



Original Software Publication

Software for biogas research: Tools for measurement and prediction of methane production



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ABSTRACT

Biogas production from organic materials by anaerobic digestion is both a developed technology and an active area of research. In this contribution we describe an R package designed to help standardize biogas research. A web-based application provides access to the main functions. The software can be used to accurately calculate biochemical methane potential (BMP) from a range of biogas measurement types. Additionally, methane potential can be predicted from substrate composition, facilitating experimental design and interpretation of results. By providing access to flexible, efficient, standardized, and transparent algorithms, this software may make biogas research more accurate and efficient.

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Current code version	1.10.3
Permanent link to code/repository used for this code version	https://CRAN.R-project.org/package=biogas
Legal Code License	GPL-2
Code versioning system used	git
Software code languages, tools, and services used	R
Compilation requirements, operating environments	Compilation not required; Windows, Mac OSX, Linux
If available Link to developer documentation/manual	https://cran.r-project.org/web/packages/biogas/biogas.pdf
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1. Motivation and significance

Anaerobic digestion is an established technology for the stabilization of organic materials and production of renewable energy. Energy is recovered in the form of biogas (a mixture of methane (CH₄) and carbon dioxide (CO₂)), and optimization of biogas production is an active area of research [1]. Research on anaerobic digestion includes laboratory and pilot-scale experiments, as well

as theoretical calculations and process modeling. Laboratory experiments are used to determine how much CH₄ can be obtained from a particular substrate, or to study the effect of a particular treatment [2,3]. Many of these experiments use biochemical methane potential (BMP) tests to estimate the maximum quantity of CH₄ that can be obtained. Transformation of laboratory measurements into BMP is done using a sequence of simple calculations [4]. Although conceptually simple, calculations differ among groups, and are seldom described in detail in publications, leading to a lack of reproducibility and a high likelihood of systematic bias in results. Many groups use custom spreadsheet templates for calculations.

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Prediction of CH₄ production can be carried out using substrate composition (simple stoichiometry) but there are multiple steps involved [5]. A simple means of quickly making these calculations would facilitate the design of experiments as well as evaluation and interpretation of results. In this contribution, we describe a package for the R environment [6] that addresses these problems and needs: the biogas package [7].

2. Software description

The biogas package is written in R and can be used directly in the R environment. The heart of the package is a set of ten functions, which require some proficiency in R for use. However, a web-based interface called OBA (from Online Biogas App, <https://biotransformers.shinyapps.io/oba1/>) provides access to the main functions, albeit with less flexibility.

2.1. Software architecture

Package functions can be divided into three groups: (1) basic vectorized functions for common conversions and calculations, (2) two data processing functions that calculate BMP or similar results from laboratory measurements, and (3) a function for predicting CH₄ production.

2.2. Software functionality

2.2.1. Basic functions

Seven functions (Table 1) assist with data processing and experimental design, and are used by the data processing functions (Section 2.2.2). Most perform a conversion of an input vector (the first argument), and are vectorized. And most include optional arguments, making them both flexible and convenient.

The `stdVol()` function is used for converting measured gas volume or pressure into a standardized volume that corresponds to a fixed quantity (44.72 mmol or 717.4 mg CH₄ per L under standard conditions of 0 °C and 1.0 atm, as calculated using the `vol2mol()` function). Standardized volume is often referred to as normal volume, and given in publications without details on the standardization conditions. However, because of inconsistency in the use of terms, correction for water vapor, and standard conditions (IUPAC now uses 1 bar = 0.9869 atm [8]), it is prudent to simply provide the conditions used for standardization. Standard conditions in the biogas package are 0 °C and 1.0 atm (101.325 kPa) by default, but can be set by the user in a function call or globally. Accurate standardization requires correction for water vapor, pressure, and temperature [9,10]. Water vapor content is based on saturation vapor pressure by default, and is calculated using a Magnus form equation [11]. This function can be used for volumetric (typically fixed pressure and variable volume) or manometric measurements (typically fixed volume and variable pressure). Multiple temperature and pressure units are supported (°C, °F, K, atm, kPa, bar, and others). Unit conversion is carried out by the hidden function `unitConvert()`.

