Calculation of methane production from gas density-based measurements

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1 BMP-methods

File version 1.4 - **DRAFT**. This file is from the GitHub repository BMP-methods. For more information, visit BMP-methods at https://github.com/sashahafner/BMP-methods.

2 Description

In the gas density BMP (GD-BMP) method, bottle mass loss and vented biogas volume from one or more time intervals are used to determine biogas density, and from that, composition. With this information, CH_4 production can be calculated from either biogas volume or bottle mass loss. This document describes calculations for the GD-BMP method (Section 3) and provides an example calculation (Section 4).

3 Calculation of CH_4 production

Using Eq. (1), biogas density (d_b, g/mL) is determined by mass loss (Δm_b, g) and standardized biogas volume (V_b, mL), corrected for water vapor content (m_{H_2O}, g/mL) in the gas.

$$d_b = \frac{\Delta m_b}{V_b} - m_{H_2O} \tag{1}$$

Standardized biogas volume is determined from measured vented biogas volume by correcting for moisture, temperature, and pressure, as described in the BMP-methods document on volumetric calculations (Hafner, 2019). Water vapor pressure (P_{H_2O}, kPa) is assumed to be at saturation, and can be calculated using a Magnus-form equation from Alduchov and Eskridge (1996)[1].

$$P_{H_2O} = 0.61094 \cdot e^{\frac{17.625T}{243.04+T}} \tag{2}$$

[1] Other options exist, and will provide nearly identical values

T_{hs} in Eq. 2 indicates the bottle headspace temperature at the time of venting (°C). The mass of the water vapor present in the vented biogas (m_{H_2O}) is then calculated from the molar mass of water (M_{H_2O} = 18.02 g/mol), the partial pressure (P_{H_2O}, kPa), the pressure of biogas in the bottle headspace just prior to venting (P_{hs}, kPa), and the molar volume of biogas at standard conditions (here, 101.325 kPa and 0°C).

$$m_{H_2O} = M_{H_2O} \cdot \frac{P_{H_2O}}{P_{hs} - P_{H_2O}} \cdot \frac{1}{v_b} \tag{3}$$

The molar volume of biogas (v_b) at standard conditions is approximated as 22300 mL/mol (Hafner et al., 2015) and the biogas pressure just prior to venting was assumed to be 150 kPa.

The molar mass of biogas (M_b, g/mol) is then obtained from the density and molar volume of the biogas.

$$M_b = d_b \cdot v_b \tag{4}$$

Finally, the mole fraction of CH_4 in biogas (x_{CH_4}, dimensionless) normalized for CH_4 and CO_2 (x_{CH_4} + x_{CO_2} = unity) is calculated from the normalized difference in molar mass of CO_2 and biogas.

$$x_{CH_4} = \frac{M_{CO_2} - M_b}{M_{CO_2} - M_{CH_4}} \tag{5}$$

From Eq. 5, the content of CH_4 in the biogas is known and can be used for calculation of BMP as with gravimetric or volumetric methods (Hafner et al., 2015). Eq. 5 is based on the assumption that biogas contains only CH_4 and CO_2.

4 Example calculation

In the following example, CH_4 production is calculated from measurements made on a single bottle in a BMP trial. For a complete BMP trial, the standardized biogas volume was 779.2 mL, and the complete total mass loss was 1.070 g.

To find the biogas density (d_b) with equation 1, water vapor partial pressure is first calculated using Eq. (2). The bottle headspace temperature (T_{hs}) was assumed to be 30°C.

$$P_{H_2O} = 0.61094 \cdot e^{\frac{17.625 \cdot 30^\circ C}{243.04 + 30^\circ C}} = 4.237\ kPa$$

Then, following equation 3, the mass of the water vapor (m_{H_2O}) is calculated.

$$m_{H_2O} = 18.016\,\mathrm{g/mol} \cdot \frac{4.237\,\mathrm{kPa}}{150\,\mathrm{kPa} - 4.237\,\mathrm{kPa}} \cdot \frac{1\,\mathrm{mol}}{22\,300\,\mathrm{mL}} = 2.348 \times 10^{-5}\,\mathrm{mg/mL}$$

With m_{H_2O} and measured biogas volume and bottle mass loss, biogas density can be calculated from Eq. (1).

$$d_b = \frac{1.070\ g}{779.2\ mL} - 2.348 \cdot 10^{-5} \frac{g}{mL} = 1.35 \cdot 10^{-3} \frac{g}{mL}$$

The molar mass of biogas (M_b, [g/mol]) is obtained from the density and molar volume of the biogas (eq. 4).

$$M_b = 1.35 \cdot 10^{-3} \frac{g}{mL} \cdot 22300 \ \frac{mL}{mol} = 30.11 \ \frac{g}{mol}$$

The mole fraction of CH_4 (x_{CH_4}, dimensionless) is calculated from the molar masses of the biogas components using Eq. (5).

$$x_{CH_4} = \frac{44.01 \ \frac{g}{mol} - 30.11 \ \frac{g}{mol}}{44.01 \ \frac{g}{mol} - 16.042 \ \frac{g}{mol}} = 0.497$$

References

[1] Hafner, S.D., 2019, Calculation of methane production from volumetric measurements, part of the BMP-methods repository, `https://github.com/sashahafner/BMP-methods`

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

[3] Hafner, S.D., Rennuit, C., Triolo, J.M., Richards, B.K., 2015, Validation of a simple gravimetric method for measuring biogas production in laboratory experiments., Biomass and Bioenergy 83: 297-301