A mechanistic model of hydrogen–methanogen dynamics in the rumen

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HIGHLIGHTS

- Model describes growth of rumen methanogens in relation to dissolved hydrogen.
- Explicit depictions of methanogen population and dissolved hydrogen pool.
- Model behaves according to biological expectations.
- Can be expanded to model multiple methanogen species with different characteristics.
- Hydrogen pool allows future incorporation of hydrogen feedback on fermentation.

ARTICLE INFO

ABSTRACT

Existing mathematical models to estimate methane production in the rumen are based on calculation of hydrogen balances without considering the presence of methanogens. In this study, a mechanistic model of methane production is proposed that depicts the interaction between hydrogen concentration and methanogens in the rumen. Analytical results show that it meets biological expectations, namely increased fractional passage rate leads to a greater growth rate of methanogens, and a greater steady state hydrogen concentration. This model provides a basis on which to develop a more comprehensive model of methane production in the rumen that includes thermodynamics and feed fermentation pathways.

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1. Introduction

The rumen is part of the digestive tract of ruminants (e.g., cattle, sheep and deer). Feed ingested by ruminants is fermented by microbes in the rumen. Feed and microbes pass through the rumen as ruminants keep ingesting feed, with the flow of material out of the rumen being commonly described as the passage or outflow rate. The microbes colonizing the rumen need to reproduce at a rate that replaces those washed out from the rumen, otherwise their populations would be eliminated. The main end products from the primary fermentation of feed are volatile fatty acids and microbial cells. These fermentation products are used by the ruminant as energy and amino acids sources, and converted into animal products (e.g., milk, wool and meat). This primary fermentation process also generates hydrogen, which is used by methanogens (a group of microbes in the rumen) to produce methane in a reaction that yields energy for the methanogens.

Methane cannot be used by ruminants. The methane emitted from the rumen to the atmosphere is a greenhouse gas (GHG). Globally, ruminants are a significant source of GHG (Ripple et al., 2014) and animal-derived protein for human consumption in the form of meat and milk products. There is growing interest in reducing the GHG emissions, while maintaining animal productivity. Thus, the long-term sustainable prosperity of pastoral agriculture requires the development of strategies to reduce GHG emissions, relative to animal product output.

Suitable mathematical models of rumen function can be cost-effective tools to support experimentation with animals for exploring mitigation strategies. There are two types of mathematical models of ruminal methane production: empirical and mechanistic. Empirical models are developed by fitting equations to experimental data and estimate methane production based on regression functions, e.g., Ellis et al. (2009); Kriss (1930); Moe and Tyrrell (1979). Mechanistic models, such as those developed by Benchaar et al. (1998) and Mills et al. (2001), estimate methane production as a stoichiometric function of the hydrogen balance of the rumen. This balance is defined as the difference between the amounts of hydrogen produced and used in reactions occurring in

the rumen. Existing empirical and mechanistic models of methane production from rumen have 20% to 50% prediction error (Ellis et al., 2010; Kebreab et al., 2008; Legesse et al., 2011) which is too large to explore potential methane mitigation strategies via modeling alone.

The model presented here represents methanogen growth using functions similar to those described for fermentative bacteria in the models of Baldwin et al. (1987) and Dijkstra et al. (1992). An advantage of representing methanogen growth using Monod kinetics (Monod, 1949) is that it allows a dynamic representation of the dissolved hydrogen pool in the rumen, which has been postulated as an area for improvement in current rumen models (Ellis et al., 2008). Because the dissolved hydrogen concentration is a key controller of fermentation pathways (Janssen, 2010), a model that describes the interaction between methanogen growth and hydrogen has utility beyond the estimation of methane, as it provides an alternative approach to current representation of fermentation based on stoichiometric profiles from feed components (e.g., Baldwin et al., 1987; Dijkstra et al., 1992). Such an approach could help overcome other known limitations of current models of rumen function, such as the prediction of volatile fatty acid profiles (Ellis et al., 2008; Morvay et al., 2011). Offner and Sauvant (2006) developed models with explicit dissolved hydrogen pool and methanogens, but their model does not directly describe the interactions between hydrogen and methanogens. A model of hydrogen–methanogen interactions could be introduced into current models to provide the basis for both the prediction of methane and the representation of the feedback of hydrogen on fermentation pathways in the rumen. In this paper we described such a model, and tested the mathematical enunciation for consistency with biological expectations described in the conceptual framework proposed by Janssen (2010).

