

Comparison of Some Mathematical Models Used in Gas Production Technique

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Abstract: The aim of this study was to compare some mathematical models used *in vitro* gas production technique. Chemical composition including Dry Matter (DM), Crude Protein (CP), Neutral Detergent Fiber (NDF), Acid Detergent Fiber (ADF) and ash contents of feedstuffs were determined. Gas productions were determined at 0, 3, 6, 12, 24, 48, 72 and 96 h incubation times and their kinetics were estimated using the four different mathematical models. The mean square error of wheat grain, vetch hay and wheat straw ranged from 5.589-10.538, 1.590-9.668 and 0.814-12.118, respectively. The adjusted coefficient of determination of wheat grain, vetch hay and wheat straw ranged from 0.979-0.989, 0.962-0.992 and 0.976-0.995, respectively. The Durbin-Watson statistic of wheat grain, vetch hay and wheat straw ranged from 1.378-2.479, 1.502-2.928 and 1.178-3.623, respectively. The best model for the gas production of wheat grain was the Von Bertalanffy and France functions when MSE and R^2_{adj} parameter was taken into consideration. The best model for the gas production of vetch is the Von Bertalanffy function when MSE parameter was taken into consideration whereas the best model for vetch hay was the Von Bertalanffy and Orskov functions when R^2_{adj} parameter was taken into consideration. The best model for the gas production of wheat straw is the Orskov, Menke and Von Bertalanffy functions when MSE parameter was taken into consideration whereas the best model for the wheat straw was the Von Bertalanffy function when the R^2_{adj} parameter was taken into consideration. The best model for the gas production of wheat grain is the Orskov and Von Bertalanffy functions when DW parameter was taken into consideration. On the other hand, the best model for the gas production of vetch hay and wheat straw is the Orskov and Menke functions when DW parameter was taken into consideration. There is no 1st order autocorrelation in errors of wheat grain and vetch hay estimated by four models used in the current study therefore, the four models can be used to fit the individual gas production data measured in different time intervals. Von Bertalanffy function is not suggested to fit the gas production data since, there is negative autocorrelation in errors of wheat straw. As a conclusion, choice of best model should be made on the basis of fitting criteria and feedstuffs since, goodness of fit of model is depended on feedstuffs tested and fitting criteria.

Key words: *In vitro* fermentation, wheat grain, vetch hay, wheat straw, mathematical model, gas production kinetics

INTRODUCTION

Recently, *in vitro* gas production technique had been used for different reason such as comparison forages (Taghizadeh *et al.*, 2006; Idikut *et al.*, 2009; Torbatinejad *et al.*, 2009; Kilic and Garipoglu, 2009; Kilic and Saricicek, 2010; Kamalak, 2010; Saricicek and Kilic, 2011), determination of anti-nutritive factors (Kamalak *et al.*, 2005) and interaction of feed ingredients in ruminant rations (Babayemi and Bamikole, 2006; Ozturk *et al.*, 2006). In addition, *in vitro* gas production methods has been reported to be more efficient than other *in vitro* methods in evaluating the potential nutritive value of tannin containing feedstuffs used in ruminant animal ration (Pashaei *et al.*, 2010). It is well known that

fermentation of feedstuffs results in production of volatile fatty acids (acetate, propionate and butyrate, etc.) and gases (carbon dioxide and methane). The amount of gas produced depends on the substrate fermented and the amount of volatile fatty acids produced (Davies *et al.*, 2000). *In vitro* gas production is based on the measurement of gas production at different time intervals such as 3, 6, 12, 24, 48, 72 and 96 h after fermentation of feedstuffs with buffered rumen liquor (Menke and Steingass, 1988). The gas production kinetics are described using different mathematical models. Although, the exponential model $Y = a + b(1 - \exp^{-ct})$ is the most popular model in mathematical model used to describe the *in vitro* gas production kinetics, there are some researchers who have used the different mathematical

models to *in vitro* gas production kinetics (Ozturk *et al.*, 2006; Ferraro *et al.*, 2009; Kamalak, 2010; Saricicek and Kilic, 2011). However, there is still limited information on the comparison of mathematical models used in describing the gas production kinetics (Noguera *et al.*, 2004; Posada and Noguera, 2007; Mello *et al.*, 2008).

Therefore, the aim of the current experiment was to compare the four mathematical models used to describe the *in vitro* gas production kinetics of several feedstuffs used in ruminant nutrition.

MATERIALS AND METHODS

This study was conducted in Kahramanmaraş Sutcu Imam University, Faculty of Agriculture, Laboratory of Department of Animal Science between January and March in 2011.

Feedstuffs: In this study, wheat grain, vetch hay and wheat straw which are the locally available and widely used feedstuffs in ruminant rations were chosen to obtain the gas production when they are subjected to fermentation *in vitro*. The samples were grounded to pass through 1 mm sieve for chemical analysis and *in vitro* gas production.

