# Calculation of methane production from gas density-based measurements*

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## 1 Introduction

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 and provides an example calculation.

## 2 Calculation of methane production

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

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

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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].

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

$T_{hs}$ 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, dry, 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 $CO_2$.

# 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 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.

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

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

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