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Validation of *in situ* disappearance curves utilizing mathematical models for incubating fish meal and cottonseed meal

Validação de curvas de desaparecimento in situ utilizando modelos matemáticos para incubação de farinha de peixe e farelo de algodão

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Highlights:
Appropriate diet formulating for ruminants requires detailed description of the nutritional value of feeds and their degradation kinetics in the rumen.
Meanwhile considering similar performance of the tested models, the biological characteristics of the models should be taken into account in order to implement the estimated parameters for practical use.
Non-linear models may help to obtain more accurate and plentiful descriptions about degradability of feeds. The optimization of models using MATLAB software has been done for the first time in this study and is novelty of the study.

Abstract

Four mathematical models were used to describe the ruminal disappearance of dry matter (DM) and crude protein (CP) of fish meal and cottonseed meal. Results of DM degradability particularity showed that all the models fitted well ($R^2 > 0.95$), however, considering that values below 0 or above 100 are not biologically justified in ruminal degradability, they are not acceptable. The models I and II were accepted to ruminal DM degradability of fish meal and cottonseed meal data. Only models I and II were successfully fitted to CP degradability of fish meal ($R^2 > 0.96$), and the I, II and III models were acceptable to ruminal CP degradability of cottonseed meal ($R^2 > 0.98$). In terms of effective degradability (ED) of DM and CP, model II generated higher values than other models. To appreciate fully the role of mathematical modelling in the biological sciences, it is necessary to consider the nature of feeds that evaluated and to review the types of models that may be constructed.

Key words: Fish meal. Cottonseed meal. In situ technique. Mathematical models.

Resumo

Quatro modelos matemáticos foram utilizados para descrever o desaparecimento ruminal da matéria seca (MS) e proteína bruta (PB) da farinha de peixe e farelo de algodão. Os resultados da particularidade da degradabilidade da MS mostraram que todos os modelos se ajustaram bem ($R^2 > 0,95$), no entanto, considerando que valores abaixo de 0 ou acima de 100 não são biologicamente justificados na degradabilidade ruminal, eles não são aceitáveis. Os modelos I e II foram aceitos para a degradabilidade ruminal da MS da farinha de peixe e e o farelo de algodão. Apenas os modelos I e II foram adaptados com sucesso à degradabilidade de PB da farinha de peixe ($R^2 > 0,96$), e os modelos I, II e III foram

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aceitáveis para a degradabilidade ruminal da PB do farelo de algodão ($R^2 > 0,98$). Em termos de degradabilidade efetiva (DE) da MS e da PB, o modelo II gerou valores mais altos que os demais. Para apreciar plenamente o papel da modelagem matemática nas ciências biológicas, é necessário considerar a natureza dos alimentos que foram avaliados e revisar os tipos de modelos que podem ser construídos.
Palavras-chave: Farinha de peixe. Farelo de algodão. Técnica in situ. Modelos matemáticos.

Introduction

Changes in digestive processes are of nutritional importance, because it determines the amount of nutrients consumed by the animal (Van Soest, 2018; Sauvant & Noziere, 2016). Dynamic digestion models not only predict the nutritional value of feeds, dietary changes, microbial populations, and livestock physiological conditions, can also be detected the limiting factors of digestion process (Gregorini, Provenza, Villalba, Beukes, & Forbes, 2018; Bannink, van Lingen, Ellis, France, & Dijkstra, 2016; Reed, Arhonditsis, France, & Kebreab, 2016). Various models have been proposed to describe the digestion and passage of feed in the digestive system of ruminants (Rochen et al., 2020; Palangi & Macit, 2019; Dijkstra, Bannink, Bosma, Lantinga, & Reijs, 2018). The amount of digestion is a function of the time it stops in the digestive tract (Oberson, Probst, & Schlegel, 2019; Lopes et al., 2018). Changes in digestion can be described by dividing feed into fast-digesting, slow-digesting, and indigestible parts (Yousefian, Teimouri Yansari, & Chashnidel, 2019; Vaga & Huhtanen, 2018; Jin et al., 2017). Digestive models due to their dependence on the nature of the feedstuffs, were contained sequential equations that includes a linear and curved distribution of differential or integral equations that must be used to indicate the type of digestion process (Chanzanagh, Seifdavati, Gheshlagh, Abdibenemar, & Seyedsharifi, 2019; Bannink et al., 2016; Reed et al., 2016).

The use of different models to estimate nutrient degradability parameters and formulating hypotheses about the biological principles governing the separation of ruminal digestion, leads to the development of mathematical models, that have ability to describing the disappearance of the rumen. Using these models ruminal digestion of feed can be estimated and different nutritional systems can be compared (Hanigan & Daley, 2019; Lapierre, Larsen, Sauvant, Van Amburgh, & Van Duinkerken, 2018).

