9   3rd Qu.:0.6418
## Max.      :228.4   Max.      :228.4   Max.      :0.7377
##   xCO2           xCH4n
## Min.      :0.0000   Min.      :0.0000
## 1st Qu.:0.2599   1st Qu.:0.6446
## Median :0.3012   Median :0.6602
## Mean     :0.2791   Mean     :0.6220
## 3rd Qu.:0.3354   3rd Qu.:0.6727
## Max.     :0.6344   Max.     :0.7637
```

```
data("sludgeTwoSetup")
```

```
dim(sludgeTwoSetup)
```

```
## [1] 18  5
```

```
head(sludgeTwoSetup)
```

```
##   id descrip  vol.hs m.inoc  m.sub.vs
## 1  1 Blank50  79.980  80.02 0.0000000
## 2  2 Blank50  79.980  80.02 0.0000000
## 3  3 Blank50  79.950  80.05 0.0000000
## 4  7 WWS75  117.575  35.02 0.3588463
## 5  8 WWS75  117.535  35.06 0.3588463
```

```
## 6 9 WWS75 117.490 35.08 0.3600578

summary(sludgeTwoSetup)

##          id          descrip          vol.hs
## Min.   : 1.00   Length:18      Min.    : 38.91
## 1st Qu.: 8.25   Class :character  1st Qu. : 63.19
## Median :12.50   Mode  :character  Median  : 80.56
## Mean   :12.00                                     Mean   : 80.05
## 3rd Qu.:16.75                                     3rd Qu.: 99.43
## Max.   :21.00                                     Max.   :117.58
##          m.inoc          m.sub.vs
## Min.   : 35.02   Min.    :0.0000
## 1st Qu.: 50.06   1st Qu. :0.3591
## Median : 72.59   Median  :0.5864
## Mean   : 68.39   Mean    :0.5605
## 3rd Qu.: 80.05   3rd Qu. :0.8130
## Max.   :100.08   Max.    :1.0191
```

The first step in processing data from a BMP trial is calculation of cumulative biogas and CH₄ production and production rates. Subsequently, BMP can be calculated by the high-level function `summBg()` included in the `biogas` package. Cumulative biogas and CH₄ production and production rates from pressure data with `sludgeTwoBiogas` and `sludgeTwoSetup` data frames as input can be calculated with `calcBgMan()`.

To calculate CH₄ production from these ‘‘longcombo’’ data, we must provide values for at least `dat` and `comp`, which is in a combined data frame (we will use `sludgeTwoBiogas`), and `temp` (biogas temperature) along with the names of a few columns in our input data frame.

We can use default values ‘‘longcombo’’, ‘‘id’’, and ‘‘pres’’ for the `data.struct`, `id.name`, and `pres.name` arguments, respectively. Whereas, the `time.name` and `comp.name` arguments need to be specified as ‘‘time.d’’ and ‘‘xCH4n’’, respectively. Similar, default values can be used for `cmethod` = ‘‘removed’’, evaluating CH₄ concentration based on normalized CH₄ and CO₂ values, for `imethod` = ‘‘linear’’, resulting in internal linear interpolation of ‘‘xCH4n’’ by calling the `interp()` function, and for `extrap` = `FALSE`.

Initial headspace temperature and pressure and post venting headspace pressure are set as constants using the `temp.init`, `pres.init`, and `pres.resid` arguments, respectively. Initial and post venting headspace pressure can be absolute or gauge depending on the value of the `absolute` argument. We will set `absolute` = `FALSE` to account for pressure measurements provided in gauge. In order to calculate absolute pressure from gauge pressure measurements when `absolute` = `FALSE`, a single absolute ambient pressure value is required. Here we will set `pres.amp` to 1013 mbar. Note the unit of the pressure data in `sludgeTwoBiogas`. Default unit is atm, but can be changed using the `unit.pres` argument. In this example we set the `unit.pres` = ‘‘mbar’’ to match unit of

`pres.name` and `pres.resid` column. Absolute ambient pressure is provided in the same unit as defined in the `unit.pres` argument.

Finally, headspace volumes are provided from `sludgeTwoSetup`. The data frame containing headspace volumes is defined using the `headspace` argument, whereas the default value `"vol.hs"` can be used for the column containing headspace volume data.

