Accuracy Analysis of Stoichiometric Models for Predicting Rumen Volatile Fatty Acid Composition in Chinese Lactating Dairy Cows (Postprint)

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Date: 2018-12-24T00:00:00+00:00

Abstract

This study aimed to evaluate the accuracy of stoichiometric models in predicting rumen volatile fatty acid (VFA) composition in Chinese lactating dairy cows and analyze the reasons affecting model prediction accuracy. This study selected three classic dairy cow rumen VFA models, namely the MUR model, DIJ model, and BAN model. Experimental data were obtained from 18 papers by major Chinese research teams, including 14 SCI papers, 3 Chinese core journal articles, and 1 unpublished English article. The paper data included animal diet, body weight, dry matter intake, feed additives, and proportions of VFA components. Two analytical methods, mean square prediction error (MSPE) and concordance correlation coefficient (CCC), were used to evaluate and analyze the estimation accuracy of the three classic dairy cow rumen VFA models. The results showed that the BAN model had the highest estimation accuracy for acetate proportion (coefficient of determination = 0.140, P = 0.007), with a root mean square prediction error of 6.8%, and the error mainly originated from deviation of overall bias (47.8%). The three models were unable to predict the proportions of propionate, butyrate, and other acids. In conclusion, the BAN model had the highest accuracy in predicting acetate proportion among the three models, but the prediction accuracy was still low, with errors originating from deviation of overall bias. There is an urgent need to establish VFA stoichiometric prediction models suitable for China' s national conditions using more data.

Full Text

Accuracy Analysis of Stoichiometric Models for Predicting Ruminal Volatile Fatty Acid Composition in Chinese Lactating Dairy Cows

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Abstract

This study evaluated the prediction accuracy of stoichiometric models for ruminal volatile fatty acid (VFA) profiles in Chinese lactating dairy cows and analyzed factors influencing model precision. Three classical ruminal VFA stoichiometric models were selected: the MUR model, DIJ model, and BAN model. Experimental data were compiled from 18 studies published by major Chinese research teams, comprising 14 SCI papers, 3 Chinese core journal articles, and 1 unpublished English manuscript. The dataset included information on animal diets, body weight, dry matter intake, feed additives, and VFA component proportions. Two analytical methods—mean squared prediction error (MSPE) and concordance correlation coefficient (CCC)—were employed to assess the prediction accuracy of the three models. The results indicated that the BAN model achieved the highest accuracy for acetate proportion estimation ($R^2 = 0.140$, $P = 0.007$) with a root mean squared prediction error of 6.8%, though error primarily stemmed from overall bias deviation (47.8%). None of the three models could satisfactorily predict propionate, butyrate, or other acid proportions. In conclusion, while the BAN model demonstrated the highest precision for acetate prediction among the three models, its overall accuracy remained low with errors derived from overall bias deviation. There is an urgent need to develop VFA stoichiometric prediction models tailored to Chinese conditions using more comprehensive datasets.

Keywords: volatile fatty acids; model; mean squared prediction error; concordance correlation coefficient; lactating dairy cows

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Volatile fatty acids (VFAs) are fermentation products of dietary carbohydrates by rumen microorganisms and represent the primary energy source for ruminants, supplying 70–80% of their energy requirements. VFAs include acetate, propionate, butyrate, and other short-chain fatty acids, with acetate, propionate, and butyrate accounting for 95% of total VFA production in the rumen. Acetate and butyrate serve as precursors for fat synthesis, while propionate is a key precursor for gluconeogenesis in ruminants. According to Brunette et al. and Seymour et al., ruminal VFA proportions significantly influence milk yield, milk protein content, and milk fat content in dairy cows, playing a critical role in maintaining normal energy metabolism.

Mathematical models for ruminal VFA proportions in dairy cows include empirical models and mechanistic models, with the latter also known as stoichiometric models. Compared to empirical models, stoichiometric models incorporate both the effective degradation rates of dietary chemical components in the rumen and conversion coefficients among VFA components, thereby better reflecting the relationship between dietary composition and ruminal VFA profiles. Consequently, international scholars have developed models to predict ruminal VFA proportions based on dietary chemical components. However, the accuracy of these models varies considerably when applied to different regions and time periods. Currently, few studies have utilized these models to estimate ruminal VFA proportions in Chinese lactating dairy cows.

