Modelling biochemical rumen functions with special emphasis on methanogenesis

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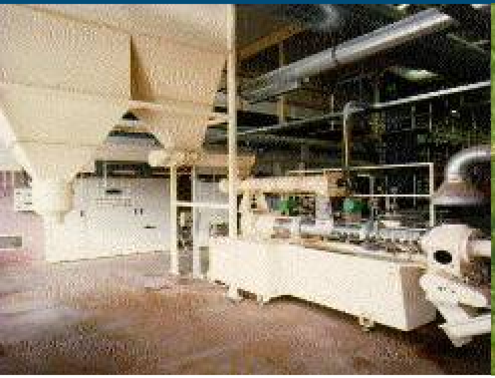


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Overview

- Principles of mathematical modelling
- Empirical models of methane production
- Mechanistic models of methane production

Prediction ~ mathematical models

- Prediction requires use of models
- A model is an equation or set of equations that represent the behaviour of a system

France and Thornley (1984)

- A model can be viewed as an idea, hypothesis or relation expressed in mathematics
- Symbiosis between experimentation and modelling

Model classification

dynamic OR static

deterministic OR stochastic

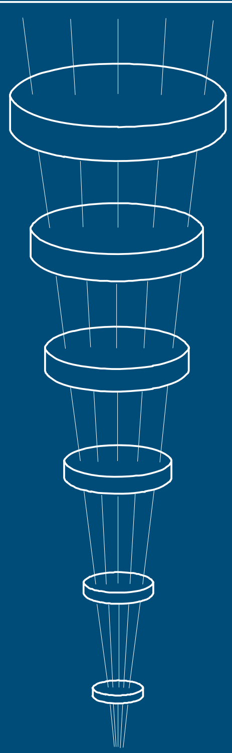
mechanistic OR empirical

To put categories into a more familiar context, a model based on:

- regression analysis → static, stochastic, empirical
- linear programming → static, deterministic, empirical
- differential eqns → dynamic, deterministic, mechanistic

Levels of organization

Level	Description of level
•	•
i + *1*	Herd / flock
i	Animal
i − *1*	Organ / tissue
i − *2*	Cell
•	•

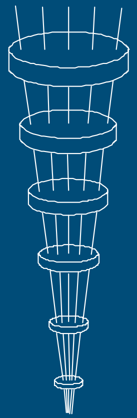


Dijkstra & France (2005)

Properties of hierarchical systems

- Each level has its own concepts and language
- Each level is an integration of items from lower levels
- Successful operation of a level requires lower levels to function properly, but not necessarily *vice versa*

Level	Description of level
•	•
i + *1*	Herd / flock
i	Animal
i - *1*	Organ / tissue
i - *2*	Cell
•	•



Contributions of modelling

- Models provide a convenient data summary, useful for interpolation and cautious extrapolation
- Models make best use of (precious) data
- Models provide quantitative description and understanding of biological problems
- Modelling provides strategic and tactical support to research programmes
- Modelling allows exploration of possible outcomes when data are not available

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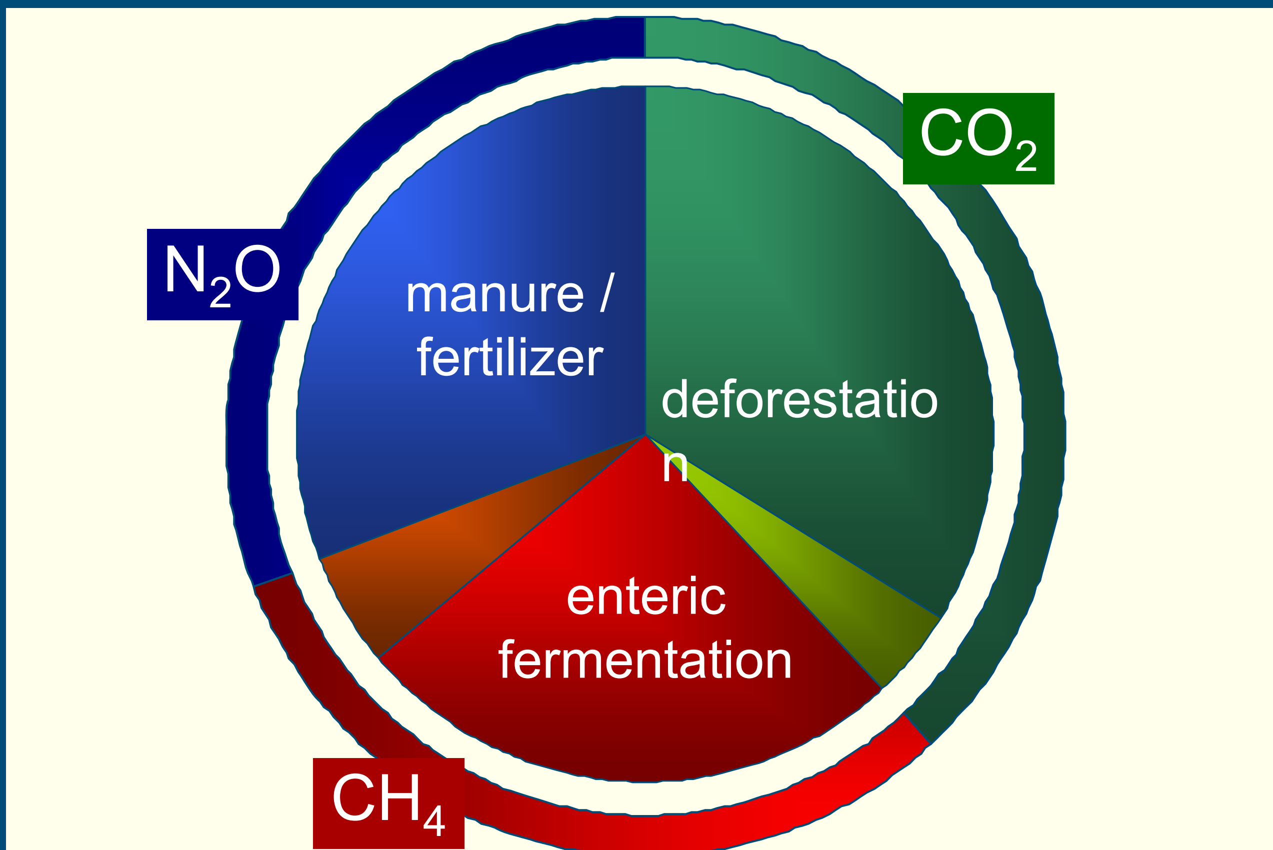
Livestock greenhouse gases

FAO (2006)



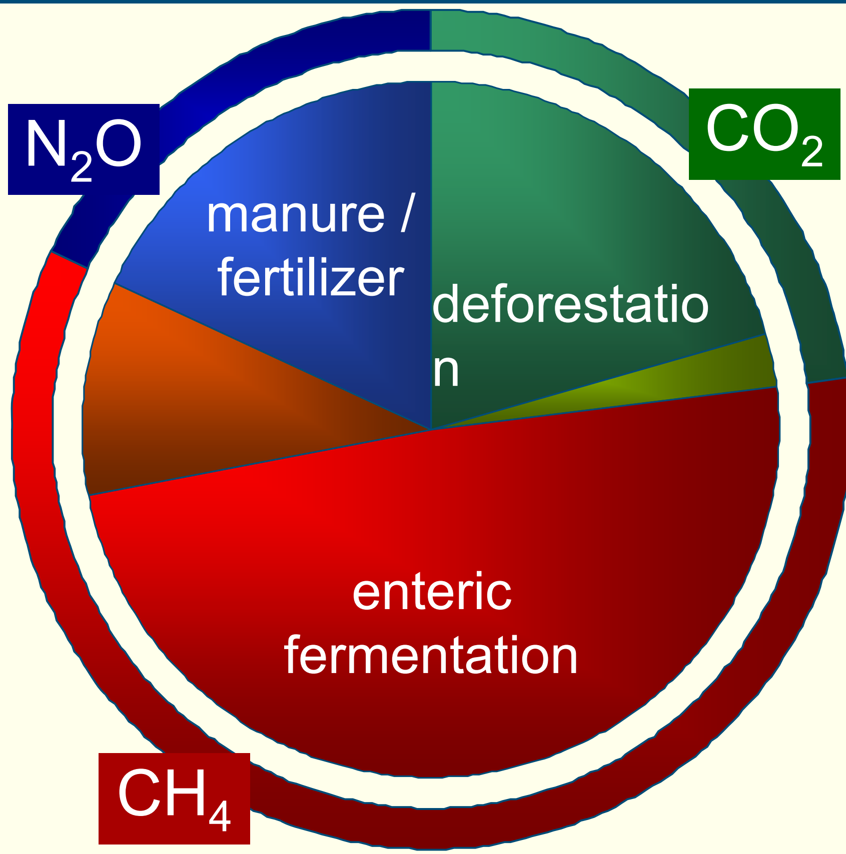
GWP*-100 yr:

CO_2	1
CH_4	25
N_2O	298

*Global Warming Potential

Livestock greenhouse gases

FAO (2006)



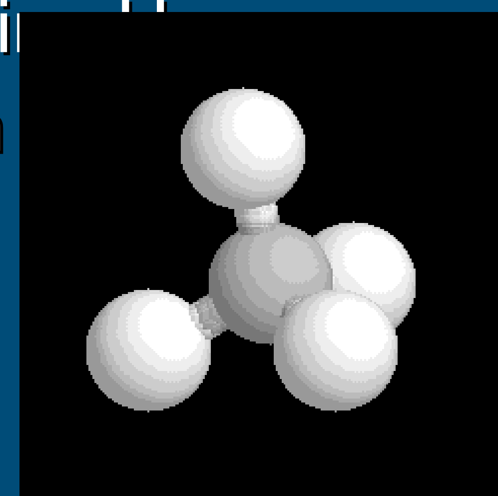
GWP*-20 yr:

