A dynamic *in silico* model of rumen microbial fermentation and methane production

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The rumen microbiota: key player of the animal

- Feed efficiency
- Ruminant production
- Health and well-being
- Environmental footprint

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Our goal: to develop mathematical models

- Enhance understanding of rumen function
- Provide virtual platform to simulate the dynamics of rumen fermentation and methane production
  - Potential use in the design of nutritional strategies to improve animal health, production, and reduce methane production

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Dynamic rumen models: longstanding research area

Journal of Dairy Science
Volume 96, Issue 6, June 2013, Pages 3867-3885

Revised digestive parameter estimates for the Molly cow model

M.D. Hanigan *, J.A.D.R.N. Appuhamy *, P. Gregorini †

Livestock Science
Volume 178, August 2015, Pages 71-80

Nordic dairy cow model Karoline in predicting methane emissions: 1. Model description and sensitivity analysis

Pekka Huhtanen [a], Mohammad Ramin [a], Peter Udén [b]

Journal of ANIMAL SCIENCE

A mechanistic model of whole-tract digestion and methanogenesis in the lactating dairy cow: model development, evaluation, and application[1]

J. A. N. Mills, J. Dijkstra, A. Bannink, S. B. Cammell, E. Kebreab, J. France

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Rumen modelling: room for improvement

Aspects for improvement (Ellis et al., 2008, J. Agric. Sci.; Janssen 2010, AFST)

- Better representation of the microbiota
- Incorporation of hydrogen dynamics
- Thermodynamic control

Dynamic component has been seldom considered in model evaluations and in model exploitation

- Assumption of steady-state
- An exception (van Lingen et al., 2019, JTB)

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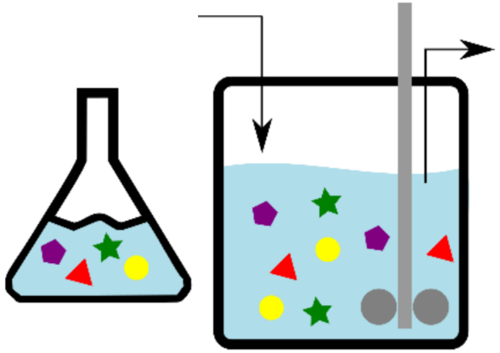
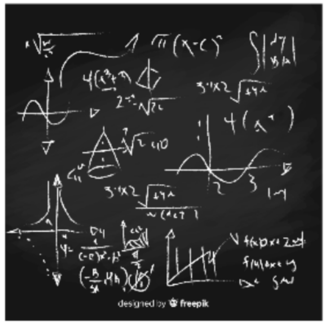
Our modelling strategy: integrating *in vitro*, *in vivo*, *in silico*