```
cum.prod.lc <- calcBgMan(sludgeTwoBiogas, temp = 30,
                        time.name = "time.d", comp.name = "xCH4n",
                        temp.init = 30, pres.init = 0.0,
                        pres.resid = 0,
                        headspace = sludgeTwoSetup,
                        pres.amb = 1013, absolute = FALSE,
                        unit.pres = "mbar")

## Pressure measurements are GAUGE. If this is incorrect, change 'absolute'
## argument to TRUE.
## Using a standard pressure of 1013.25 mbar and standard temperature
## of 0 C for standardizing volume.
```

Note the message about standard temperature and pressure. It is important to make sure these values are correct, therefore users are reminded by a message². Also, note warning about pressure unit. This warning is to make sure all pressure measurements are gauge, as absolute is set to `FALSE`, meaning all pressure data are corrected to absolute pressure by the `calcBgMan()` function.

The output becomes:

```
head(cum.prod.lc)

##   id   time.d pres mass.init mass.final  xCH4  xCO2  xCH4n
## 1  1 0.000000   0  187.4168  187.4168 0.0000 0.0000 0.0000000
## 2  1 0.6270833 368  187.4149  187.3814 0.1010 0.1004 0.5014896
## 3  1 1.6027778 286  187.3823  187.3568 0.2253 0.1610 0.5832255
## 4  1 1.9972222 134  187.3538  187.3447 0.2485 0.1800 0.5799300
## 5  1 2.7152778 142  187.3406  187.3287 0.3246 0.2062 0.6115298
## 6  1 3.6180556 168  187.3295  187.3150 0.3674 0.2222 0.6231343
##   vol.hs temperature pres.resid pres.abs pres.resid.abs
## 1  79.98           30           0    1013           1013
## 2  79.98           30           0    1381           1013
## 3  79.98           30           0    1299           1013
## 4  79.98           30           0    1147           1013
## 5  79.98           30           0    1155           1013
## 6  79.98           30           0    1181           1013
##   rh.resid pres.resid.prev rh.resid.prev temp.prev xCH4n.prev
```

²Remember that standard conditions can be set in the function call with `temp.std` and `pres.std`, or globally with `options()`.


```
## 1 1.0000000          1013      1.0000000          30 0.0000000
## 2 0.7335264          1013      1.0000000          30 0.0000000
## 3 0.7798306          1013      0.7335264          30 0.5014896
## 4 0.8831735          1013      0.7798306          30 0.5832255
## 5 0.8770563          1013      0.8831735          30 0.5799300
## 6 0.8577477          1013      0.8770563          30 0.6115298
##           vBg           vCH4           cvBg           cvCH4           rvBg           rvCH4
## 1 0.0000000 0.0000000 0.000000 0.000000          NA          NA
## 2 26.168144 13.123052 26.16814 13.12305 41.72993 20.927125
## 3 19.530015 11.390402 45.69816 24.51345 20.01653 11.674149
## 4  8.861695  5.139163 54.55985 29.65262 22.46627 13.028864
## 5  9.743608  5.958506 64.30346 35.61112 13.56943  8.298113
## 6 11.573914  7.212103 75.87738 42.82323 12.82034  7.988791

