# Mathematical Models Comparison for Illustration of Ruminal Degradability Curves of Citrus Pulp

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## Abstract

*Food security is of global concern, which requires more attention on the identification of alternative sources. To combat and marginally prevent the issue, human edible grains can be excluded from the livestock feed. These grains can be substituted by nutrient rich process discards and by-products such as citrus pulp. In this study, four mathematical models were used to describe the ruminal disappearance of dry matter (DM) and crude protein (CP) of orange, grapefruit, lemon, and tangerine pulps: (I) non-lagged simple Mitscherlich or exponential, (II) lagged simple Mitscherlich or exponential, (III) Gompertz and (IV) generalized Mitscherlich. Results of DM and CP degradability characteristics showed that all the models fitted well ($r^2 > 0.95$) to the disappearance data and there were minor differences between the models in terms of statistical evaluations. Results also revealed that the models differed in the estimated parameters depending on the nature and structure of the model, and parameters included. Model III estimated negative values for the studied parameters making those biologically unacceptable. Only models I and II can be used for estimating the degradability of DM and CP of citrus pulps. Citrus pulps, containing a large amount of ruminal degradable fractions, can be used as feed source in ruminants.*

***Keywords**:* citrus pulps, model selection, nonlinear regression

## 1. Introduction

The use of agro-industrial by-products as animal feeds has been a matter of interest for the last few decades because of discarding or burning wastes or agro-industrial by-products causes potential air and water pollution problems (Palangi *et al*., 2013). Food processing discards and or by-products have successfully been used to improve the sustainability of the dairy industry (Fessenden *et al*., 2019). For instance, in 2016, 124.246 kt of citrus pulp was produced that could have been utilized as feed and or feed additive (Food and Agriculture, 2017; Nogales-Mérida *et al.*, 2019).

Not only that citrus pulp is rich in nutrients, but it also contains soluble carbohydrates as well as readily digestible neutral detergent fiber (NDF) that could be used up by ruminal microbes as energy substrates (Ammerman and Henry, 1991; Miron *et al.*, 2002). This by-product has been previously used as high energy feed to boost the growth and lactation of cattle (Pang *et al.*, 2018; Karlsson *et al.*, 2020).

Generally, fermentation of feedstuff in ruminants is studied by in-vivo, in-situ and in-vitro techniques. In the one hand, in-situ technique (Dacron polyester), as a rather simple and an inexpensive method, has been used widely for estimating the ruminal nutrient degradation worldwide. On the other hand, with the nylon-bag technique, a rather complex method, potential degradability of feedstuffs and feed constituents as well as its rates of disappearance could be estimated (Taghizadeh *et al*., 2008). In contrary to the above-mentioned techniques, dynamic digestion models not only would predict the nutritional value of the feed, microbial populations, and physiological status of livestock but could also facilitate investigating the digestion process limiting factors (Palangi and Macit, 2019). It is of note that digestion rate is the function of feed retention time in the digestive tract; thus, changes in the digestion process can be illustrated by dividing feed into (1) easily digested, (2) slowly digested and (3) indigestible part.

To date, various methods have been suggested for the estimation of quality proportions of feeds. Nonetheless, identifying digestible models and plotting their degradation curves would provide more useful information for feed evaluation. The aim of present study was to investigate the in-situ digestion parameters of citrus pulps as an alternative fibrous feedstuff, and to compare different mathematical models to select the best model for fitting the ruminal degradability data.

## 2. Methodology

Samples were dried in controlled conditions to avoid excessive dehydration and heat damage, which could result in formation of indigestible protein. Subsequently, samples were ground, sieved (Willy® Mill, 2 mm screen sieve) and combined for chemical analysis and in-situ degradability assays. Two yearling ruminal cannulated wethers (35±1.8 kg) were used for in-situ degradability experiment.

Models I and II are simple negative exponential curve models (monomolecular, Mitscherlich, or first-order kinetics model) without and with a lag phase, respectively. Model III is Gompertz curve, asymmetrical about an inflection point M, which can be calculated from K = exp (cM). Model IV is generalized Mitscherlich, generalization of the model I (results in the model I for d = 0), with the addition of a square root time dependence component (Palangi, 2020). Mathematically, models I, II, III, and IV are specified in Equations 1, 2, 3 and 4, respectively.

