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Assessing the predictive capabilities of a dynamic mechanistic model of *in vitro* rumen fermentation and methane production

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Application Mathematical modelling of rumen *in vitro* fermentation offers a potential tool for the design of methane mitigation strategies.

Introduction We have previously developed a mechanistic dynamic model of *in vitro* rumen fermentation (Muñoz-Tamayo *et al.*, 2016). The model was efficient to represent calibration data from experiments using rumen inocula from goats. The objective of this work was to assess further the robustness of the model by challenging the model against an independent data set.

Material and methods The experimental data set was obtained using rumen inocula sampled from the rumen of two cannulated dry cows fed at maintenance. Five total mixed rations (TMR) were collected from different dairy farms and characterized for chemical parameters, along with NDF, crude protein and starch degradability rates determined by previously developed enzymatic based methods (Gallo et al. 2018). Each TMR was incubated in diluted rumen fluid. The dynamics of fermentation were tracked at six sampling times (2, 5, 9, 24, 36, and 48 h) by measuring gas production and composition, as well as the concentrations of acetate, butyrate, propionate, and ammonia. The developed mathematical model (Muñoz-Tamayo *et al.*, 2016) was calibrated using volatile fatty acids (VFA) and CH₄ data. Model calibration was performed with the IDEAS Matlab toolbox (Muñoz-Tamayo *et al.*, 2009) using a maximum likelihood estimator.

Results The figure 1 shows the experimental data for one TMR compared against the model predicted variables. The model represented satisfactorily VFA concentrations and CH₄ production with Lin's concordance correlation coefficient (CCC) of 0.93 in average. We further assessed whether the hydrolysis rate constants of dietary carbohydrates and proteins determined enzymatically could be used as known parameters in the model while keeping satisfactory predictions. When using the enzymatically determined hydrolysis rate constants, the CCC was in average of 0.89. indicating the need of further improvements.



Figure 1. Experimental data of rumen fermentation (•) are compared against model predicted responses (-). Ac = Acetate; Bu = butyrate; Pr = Propionate.

Conclusion The model evaluation performed in this work strengthen the capabilities of our model structure to predict the *in vitro* fermentation pattern and CH₄ production from rumen microbiota. Further model extensions are currently undertaken to enhance the model capabilities for the assessment of strategies for methane mitigation.

References

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