CO_2	1
CH_4	72
N_2O	289

*Global Warming Potential

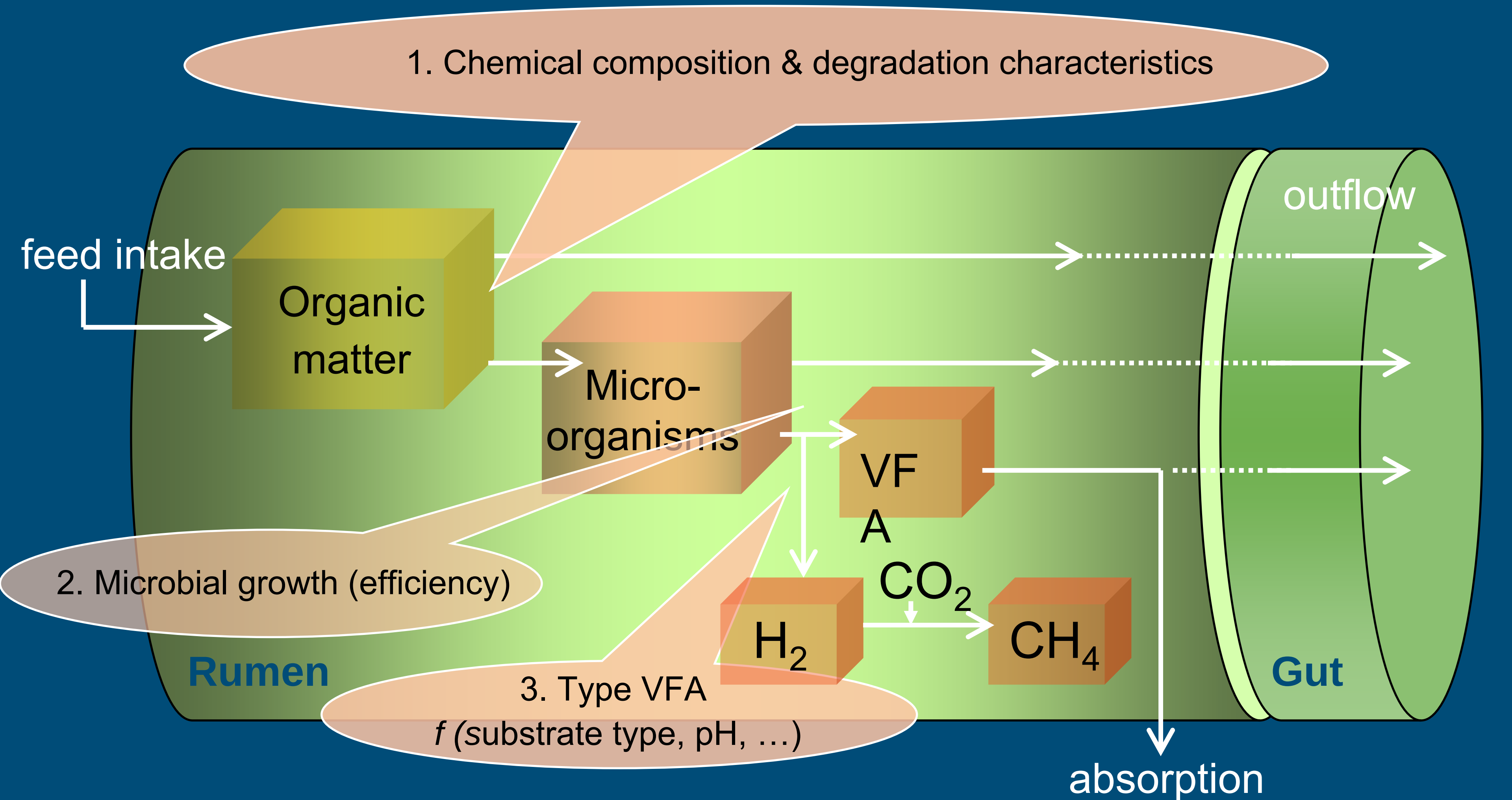
Rumen methanogenesis

- Fermentative micro-organisms utilize dietary organic matter to produce VFA plus gases (e.g., CO_2, H_2)
  - amount of H_2 depends on type of VFA
- Methanogens reduce CO_2 to CH_4 usi
  keeping H_2 partial pressure in rumen



- H_2 is used up as it is produced
- CH_4 production:
  - 2 – 12% of GE intake
  - 10 – 35 g/kg DM intake

Factors involved in rumen methanogenesis



Empirical models of methane production

- > 30 empirical models available
  - inventory
  - mitigation strategy
- Independent variables include live weight, milk production, feed intake, dietary components, digestibility
- Applied in models of greenhouse gas emissions in whole farm setting

Assessment of accuracy of empirical models

Ellis et al. (2010) *Global Change Biology*

- 9 methane equations applied in 8 whole farm models
- 169 observations from 9 studies

	Mean	SD	Min	Max
Feed intake (kg DM/d)	19.6	4.0	11.2	32.0
Milk production (kg/d)	30.3	9.05	8.8	49.4
Methane production (g/d)	371	77.1	117	698

Empirical models of methane production - 1

CH_4 production (g/d) estimated as:

- 274 (Europe) or 323 (N-America)

  IPCC (1997) Tier I

- 0.06 x GE intake / 55.65

  IPCC (1997) Tier II

- 137 + 10 x milk yield

  Corre (2002)

- 10 + 4.9 x milk yield + 1.5 x $LW^{0.75}$

  Kirchgeßner et al. (1995) - 1

Empirical models of methane production - 2

CH_4 production (g/d) estimated as:

- (45 – 0.02 x DMI² – 1.8 x C18:2 – 84 x C≥20) x DMI
- [1.3 + 0.11 x Dig_m + Mn x (2.4 – 0.05 x Dig_m)] x GEI

  Giger-Reverdin et al. (2003)
- (3 + 0.5 x NSC + 1.7 x HC + 2.7 x CEL)/55.65

  Blaxter & Clapperton (1965)

  Moe & Tyrrell (1979)
- 63 + 79 x CF + 10 x NFE + 26 x CP – 212 x FAT

  Kirchgeßner et al. (1995) - 2
- 20 x concentrate + 22 x maize sil + 27 x grass (sil)

Evaluation of empirical methane models

Ellis et al. (2010)

	Pred CH_4 (g/d)
IPCC (1997) Tier I	304
IPCC (1997) Tier II	399
Corre (2002)	440
Kirchgeßner et al. (1995) – 1	404
Giger-Reverdin et al. (2003)	230
Blaxter & Clapperton (1965)	332
Moe & Tyrrell (1979)	391
Kirchgeßner et al. (1995) – 2	345
Schils et al. (2006)	483

Observed CH_4
371 g/d

Evaluation of empirical methane models

Ellis et al. (2010)

	Pred CH_4 (g/d)	RMSPE (%)
IPCC (1997) Tier I	304	27.6
IPCC (1997) Tier II	399	20.9
Corre (2002)	440	34.2
Kirchgeßner et al. (1995) – 1	404	29.5
Giger-Reverdin et al. (2003)	230	52.5
Blaxter & Clapperton (1965)	332	21.2
Moe & Tyrrell (1979)	391	20.2
Kirchgeßner et al. (1995) – 2	345	20.9
Schils et al. (2006)	483	39.5

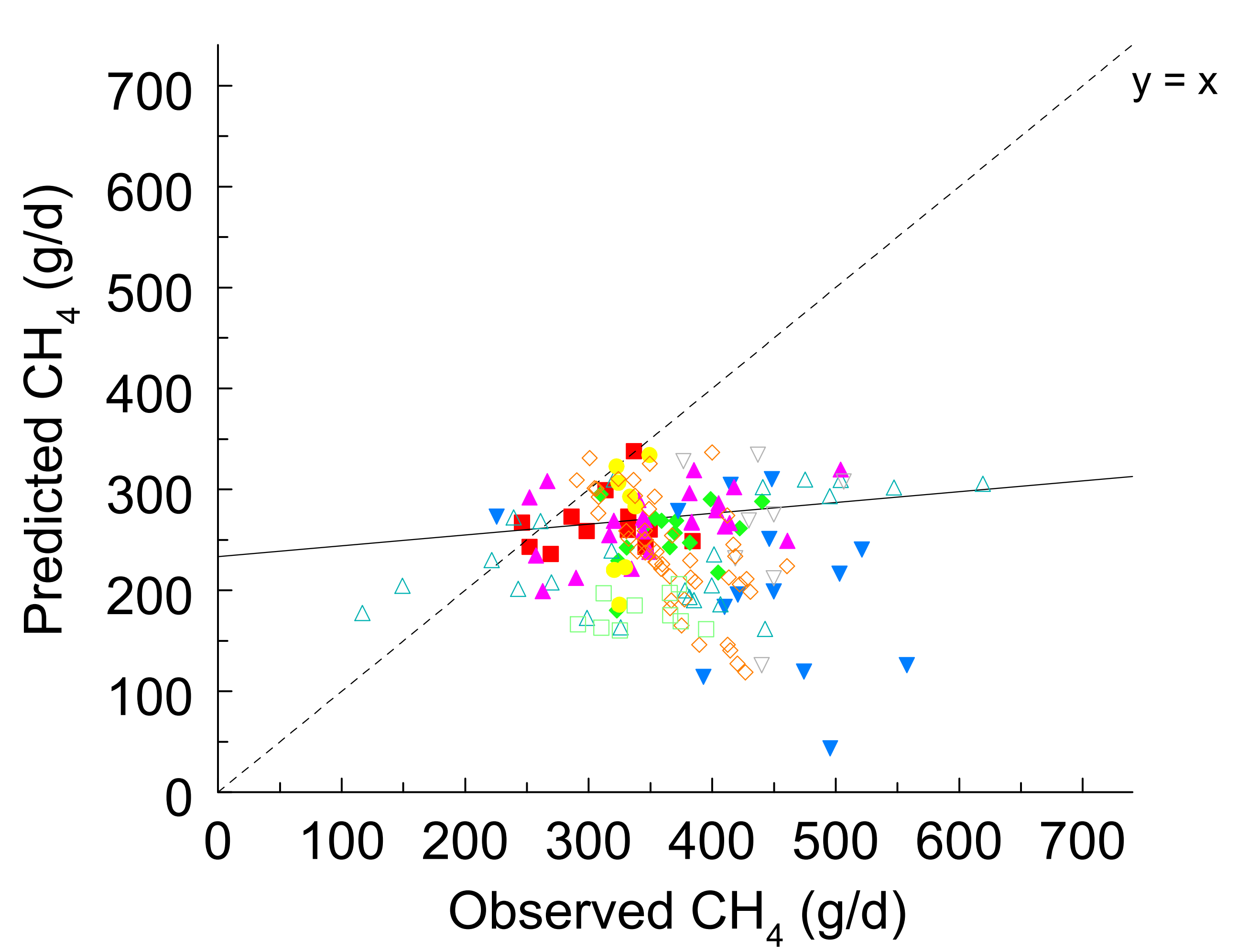
Evaluation of empirical methane models

Ellis et al. (2010)

	Pred CH_4 (g/d)	RMSPE (%)	CCC
IPCC (1997) Tier I	304	27.6	0.01
IPCC (1997) Tier II	399	20.9	0.49
Corre (2002)	440	34.2	0.13
Kirchgeßner et al. (1995) – 1	404	29.5	0.29
Giger-Reverdin et al. (2003)	230	52.5	0.12
Blaxter & Clapperton (1965)	332	21.2	0.27
Moe & Tyrrell (1979)	391	20.2	0.46
Kirchgeßner et al. (1995) – 2	345	20.9	0.22
Schils et al. (2006)	483	39.5	0.25

Evaluation of empirical methane models

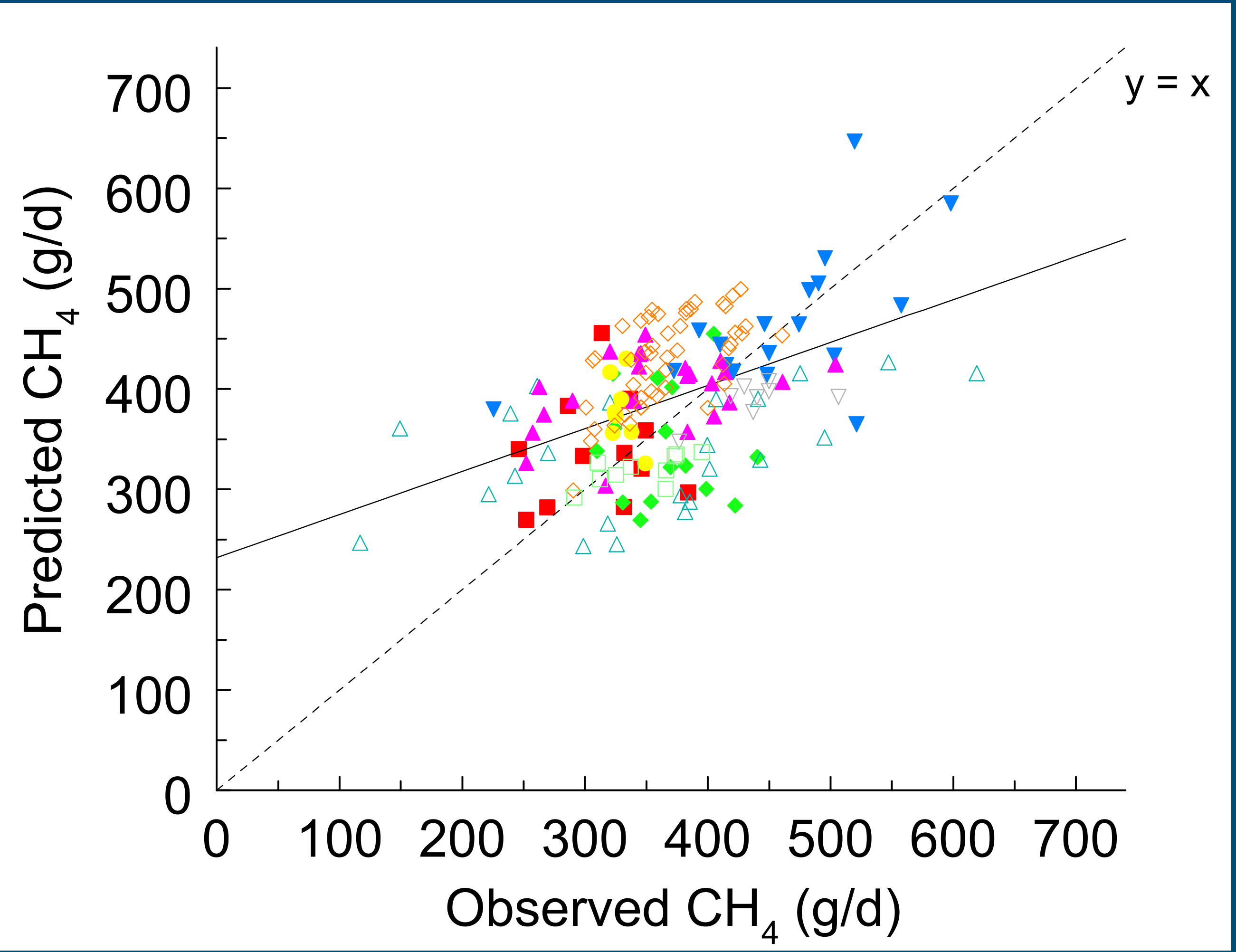
Ellis et al. (2010)



