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Sensitivity analysis of a mechanistic model of the rumen in-vitro fermentation: Study of the impact of 3 sampling methods on Sobol indices of accuracy

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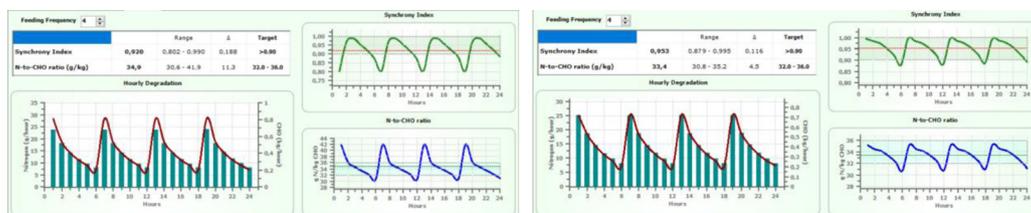


Fig. 2. Case study 2 as shown in NDS Professional before and after the reformulation (i.e., sunflower replaced by soymeal and molasses introduced).

Conclusion and implications

The index and the other parameters utilized can represent a way to represent asynchrony and possibly assist in a decision making process if associated with the CNCPS fractionation and prediction system. The tool would need to be validated *in vivo*. However, it is well known that the animal has a system to temporary manage lacks or surplus of either N or CHO. In fact the tool presents the potential as well to be improved with the prediction of, for example, the recycled N influx and the effects of low pH on fiber degradation across the 24 h.

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20. Sensitivity analysis of a mechanistic model of the rumen *in-vitro* fermentation: Study of the impact of 3 sampling methods on Sobol indices of accuracy

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Introduction

Biological systems are often described by complex models involving many input parameters, linked by non-linear relationships. Sensitivity analysis (SA) methods were developed to identify the contribution of input parameters (IP) to model's variance, using sensitivity indices (SI) (Sobol 1993). To accurately estimate SI, the sampling step is crucial to widely explore the variability space of IP, using techniques such as the Sobol sequences (SSeq), the latin hypercube sampling (LHS) or the Monte-Carlo method (MC). This work aims to study the impact of these 3 sampling methods on the accuracy of SI estimation of IP from an *in-vitro* mechanistic model of the rumen fermentation (Muñoz-Tamayo et al. 2016).

Material and methods

We applied the Sobol method with 3 sampling methods. The MC technique is commonly used to generate random and independent IP values following a probability distribution function. However, when applying MC, there is no control that the variability space is fully explored especially for a low number of simulations. To manage that, SSeq and LHS generate deterministic sequences that explore more evenly the IP variability space. We used as case study the model of rumen *in vitro* fermentation developed by Muñoz-Tamayo et al. (2016). The 9 IP considered for the SA were hydrolysis rate parameters (k_{hyd} , h^{-1}) associated to 3 polymer components in the diet (neutral detergent fiber, non-structural carbohydrates and proteins) and kinetic rate parameters (k_m , mol substrate/ (mol biomass h) and k_s , mol/L) associated to the utilization of 3 soluble substrates (sugars, amino acids and hydrogen). Methane concentration (CH_4 , μmol) at time $t = 24h$ was the output. First-order Sobol index (S_i) and total SI (T_i) (Homma and Saltelli 1996) were considered. For each sampling method, simulations number N varied from 100 to 1500 (step = 50). The IP sampling and indices were computed using *sensobol* R package (Puy et al. 2022).

Results and discussion

The parameter k_{m,H_2} contributed the most to CH_4 concentration variability ($S_{K_{m,H_2}} = 0.59$) followed by k_{s,H_2} ($S_{K_{s,H_2}} = 0.21$) and $k_{hyd,ndf}$ ($S_{K_{hyd,ndf}} = 0.10$), for $N = 100$ simulations with SSeq (Table 1). Moreover, interactions' contribution between IP x_i and other IP to model output variability was low ($T_i - S_i \leq 7\%$). For k_{m,H_2} , using the 3 sampling methods, S_i converged to the same value when simulation number N increased ($S_{K_{m,H_2}}$ was 0.65 – 0.66) (Fig. 1). The SSeq and LHS providing the closest S_i estimations for $N = 100$ simulations (Fig. 1). When increasing N, SSeq provided more stable estimations and lower SD, in comparison to LHS and MC (0.01 vs 0.02 and 0.04, respectively) (Fig. 1). Moreover, SSeq requires less simulations to provide a stable SI estimation. However, SSeq can have larger CI than LHS (High CI – Low CI = 0.34 vs 0.16 for $N = 100$ simulations, respectively).

