Calculation of methane production from manometric measurements

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Description

This document describes calculations for manometric measurment of biogas. Two methods are commonly used and both are described here: one based on normalized CH_4 concentrations (method 1) and one that explicitly includes estimation of CH_4 in the bottle headspace (method 2). Expected results from the two methods are identical; differences are due only to error in measurement of biogas composition or headspace volume. Both methods are available through the `cumBg()` function in the biogas package [1] and through the web application OBA (`https://biotransformers.shinyapps.io/oba1/`) and can be easily added to, e.g., a spreadsheet template.

1 Standardization of measured gas volume

Both methods use the same approach for standardization of gas volume. Dry biogas volume in a bottle's headspace before and after venting is calculated by correcting for water vapor, temperature, and pressure. First the volume of headspace gas is converted to dry conditions at standard pressure:

$$V_{dry} = V_{headspace}(P_{meas} - P_{H_2O})/101.325\,\text{kPa} \tag{1}$$

where P_{meas} is the measured headspace pressure and P_{H_2O} the water vapor partial pressure (both in kPa). Eq. (1) is an expression of Boyle's law. The value of P_{H_2O} is assumed to be the saturation vapor pressure prior to venting, and can be calculated using, e.g., the Magnus-form equation given below (Eq. 21 in [2]):

$$P_{H_2O} = 0.61094e^{(17.625T/(243.04+T))} \tag{2}$$

where T is temperature in °C. After venting, when water vapor has been lost and water evaporation has not yet attained equilibrium, relative humidity is taken as the ratio of post- to pre-venting absolute pressure. Volume is then further standardized to 273.15 K by application of Charles's law:

$$V_{std} = V_{dry} 273.15\,\mathrm{K}/T_{meas} \tag{3}$$

where V_{std} is the standardized volume of gas within a bottle's headspace at the time of pressure measurement.

Interval biogas production is calculated as:

$$V_{biogas,i} = V_{std,pre,i} - V_{std,post,i-1} \tag{4}$$

where all V is standardized gas volume in a bottle's headspace, *pre* and *post* refer to before and after venting, respectively, i indicates the current interval and $i-1$ the previous one.

2 Calculation of CH_4 production

2.1 Method 1

In the first method, biogas is assumed to consist of only CH_4 and CO_2 at the time of production (i.e., as produced by the microbial community) and CH_4 production is calculated from vented (removed) biogas only. This method is described in [3]. Coupled with the assumption that all gas production is biogas (Eq. 4), this provides the simplest approach for calculating CH_4 production.

First, concentrations of CH_4 and CO_2 are adjusted so they sum to 1.0:

$$x_{CH_4,n} = x_{CH_4}/(x_{CH_4} + x_{CO_2}) \tag{5}$$

where x_{CH_4} and x_{CO_2} are the measured CH_4 and CO_2 concentrations as volume (mole) fraction (possibly including a correction for water vapor–this has no effect here) and $x_{CH_4,n}$ is the normalized CH_4 volume fraction.

Methane production in an interval i is then calculated as

$$V_{CH_4,i} = x_{CH_4,n} V_{biogas,i} \tag{6}$$

Cumulative production is taken as the cumulative sum of interval values.

2.2 Method 2

Method 2 relies on fewer assumptions, but requires the true concentration of CH_4 (volume fraction) of CH_4 within the bottle headspace, with correction only for water vapor. Here, CH_4 production in an interval has two components: a vented part that is naturally interval, and a residual headspace part, that is naturally cumulative:

$$V_{CH_4,i} = V_{CH_4,v,i} + (V_{CH_4,HSR,i} - V_{CH_4,HSR,i-1}) \tag{7}$$

where the subscript v indicates vented volume and HSR = residual headspace volume (post-venting).

Vented CH_4 is calculated from:

$$V_{CH_4,v,i} = x_{CH_4,n,i} V_{biogas,i} \tag{8}$$

Headspace CH_4 is calculated from:

$$V_{CH_4,HSR,i} = x_{CH_4,n,i} V_{post,i} \tag{9}$$

Cumulative production is taken as the cumulative sum of interval values.

References

[1] 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

[2] Alduchov, O.A., Eskridge, R.E. 1996 Improved Magnus form approximation of saturation vapor pressure. Journal of Applied Meteorology 35: 601-609

[3] Richards, B.K., Cummings, R.J., White, T.E., Jewell, W.J. 1991 Methods for kinetic-analysis of methane fermentation in high solids biomass digesters. Biomass and Bioenergy 1: 65-73