Model: Giger-Reverdin et al. (2003)

Evaluation of empirical methane models

Ellis et al. (2010)



Model:

Moe & Tyrrell (1979)

Conclusions empirical methane models

- Simple, generalized models performed worse than models based on diet composition
- Predictions poor; significant bias and deviation of regression slope from unity
- Substantial errors into inventories of whole farm greenhouse gas emissions are likely
- Low prediction error may lead to incorrect mitigation recommendations

Overview

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- Empirical models of methane production
- Mechanistic models of methane production

Rate : state formalism

- State variables: $Q_1, Q_2, \ldots\ldots, Q_n$
- Change of state variables with time t:

$$dQ_1/dt = f_1\,(Q_1, Q_2, \ldots, Q_n; P\,)$$

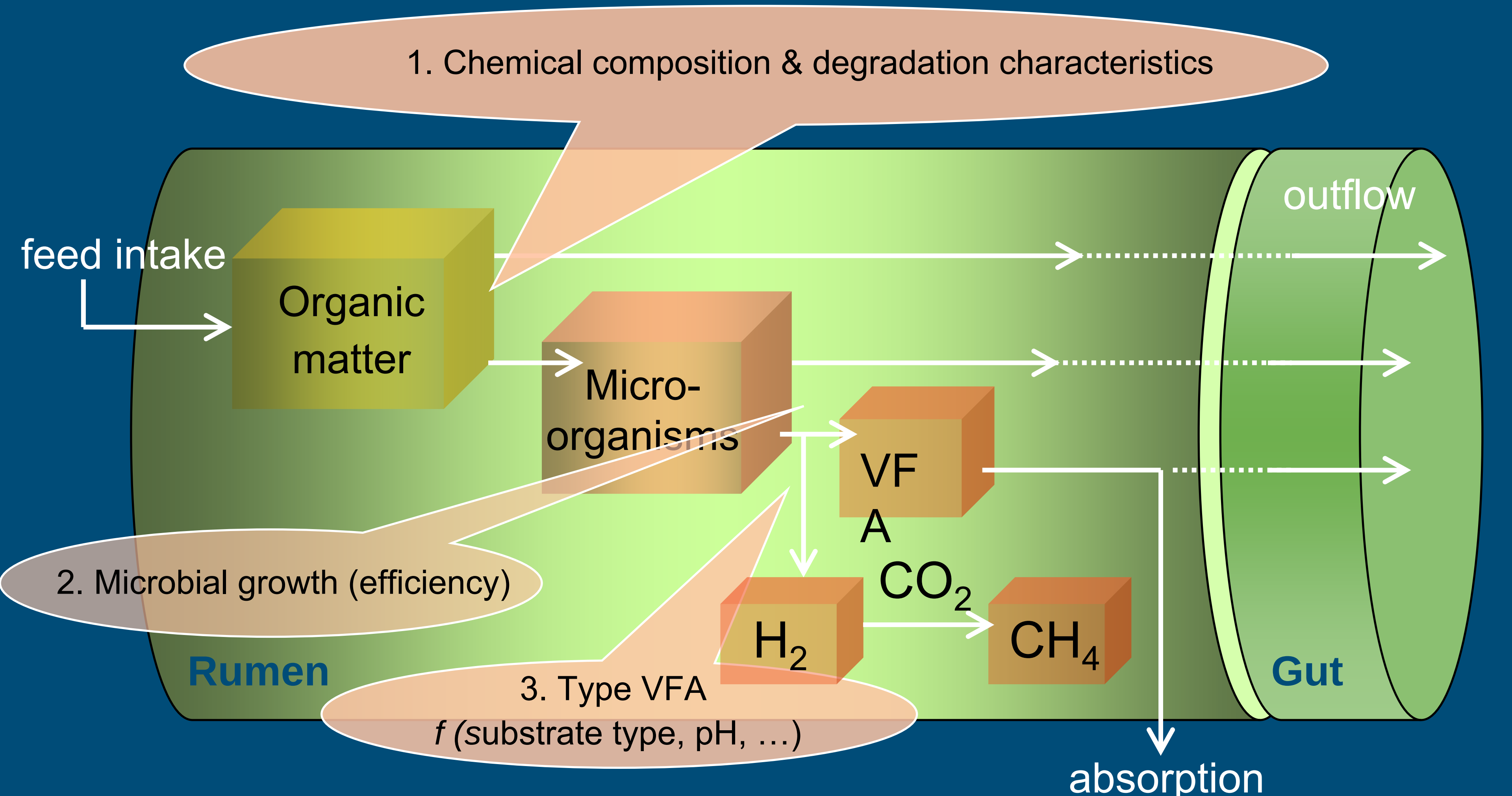
$$dQ_2/dt = f_2\,(Q_1, Q_2, \ldots, Q_n; P\,)$$

$$\vdots \qquad\qquad\qquad \vdots$$

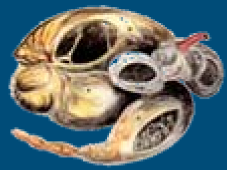
$$dQ_n/dt = f_n\,(Q_1, Q_2, \ldots, Q_n; P\,)$$

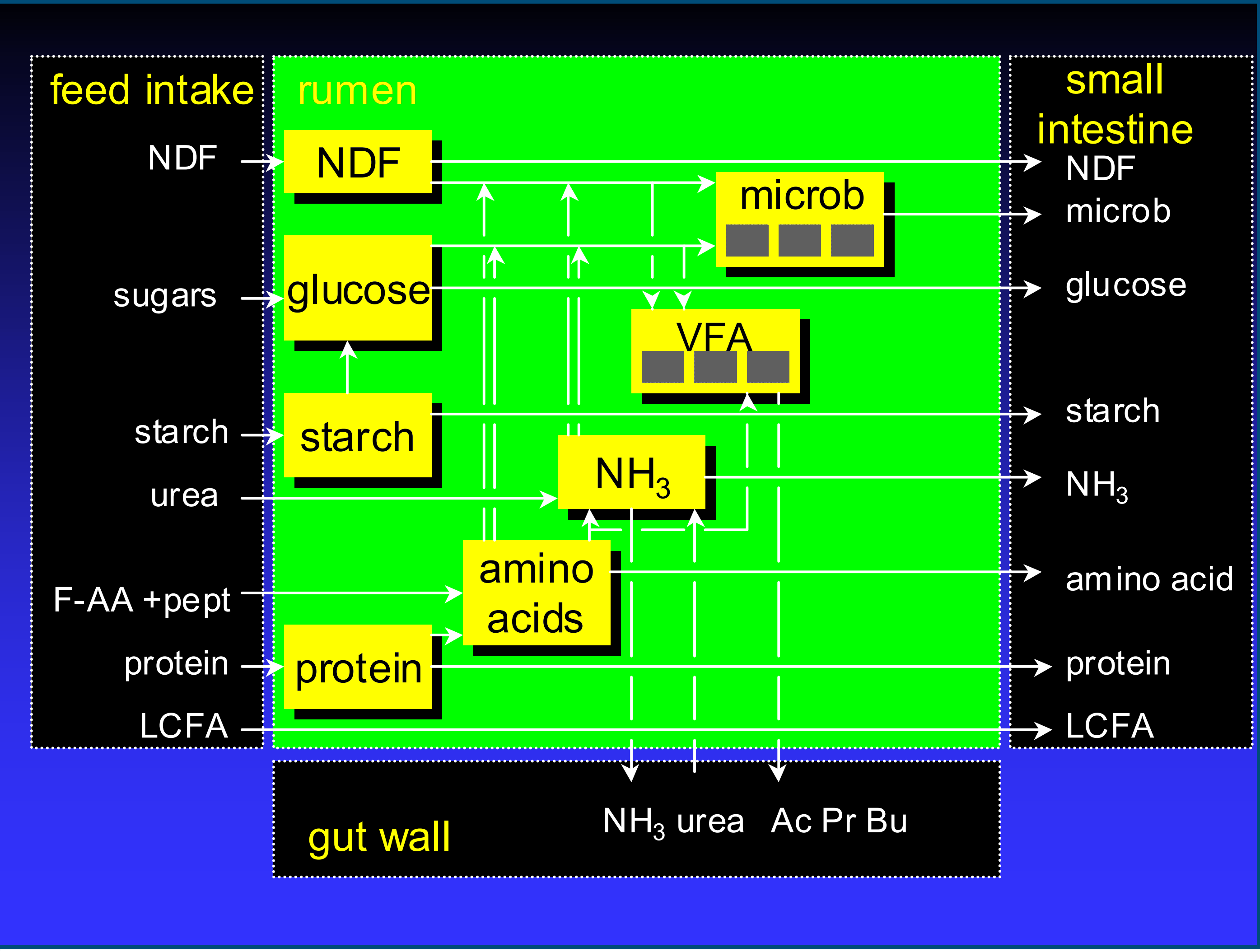
- Differential equations based on law of mass conservation, 1st law of thermodynamics, etc

Factors involved in rumen methanogenesis



Mechanistic rumen module





Dijkstra et al. (1992)

Modifications:

- Dijkstra (1994)
- Mills et al. (2001)
- Dijkstra et al. (2002)
- Kebreab et al. (2004)
- Bannink et al. (2006)

In use in:

- Netherlands
- UK
- Australia
- Brazil
- Canada
- USA
- and many more

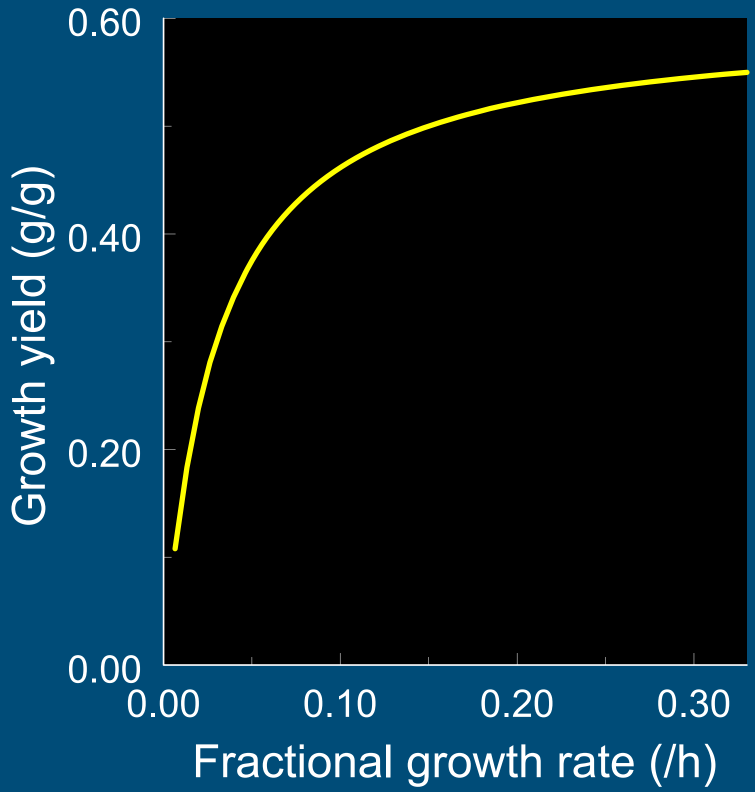
Efficiency of microbial growth

- Substrate is used for
  - ✓ non-growth purposes ('maintenance')
  - ✓ growth purposes