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

$$P = a + b\,(1 - e^{-c(t + L)}) \tag{2}$$

$$P = a + b\,(K - K^{\exp(-ct)}/K - 1) \tag{3}$$

$$\mathrm{P} = a + b\,(1 - e^{-c(t - L) - d(\sqrt{t} - \sqrt{L})}) \tag{4}$$

Data of the DM and CP disappearance were fitted to each model by nonlinear regression using the Levenberg-Marquardt procedure of the MATLAB (MATLAB, 2019). In this study, optimization method was proposed, which combines MATLAB curve fitting toolbox and the numerical algorithm based on the Levenberg-Marquardt method. The models were identified through the editor toolstript, and the starting points and ranges required for the models were defined. The study used goodness-of-fit measure function to measure the error values of the fit curves in studied models. The mathematical model fitting was stopped when change in residuals were less than the tolerance. Effective degradability (ED) was calculated using Equation 5 (Ørskov *et al*., 1980).

$$ED = a + [bc/(c+k)] \tag{5}$$

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).

## 3. Results and Discussion

### *3.1 Statistical Models Output*

The results of the different digestible models on the DM degradability of citrus pulps are presented in Table 1. The comparison of various fitted models for DM degradability of citrus pulps based on the coefficient of determination ($r^2$) and adjusted R square ($r^2$) showed that model III was fitting the best for orange and tangerine but not biologically acceptable for grapefruit and lemon due to estimated negative values. Correspondingly, models I and II were best fitted for grapefruit and lemon. The challenge for the mathematical modeler is to develop a meaningful equation capable of describing such a group of accumulation curves. In this study, models I and II showed highest goodness parameters, which better describe the properties of citrus pulps. The process of fitting continued until change in residuals were less than tolerance, and then fitting was stopped. According to fitted model (model II), there was part of the lag time in degradability. This may mean that the degradability of citrus pulps takes some hours to start. Thus, it can be concluded that the formation of secondary structure of the cell wall in the citrus pulps would lead to an increase in structural compounds, increased pectin and cellulose content impeding the initiation of microbial degradation.

Comparison of different models for estimating ruminal CP degradation parameters of citrus pulps revealed that models I and II reported by Ørskov and McDonald (1979) reach convergence, while others, due to estimated negative values, were not biologically acceptable (Table 2). The results of this study demonstrated that model I is the best one among all fitted models given the higher value of adjusted R square ($r^2$).

According to Silva *et al*. (1997) values of soluble (a) and insoluble (b) fraction for DM of orange were 30.06 and 69.94, respectively. The present results were not in agreement with the findings of Silva *et al*. (1997). Values for CP soluble and insoluble fractions, reported by Pereira and Gonzalez (2004), were 39.5 and 55.5, respectively. These values were higher than our findings. These variations can be due to various factors such as citrus variety, drying processes, climate conditions and maturity.

Table1. Estimated DM degradability parameters of citrus pulps using different mathematical models with MATLAB

