## Biochemical rumen functions: facts and modelling

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Modelling is an integral part of the scientific method in nutritional research. A mathematical equation or model can be viewed as an idea, hypothesis or relation expressed in mathematics. Models of rumen function aim at an improved prediction of fermentation in the rumen for practical purposes (e.g., microbial representations in protein evaluation systems) or at an improved understanding and integration for research purposes. Such quantitative approaches may be broadly classified into empirical and mechanistic models. Empirical models use experimental data to quantify relationships directly. In contrast, mechanistic models are constructed by examining the structure of a system and analysing the behaviour of the system in terms of its individual components and their interactions. This contribution considers models of rumen fermentation processes with special emphasis on methanogenesis.

Methane, in addition to being a significant source of energy loss to the animal that can range from 0.02 to 0.12 of gross energy intake in ruminants, is one of the major greenhouse gases (GHG). Methane is produced predominantly in the rumen and to a small extent in the large intestine of ruminants. Conversion of feed material to methane in the rumen involves the integrated activities of several different microbial species, the final step being carried out by methanogenic archaea. Various empirical models to predict methane emissions have been developed based on commonly measured dietary inputs or animal characteristics including body weight and milk production. The importance of evaluating GHG emissions from dairy cows within the whole farm setting is being realized as more important than evaluating these emissions in isolation. Thus, such empirical models provide a tool for evaluating methane mitigation strategies in whole farm models. Recently, the performance of nine methane prediction equations that are currently being used in whole farm GHG models have been evaluated against actual observed methane production of dairy cattle. In general, predictions are poor. Results show that the simple more generalized equations perform worse than those that attempt to represent important aspects of diet composition, but in general significant amounts of bias and deviation of the regression slope from unity exist for all equations. The low prediction accuracy of empirical methane prediction models in whole farm models may introduce substantial error into inventories of GHG emissions and lead to incorrect mitigation recommendations.

The impact of mitigation strategies to reduce methane emissions has to be assessed holistically, and empirical models lack the biological basis for such an assessment. Various mechanistic models have been developed that account for the most important features of ruminal digestion and microbial metabolism. The majority of dynamic mechanistic models appearing in the nutritional literature are based on systems of ordinary differential equations. The standard way of representing such models is the rate: state formalism. The system is defined by a number of state variables and a set of differential equations describe the change of the state variables with time. In general, the differential equations are formed through direct application of the laws of science (for example, the law of mass conservation, the first law of thermodynamics) or by application of a continuity equation derived from more fundamental scientific laws. Several mechanistic models of rumen function contain a hydrogen gas balance sub-model from which methane can be predicted. Central to methane prediction in these mechanistic models is the accurate prediction of hydrogen production from fermentation of substrates to volatile fatty acids (VFA) and subsequent hydrogen utilization for various purposes. The representation of VFA stoichiometry is likely to have the largest impact on methane prediction. In recent developments, the type of VFA formed is related to the type of substrate fermented, and further improvements include the introduction of pH-dependent stoichiometric parameters for rapidly fermentable carbohydrates. These mechanistic models predict methane production more accurate than linear empirical models, but benefit from further development. Mechanistic models are important tools for assessing mitigation options and for directing experimental research towards options most likely to result in significant reduction of methane emissions from enteric fermentation.