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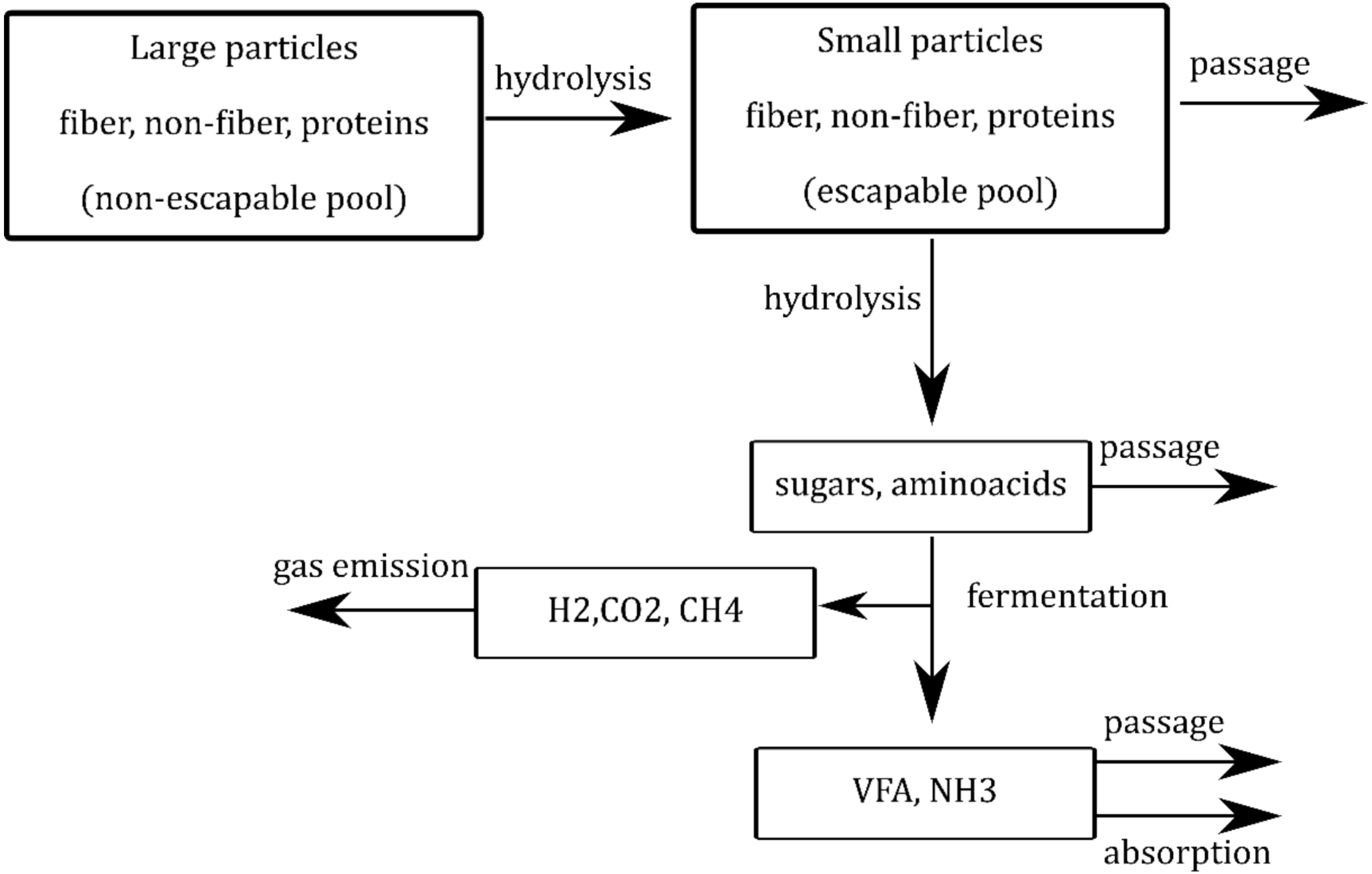
Our model in figures: mass fluxes



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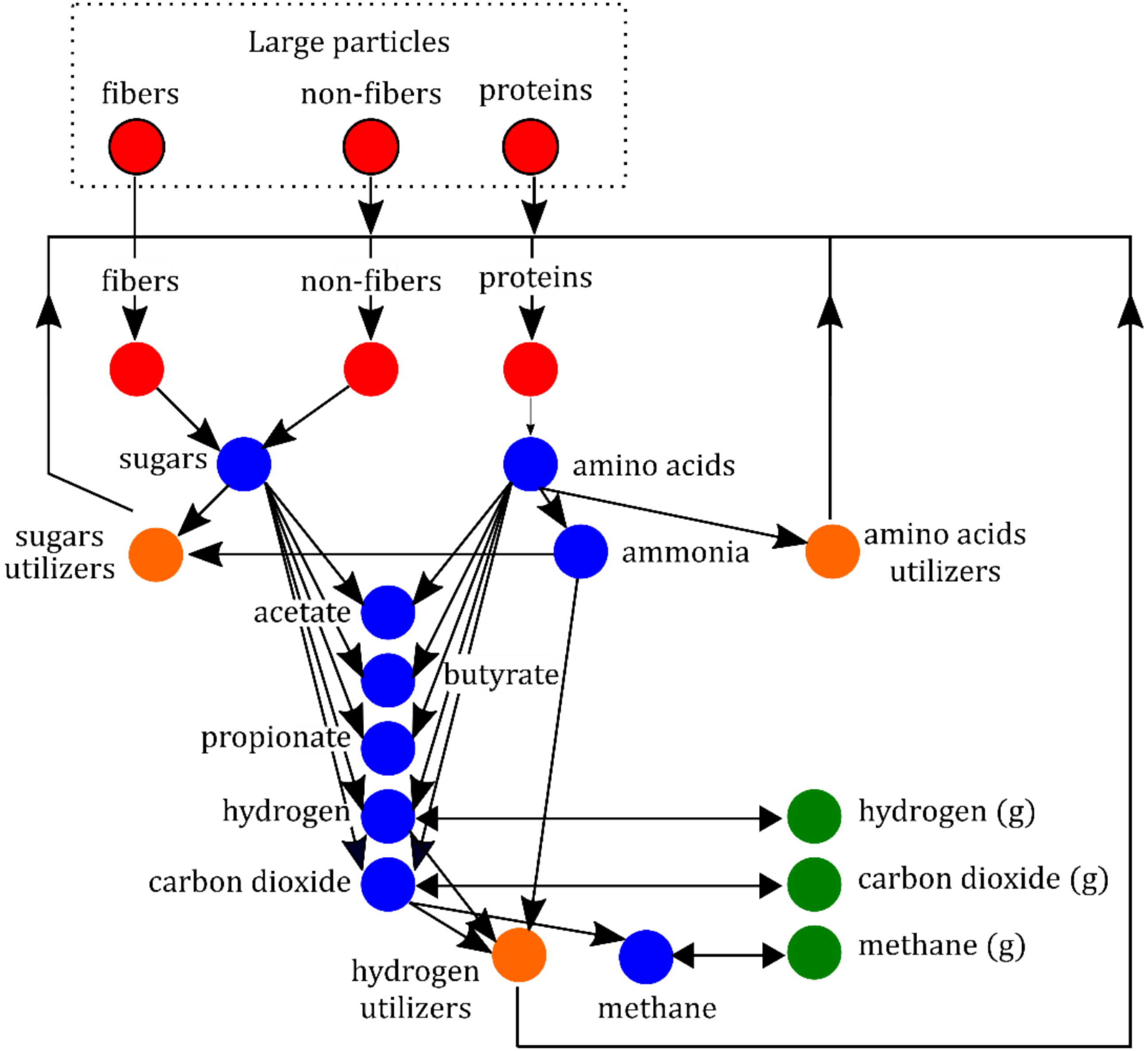
Our model in figures: fermentation pathway