dim(cum.prod.lc)
## [1] 324 24
```

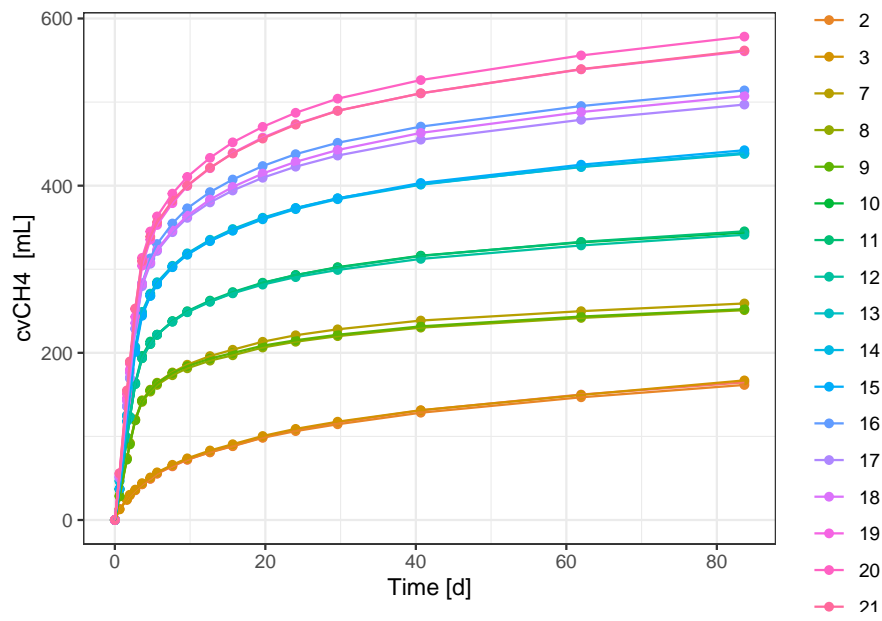
The data frame that is returned has maintained the ‘‘longcombo’’ structure with all the original columns in `sludgeTwoBiogas`, plus additional columns from manometric biogas calculations.

`v` stands for (standardized) volume, `cv` (standardized) cumulative volume, `rv` stands for (standardized) volume production rate, and `Bg` and `CH4` for biogas and methane. `cvBg` contains standardized cumulative biogas production and `cvCH4` contains standardized cumulative CH_4 production.

Graphical illustrations often increases interpretability. Here we will use the `ggplot` function from the `ggplot2` package to plot it.

```
library(ggplot2)

ggplot(cum.prod.lc, aes(time.d, cvCH4, colour = factor(id))) +
  geom_point() +
  geom_line(aes(group = id)) +
  labs(x = "Time [d]", y = "cvCH4 [mL]", colour = "Bottle id") +
  theme_bw()
```



3.2 ‘‘long’’ Data Structure

In this example, we will use ‘‘long’’ example data set included in the biogas package: `strawPressure` for headspace pressure in batch bottles, `strawComp` for methane content of biogas, and `strawSetup` for grouping and headspace volumes.

These data are interval-based BMP measurement of headspace pressure in 12 bottles with straw as the substrate. The experiment included 12 batch bottles:

- Two bottles with inoculum and straw treated with treatment r3
- Two bottles with inoculum and straw treated with treatment r5
- Two bottles with inoculum and straw treated with treatment r6.5
- Two bottles with inoculum and straw treated with treatment r8
- Two bottles with inoculum and straw treated with treatment r8 no buff
- Two bottles with inoculum and straw treated with treatment r9

Bottles were ca. 600 mL glass serum bottles with butyl rubber septa and screw caps. Pressure was measured using an electronic manometer. Data in `strawMass`, `strawSetup`, and `strawComp` are from the same bottles. More details can be found in the helpfiles for these data.