Table 1
First-order Sobol (S_i) and total (T_i) indices estimated, with the confidence intervals (CI) associated for the Sobol sequences sampling (SSeq) method and 100 simulations.

| | S_i | Low CI | High CI | T_i | Low CI | High CI |
|----------------------------|-------|--------|---------|-------|--------|---------|
| k_{m,H_2} (mol/(mol.h)) | 0.59 | 0.44 | 0.78 | 0.62 | 0.34 | 0.85 |
| k_{s,H_2} (mol/L) | 0.21 | 0.01 | 0.48 | 0.14 | 0.09 | 0.19 |
| $k_{hyd,ndf}$ (h^{-1}) | 0.10 | -0.10 | 0.36 | 0.12 | 0.05 | 0.18 |
| $k_{hyd,pro}$ (h^{-1}) | 0.09 | -0.14 | 0.33 | 0.08 | 0.02 | 0.12 |
| $k_{s,aa}$ (mol/L) | 0.03 | -0.21 | 0.28 | 0.02 | 0.01 | 0.03 |
| $k_{m,aa}$ (mol/(mol.h)) | 0.02 | -0.20 | 0.25 | 0.02 | 0.01 | 0.04 |
| $k_{m,su}$ (mol/(mol.h)) | 0.02 | -0.20 | 0.26 | 0.00 | 0.00 | 0.01 |
| $k_{hyd,nsc}$ (h^{-1}) | 0.01 | -0.19 | 0.22 | 0.04 | 0.02 | 0.07 |
| $K_{s,su}$ (mol/L) | 0.01 | -0.22 | 0.26 | 0.01 | 0.00 | 0.02 |

$k_{hyd,j}$: hydrolysis rate constant associated to polymer components fiber carbohydrates (ndf), non-fiber carbohydrates (nsc) or proteins (pro).
 $k_{m,j}$: maximum specific utilization rate of soluble substrates sugars (su), amino acids (aa) or hydrogen (H_2).

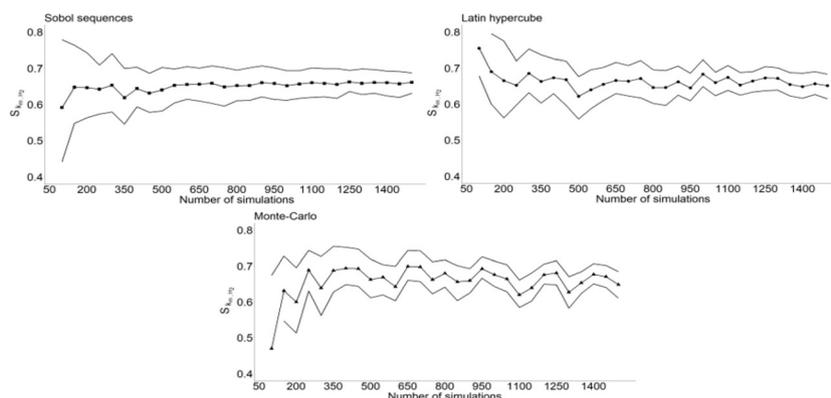


Fig. 1. Dynamic of the first-order Sobol index of k_{m,H_2} ($S_{k_{m,H_2}}$), with the confidence intervals (CI) associated according to the number of simulations for the 3 sampling methods.

Conclusion and implications

The IP k_{m,H_2} contributed the most to the variation of CH_4 concentration. The SSeq sampling method provided more stable estimations of IP's contribution than other methods, with a low number of simulations. Therefore, SSeq should be a more suitable sampling method, especially for models with a high computation time (models associated with numerous parameters and/or a high level of complexity). These models usually cannot afford a large number of simulations (of the order of a hundred). However, SSeq showed large confidence intervals and for a high number of simulations the 3 methods showed similar results. Based on this work, one research perspective is to conduct the sensitivity analysis of an *in-vivo* mechanistic model of the rumen fermentation with a high complexity level.

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