

Standardization of Biochemical Methane Potential Calculations in R

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Summary of an R&D project The purpose of this document is to provide an overview of a R&D project about standardization of biochemical methane potential calculations in R and what products resulted from this project.

As the major product of this R&D project, I created two functions: one for processing manometric measurements and one for processing volumetric measurements. The idea with these functions is to simplify functions within the biogas package, making it easier for new biogas package users to work with and process their data. In the process of creating these functions, a third function was created to enhance the simplification of each new function. The purpose of the third function is to process (sorting and restructuring) all data prior to biogas calculations. To support the new functions, I created help files describing usage of the functions and R scripts for new example datasets (including associated helpfiles) and test files to test the functions. Additionally, I have updated BMP methods documents for volumetric and manometric calculation to include example calculations. This document provides a brief description of the objective of this project and a summary of the work process and topics included.

1 Introduction

Biochemical methane potential (BMP) has become an important number in the biogas industry, as it can reveal essential knowledge of several factors of concern when producing biogas, such as substrate, product and inoculum behavior, or more process related variables (temp., pres., stirring, etc.). It is commonly used to determine the methane potential and anaerobic biodegradability of a given substrate. BMP is a measure of the potential yield of methane (CH_4) from a substrate treated by anaerobic digestion and is most commonly evaluated by monitoring the production of biogas. Several methods are available for measurement of BMP including gravimetric, manometric, volumetric, and gas density approaches. Each method requires a specific set of calculations to go from raw measurements to standardized CH_4 volume, which can then be used to calculate BMP. This R&D project will focus on standardization of BMP calculations and refinement of a software tool for BMP data processing.

The aim of the project is to create and test a volumetric and manometric BMP functions for R, a public environment for statistical computing. These developments will include writing new and improving functions within the already existing biogas package. Testing will include writing R scripts for example datasets from existing Excel sheets (creating csv and Rda files) and evaluating results visual and comparing qualitatively and quantitative with the existing `cumBg` function through analysis of existing data and newly created Rda files.

2 Objective

Results from a recent large inter-laboratory comparison of BMP measurement show that manual volumetric and manometric measurements of biogas production in laboratory experiments are handled differently from one laboratory to another. These different calculation approaches have shown to give minor deviations (up to about 10 percentage in results from the same measurements). In order to eliminate these completely avoidable deviations, a set of standard approaches for calculations is essential. Documentation of a standardized mathematical approach for calculations used for at least one measurement method is one objective of this project.

A newly developed software package for biogas calculations, known as the biogas package, is available for the R environment (Hafner et al., 2018). This package address issues with time-consuming calculations and lack of reproducible among laboratories for obtaining BMP. The biogas package consists of ten function including `cumBg()`, which is used for processing all the types of BMP measurements listed above. The resulting biogas and methane production values and production rates can be further used to calculate BMP. `cumBg()` is a large and rather somewhat complex function, which requires some proficiency in R for use. A second objective of this project is the development of simpler method-specific versions of the `cumBg()` function: one for volumetric data and one for manometric data.

A complete list of project objectives is shown below:

- Contribute to documentation of calculation methods through example calculations.
- Develop new R functions for calculation biogas and methane production and production rates from volumetric and manometric BMP measurements.
- Create related files for testing and documentation of the new functions

3 Project summary

In total, in this project I created: three new R functions and three associated help files, three new R scripts to test functions, four new R datasets from existing Excel files, four associated help files, two vignettes to describe the new

functions, and I also contributed new example calculations to two documents on BMP methods. A complete list is shown below (refer to Table 1). For most documents, existing files were used as a starting point or template for creating the new files: `cumBg()` was the starting point for `cumBgVol()`, `cumBgMan()`, and `cumBgDataPrep()` and `biogas_quick_start.Rnw` was used as a template for the two vignettes `cumBgVol_function.Rnw` and `cumBgMan_function.Rnw`.

The most significant products were the two new functions for calculation of biogas and methane production and production rates from volumetric and manometric BMP measurements. These functions are described in detail (including relevant examples) in two separate vignettes.

This document (project summary) and the two above mentioned vignettes were submitted in lieu of a more classical report.

3.1 Project products

Table 1: Project Products

Topic	Document name
Example datasets for volumetric methods	<code>feedVol</code>
Example datasets for volumetric methods	<code>feedSetup</code>
Example datasets for manometric methods	<code>sludgeTwoBiogas</code>
Example datasets for manometric methods	<code>sludgeTwoSetup</code>
Function for volumetric biogas calculations	<code>cumBgVol()</code>
Function for manometric biogas calculations	<code>cumBgMan()</code>
Function for data preparation	<code>cumBgDataPrep()</code>
Test file for <code>cumBgVol()</code>	<code>cumBgVol.R</code>
Test file for <code>cumBgMan()</code>	<code>cumBgMan.R</code>
Test file for <code>cumBgDataPrep()</code>	<code>cumBgDataPrep.R</code>
Help file for <code>cumBgVol()</code>	<code>cumBgVol.Rd</code>
Help file for <code>cumBgMan()</code>	<code>cumBgVol.Rd</code>
Help file for <code>cumBgDataPrep()</code>	<code>cumBgVol.Rd</code>
Help file for <code>sludgeTwoBiogas</code>	<code>cumBgVol.Rd</code>
Help file for <code>sludgeTwoSetup()</code>	<code>cumBgVol.Rd</code>
Help file for <code>feedVol()</code>	<code>feedVol</code>
Help file for <code>feedSetup()</code>	<code>feedSetup</code>
Example calc. in BMP methods documents (vol)	<code>volumetric_calculations.tex</code>
Example calc. in BMP methods documents (vol)	<code>manometric_calculations.tex</code>
Vignette describing <code>cumBgVol()</code>	<code>cumBgVol_function.Rnw</code>
Vignette describing <code>cumBgMan()</code>	<code>cumBgMan_function.Rnw</code>

References