In 1982, Murphy et al. developed the first international stoichiometric model (MUR model) using five chemical components through infinite iteration and least squares methods. In 1992, Dijkstra et al. enhanced the MUR model by incorporating ruminal pH and VFA absorption rates, creating the DIJ model. In 2006, Bannink et al. further refined the DIJ model by introducing biochemical pathways of VFA production, establishing the BAN model. This study aims to evaluate the accuracy of these three classical models in predicting ruminal VFA proportions in Chinese lactating dairy cows and to explore factors affecting model precision. By reviewing published studies from Chinese researchers and compiling data on animal body weight, dry matter intake, dietary components, and VFA profiles, we employed MSPE and CCC methods to assess the prediction accuracy of the three models. The findings will contribute to the selection and development of stoichiometric models suitable for predicting ruminal VFA profiles in Chinese dairy cows.

1.1 Model Selection

Three classical ruminal VFA stoichiometric models for ruminants were selected: the MUR model, DIJ model, and BAN model. According to the data requirements of each model, diets were classified into concentrate diets (C diets, concentrate proportion 50%) and forage diets (R diets, concentrate proportion $<$ 50%). Common parameters required by all three models included: contents of five major dietary chemical components (soluble carbohydrates, starch, cellulose, hemicellulose, and crude protein), intake levels, ruminal effective degradation rates of these five components, and ruminal VFA proportions. All three models employed infinite iteration and least squares methods to establish conversion coefficients between the five chemical components (independent variables) and VFA proportions (dependent variables).

1.2 Dairy Cow Experimental Data

Chinese and English articles were retrieved from CNKI and Web of Science, respectively, using search terms including "dairy cows," research team names, and institutional affiliations, with publication dates ranging from 2000 to 2016. The research teams and institutions included: Tan Zhiliang (Institute of Subtropical Agriculture, Chinese Academy of Sciences), Wang Jiaqi (Institute of Animal Science, Chinese Academy of Agricultural Sciences), Liu Jianxin (Zhejiang University), Diao Qiyu (Institute of Feed Research, Chinese Academy of Agricultural Sciences), Li Shengli (China Agricultural University), Meng Qingxiang (China Agricultural University), Wang Hongrong (Yangzhou University), and Zhu Weiyun (Nanjing Agricultural University). The searches yielded 10, 7, 5, 16, 7, 12, 2, and 2 Chinese articles, and 2, 12, 32, 1, 19, 2, 2, and 2 English articles, respectively. Only lactating dairy cow feeding trials were retained (excluding 2 calf studies), and articles had to provide data on animal diets, body weight, dry matter intake, feed additives, and VFA component proportions. Additionally, studies with acetate proportions exceeding 70% in C diets were excluded (1 article). The final dataset comprised 14 SCI papers, 3 Chinese core journal articles, and 1 unpublished manuscript from Tan Zhiliang' s team. The utilized studies included: 1 from Tan Zhiliang (Wang et al.), 7 from Wang Jiaqi (Wang et al., Sun et al., Yang et al., Peng et al., Guo et al., Pan et al., and Zhao et al.), 2 from Liu Jianxin (Wang et al., Zhang et al.), 6 from Li Shengli (Zhang et al., Zeng et al., Guo et al., Sun et al., Chen et al., Cao et al.), and 1 from Zhu Weiyun (Wang et al.).

1.3 Dietary Information

Among the 17 published and 1 unpublished Chinese studies, nutrient composition in Chinese core journal articles was determined according to methods described by Zhang Liying, while organic matter (OM), crude protein (CP), ash, and ether extract (EE) in 13 English articles were analyzed following AOAC methods. Neutral detergent fiber (NDF) and acid detergent fiber (ADF) contents were measured using Van Soest et al.' s methods. For 3 articles lacking complete dietary component information, values were estimated using the International Tables of Feed Composition for Ruminants and the CNCPS System Evolution Model and Feed Composition Tables. Soluble carbohydrates, hemicellulose, and cellulose were calculated using the following formulas:

Soluble carbohydrates = OM - EE - starch - NDF - CP
Hemicellulose = NDF - ADF
Cellulose = ADF - acid detergent lignin (ADL)

1.4 Rumen Effective Degradation of Dietary Components

The selected models require ruminal effective degradation amounts of the five major chemical components. Effective degradation was calculated using rumen passage rate, rapidly degradable fraction, and slowly degradable fraction. The calculation formula was:

$P_t = a + b \times \frac{c}{c+k} \times e^{-(c+k)t}$

Where: P_t is the effective degradation of a chemical component (%); a is the rapidly degradable fraction content (%); b is the slowly degradable fraction content (%); c is the ruminal degradation rate (h ^{1}); k is the ruminal passage rate (h ^{1}); and t is time (set at 24 h).