- Yield is related to fractional growth rate (Pirt, 1965)

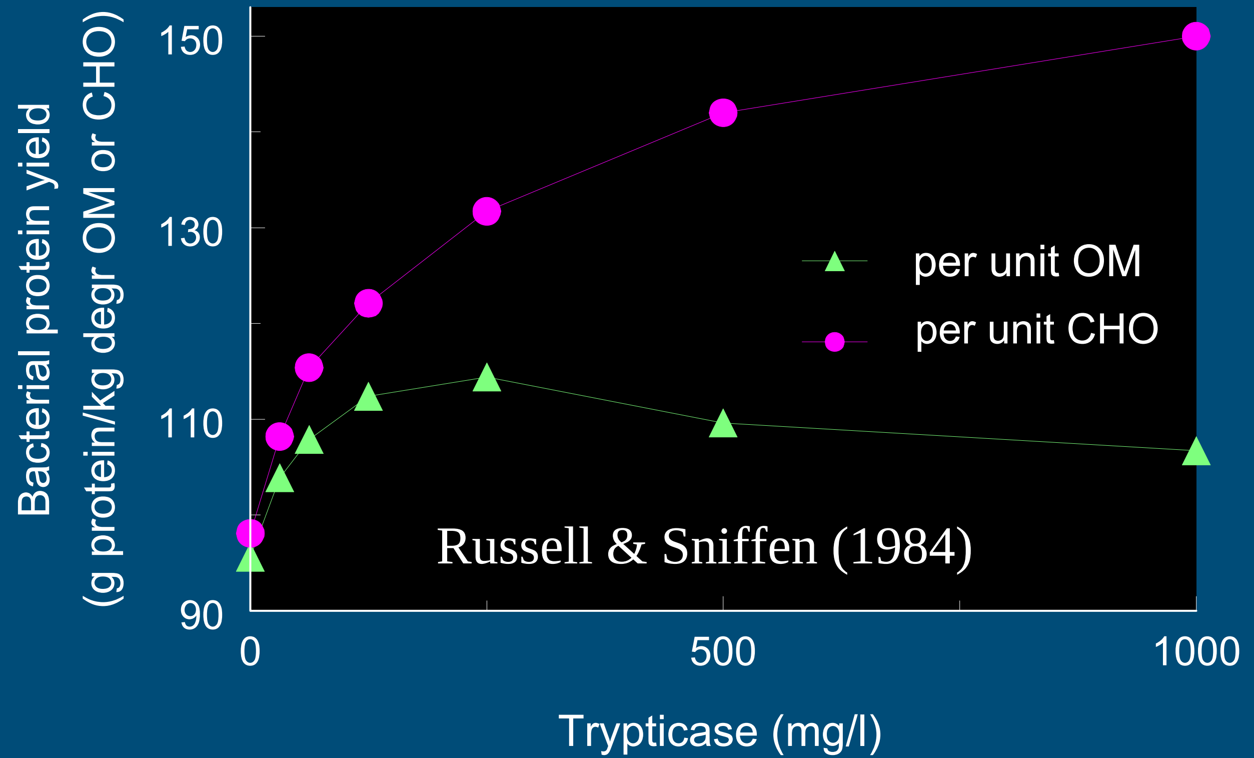
$$1 / Y = M / \mu + 1 / Y_{max}$$

Y = growth yield
M = maintenance requirement
Y_{max} = maximum yield
μ = fractional growth rate



Microbial metabolism: N source

Yield affected by availability of preformed molecules



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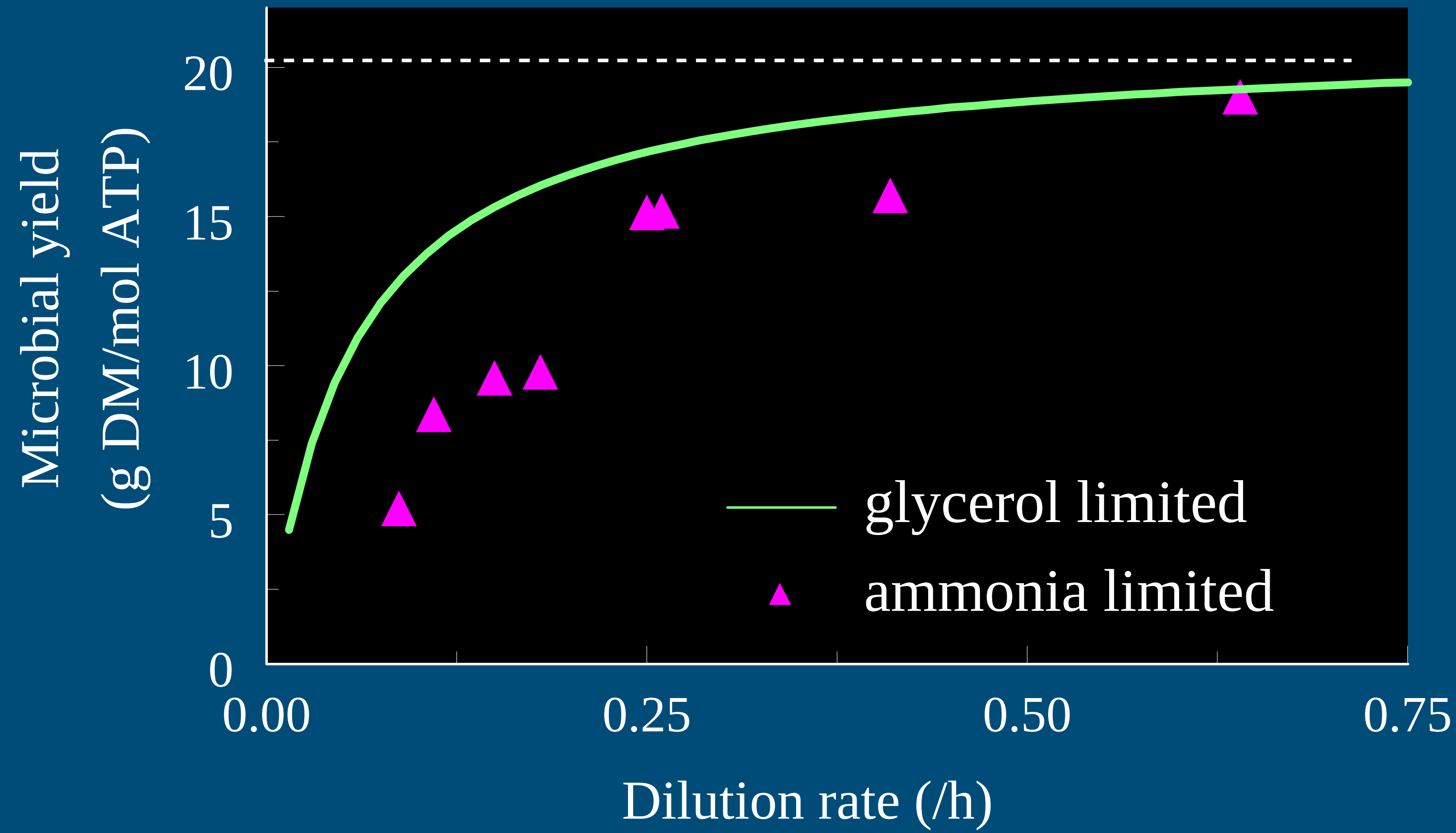
Energy and N synchrony: energy spilling

K. aerogenes; Neijssel & Tempest (1976)

$$U_{glycerol\ in\ energy\ spilling} = v_{max}\ Q_{microbes} / (1+[ammonia]/J_{ammonia})$$



Significance of VFA molar proportion

$C_6H_{12}O_6 + 2H_2O \rightarrow 2C_2H_4O_2$ (acetate) $+ 2CO_2 + 4H_2$

$C_6H_{12}O_6 + 2H_2 \rightarrow 2C_3H_6O_2$ (propionate) $+ 2H_2O$

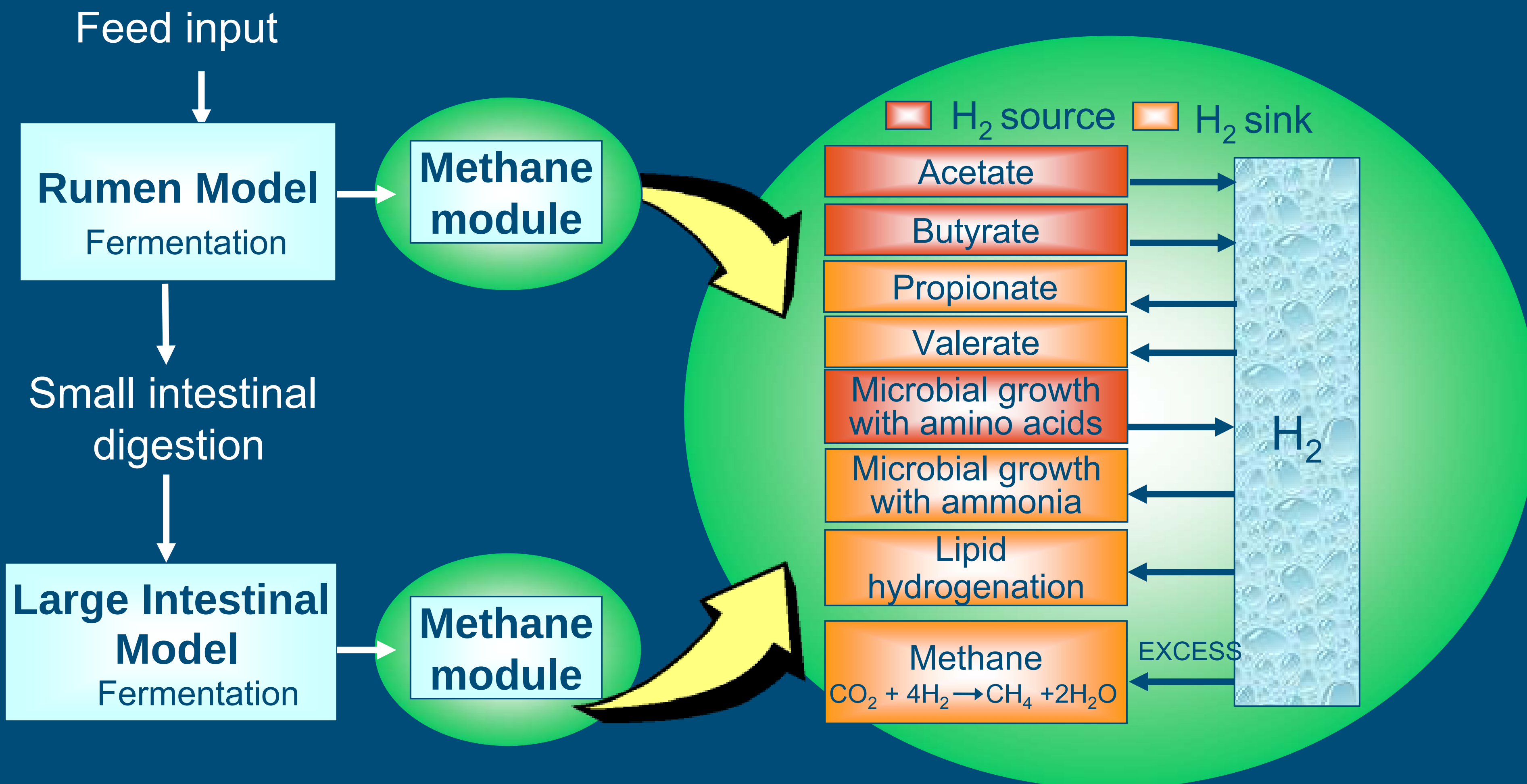
$C_6H_{12}O_6 \rightarrow C_4H_8O_2$ (butyrate) $+ 2CO_2 + 2H_2$