The objective of this study was to determine ruminal disappearances of fish meal and cottonseed meal in the rumen by *in situ* and to estimate their degradability parameters using different mathematical models fitted by MATLAB and to identify the best model fitting the data.

Materials and Methods

Mathematical modeling with MATLAB

The models, I and II, are Simple negative exponential curve models (monomolecular, Mitscherlich, or first-order kinetics model) without and with a lag phase (Ørskov & McDonald, 1979). Model III is Gompertz curve, asymmetrical about an inflection point M, which can be calculated from K=exp (cM) (France et al., 1990). Model IV is Generalised Mitscherlich, generalization of the model I (results in the model I for d = 0), with the addition of a square root time dependence component (Dhanoa, France, Siddons, Lopez, & Buchanan, 1995). The models that we used included:

First-order kinetics model without lag phase

$$P = a + b\,(1-e^{-ct})$$

First-order kinetics model with lag phase

$$P = a + b\,(1-e^{-c(t+L)})$$

Gompertz model

$$P = a+b\,(K - K^{\exp(-ct)}/K - 1)$$

Generalised Mitscherlich model

$$P = a + b\,(1 - e^{-c(t-L)-d(\sqrt{t}-\sqrt{L})})$$

Nowadays, optimization methods are widely used in various sciences (Milani, Çavdar, & Aghjehkand, 2012; Çavdar, Mohammad, & Milani, 2013), an optimization method combining MATLAB curve fitting toolbox and the numerical algorithm based on the Levenberg-Marquardt method was used. The models were identified through the editor toolstript, and the starting points and ranges required for the models were defined. We used a goodness of fit measure function to measure the error values of the fit curves in studied models.

Effective degradability

Effective degradability (ED) was calculated according to (Ørskov, Hovel, & Mould, 1980) equation:

$$ED = a + [bc/(c+k)]$$

where 'a', 'b' and 'c' are the constants as described earlier in the different mathematical models above and 'k' is the rumen fractional outflow rate (0.02/h, 0.03/h, 0.04/h, 0.05/h or 0.06/h).

Results

Statistical models output

The results of the different models on the DM and CP degradability of fish meal and cottonseed meal were presented in Table 1 and 2. The comparison of various fitted models for DM degradability of fish meal and cottonseed meal, based on the coefficient of determination (R^2) and Adjusted (R^2) showed that models I and II was the best model. It may be concluded that the model with lag time (Model III) was the best model for description of degradability trends in CP of the cottonseed meal, because it was showed higher r^2 and Adjusted r^2.

Table1
Estimated DM degradability parameters of fish meal and cottonseed meal using different mathematical models with MATLAB

	Prameter[1]						SSE[2]	R-Square	Adj R-Square	Iter
	a	b	c	L	d	k				
Fish meal										
Model I[3]	6.51	22.69	0.0627	-	-	-	13.673	0.9600	0.9400	22
Model II	7.10	22.10	0.0627	0.2636	-	-	13.673	0.9600	0.9200	6
Model III	-134.5	22.48	0.0669	-	-	0.8445	13.786	0.9597	0.9194	109
Model IV	21.19	54.12	0.0075	210.3	-0.0748	-	14.135	0.9587	0.8760	92
Cottonseed meal										
Model I	15.50	42.96	0.0219	-	-	-	11.947	0.9779	0.9668	22
Model II	21.73	36.73	0.0219	0.1566	-	-	11.947	0.9779	0.9557	12
Model III	-35.41	36.50	0.0359	-	-	0.4785	10.827	0.9799	0.9599	109
Model IV	136.30	197.60	0.0015	277.6	-0.0055	-	21.028	0.9610	0.8831	92

[1]*a* = rapidly soluble fraction (%); *b* = slowly degradable fraction (%); *c* = degradation rate constant (%/h) of fraction 'b'; *L* = lag time (h); *d*= is the parameter pertaining to the variable fractional rate of degradation; *k* = slope, or degradation rate coefficient (h^{-1}); [2]SSE = Sum of Squares Due to Error; R-Square= the square of the correlation between the response values and the predicted response values; Adj R-Square= Degrees of Freedom Adjusted R-Square; Iter = iteration number of MATLAB.
[3] Model I, First-order kinetics model without lag phase; Model II, First-order kinetics model with lag phase; Model III, Gompertz model; Model IV, Generalised Mitscherlich model.