Two functions convert between biogas mass and volume: `mass2vol()` and `vol2mass()`. These functions are intended for gravimetric measurement of biogas production (`mass2vol()`), and checking for leaks (`vol2mass()`). The `vol2mol()` function facilitates standardization to molar quantity, and is based on molar volume data from NIST [12].

Given the importance of substrate energy content, it is useful to be able to easily determine the oxygen demand of any substrate. The `calcCOD()` function returns the theoretical (or “calculated” [5]) oxygen demand COD’ based on a chemical formula [5]. The `molMass()` function calculates molar mass based on a chemical formula. An internal database of atomic weights is from [13] (for

Table 1

Basic functions in the biogas package.

Operation	Function
Calculate oxygen demand of a compound	<code>calcCOD()</code>
Interpolate composition etc.	<code>interp()</code>
Calculate biogas volume from mass loss	<code>mass2vol()</code>
Calculate molar mass of a compound	<code>molMass()</code>
Standardize gas volume	<code>stdVol()</code>
Calculate mass loss from biogas volume	<code>vol2mass()</code>
Convert gas volume to moles	<code>vol2mol()</code>

“normal materials”). Both functions rely on a hidden function (`readFormula()`) for reading chemical formulas. Interpolation of biogas composition, cumulative production, or any other variable can be done using `interp()`, which provides a simple integrated interface to both linear interpolation and spline functions from the stats package [6].

2.2.2. Functions for biogas data processing

Calculation of BMP (or related measures of biogas production) from laboratory data is done using two functions sequentially: `cumBg()` (for cumulative biogas) and `summBg()` (for summarize biogas). Their use requires some familiarity with the design of BMP experiments [4,14,15]. Inputs, outputs, and operations are shown in Fig. 1. These functions carry out data manipulation, and calls to basic functions perform the necessary conversions.

Input data will generally consist of one or two data files (once in the R environment, data frames), containing original measurements of biogas quantity and composition (“biogas” and “composition” data, respectively (Fig. 1)). All files must contain a unique key to identify individual bottles. Any type of file that can be read by R can be used (spreadsheet files, tab- or comma-delimited text files, and others). Spreadsheets are convenient for data entry, but data import is simpler with text files. Measurement data and related variables such as biogas measurement temperature are passed to `cumBg()` to calculate biogas production. Input and output data are interval-level, meaning each observation corresponds to a single measurement interval. Calculated cumulative CH₄ production is primarily an intermediate object that is used to calculate BMP with `summBg()`. However, some users may work with these data directly to study kinetics, and users interested in BMP may check the shape of the CH₄ production curves by plotting cumulative production. Model fitting and plotting tasks can currently be carried out with functions from other packages.

Measurements may be volumetric [16], manometric [16], gravimetric [9], or gas-chromatography-based [17]. Both cumulative (biogas quantity is the total up to the end of the interval represented by a row in a data frame) and interval (biogas quantity is only that produced during a single interval) data can be handled by `cumBg()`. For most methods, there are two options for calculating CH₄ production. If measured CH₄ concentrations are normalized so the sum of CH₄ and CO₂ concentration is unity, calculations can be based on the volume of gas that exited each bottle [18]. With absolute CH₄ concentrations, production is determined as the sum of the volume of CH₄ that exited the bottle and CH₄ in the bottle headspace. These two methods will give identical results if headspace volume is accurately known and biogas contains only CH₄, CO₂, H₂O, and flushing gas.

Structure of input data is flexible: “wide” and “long” formats [19] can be used for biogas and composition data, or the two can be combined. The default long format is the most flexible (because sampling times may differ among bottles) but the wide format is more compact when measurements are made at fixed times, and is used in the automated AMPTS II system (Bioprocess Control, Lund, Sweden).

The final data file required for calculating BMP (“setup” data (Fig. 1)) is bottle-level, and contains at least the bottle key, a

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