Calculation of Methane Production from Gas Density-Based Measurements*

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1 Introduction

Biochemical methane potential (BMP) can be measured using several different methods. 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. Development and validation of the method is described in Justesen et al. [2019]. This document describes calculations for the GD-BMP method and provides an example calculation.

2 Calculation of methane production

Using Eq. (1), biogas density (ρ_b, g/mL) is determined by mass loss (Δm_b, g) and standardized biogas volume (V_b, mL), corrected for water vapor content

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(c_{H_2O}, g/mL) in the gas.

$$\rho_b = \frac{\Delta m_b}{V_b} - c_{H_2O} \tag{1}$$

Standardized biogas volume is determined from measured vented biogas volume by correcting for moisture, temperature, and pressure, as described in the BMP-methods document 201, on volumetric calculations [Hafner et al., 2020]. 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].

$$p_{H_2O} = 0.61094 \cdot e^{\frac{17.625 T_{hs}}{243.04 + T_{hs}}} \tag{2}$$

T_{hs} in Eq. (2) indicates the bottle headspace temperature at the time of venting (°C). The concentration of the water vapor present in the vented biogas (c_{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, dry, 101.325 kPa, and 0°C).

$$c_{H_2O} = M_{H_2O} \cdot \frac{p_{H_2O}}{p_{hs} - p_{H_2O}} \cdot \frac{1}{v_b} \tag{3}$$

The molar volume of biogas (v_b) at standard conditions is approximated as 22300 mL/mol [Hafner et al., 2015].

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 density of CO_2 and biogas[2].

$$x_{CH_4} = \frac{\rho_{CO_2} - \rho_b}{\rho_{CO_2} - \rho_{CH_4}} \tag{4}$$

In Eq. (4) ρ_{CH_4} and ρ_{CO_2} are pure gas densities at standard conditions, which are 0.0007174 and 0.001977 g mL^{-1} for CH_4 and CO_2, respectively. From Eq. (4), 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. (4) is based on the assumption that biogas contains only CH_4 and CO_2. Over a complete BMP incubation, this is generally a reasonable approximation, but a correction is available [Justesen et al., 2019].

3 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 [Hafner et al., 2020] was 779.2 mL, and the complete total mass loss was 1.070 g.

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

[2] In the original work [Justesen et al., 2019] molar mass was calculated as an intermediate step, but this is not needed.

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

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

Then, following Eq. (3), the concentration of the water vapor ($c_{\mathrm{H_2O}}$) is calculated.

$$c_{\mathrm{H_2O}} = 18.016\,\mathrm{g\ mol^{-1}} \cdot \frac{4.237\,\mathrm{kPa}}{150\,\mathrm{kPa} - 4.237\,\mathrm{kPa}} \cdot \frac{1\,\mathrm{mol}}{22300\,\mathrm{mL}} = 2.348 \cdot 10^{-5}\,\mathrm{g\ mL^{-1}}$$

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

$$\rho_b = \frac{1.070\,\mathrm{g}}{779.2\,\mathrm{mL}} - 2.348 \cdot 10^{-5}\,\mathrm{g\ mL^{-1}} = 1.349 \cdot 10^{-3}\,\mathrm{g\ mL^{-1}}$$

The mole fraction of $\mathrm{CH_4}$ ($x_{\mathrm{CH_4}}$, dimensionless) is calculated from the density of the biogas components using Eq. (4).

$$x_{\mathrm{CH_4}} = \frac{1.977 \cdot 10^{-3}\,\mathrm{g\ mL^{-1}} - 1.349 \cdot 10^{-3}\,\mathrm{g\ mL^{-1}}}{1.977 \cdot 10^{-3}\,\mathrm{g\ mL^{-1}} - 7.174 \cdot 10^{-4}\,\mathrm{g\ mL^{-1}}} = 0.498$$

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