| | Prameter[1] | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | *a* | *b* | *c* | *L* | *d* | *k* | SSE[2] | R-Square | Adj R-Square | Iter |
| *Orange* | | | | | | | | | | |
| Model I[3] | 30.02 | 60.52 | 0.1274 | - | - | - | 78.918 | 0.9718 | 0.9638 | 4 |
| Model II | 44.26 | 46.27 | 0.1274 | 0.2685 | - | - | 78.918 | 0.9718 | 0.9578 | 3 |
| Model III | 44.98 | 44.22 | 0.3186 | - | - | 0.0006 | 46.025 | 0.9836 | 0.9754 | 22 |
| Model IV | 42.14 | 44.6 | 0.1398 | 1.806 | -0.0134 | - | 75.178 | 0.9732 | 0.9517 | 5 |
| *Grapefruit* | | | | | | | | | | |
| Model I | 32.17 | 60.29 | 0.1837 | - | - | - | 26.220 | 0.9868 | 0.9830 | 6 |
| Model II | 51.28 | 41.18 | 0.1837 | 0.3812 | - | - | 26.220 | 0.9868 | 0.9802 | 6 |
| Model III | -134.3 | 58.35 | 0.1994 | - | - | 0.6873 | 28.453 | 0.9857 | 0.9785 | 105 |
| Model IV | 47.5 | 38.38 | 0.2365 | 1.725 | -0.0285 | - | 8.836 | 0.9956 | 0.9920 | 5 |
| *Lemon* | | | | | | | | | | |
| Model I | 24.32 | 61.38 | 0.0763 | - | - | - | 60.939 | 0.9840 | 0.9794 | 5 |
| Model II | 47.81 | 37.89 | 0.0763 | 0.4825 | - | - | 60.939 | 0.9840 | 0.9759 | 5 |
| Model III | -101.0 | 59.64 | 0.0882 | - | - | 0.6031 | 60.409 | 0.9841 | 0.9761 | 109 |
| Model IV | 40.17 | 43.17 | 0.0800 | 3.916 | -0.0083 | - | 60.443 | 0.9841 | 0.9714 | 5 |
| *Tangerine* | | | | | | | | | | |
| Model I | 32.44 | 57.64 | 0.1041 | - | - | - | 75.862 | 0.9739 | 0.9664 | 3 |
| Model II | 50.03 | 40.04 | 0.1041 | 0.3642 | - | - | 75.862 | 0.9739 | 0.9608 | 4 |
| Model III | 40.69 | 46.53 | 0.2265 | - | - | 0.0151 | 70.057 | 0.9759 | 0.9638 | 18 |
| Model IV | 40.63 | 42.98 | 0.1222 | 1.61 | -0.0226 | - | 68.215 | 0.9765 | 0.9577 | 4 |

[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, generalized Mitscherlich model.

Table 2. Estimated CP degradability parameters of citrus pulps using different mathematical models with MATLAB

| | Prameter[1] | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | *a* | *b* | *c* | *L* | *d* | *k* | SSE[2] | R-Square | Adj R-Square | Iter |
| *Orange* | | | | | | | | | | |
| Model I[3] | 7.002 | 30.58 | 0.0605 | - | - | - | 33.663 | 0.9672 | 0.9578 | 8 |
| Model II | 10.96 | 26.62 | 0.0605 | 0.1387 | - | - | 33.663 | 0.9672 | 0.9508 | 9 |
| Model III | -135.6 | 30.09 | 0.0642 | - | - | 0.7982 | 36.064 | 0.9648 | 0.9472 | 109 |
| Model IV | 4.78 | 16.75 | 0.1822 | 1.119 | -0.127 | - | 6.724 | 0.9934 | 0.9882 | 5 |
| *Grapefruit* | | | | | | | | | | |
| Model I | 9.19 | 27.02 | 0.0538 | - | - | - | 29.105 | 0.9644 | 0.9542 | 7 |
| Model II | 11.45 | 24.76 | 0.0538 | 0.0873 | - | - | 29.105 | 0.9644 | 0.9466 | 9 |
| Model III | -116. 6 | 26.58 | 0.0567 | - | - | 0.7979 | 30.938 | 0.9622 | 0.9432 | 109 |
| Model IV | 4.47 | 15.3 | 0.2135 | 0.7401 | -0.1353 | - | 10.206 | 0.9875 | 0.9775 | 7 |
| *Lemon* | | | | | | | | | | |
| Model I | 2.53 | 27.24 | 0.0888 | - | - | - | 11.628 | 0.9834 | 0.9787 | 6 |
| Model II | 7.38 | 22.39 | 0.0888 | 0.1961 | - | - | 11.628 | 0.9834 | 0.9751 | 6 |
| Model III | -78.16 | 26.73 | 0.0992 | - | - | 0.6999 | 12.102 | 0.9827 | 0.9741 | 109 |
| Model IV | 6.57 | 18.34 | 0.1158 | 2.02 | -0.0393 | - | 8.107 | 0.9884 | 0.9792 | 4 |
| *Tangerine* | | | | | | | | | | |
| Model I | 6.28 | 28.77 | 0.0574 | - | - | - | 16.511 | 0.9817 | 0.9765 | 5 |
| Model II | 9.86 | 25.19 | 0.0574 | 0.1331 | - | - | 16.511 | 0.9817 | 0.9726 | 9 |
| Model III | -121.4 | 28.31 | 0.0612 | - | - | 0.7887 | 18.105 | 0.9799 | 0.9699 | 109 |
| Model IV | 5.32 | 16.75 | 0.1226 | 1.02 | -0.0989 | - | 7.1358 | 0.9921 | 0.9858 | 5 |

[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, generalized Mitscherlich model.