2. Model

2.1. Assumptions

1. Methanogens and hydrogen are *uniformly distributed* in the rumen liquid contents.
2. Methanogens capture hydrogen *randomly with no competition* among methanogens for hydrogen.
3. *No other microbes compete* for hydrogen with the methanogens.
4. Hydrogen is the *only* energy source of methanogens, which *instantaneously* metabolize hydrogen to gain energy (i.e., adenosine triphosphate, ATP).
5. *Each methanogen cell* metabolizes hydrogen at the *same rate* to generate ATP and needs the *same* amount of ATP for maintenance.
6. The ATP generated is used either to maintain existing methanogens *or* to reproduce, and new methanogens are *biologically identical* to existing methanogens.
7. Methanogens cannot reproduce unless there is an *excess* of ATP beyond what is needed for their maintenance.
8. Hydrogen is lost through consumption by methanogens *or* exiting from the rumen (passage rate).
9. Methanogens are lost by either passage rate *or* "starvation" (i.e., there are no predators).
10. The passage rate in the rumen is *constant*.
11. The hydrogen generation rate in the rumen is *constant*.

These assumptions are a simplified representation of the complex nature of the rumen function. For example, methanogens can attach to the rumen epithelium and feed particles and so have passage rates different to the liquid; there are multiple types of

methanogens that compete for hydrogen and with different substrate requirements (Ellis et al., 2008); hydrogen can escape the rumen by eructation (Takenaka et al., 2008); rates of passage and hydrogen generation are not constant. Rather than trying to incorporate this complexity in this paper, we propose that implementation of our work into models of whole rumen function could be an alternative approach to address more complex assumptions.

2.2. Model formulation

Methane produced in the rumen is formed from the consumption of hydrogen by methanogens (Janssen, 2010). The chemical reaction is

$$4H_2 + CO_2 \rightarrow CH_4 + 2H_2O. \tag{1}$$

There is an excess of carbon dioxide in the rumen (McArthur and Miltimore, 1961) and hydrogen is the limiting energy source for methanogens. Thus, in our model, the reproduction of methanogens and hence growth of the methanogen population is dependent on hydrogen as the growth rate-limiting substrate, and the Monod model of microbial growth (Monod, 1949) can be adapted to model the rate of hydrogen metabolism by methanogens as a function of the hydrogen concentration.

Let S_h be the dissolved hydrogen concentration (mol_h ml^{-1}) and X_m be the methanogen population density (cell ml^{-1}) in the rumen liquid at time t. S_h' (mol_h ml^{-1} s^{-1}) and X_m' (cell ml^{-1} s^{-1}), are the *rates of change* of hydrogen concentration and methanogen population density, respectively. Here ' denotes differentiation with respect to time. Subscripts h and m indicate that the parameters are related to hydrogen and methanogens, respectively. Let q (mol $cell^{-1}$ s^{-1}) be the rate at which a methanogen metabolizes hydrogen. From the Monod model, the rate of hydrogen metabolism at a given hydrogen concentration is

$$q = \frac{q_m}{K_m + S_h} S_h \; (mol_h \; cell^{-1} \; s^{-1}), \tag{2}$$

where q_m (mol_h $cell^{-1}$ s^{-1}) is the maximal rate at which a methanogen can metabolize hydrogen and K_m (mol_h ml^{-1}) is the hydrogen concentration at half of q_m. Under assumptions 1–5, the hydrogen consumed by X_m methanogens is

$$qX_m = \frac{q_m}{K_m + S_h} S_h X_m \; (mol_h \; ml^{-1} \; s^{-1}). \tag{3}$$

Let α (s^{-1}) denote the (fractional) passage rate through the rumen. Then, the hydrogen concentration will decrease by αS_h per unit of time due to passage of dissolved hydrogen in the liquid that exits from the rumen. Let β_h (mol_h ml^{-1} s^{-1}) denote the hydrogen generation rate. Thus, S_h' is the sum of the loss of hydrogen metabolized by methanogens and passage rate, and the hydrogen generation rate in the rumen is

$$S_h' = -\frac{q_m}{K_m + S_h} S_h X_m - \alpha S_h + \beta_h \; (mol_h \; ml^{-1} \; s^{-1}). \tag{4}$$

Methanogens gain n_m (mol_{ATP} mol_h^{-1}) amount of ATP per unit of hydrogen metabolized. The total ATP gained for the whole methanogen population is

$$\frac{n_m q_m}{K_m + S_h} S_h X_m \; (mol_{ATP} \; ml^{-1} \; s^{-1}). \tag{5}$$

Let m_m (mol_{ATP} $cell^{-1}$ s^{-1}) be the maintenance requirement for ATP of a single methanogen per unit of time. Assumption 5 indicates that the total maintenance requirement of X_m methanogens is $m_m X_m$. The net ATP available, Δ, is thus

$$\Delta = \frac{n_m q_m}{K_m + S_h} S_h X_m - m_m X_m = \Delta_m X_m \; (mol_{ATP} \; ml^{-1} \; s^{-1}), \tag{6}$$