Table2
Estimated CP degradability parameters of fish meal and cottonseed meal using different mathematical models with MATLAB

	Prameter[1]						SSE[2]	R-Square	Adj R-Square	Iter
	a	b	c	L	d	k				
Fish meal										
Model I[3]	6.74	25.78	0.0611	-	-	-	14.363	0.9669	0.9503	17
Model II	8.76	23.76	0.0611	0.0816	-	-	14.363	0.9669	0.9337	5
Model III	-101.7	25.39	0.0672	-	-	0.7776	14.944	0.9655	0.9310	109
Model IV	-204.5	249	-0.114	87.09	-0.0167	-	9.824	0.9773	0.9320	92
Cottonseed meal										
Model I	14.18	42.74	0.0298	-	-	-	13.657	0.9813	0.9719	17
Model II	20.95	35.97	0.0298	0.1725	-	-	13.657	0.9813	0.9626	11
Model III	8.62	32.65	0.0814	-	-	0.0947	8.742	0.9880	0.9760	55
Model IV	132.6	197.6	0.0014	251.3	-0.0110	-	31.281	0.9572	0.8715	92

[1]*a* = rapidly soluble fraction (%); *b* = slowly degradable fraction (%); *c* = degradation rate constant (%/h) of fraction 'b'; *L* = lag time (h); *d*= is the parameter pertaining to the variable fractional rate of degradation; *k* = slope, or degradation rate coefficient (h^{-1});
[2]SSE = Sum of Squares Due to Error; R-Square= the square of the correlation between the response values and the predicted response values; Adj R-Square= Degrees of Freedom Adjusted R-Square; Iter = iteration number of MATLAB.
[3] Model I, First-order kinetics model without lag phase; Model II, First-order kinetics model with lag phase; Model III, Gompertz model; Model IV, Generalised Mitscherlich model.

Effective degradability

Table 3 shows the fish meal and cottonseed meal main effect means for effective degradability (ED) at the five rates of passage considered (0.02/h, 0.03/h, 0.04/h, 0.05/h or 0.06/h).

Table 3
Estimated effective degradability (ED) of dry matter and crude protein of fish meal and cottonseed meal using different mathematical models

	DM[1]					CP				
	k[2]=0.02	k=0.03	k=0.04	k=0.05	k=0.06	k=0.02	k=0.03	k=0.04	k=0.05	k=0.06
Fish meal										
Model I[3]	23.72	21.86	20.37	19.14	18.11	26.16	24.02	22.31	20.91	19.74
Model II	23.86	22.06	20.60	19.40	18.40	26.66	24.69	23.11	21.82	20.74
Model III	-	-	-	-	-	-	-	-	-	-
Model IV	-	-	-	-	-	-	-	-	-	-
Cottonseed meal										
Model I	37.98	33.65	30.73	28.61	27.01	39.77	35.49	32.44	30.15	28.38
Model II	40.95	37.25	34.75	32.94	31.57	42.48	38.89	36.32	34.40	32.90
Model III	-	-	-	-	-	34.83	32.48	30.51	28.85	27.42
Model IV	-	-	-	-	-	-	-	-	-	-

[1]*DM* = effective ruminal degradability of dry matter; *CP* = effective ruminal degradability of crude protein
[2]*k* = the rumen fractional passage rate
[3] Model I, First-order kinetics model without lag phase; Model II, First-order kinetics model with lag phase; Model III, Gompertz model; Model IV, Generalised Mitscherlich model.

Discussion

Statistical models output

According to fitted model (model II), there was part of the hour lag time in degradability, it can be said that the degradability of fish meal and cottonseed meal takes some h to be started.

Comparison of different models for estimating ruminal CP degradation parameters of fish meal revealed that models I and II reported by Ørskov and McDonald (1979) reach convergence, while other models because of estimated negative values, they were not biologically acceptable. Despite that the I, II and III models were reached convergence for CP degradability of cottonseed meal, based on the coefficient of determination (R^2) and Adjusted (R^2) showed that models III was fitting the best model.

Effective degradability

The ED declined as passage rates increased, because if the passage rates increased the rumen microorganisms will not have enough time to effect on the feed. According to the results, model II showed a higher amount of DM and CP effective degradability in fish meal and cottonseed meal. The ruminal biodegradability of CP affects the efficiency of nitrogen use for microbial protein synthesis. Starch fermentation rates can also affect the rate of ammonia consumption by altering the energy supply for microbial growth.

Conclusions

It can be concluded that only models I and II can be used for estimating the degradability of DM of fish meal and cottonseed meal, but in cottonseed protein, in addition to these models, the III model showed the good behavior.

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Authors' contributions

VP collected the data for this study, conducted the statistical analyses, VP and MB developed the original hypotheses and designed the experiments, VP collaborated in interpreting the results and finalized the manuscript. Both authors have read and approved the finalized manuscript

Conflict of Interest Declaration

The authors declare that they have no known competing financial interests or personal relationship that could have appeared to influence the work reported in this paper.

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