$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$

acetate	70%	60%
propionate	15%	25%
butyrate	15%	15%
CH_4	0.39 mol/mol VFA	0.31 mol/mol VFA

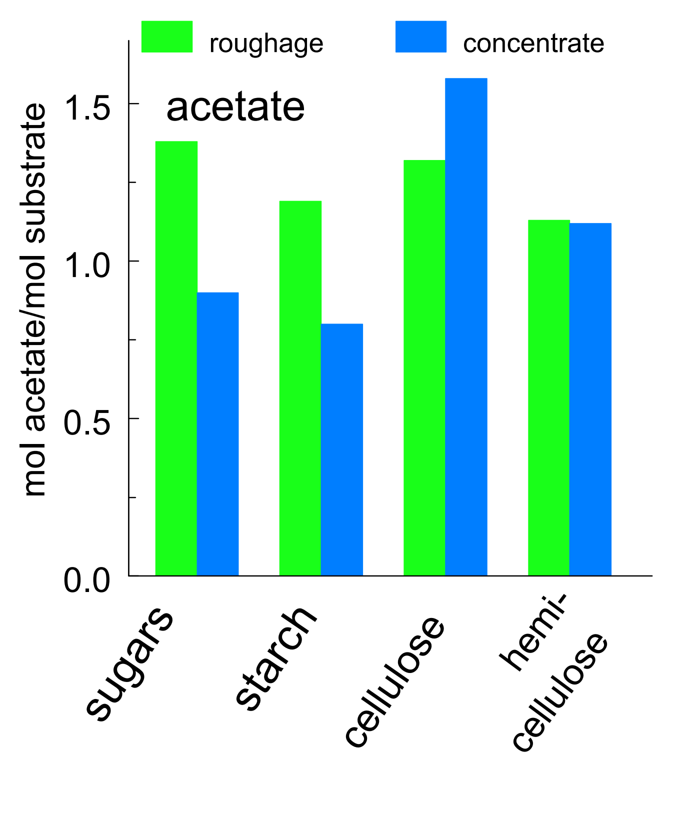
Mechanistic model methane production

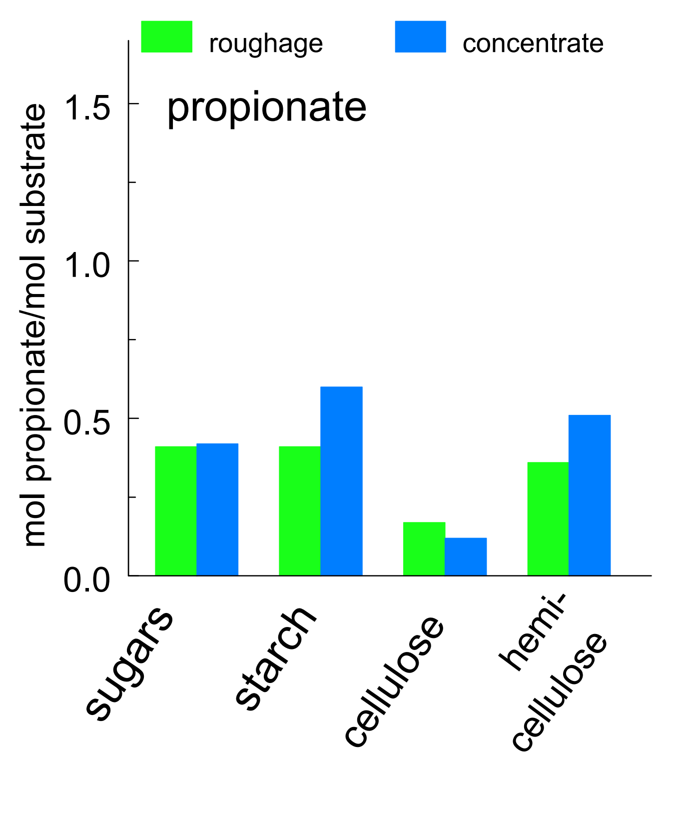
(Dijkstra et al. 1992; Mills et al. 2001; Bannink et al. 2006)



VFA stoichiometry

- Type of VFA formed related to substrate fermented, rumen pH, roughage vs concentrate

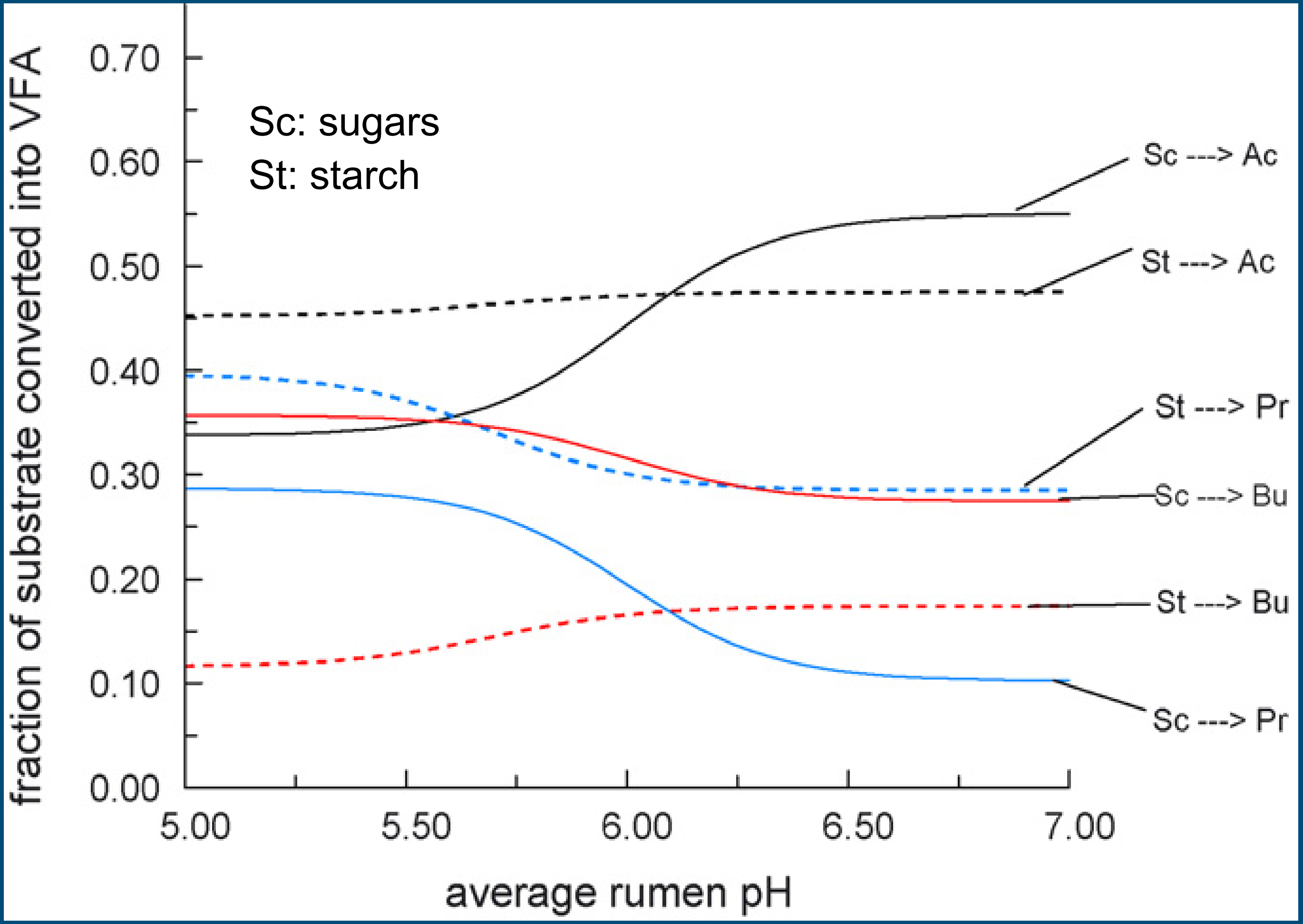




Murphy et al. (1984)

VFA stoichiometry and rumen pH

Bannink et al. (2008)



In vivo data

rumen digestion lactating cows

Analysis

substrate type

roughage vs. concentrates

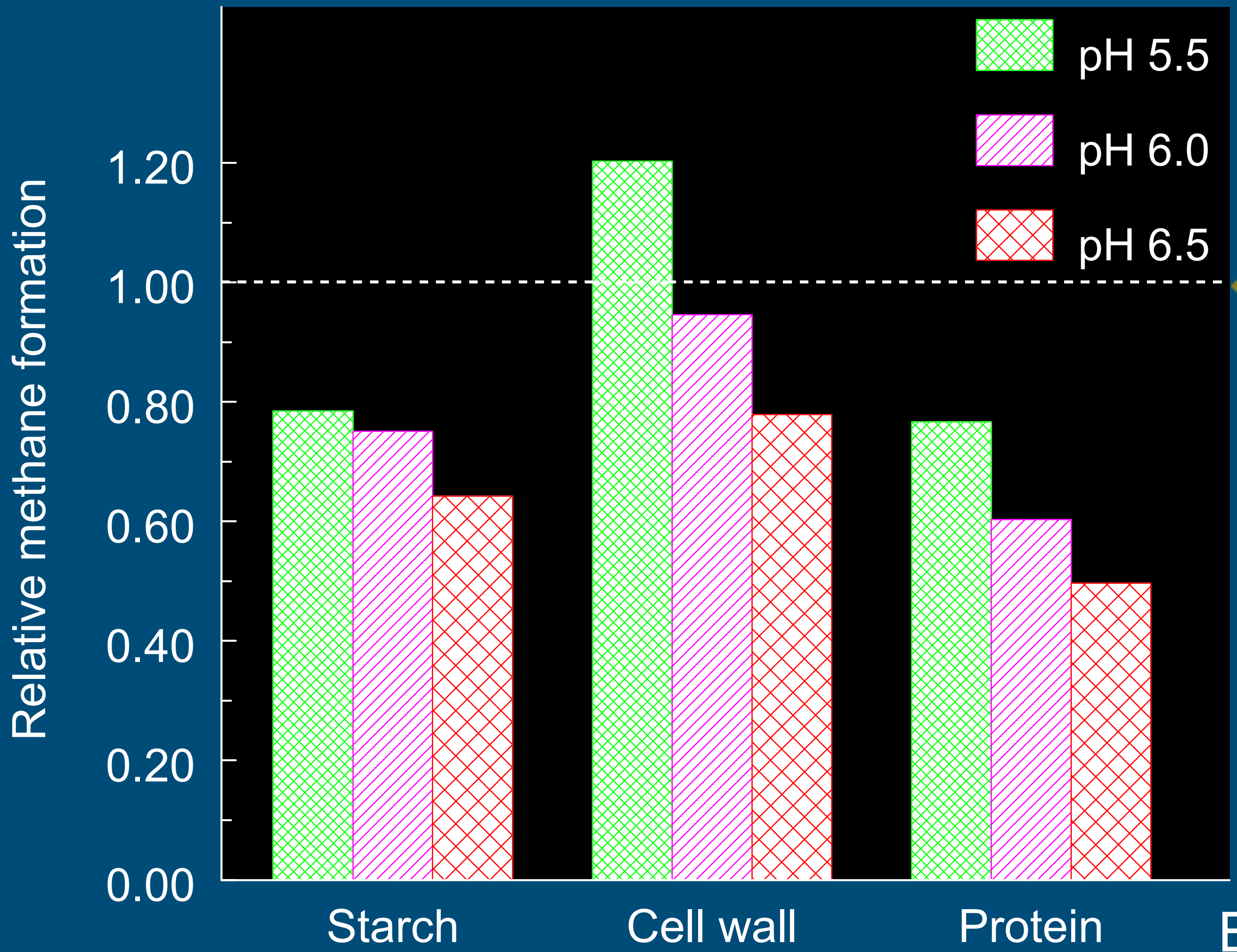
efficiency microbial growth

kinetics

VFA-absorption

pH

Methane formation from various substrates



CH_4 from soluble carbohydrates set at unity

Bannink et al. (2008)