```
data("strawPressure")

dim(strawPressure)

## [1] 72 5

head(strawPressure)

##   bottle      date.time time      pres pres.resid
## 1     1 2016-04-28 10:30:00.00 1.9 153.2034 101.629
## 2     2 2016-04-28 10:30:00.00 1.9 152.0888 101.629
## 3     3 2016-04-28 10:30:00.00 1.9 142.0576 101.629
## 4     4 2016-04-28 10:30:00.00 1.9 142.1590 101.629
## 5     5 2016-04-28 10:30:00.00 1.9 138.7139 101.629
## 6     6 2016-04-28 10:30:00.00 1.9 139.5245 101.629

summary(strawPressure)

##      bottle      date.time      time
## Min.   : 1.00 2016-04-28 10:30:00.00:12  Min.   : 1.900
## 1st Qu.: 3.75 2016-04-29 16:00:00.00:12  1st Qu.: 3.120
## Median : 6.50 2016-04-30 13:20:00.00:12  Median : 4.965
## Mean   : 6.50 2016-05-02 11:00:00.00:12  Mean   : 5.987
```

```
## 3rd Qu.: 9.25 2016-05-04 14:30:00.00:12 3rd Qu.: 8.060
## Max. :12.00 2016-05-09 10:45:00.00:12 Max. :12.910
## pres pres.resid
## Min. :103.9 Min. :101.0
## 1st Qu.:125.3 1st Qu.:101.6
## Median :138.8 Median :101.8
## Mean :140.2 Mean :101.7
## 3rd Qu.:155.0 3rd Qu.:102.0
## Max. :180.7 Max. :102.1
```

```
data("strawComp")
```

```
dim(strawComp)
```

```
## [1] 63 4
```

```
head(strawComp)
```

```
## bottle date.time time xCH4
## 1 1 2016-04-28 10:30:00.00 1.9 0.4189
## 2 2 2016-04-28 10:30:00.00 1.9 0.4219
## 3 3 2016-04-28 10:30:00.00 1.9 0.3395
## 4 4 2016-04-28 10:30:00.00 1.9 0.3015
## 5 5 2016-04-28 10:30:00.00 1.9 0.2769
## 6 6 2016-04-28 10:30:00.00 1.9 0.2850
```

```
summary(strawComp)
```

```
## bottle date.time time
## Min. : 1.000 2016-04-28 10:30:00.00:12 Min. : 1.900
## 1st Qu.: 3.000 2016-05-04 14:30:00.00:11 1st Qu.: 3.120
## Median : 6.000 2016-04-30 13:20:00.00:10 Median : 4.010
## Mean : 6.175 2016-05-09 10:45:00.00: 9 Mean : 5.724
## 3rd Qu.: 9.000 2016-04-29 15:35:00.00: 1 3rd Qu.: 8.060
## Max. :12.000 2016-04-29 15:40:00.00: 1 Max. :12.910
## (Other) :19
## xCH4
## Min. :0.01187
## 1st Qu.:0.30020
## Median :0.43490
## Mean :0.39450
## 3rd Qu.:0.48925
## Max. :0.88720
##
```

```

data("strawSetup")

dim(strawSetup)

## [1] 12 6

head(strawSetup)

##   bottle treatment          start sub.mass inoc.mass
## 1     1         r3 2016-04-26 13:00:00.00    5.27    45.36
## 2     2         r3 2016-04-26 13:00:00.00    5.27    43.88
## 3     3         r5 2016-04-26 13:00:00.00    5.28    26.27
## 4     4         r5 2016-04-26 13:00:00.00    5.30    26.95
## 5     5        r6.5 2016-04-26 13:00:00.00    5.31    20.37
## 6     6        r6.5 2016-04-26 13:00:00.00    5.29    20.61
##   headspace
## 1     491.3
## 2     493.3
## 3     502.9
## 4     502.4
## 5     502.4
## 6     505.8

summary(strawSetup)