Table 3. Estimated ED of dry matter and crude protein of citrus pulps 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 |
| *Orange* | | | | | | | | | | |
| Model I[3] | 82.33 | 79.01 | 76.08 | 73.48 | 71.16 | 29.98 | 27.44 | 25.41 | 23.74 | 22.36 |
| Model II | 84.25 | 81.71 | 79.47 | 77.49 | 75.72 | 30.97 | 28.76 | 26.98 | 25.53 | 24.32 |
| Model III | 86.59 | 85.39 | 84.27 | 83.20 | 82.19 | - | - | - | - | - |
| Model IV | 81.16 | 78.86 | 76.82 | 74.99 | 73.35 | 19.87 | 19.16 | 18.51 | 17.92 | 17.38 |
| *Grapefruit* | | | | | | | | | | |
| Model I | 86.54 | 84.00 | 81.68 | 79.56 | 77.62 | 28.89 | 26.54 | 24.69 | 23.20 | 21.97 |
| Model II | 88.42 | 86.68 | 85.10 | 83.65 | 82.32 | 29.50 | 27.35 | 25.66 | 24.29 | 23.16 |
| Model III | - | - | - | - | - | - | - | - | - | - |
| Model IV | 82.89 | 81.56 | 80.33 | 79.18 | 78.11 | 18.46 | 17.88 | 17.35 | 16.86 | 16.41 |
| *Lemon* | | | | | | | | | | |
| Model I | 72.96 | 68.38 | 64.59 | 61.40 | 58.68 | 24.77 | 22.90 | 21.32 | 19.96 | 18.79 |
| Model II | 77.83 | 75.01 | 72.67 | 70.70 | 69.02 | 25.66 | 24.12 | 22.82 | 21.71 | 20.74 |
| Model III | - | - | - | - | - | - | - | - | - | - |
| Model IV | 74.71 | 71.57 | 68.95 | 66.74 | 64.84 | 22.21 | 21.14 | 20.20 | 19.38 | 18.65 |
| *Tangerine* | | | | | | | | | | |
| Model I | 80.79 | 77.18 | 74.08 | 71.38 | 69.01 | 27.61 | 25.17 | 23.23 | 21.65 | 20.34 |
| Model II | 83.62 | 81.11 | 78.96 | 77.08 | 75.43 | 28.54 | 26.40 | 24.70 | 23.32 | 22.17 |
| Model III | 83.44 | 81.78 | 80.24 | 78.81 | 77.48 | - | - | - | - | - |
| Model IV | 77.56 | 75.14 | 73.01 | 71.13 | 69.46 | 19.72 | 18.78 | 17.95 | 17.22 | 16.57 |

[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, Generalized Mitscherlich model

### *3.2 Effective Degradability*

Table 3 shows the effective degradability of citrus pulps in the assumed values of ruminal rate of passage rate (0.02/h, 0.03/h, 0.04/h, 0.05/h or 0.06/h). The ED declined as passage rates increased; if the passage rates increased, the rumen microorganisms will not have enough time to affect the feed. The amount of ED for crude protein in model II was greater. This is due to the dissimilar behavior of different models for the degradability of dry matter and crude protein. On the one hand, the ruminal biodegradability of CP affects the efficiency of nitrogen use for microbial protein synthesis. On the other hand, starch fermentation rates can also affect the rate of ammonia consumption by altering the energy supply for microbial growth (Owens and Basalan, 2016).

## 4. Conclusion

It can be concluded that only models I and II can be used for estimating the degradability of DM and CP of citrus pulps. However, 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. In addition, citrus pulp may be used in ruminant rations as an alternative feed source to roughage. Nevertheless, more in-vivo along with in-situ and in-vitro studies are required to determine the actual nutritive value of citrus pulp for ruminant animals.

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