Mechanistic models of methane formation

- Prediction based on description of the rumen in terms of components and associated processes
- Mechanistic models superior predictive power

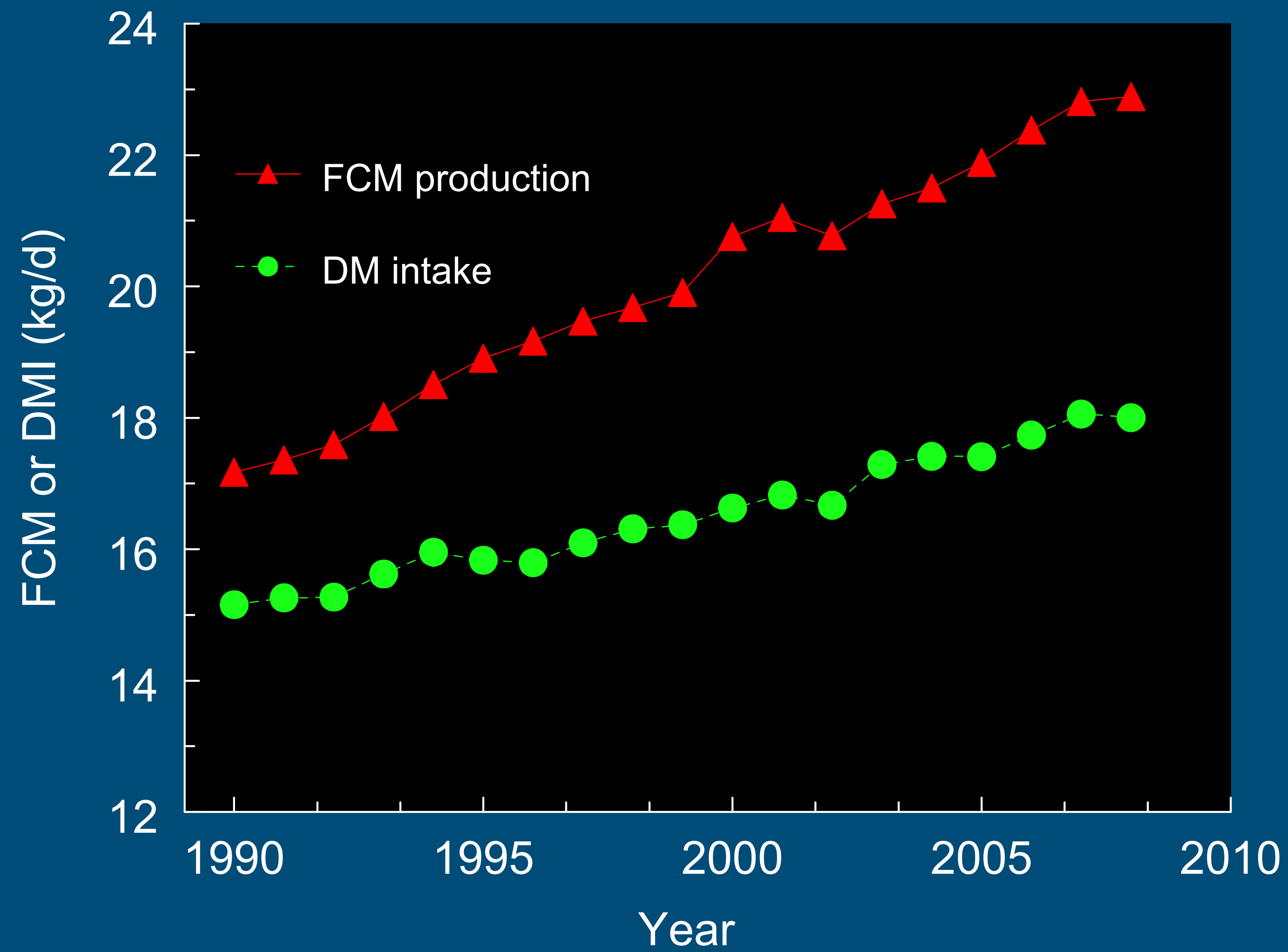
  Benchaar et al. (1998); Mills et al. (2001); Kebreab et al. (2006)
- Allows evaluation of dietary mitigation options
  - Inventories under Kyoto protocol

Example: Netherlands, database 1990 - 2008

- Milk production and composition data
- Feed intake data
  - feed categories: fresh grass, grass silage, maize silage, wet byproducts, concentrates
  - concentrate chemical composition from central database
  - roughage chemical composition from Laboratory for Soil and Crop Testing

- Dietary changes in 1990 – 2008
  - more maize silage and less fresh grass
  - crude protein content decreased

DM intake and fat corrected milk (FCM)



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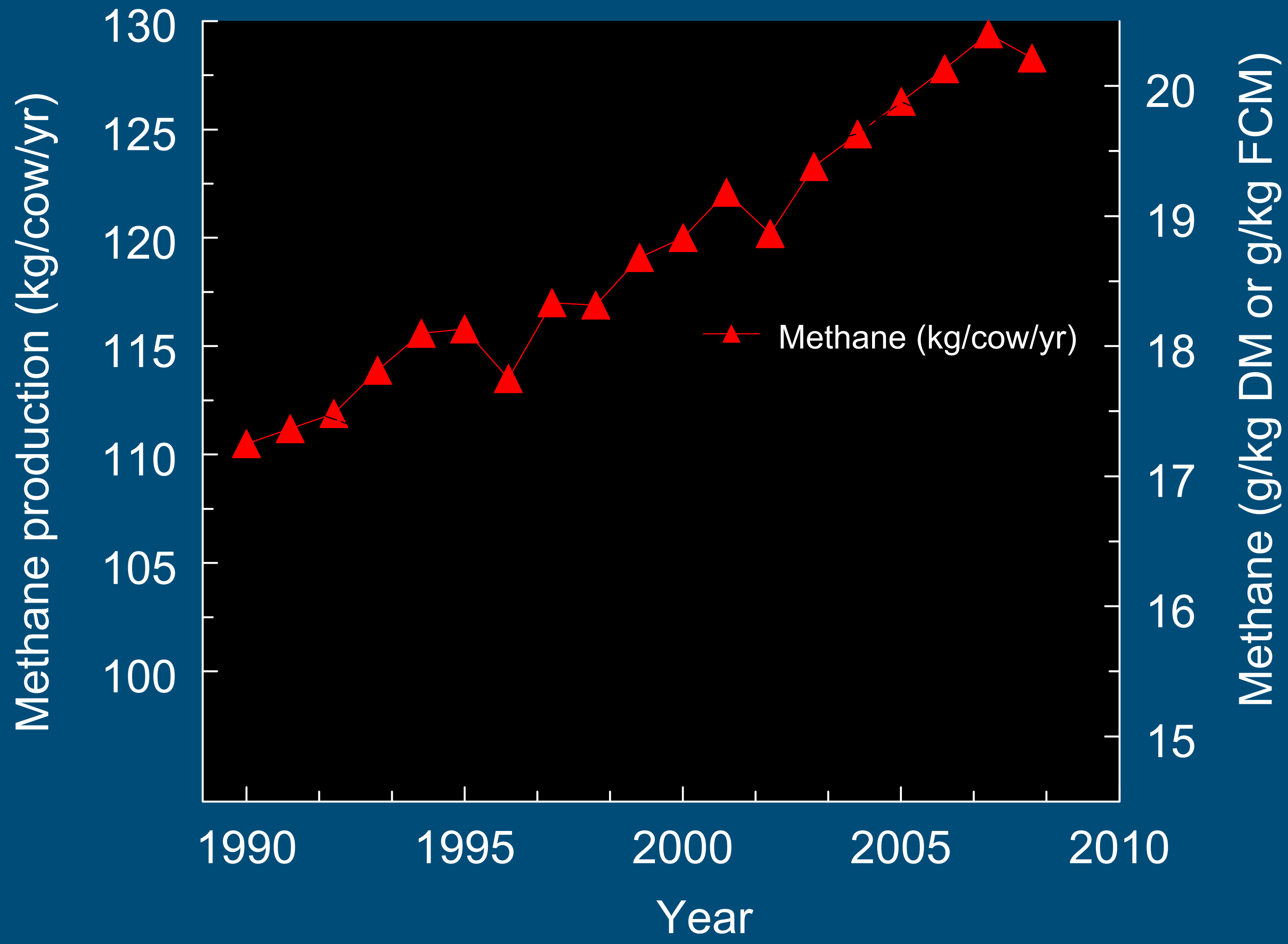
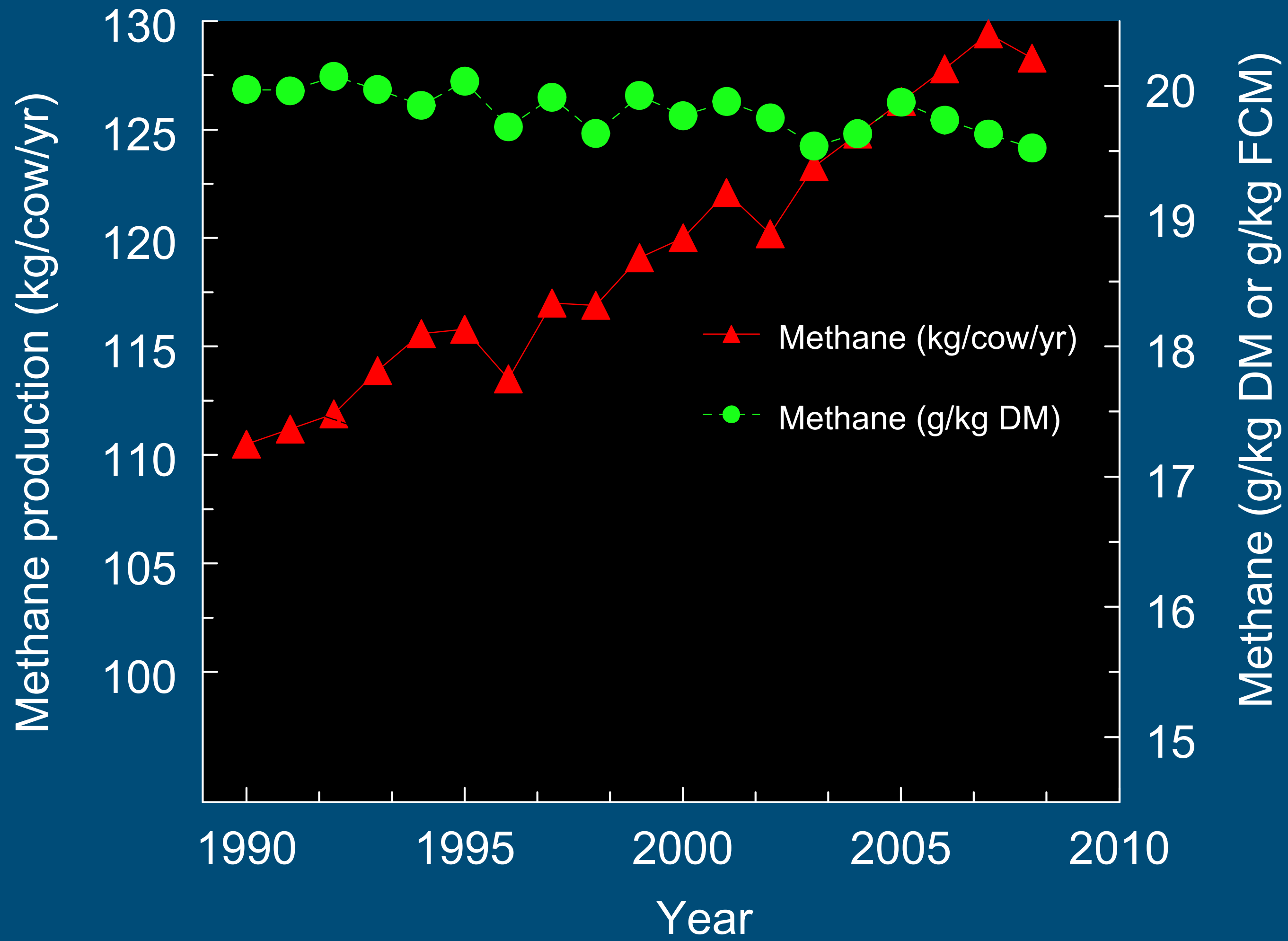
J. Dijkstra
Modelling methane emissions