##   bottle      treatment          start
## Min.   : 1.00   r3           :2 2016-04-26 13:00:00.00:12
## 1st Qu.: 3.75   r5           :2
## Median : 6.50   r6.5         :2
## Mean   : 6.50   r8           :2
## 3rd Qu.: 9.25   r8 no buff :2
## Max.   :12.00   r9           :2
##   sub.mass      inoc.mass      headspace
## Min.   :5.240   Min.   :14.57   Min.   :491.3
## 1st Qu.:5.270   1st Qu.:16.48   1st Qu.:502.4
## Median :5.280   Median :18.76   Median :502.9
## Mean   :5.284   Mean   :23.31   Mean   :503.1
## 3rd Qu.:5.300   3rd Qu.:26.44   3rd Qu.:507.5
## Max.   :5.340   Max.   :45.36   Max.   :509.5

```

As with the ‘‘longcombo’’ data, cumulative production of CH₄ is needed in order to calculate BMP. Again, we can calculate these with the `calcBgMan` function, using `strawPressure`, `strawComp`, and `strawSetup` data frames as input.

To calculate CH₄ production from these ‘‘long’’ structured data, we must provide values for at least `dat`, `comp`, and `temp` along with the names of a few

columns in our input data frame. The `dat` and `comp` arguments are set as the data frames: `strawPressure` and `strawComp`, respectively, whereas `temp` is set as single values of 31 °C. For `data.struct != 'longcombo'` the data structure needs to be specified. Here we set `data.struct = 'long'`. Furthermore, we need to specify the name of the id column in `strawPressure` as `bottle` using the `id.name` argument.

We can use default values `'time'`, `'pres'`, and `'xCH4'` for the `time.name`, `pres.name` and `comp.name` arguments, respectively. The id and time columns create a link between the two data frames. Observations from different times can be solved by the external `interp()` function by interpolation. Similar, default values can be used for `cmethod = "removed"`, evaluating CH₄ concentration based on normalized CH₄ and CO₂ values and for `imethod = 'linear'`, resulting in internal linear interpolation of `'xCH4'` by calling the `interp()` function. Additionally, the response variables are interval data only and hence, we can use the default `interval = TRUE`.

In addition to interpolation for later observations, an extrapolation argument (`extrap`) can be provided if required. We do not have initial biogas composition (compare the heads of `strawPressure` and `strawComp`) so extrapolation is required to calculate initial volumes and rates. Therefore, we need to set `extrap = TRUE`.

Initial headspace temperature and pressure are set as constant values using the `temp.init` and `pres.init` arguments, respectively. Headspace pressure after venting is provided from the `strawPressure` data frame and can be defined by assigning the column name to the `pres.resid` argument. Similar to the `'longcombo'` data example, we will set `absolute = FALSE` to account for pressure measurements provided in gauge. In order to calculate absolute pressure from gauge pressure measurements when `absolute = FALSE`, a single absolute ambient pressure value is required. To correct gauge pressure data to absolute pressure, we will set `pres.amb` to 101.3 kPa. Again, note the unit of the pressure data in `strawPressure`. Pressure unit is set as atm by default, but this can be changed using the `unit.pres` argument. In this example we will set the `unit.pres = "kPa"` to match unit of `pres.name` and `pres.resid` column.

Finally, headspace volumes are provided from `strawSetup`. The data frame containing these volumes is defined using the `headspace` argument, whereas the column is set as `vol.hs.name = "headspace"`.

The output becomes:

```
cum.prod.l <- calcBgMan(strawPressure, comp = strawComp, temp = 31,
                        data.struct = "long",
                        time.name = "time", id.name = "bottle", comp.name = "xCH4",
                        temp.init = 21.55, pres.resid = "pres.resid",
                        pres.init = 0.0,
                        headspace = strawSetup, vol.hs.name = "headspace",
                        pres.amb = 101.3, absolute = FALSE,
                        extrap = TRUE,
                        unit.pres = "kPa")
```

```

## Biogas composition is interpolated.
## Pressure measurements are GAUGE. If this is incorrect, change 'absolute'
## Using a standard pressure of 101.325 kPa and standard temperature
## of 0 C for standardizing volume.

head(cum.prod.l)