Ruminal passage rates for dietary components were estimated using Fox et al.' s model:

$k_{forage} = 3.362 + 0.479 \times DMI - 0.017 \times BW^{0.75} - 0.007 \times F$
$k_{concentrate} = 2.904 + 1.375 \times DMI - 0.020 \times BW^{0.75} - 0.008 \times F$

Where: k_{forage} is the passage rate of forage (h ^{1}); $k_{concentrate}$ is the passage rate of concentrate (h ^{1}); DMI is dry matter intake (kg/d); $BW^{0.75}$ is metabolic body weight (kg); and F is the proportion of forage in the diet (%).

1.5 Model Analysis

This study employed MSPE and CCC methods to evaluate the prediction accuracy of the three models. The MSPE analysis comprises three components: error due to overall bias (ECT), error due to regression slope deviation from unity (ER), and random error (ED), expressed as percentages of observed values. The CCC analysis includes four components: bias correction factor (Cb), correlation coefficient between predicted and observed values (r), ratio of standard deviations (v), and shift in location (u). Calculation formulas for both methods followed Xie Tianyu. Linear regression analysis between observed and predicted VFA values and between residuals and predicted values was performed using SPSS 18.0, with significance set at $P < 0.01$.

2.1 Summary of Dairy Cow Dietary Information

Data on cow body weight, diet composition, and dry matter intake are summarized in Table 1 . Dry matter intake ranged from 10.5 to 24.0 kg/d, averaging 17.6 kg/d. Body weight ranged from 474 to 700 kg, averaging 560 kg. The C diet group had higher starch content (172-387 g/kg) and lower NDF content (253-539 g/kg) compared to the R diet group (86-244 g/kg starch and 371-521 g/kg NDF).

2.2 Effective Rumen Degradation of Five Major Dietary Components

The ranges of effective ruminal degradation for soluble carbohydrates, starch, cellulose, hemicellulose, and crude protein were 0.60-3.13, 1.37-3.52, 0.59-2.59, 0.46-1.42, and 0.33-1.99 kg/d, respectively, in the C diet group, and 0.74-2.73, 0.96-2.55, 0.80-1.43, 0.38-1.16, and 0.66-1.75 kg/d, respectively, in the R diet group (Table 2).

2.3 Summary of VFA Component Proportions

Measured ruminal VFA proportions were as follows: acetate ranged from 57.2% to 72.9% (mean 65.5%); propionate ranged from 15.5% to 25.4% (mean 20.2%); butyrate ranged from 7.5% to 13.6% (mean 11.0%); and other acids (including valerate, isovalerate, and isobutyrate) ranged from 0.8% to 9.6% (mean 4.1%) (Table 2).

2.4 MSPE Analysis Results

As shown in Table 3 and Figure 1 [Figure 1: see original paper], the BAN model exhibited the smallest RMSPE for acetate proportion (6.8%) and the largest coefficient of determination ($R^2 = 0.140$). The MUR model showed the largest RMSPE (21.6%). The regression line between predicted and observed values for the BAN model was closest to the 1:1 standard line, with error primarily attributed to overall bias deviation (47.8%). All three models failed to predict propionate, butyrate, and other acid proportions, with R^2 values below 0.100 and no significant correlations ($P > 0.01$).

2.5 Residual Analysis Results

Linear regression results between residuals and predicted values are presented in Table 4 . The slopes and intercepts of regression equations for residuals versus predicted values differed significantly from zero ($P < 0.01$) for acetate, propionate, and other acids in the MUR and DIJ models, and for propionate in the BAN model. The R^2 values for these relationships ranged from 0.019 to 0.749.

2.6 CCC Analysis Results

As shown in Table 5 and Figure 2 [Figure 2: see original paper], the BAN model achieved the highest CCC value for acetate proportion (0.178), while the MUR model had the lowest (0.044). The regression equation for residuals versus predicted values in the BAN model was closest to the zero standard line. For propionate, butyrate, and other acids, all models exhibited CCC values below 0.120, with regression lines crossing the zero standard line. The Cb values for propionate prediction exceeded 0.200 across all models, with u values below zero, indicating systematic overestimation of propionate proportions.