Simulated methane production



Simulated methane production



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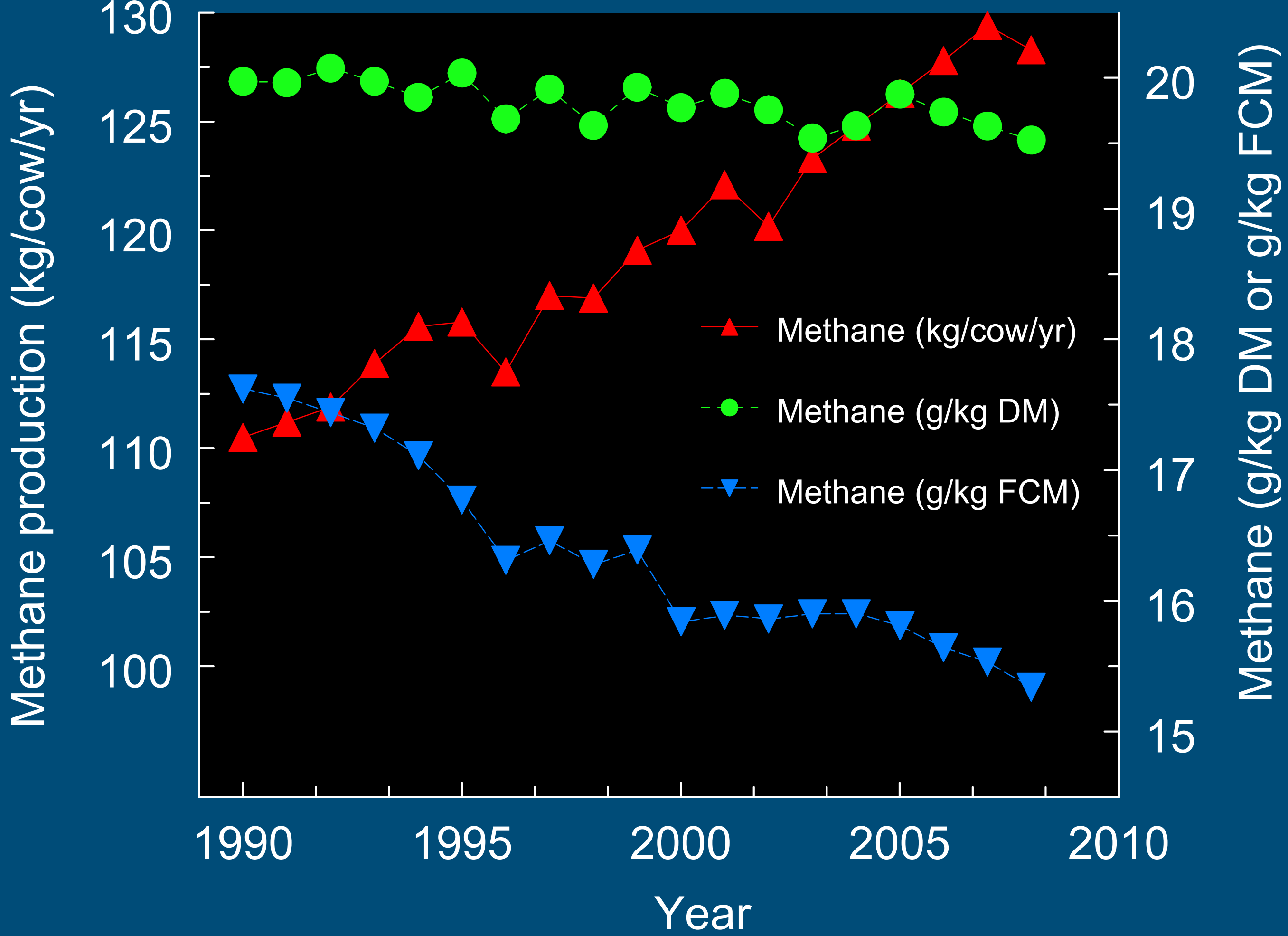

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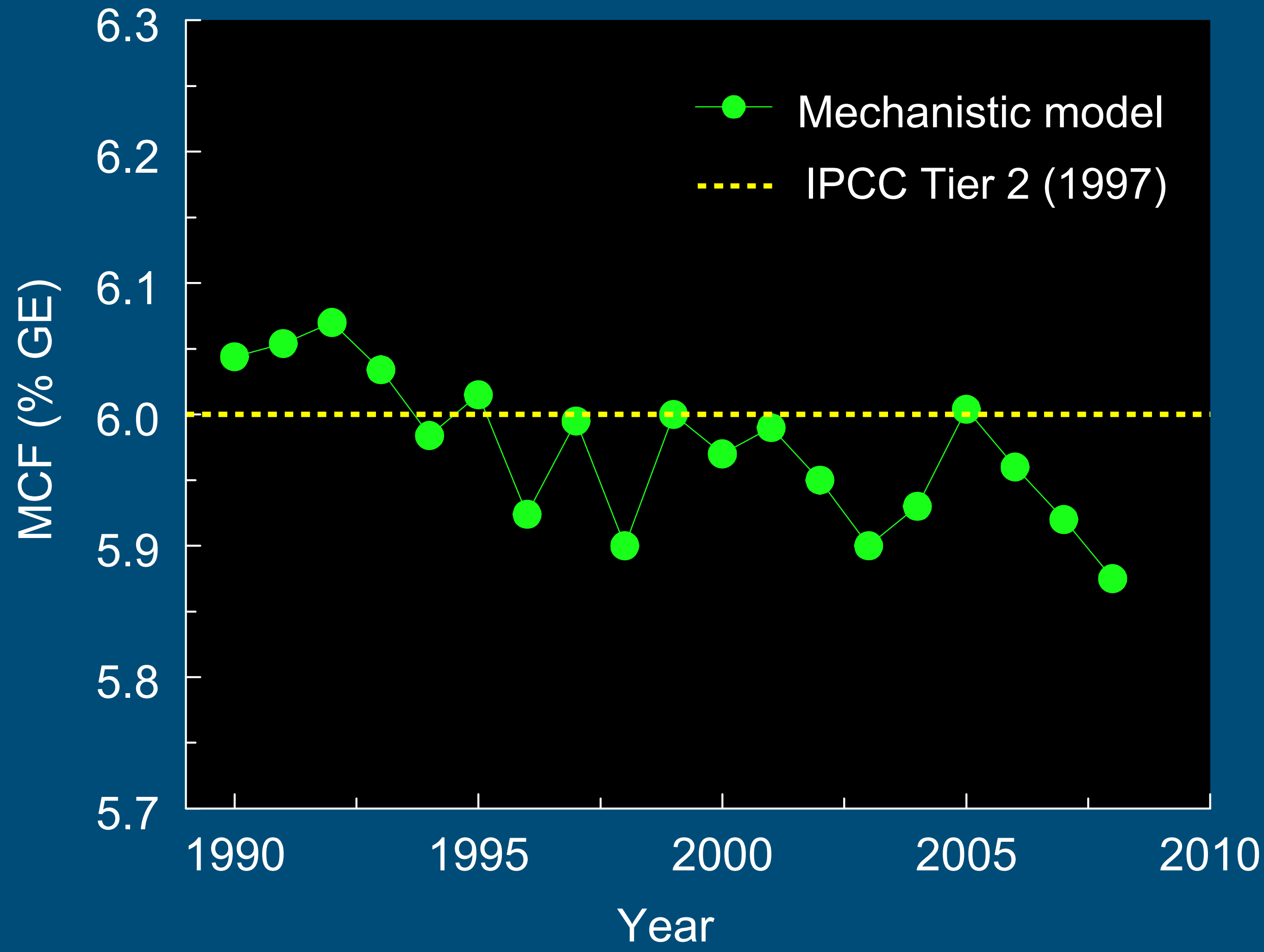
Methane Conversion Factor (MCF)



Trend methane production (kg/cow/yr):

IPCC 1.38

model 1.05

Conclusions mechanistic methane models

- Mechanistic methane models enable prediction based on understanding of the system
- Continued interaction between mechanistic modelling and experimentation allows faster progress
  - combine expertise in traditional fermentation parameters, molecular microbiological tools, and mathematics

Acknowledgements

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- Jennifer Ellis – Univ Guelph, Canada
- James France – Univ Guelp, Canada
- Ermias Kebreab – Univ Davis, USA
- Secundino Lopez – Univ Leon, Spain

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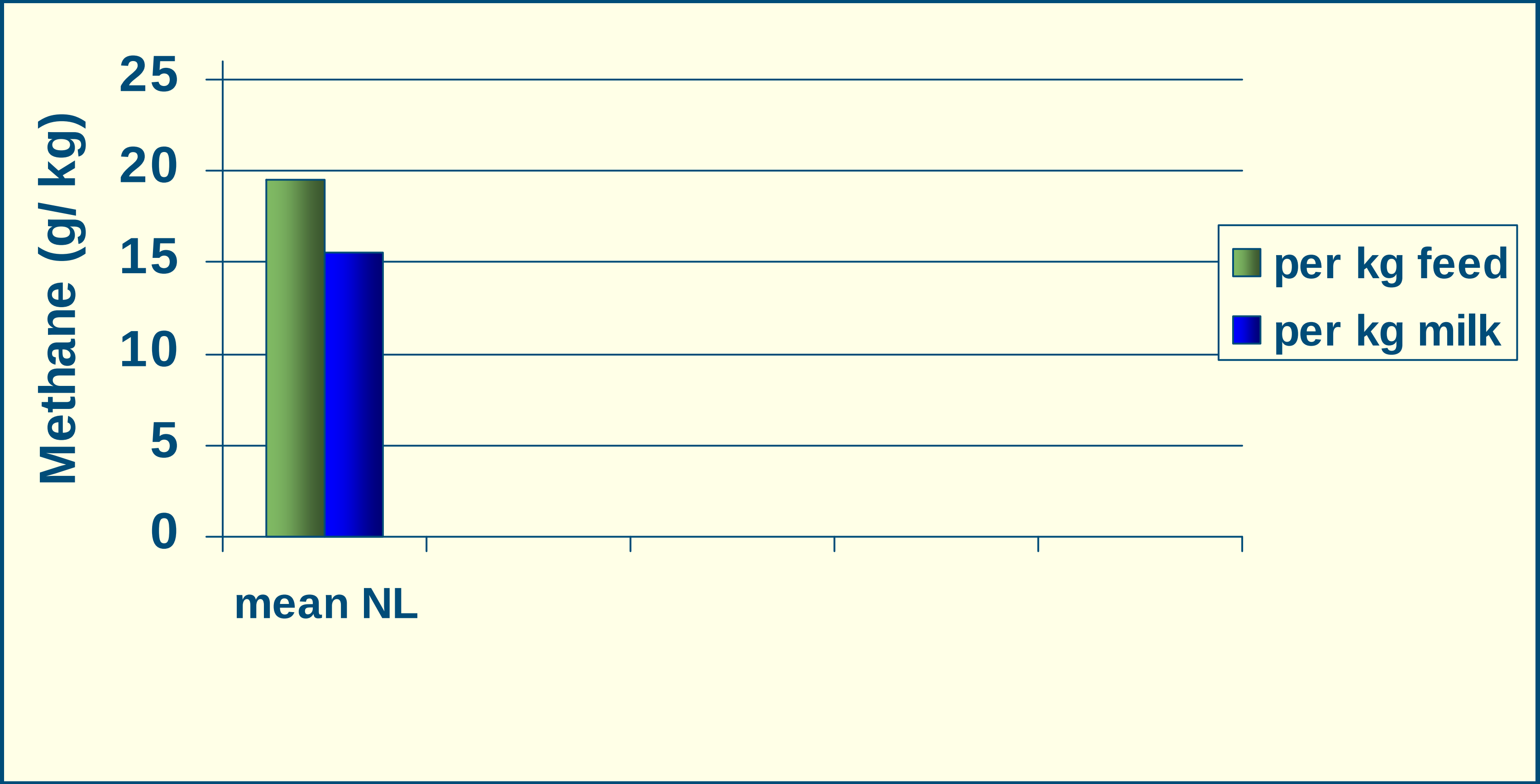
Practical solutions: model results