##   bottle          date.time time      pres pres.resid
## 1      1              <NA> 0.00      NA      NA
## 2      1 2016-04-28 10:30:00.00 1.90 153.2034 101.6290
## 3      1 2016-04-29 16:00:00.00 3.12 171.9485 101.8316
## 4      1 2016-04-30 13:20:00.00 4.01 140.7404 101.8316
## 5      1 2016-05-02 11:00:00.00 5.92 168.7061 102.1356
## 6      1 2016-05-04 14:30:00.00 8.06 168.4022 102.0343
##   xCH4 headspace temperature pres.abs pres.resid.abs
## 1      NA      NA      NA      NA      NA
## 2 0.4189000    491.3      31 254.5034    202.9290
## 3 0.4363556    491.3      31 273.2485    203.1316
## 4 0.4413000    491.3      31 242.0404    203.1316
## 5 0.5014287    491.3      31 270.0061    203.4356
## 6 0.5152000    491.3      31 269.7022    203.3343
##   rh.resid pres.resid.prev rh.resid.prev temp.prev xCH4.prev
## 1      NA      NA      NA      NA      NA
## 2 0.7973527    101.3000    1.0000000    21.55 0.0000000
## 3 0.7433951    202.9290    0.7973527    31.00 0.4189000
## 4 0.8392467    203.1316    0.7433951    31.00 0.4363556
## 5 0.7534481    203.1316    0.8392467    31.00 0.4413000
## 6 0.7539216    203.4356    0.7534481    31.00 0.5014287
##   vBg      vCH4      cvBg      cvCH4      rvBg      rvCH4
## 1 0.0000 0.00000 0.0000 0.0000      NA      NA
## 2 644.8100 270.11092 644.8100 270.1109 339.3737 142.16364
## 3 302.1496 131.84467 946.9597 401.9556 247.6636 108.06940
## 4 164.3333 72.52027 1111.2929 474.4759 184.6441 81.48345
## 5 287.9775 144.40021 1399.2705 618.8761 150.7736 75.60220
## 6 283.6379 146.13027 1682.9084 765.0063 132.5411 68.28517

```

Note the message about standard temperature and pressure. It is important to make sure these values are correct, therefore users are reminded by a message³. Also, note that a “time zero” value is added to each bottle. This is due to the default value `addt0 = TRUE`, enabling calculation of production rates for the first observation.

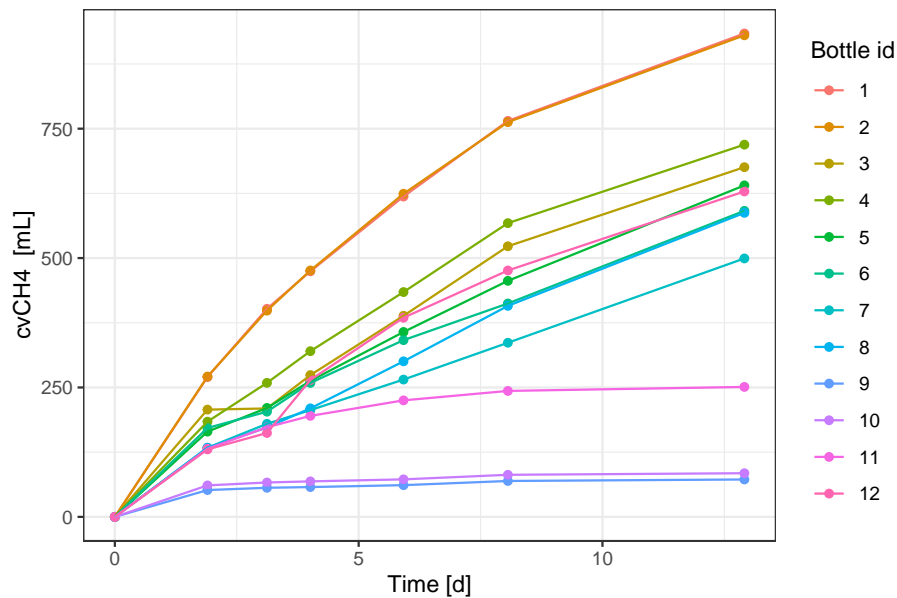
The data frame that is returned has been restructured to “`longcombo`” structure and contains all the original columns in `strawPressure`, plus addi-

³Remember that standard conditions can be set in the function call with `temp.std` and `pres.std`, or globally with `options()`.

tional columns from volumetric biogas calculations (refer to Section 3.1)

As with the ‘‘longcombo’’ data example, the `ggplot` function from the `ggplot2` package is used to increase interpretability of the results.