Chemical analysis: Dry matter content was determined by drying the samples at 105°C overnight and the ash content was determined by igniting the samples in a muffle furnace at 525°C for 8 h. Nitrogen (N) content was measured by the Kjeldahl method (AOAC, 1990). The CP was calculated as Nitrogen x 6.25. The Neutral Detergent Fiber (NDF) and Acid Detergent Fiber (ADF) of pepper leave sample were analyzed with the ANKOM fiber analyzer using reagents described by Van Soest (1963) and Van Soest and Robertson (1985), respectively. All chemical analyses were carried out in triplicate.

In vitro gas production: The samples milled through a 1 mm sieve were incubated *in vitro* rumen fluid in glass bottles following the procedures of Theodorou *et al.* (1994). Each model shown in Table 1 was fitted to the *in vitro* gas production curves by non-linear regression using the PROC NLIN of SAS (1999). Several possible starting values were indicated for each parameter, so that the NLIN procedure evaluated the model at each

Table 1: The mathematical model used to describe the *in vitro* gas production

Models suggested by	Equations
Orskov (exponential)	$Y = a+b (1 - e^{-ct})$
Menke and Steingass (Logistic model)	$Y = a_1/(1+e^{(2.4c - t) \cdot D})$
Von Bertalanffy	$Y = a_1 + b_1 (1 - e^{-ct})^{1/v}$
France	$Y = a_2 (1 - e^{-(b_2(t-T_0) - c_1(\sqrt{t-T_0}))})$

combination of initial values on the grid using for the 1st iteration of fitting process, the combination yielding the smallest residual sum of squares (Nasri *et al.*, 2006).

Statistical analysis: Mean Square Error (MSE) adjusted coefficient of determination (R^2_{adj}) and Durbin-Watson statistic were obtained by analyzing the data of gas volume and used to evaluate goodness of fit of each model. Mean square prediction error was estimated as the sum of squared differences between observed and predicted values divided by the number of experimental observation. Adjusted coefficient of determination (R^2_{adj}) was estimated as follows:

$$R^2_{adj} = 1 - \left(\frac{MS_{residual}}{MS_{corrected total}} \right)$$

The Durbin-Watson statistic (DW) was estimated as follows:

$$DW = \frac{\sum_{i=2}^n (e_i - e_{i-1})^2}{\sum_{i=1}^n e_i^2}$$

Residual (e_i) is the difference between the observed value and the predicted value at a certain level of X:

$$e_i = y_i - \hat{y}_i$$

Data on chemical composition of feedstuffs, MSE, R^2_{adj} and the critical value of Durbin-Watson statistic were subjected to one way of ANOVA using GLM of SPSS for Windows. Significance between individual means was identified using the Duncan multiple range test. Mean differences were considered significant at $p < 0.05$. Standard errors of means were calculated from the residual mean square in the analysis of variance.

RESULTS AND DISCUSSION

The chemical composition of feedstuffs used in the current study is shown in Table 2. There is considerable variation among feedstuffs used in the current experiment.

Table 2: The chemical composition of feedstuffs used in the current study

Composition	Feedstuffs			SEM	Sig.
	WG	VH	WS		
Ash	1.80 ^a	6.53 ^b	8.36 ^a	0.090	***
CP	17.46 ^b	21.68 ^a	3.48 ^c	0.531	***
NDF	24.66 ^c	35.26 ^b	74.98 ^a	0.591	***
ADF	1.53 ^c	25.26 ^b	48.25 ^a	0.297	***

^{a-c}Row means with common superscripts do not differ ($p > 0.05$); SEM: Standard Error Mean; Sig.: Significance level; WG: Wheat Grain; VH: Vetch Hay; WS: Wheat Straw; DM: Dry Matter; CP: Crude Protein; NDF: Neutral Detergent Fiber; ADF: Acid Detergent Fiber

Cell wall contents (NDF and ADF) of VH and WS were significantly higher than that of wheat grain. The CP contents of WG and VH were significantly higher than that of WS. The CP ranged from 3.48-17.46%. The NDF and ADF contents ranged from 24.66-74.98 and 1.53-48.28%, respectively. The time course of gas production of WG, VH and WS and fit to Orskov, Menke, Bertalanffy and France models are shown in Fig. 1-3. In

Fig. 1, the actual time course gas production of wheat grain well coincided with the gas production estimated by using the Von Bertalanffy and France models. In Fig. 2, the actual time course gas production of vetch hay well coincided with the gas production estimated by using the Von Bertalanffy model.

On the other hand, the actual time course gas production of wheat straw well coincided with the gas production estimated by using the Orskov, Menke and Von Bertalanffy models (Fig. 3). Mean Square Error (MSE), adjusted coefficient of determination (R^2_{adj}) and Durbin-Watson statistic are shown in Table 3. The mean square error of wheat grain, vetch hay and wheat straw ranged from 5.589-10.538, 1.590-9.668 and 0.814-12.118, respectively. The MSE obtained current study were considerably lower than those obtained by Posada and Noguera (2007) who found that the MSE values for France and Menke models 45.20-295.38, respectively. The differences in MSE between two studies may be associated with differences in forage used.