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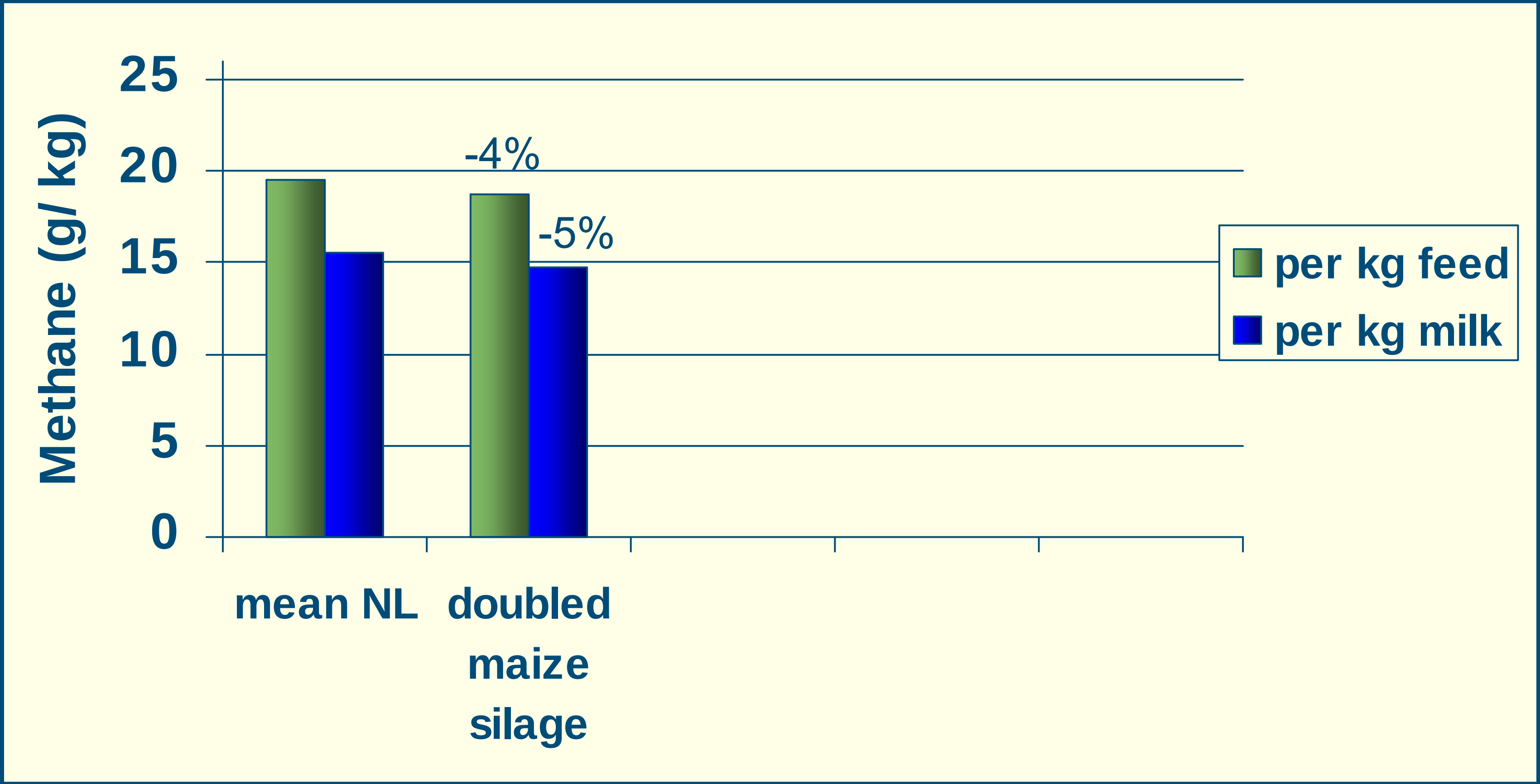

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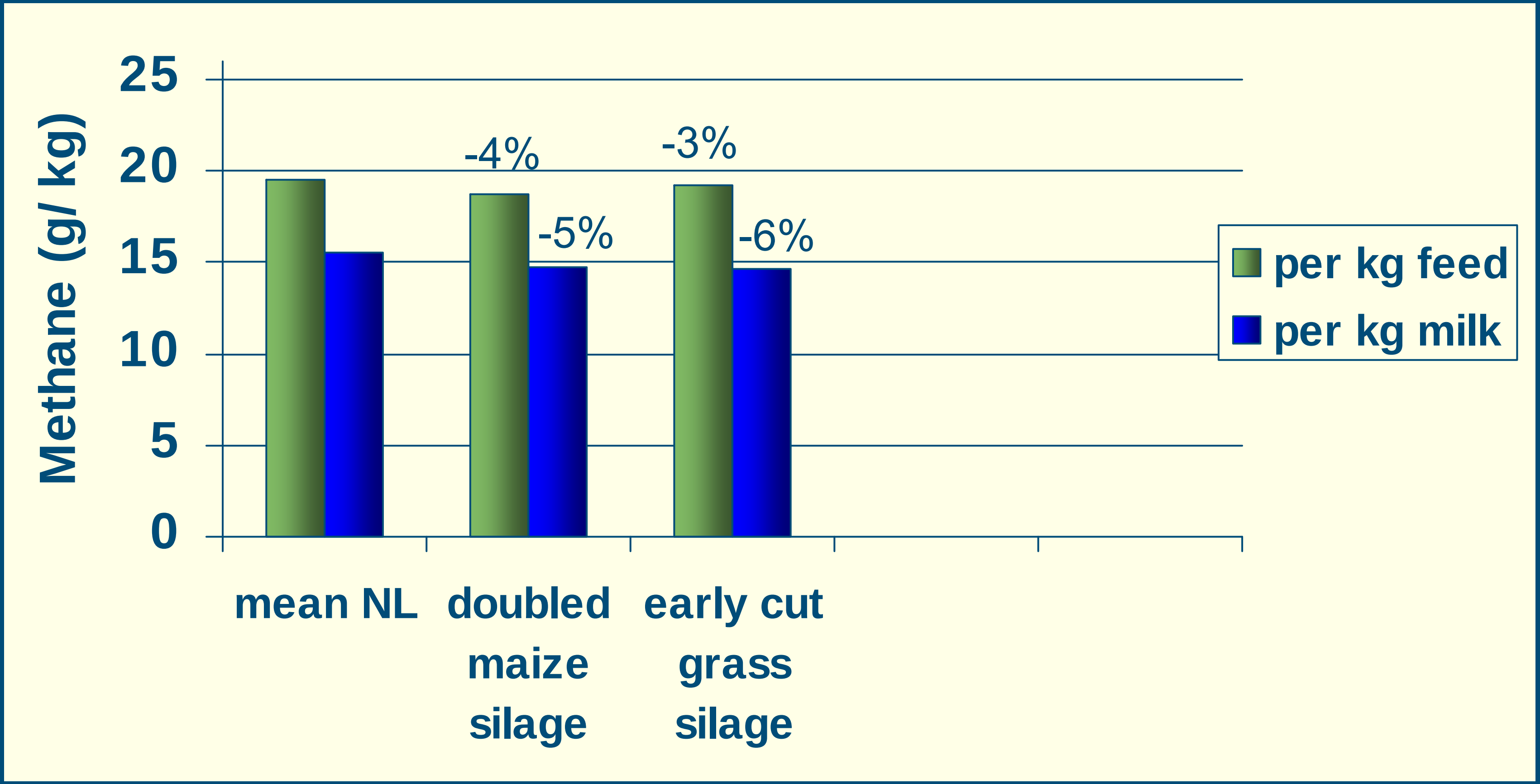

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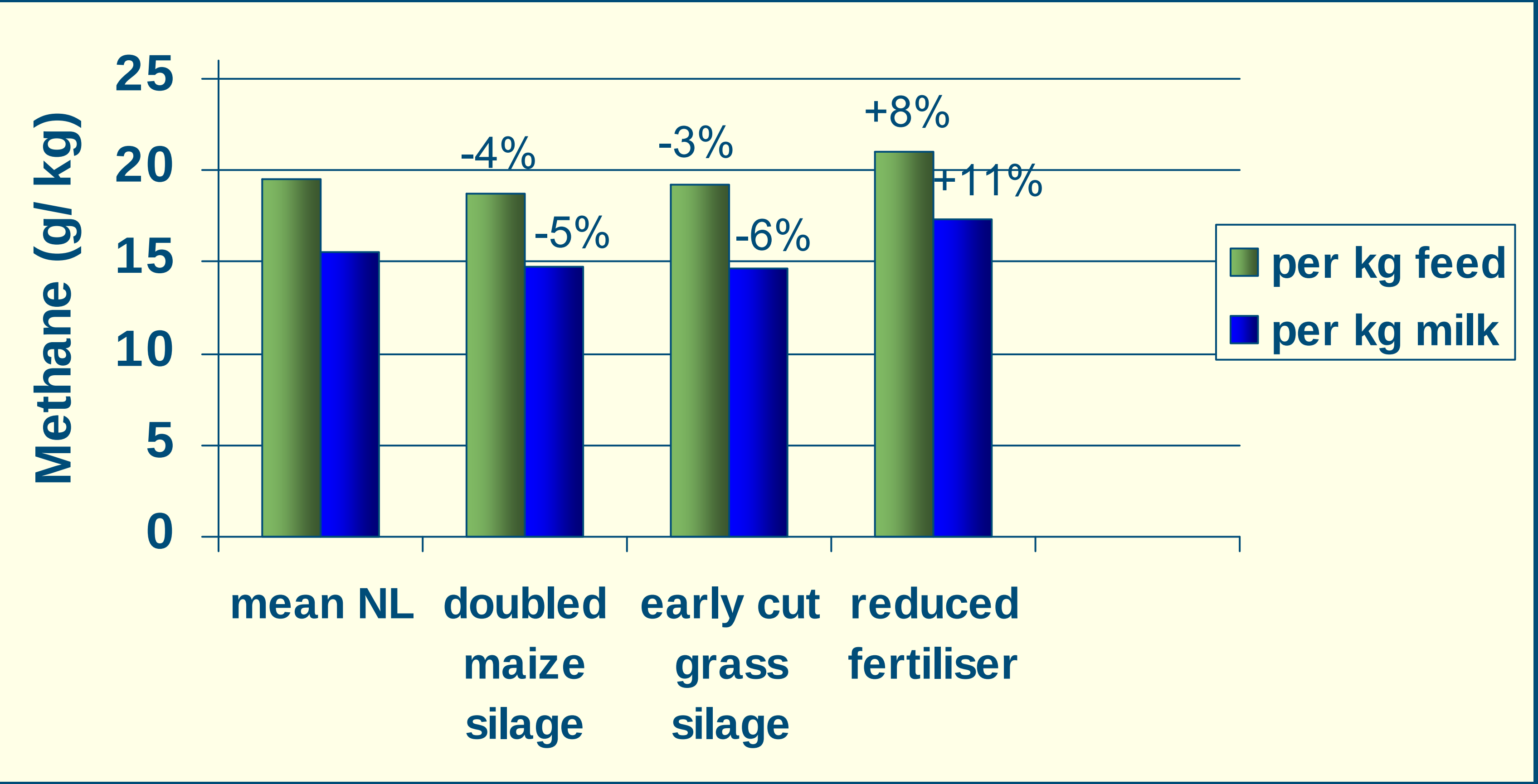

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