```
ggplot(cum.prod.l, aes(time, cvCH4, colour = factor(bottle))) +  
  geom_point() +  
  geom_line(aes(group = bottle)) +  
  labs(x = "Time [d]", y = "cvCH4 [mL]", colour = "Bottle id") +  
  theme_bw()
```



Plotting results is recommended, and can be used to catch strange responses like for bottle # 2 here.

3.3 Additional Examples

For examples using ‘‘wide’’ structured input data frame and varying settings of other arguments (e.g. `addt0` and `showt0`), refer to vignette for volumetric `cumBg` function (`cumBgVol.function.Rnw`).

4 Continuing With the `calcBgMan()` Function

The `calcBgMan()` function is one of several `cumBg*`() functions within the biogas package. Results from the `cumBg*`() functions can be used directly in the `summBg()` function from the biogas package to calculate BMP for the data in question. Though, this operation often requires additional setup information (e.g. inoculum and substrate mass), which is most commonly provided in an

external data frame (`setup`). More details can be found in the associated help file

5 Function Internals

In general, `cumBg*`(`)` functions consist of four sections: argument checks, restructuring and sorting data, interpolation if needed, and biogas standardization and calculations. Restructuring and sorting of data and interpolation are handled by the external functions `cumBgDataPrep()` and `interp()`, respectively. From `interp()` gas composition, cumulative biogas production, and other variables can be interpolated to a specified time if required. From `cumBgDataPrep()` ‘‘wide’’ and ‘‘long’’ data structure are restructured to ‘‘longcombo’’ data, which is required for `calcBgMan()` for further data processing. Additionally, data are sorted, headspace is added if provided, and composition data is corrected if it seems to be a percentage. Subsequently, the restructured and sorted data is standardized in `cumBgVol()` by an external function called `stdVol()`.

`calcBgMan()` accepts all data structures, but the manometric calculation methods within `calcBgMan()` only process ‘‘longcombo’’ data. ‘‘wide’’ and ‘‘long’’ data are restructured internally by the ‘‘low-level’’ function `cumBgDataPrep()`. `cumBgDataPrep()` sorts and restructures biogas data for further calculation of cumulative biogas and methane production and production rates. The `data.struct` argument is internally passed to `cumBgDataPrep()` and restructured to ‘‘longcombo’’ structure prior to being processed by volumetric calculation methods.

Table 1: Operations done with the ‘‘low-level’’ functions in `calcBgMan()`. All functions are vectorized. See help files for more details.

Operation	Function
Standardize gas volume	<code>stdVol()</code>
Interpolate composition etc.	<code>interp()</code>
Structurize and sort data	<code>cumBgDataPrep()</code>

References

- [1] J. Filer, H. H. Ding and S. Chang Biochemical Methane Potential (BMP) Assay Method for Anaerobic Digestion Research. *Water*, 11, 921, 2019.
- [2] Hafner, S.D., Koch, K., Carrere, H., Astals, S., Weinrich, S., Rennuit, C. 2018 Software for biogas research: Tools for measurement and prediction of methane production. *SoftwareX* 7: 205-210
- [3] B.K. Richards, R.J. Cummings, T.E. White, and W.J. Jewell. Methods for kinetic-analysis of methane fermentation in high solids biomass digesters. *Biomass & Bioenergy*, 1(2):65–73, 1991.