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38. A theoretical optimal experiment design for accurate estimation of key parameters of a dynamic mechanistic model representing the effect of *Asparagopsis taxiformis* on rumen fermentation and methane production under *in vitro* continuous conditions

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Introduction: Reducing methane (CH₄) emissions from ruminants is a major target for the livestock sector. Synergy between *in vitro* studies and models can be useful to provide high quality data enabling to quantify the mode of action of anti-methanogenic additives and thus robust mitigation solutions. The objective of this work was to conduct a theoretical optimal experiment design (OED) to identify experimental conditions for attaining accurate estimates of key parameters of a model we previously developed representing the impact of the anti-methanogenic macroalgae *Asparagopsis taxiformis* on rumen fermentation and CH₄ production under *in vitro* continuous conditions (Blondiaux et al. 2024).

Material and methods: *A. taxiformis* contains the anti-methanogenic compound bromoform (we assumed a bromoform content in the macroalgae of 0.684 % in the DM). CH₄ inhibition results in hydrogen (H₂) accumulation. H₂ exerts thermodynamic control on the fermentation via the flux allocation towards volatile fatty acids production. We applied the OED to 5 model parameters related to the mode of action of *A. taxiformis*: k_i (inhibitor bromoform constant) and p_1, p_2, p_3, p_4 (parameters of affine functions representing flux allocation factors). We assessed the parameter identifiability with GenSSI (Ligon et al. 2018) assuming that the measurements are the concentrations of acetate, butyrate, propionate and bromoform in the liquid phase, and CH₄, H₂, CO₂ in the gas phase. Then, we solved an OED problem for parameter estimation for a 24 h run allowing an accurate parameter estimation. For that, we used the D-optimality criterion that maximizes the determinant of the Fisher information matrix (**FIM**). The OED problem was set as $\min_{\varphi_d} -\text{Det}(\mathbf{FIM})$, with φ_d the design vector.

$\varphi_d = [w_{br}, t_1, t_2, \dots, t_{10}]$, with w_{br} the bromoform content in the feed, t_i the sampling times (h). The **FIM** was calculated by symbolic manipulation in Matlab. The optimization was done using the Matlab function `fminsearch` (Nelder-Mead Simplex Method).

Results and discussion: The parameters are globally identifiable. The optimal sampling were [0; 3.6; 5.7; 7.8; 11.4; 13; 15.4; 19.3; 22.4; 24] and the optimal bromoform content was 0.0020 % DM. Table 1 shows the standard deviations (s.d.) of the parameters by the OED compared to a classical equidistant sampling (ES) with a w_{br} of 0.0034 % DM. In average the s.d of the OED are 58 % of the s.d. with equidistant sampling.

Table 1 Ratio of the s.d. of the parameter estimates from the OED to the s.d. from an equidistant sampling (ES).

	k_i	p_1	p_2	p_3	p_4
100.s.d OED/s.d. ES	102	33	60	35	61

Conclusion and implications: We showed the benefits of OED for accurate parameter estimates. Applying OED can be instrumental for conducting experiments whose data will allow the construction of robust rumen fermentation models for helping the design of CH₄ mitigation strategies.

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39. Modelling collective manure management scenario and their environmental impacts

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