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**Microbial co-existence and stable equilibria
in a mechanistic model of enteric methane
production**

A thesis presented in partial fulfillment of the requirements
for the degree of

Doctor of Philosophy

in

Mathematics

at Massey University, Manawatū Campus,
New Zealand

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2016

Abstract

Globally, 14.5% of all anthropogenic greenhouse gases come from ruminants. One of these is methane, which is produced in the rumen of ruminant animals. Feed is degraded by microbes to produce volatile fatty acids (which are absorbed by the animal) and hydrogen (which is metabolized by methanogens to form methane). The dynamics of hydrogen production and metabolism are subject to thermodynamic control imposed by the hydrogen concentration. Existing models to estimate methane production are based on calculation of hydrogen balances without considering the presence of methanogens and do not include thermodynamic control. In this project, a model is developed based on glucose-hydrogen-methanogen dynamics to estimate methane production and illustrates a co-existence of microbes that employs different fermentation pathways competing for the same food source in the rumen. Glucose was chosen as an example of a fermentable feed component. A thermodynamic term was integrated into a Monod-type model to represent the thermodynamic control of hydrogen concentration on the rates of hydrogen generation and hydrogen metabolism. Results of this model suggest that the microbial community composition and the combination of the different pathways are determined by the rumen environment, biological parameters of the microbes and the feedback imposed by substrate and product concentrations. The mathematical enunciation of this model is therefore consistent with biological expectations. This model could be expanded to include plant polymer degradation rate, feeding level and feeding frequency to explore their effects on methane production. This model could also be integrated into models of whole rumen function to address more complex questions. It would also support experimentation

with animals for understanding factors that control methane formation and to explore methane mitigation strategies.

Acknowledgements

This project would not have been possible without the contributions of people along the journey of this research. My sincere thanks go to my parents for their continuous support. I would like to express my gratitude to my supervisors: Dr. Tammy A. Lynch, Associate Professor Bruce Van Brunt, Dr. Peter H. Janssen and Dr. David Pacheco, for their guidance and inspiration throughout this challenge. I enjoyed learning and working with this team. Thank you for your effort and time on proofreading reports, manuscripts, and this thesis. The visit of Dr. Mark I. Nelson, University of Wollongong, to discuss my works is greatly appreciated. Many thanks to Dr Indrakumar Vetharaniam and Dr Ronaldo Vibart, AgResearch, for valuable feedback on the manuscript. I would like to acknowledge the stipend from the New Zealand Agricultural Greenhouse Gas Research Centre (NZAGRC) and the combined methane mitigation program of the NZAGRC and the Pastoral Greenhouse Gas Research Consortium. Thanks to the Institute of Fundamental Sciences of Massey University, Manawatū Campus and AgResearch, Grassland Research Centre, for hosting my study. Thanks are also due to the IT, academic and administrative staff at the Institute of Fundamental Sciences and AgResearch for their direct and indirect assistance. The interactions with my office mates and other PhD students including: Ali Ashher Zaidi, Saima Gul, Yang Li, Nick Palevich and Preeti Raju are treasured. It is my privilege to present this work combining all these efforts to you.

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Abbreviations

ADP	Adenosine diphosphate
ATP	Adenosine triphosphate (used by microbes for maintenance and reproduction)
VFA	Volatile fatty acids (e.g., acetate, propionate and butyrate)
HM	Hydrogen-methanogen dynamics
HM ^θ	Hydrogen-methanogen dynamics with thermodynamic term
GHM ^θ	Glucose-hydrogen-methanogen dynamics with thermodynamic term

Nomenclature

Subscript

Substrate	Description
h	hydrogen
g	glucose
A	acetate
P	propionate
B	butyrate

Microbe	Description
m	methanogens
i	glucose fermenters

Superscript

Notation	Description
*	equilibrium point (steady state solution) of variables

Variables

Notation	Description	Unit
t	time	s
S	substrate concentration	mol ml ⁻¹
X	microbe population density	cell ml ⁻¹
θ	thermodynamic term	unitless
M	estimated methane production	rumen ⁻¹ d ⁻¹

Parameters

Rumen environment	Description	Unit
α	passage rate through the rumen	s ⁻¹
β	rate of substrate generation	mol ml ⁻¹ s ⁻¹
γ	absorption rate of substrate	s ⁻¹

Microbe	Description	Unit
q	maximal rate at which a microbe can metabolize substrate	mol cell ⁻¹ s ⁻¹
K	substrate concentration at half of q assuming no thermodynamic feedback	mol ml ⁻¹
w	moles of product generated from metabolizing per mole of substrate	unitless
n	ATP gained by microbe from metabolizing per mole of substrate	mol _{ATP} mol ⁻¹
m	maintenance requirement of a microbe	mol _{ATP} cell ⁻¹ s ⁻¹
Y	reproduction coefficient of microbe	cell mol _{ATP} ⁻¹
μ	reproduction rate of microbe	s ⁻¹
d	death coefficient of microbe	s ⁻¹

Thermodynamic term	Description	Unit
T	temperature	K
\mathcal{R}	ideal gas constant	kJ mol ⁻¹ K ⁻¹
ΔG_T^o	Gibbs free energy of a chemical reaction at T under standard conditions	kJ mol ⁻¹
$\Delta \mathcal{G}_{ATP}$	energy required to generate one unit of ATP	kJ mol _{ATP} ⁻¹