3 Discussion

Alemu et al. evaluated four VFA models using 141 datasets from dairy cows and reported low prediction accuracy for the MUR model, consistent with our findings. In this study, the MUR model yielded R^2 values below 0.1 with no significant correlations. MSPE component analysis revealed that overall bias and slope errors accounted for over 50% of prediction errors for acetate, propionate, butyrate, and other acids. Residual plots showed clear deviation from the zero standard line, with significant differences in slope and intercept for acetate, propionate, and other acids. The MUR model does not account for VFA production rates, interconversions, or absorption rates. Furthermore, it was developed using VFA data from beef cattle and sheep. Chamberlain et al. and Loncke et al. demonstrated that the acetate-to-propionate ratio differs between beef cattle and sheep, with higher ratios in beef cattle. Morvay et al. evaluated six VFA models using 101 dairy cow datasets and concluded that models based on beef cattle and sheep data poorly predict VFA profiles in dairy cows. Therefore, the low accuracy of the MUR model in this study can be attributed to two factors: (1) the model' s failure to consider VFA production rates, interconversions, and absorption; and (2) the inappropriateness of conversion coefficients derived from beef cattle and sheep data for dairy cow applications.

Dijkstra et al. recognized that a portion of ruminal VFAs is absorbed by the rumen wall, leading the DIJ model to incorporate absorption rates for acetate, propionate, butyrate, and other VFAs as reported by Hogan and Danielli. The model also included ruminal pH as a factor influencing VFA production. However, our CCC analysis revealed low prediction accuracy for the DIJ model (all values below 0.160) with R^2 values below 0.100 and no significant correlations. Residual plots showed marked deviation from the zero standard line, with significant slope and intercept differences for acetate, propionate, and other acids. Additionally, distinct stratification was observed between R and C diets for acetate, propionate, and other acids. Bannink et al. similarly reported low accuracy for the DIJ model and observed stratification between diet types when evaluating three models with dairy cow data. The poor performance of the DIJ model may stem from: (1) consideration of VFA absorption rates without accounting for interconversions and production rates; and (2) failure to incorporate the influence of microbial fermentation biochemical pathways on VFA proportions.

The BAN model introduced biochemical pathways of hexose degradation to VFA components. For instance, 1 mol of carbohydrate hexose units (from soluble carbohydrates, starch, cellulose, hemicellulose) degrades to produce 2 mol of acetate and propionate, and 1 mol of butyrate and other acids, while 1 mol of protein is equivalent to 0.55 mol of carbohydrate hexose. Consequently, the BAN model multiplied the conversion equations for the five chemical components to acetate and propionate by 2. The model also incorporated VFA absorption and passage rates. By refining the biochemical processes of ruminal hexose degradation, the BAN model improved VFA proportion prediction accuracy. Morvay et al. reported that the BAN model enhanced acetate prediction accuracy compared to the MUR and DIJ models, consistent with our results. In this study, the regression between predicted and observed acetate proportions was significant, and both MSPE and CCC analyses confirmed that the BAN model achieved the highest acetate prediction accuracy among the three models.

However, despite improved acetate prediction, the BAN model' s overall accuracy remained low (CCC < 0.200, $R^2 < 0.200$). MSPE component analysis indicated that overall bias and slope errors exceeded 45% of total prediction error. Previous research has confirmed that ruminal VFA proportions are influenced by dietary chemical components. In this study, starch intake in both C and R diet groups was lower than that used in the BAN model development, while NDF content was higher than in the original BAN model diets, reflecting lower feeding levels in Chinese dairy production compared to the Netherlands. Additionally, the BAN model assumed identical absorption and passage rates for all VFA components. Murphy reported that VFA absorption rates increase with carbon chain length, suggesting this assumption may overestimate acetate proportions and compromise model accuracy.

4 Conclusion

1. Although the BAN model achieved the highest accuracy for acetate proportion prediction, its precision remained low, with errors primarily derived from overall bias deviation.

2. The MUR, DIJ, and BAN models were unable to predict propionate, butyrate, and other acid proportions.

3. All three models were developed using data from foreign dairy farms and are unsuitable for estimating ruminal VFA composition in Chinese dairy cows. There is an urgent need to develop VFA stoichiometric prediction models tailored to Chinese conditions using more extensive datasets.

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Note: Figure translations are in progress. See original paper for figures.