ELSEVIER
Animal Feed Science and Technology
Volume 220, October 2016, Pages 1-21

Mechanistic modelling of *in vitro* fermentation and methane production by rumen microbiota

Rafael Muñoz-Tamayo, Sylvie Giger-Reverdin, Daniel Sauvant

Peer Community Journal
Animal Science

Modelling the impact of the macroalgae *Asparagopsis taxiformis* on rumen microbial fermentation and methane production

Muñoz-Tamayo, Rafael[1]; Chagas, Juana C.[2]; Ramin, Mohammad[2]; Krizsan, Sophie J.[2]

10.24072/pcjournal.11 - Peer Community Journal, Volume 1 (2021), article no. e7.

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Our model: some equations

- Mass balance equations: ordinary differential equations

$$\frac{d\mathbf{x}}{dt} = \mathbf{S} \cdot \boldsymbol{\rho}(\mathbf{x}, \mathbf{p}) - \mathbf{g}(\mathbf{x}, \mathbf{p})$$

$\mathbf{x}$: vector of metabolites concentrations
$\mathbf{S}$: stoichiometry matrix
$\boldsymbol{\rho}(\mathbf{x}, \mathbf{p})$: vector of reaction rates
$\mathbf{g}(\mathbf{x}, \mathbf{p})$: function vector of tranport phenomena

- 21 state variables (compartiments)
- 37 parameters
  - Physicochemical and fermentation parameters (yield factors, Monod parameters of the kinetic rates): Muñoz-Tamayo et al., (2016), AFST
  - absorption rate constants: initial guess from Dieho et al., (2016), JDS
  - microbial biomass data: Ahvenjärvi et al. (2002), JAS; (2018) JDS
  - passage rates: Bayat et al., (2011), AFST

MATLAB

Implementation

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Model calibration (parameter estimation)

- Experimental data from 4 Nordic-Red dairy cows rumen fistula (2 days)
  - Dry matter intake: 3 h
  - Rumen sampling for VFA (acetate, butryrate, propionate) determination: 3 h
  - Methane in respiration chambers: 17 min

- Maximum likelihood estimation
  - 5 parameters:
    - absorption rate constants of VFAs
    - Hydrolysis rate constants of NSC and protein
  - Check for identifiability

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IFAC Proceedings Volumes

Volume 42, Issue 10, 2009, Pages 1271-1276

IDEAS: a Parameter Identification Toolbox with Symbolic Analysis of Uncertainty and its Application to Biological Modelling

R. Muñoz-Tamayo *, ¶, § ✉, B. Laroche * ✉, M. Leclerc ¶ ✉, E. Walter * ✉

https://doi.org/10.3182/20090706-3-FR-2004.00211

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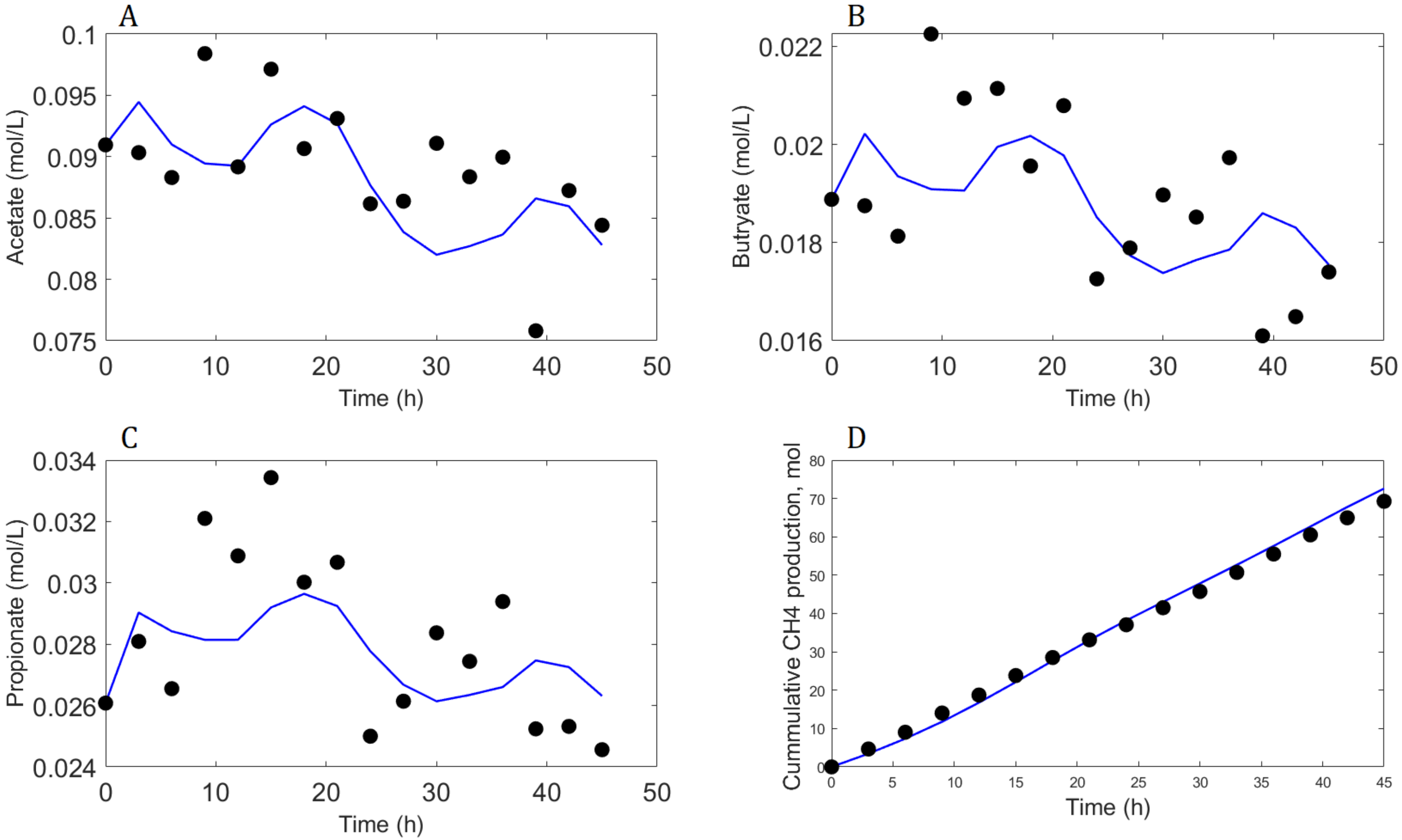
Example results: one cow

Experimental data (•) , ____ predicted variables



Capability of the model to represent the dynamic pattern of fermentation

	CVRMSE
Acetate	9%
Butyrate	11%
Propionate	13%
CH4	21%
Cummulative CH4	5%

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Take home message

- Our mathematical model represents satisfactorily the rumen fermentation and CH4 production by dairy cows

- Ongoing work
  - Include mechanistic description of pH (Muñoz-Tamayo et al., 2016, AFST)
  - Include hydrogen thermodynamic control (Muñoz-Tamayo et al., 2021, PCJ)
  - Make the code Open Source and available for the scientific community
    - User interface: R or Python

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Diet

- Cows were offered total mixed ration at 7:00, 13:00 and 19:00 h consisting of grass silage (timothy-meadow fescue sward) provided at 45:55 forage to concentrate ratio on a dry matter basis.

  TMR = 58 kg/dDMI = 26 kg/d

- NDF = 39%, NSC = 36% , PRO = 15%

- Acclimatisation period in chambers: 1 day

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