The adjusted coefficient of determination of wheat grain, vetch hay and wheat straw ranged from 0.979-0.989, 0.962-0.992 and 0.976-0.995, respectively. The adjusted coefficient of determination of obtained current study

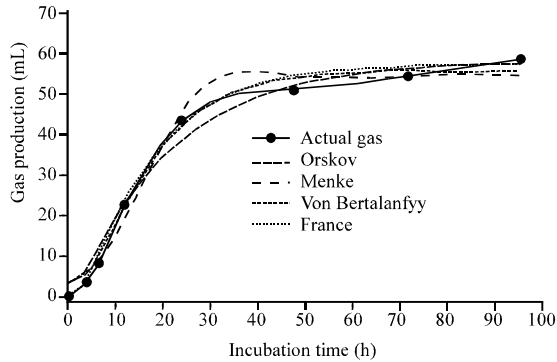


Fig. 1: The time course of gas production of wheat grain and fit to Orskov, Menke, Von Bertalanffy and France models

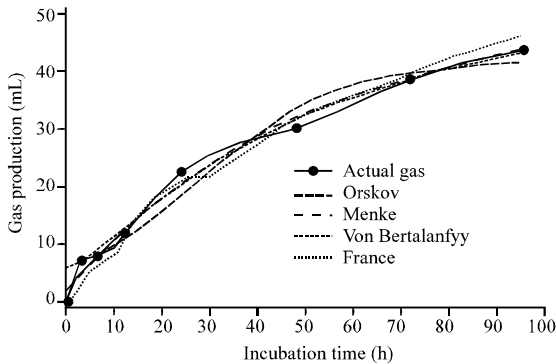


Fig. 2: The time course of gas production of vetch hay and fit to Orskov, Menke, Von Bertalanffy and France models

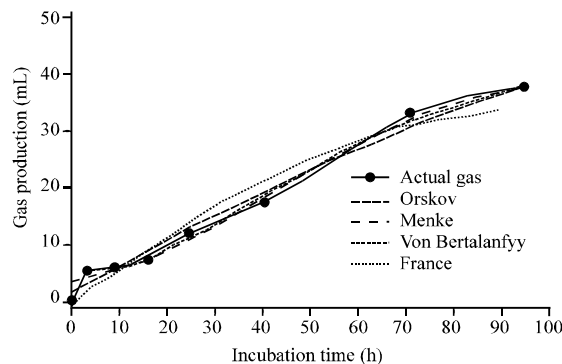


Fig. 3: The time course of gas production of wheat straw and fit to Orskov, Menke, Von Bertalanffy and France models

Table 3: The mean square error adjusted coefficient of determination and Durbin-Watson test critical values of mathematical models used in the current experiment

Parameters	Feedstuff	Models				SEM	Sig.
		Orskov	Menke	Von Bertalanffy	France		
MSE	Wheat grain	10.538 ^a	10.161 ^a	6.327 ^b	5.589 ^b	1.5790	*
	Vetch hay	2.784 ^{ab}	9.668 ^a	1.590 ^b	6.957 ^{ab}	2.9090	*
	Wheat straw	3.055 ^b	3.447 ^b	0.814 ^b	12.118 ^a	1.6020	**
R^2_{adj}	Wheat grain	0.979 ^b	0.980 ^b	0.986 ^b	0.989 ^a	0.0024	**
	Vetch hay	0.989 ^a	0.962 ^a	0.992 ^a	0.973 ^a	0.0117	NS
	Wheat straw	0.980 ^b	0.976 ^b	0.995 ^a	0.921 ^c	0.0035	**
DW	Wheat grain	1.919 ^b	1.378 ^c	1.877 ^b	2.479 ^a	0.0476	**
	Vetch hay	2.630 ^a	1.751 ^b	2.928 ^a	1.502 ^b	0.2205	**
	Wheat straw	2.342 ^b	1.671 ^c	3.623 ^a	1.178 ^d	0.1378	**

MSE: Mean Square Error; R^2_{adj} : Adjusted coefficient of determination; DW: Durbin-Watson test (the critical values) for $D > 2.997$; SEM: Standard Error of the Mean; ** $p < 0.01$; * $p < 0.05$. NS = Non Significant; Sig: Significance level

were comparable with Posada and Noguera (2007) who found that the adjusted coefficient of determination ranged from 0.998-0.983. The Durbin-Watson statistic of wheat grain, vetch hay and wheat straw ranged from 1.378-2.479, 1.502-2.928 and 1.178-3.623, respectively.

The best model for the gas production of wheat grain was the Von Bertalanffy and France functions when MSE and R^2_{adj} parameter was taken into consideration. The best model for the gas production of vetch hay is the Von Bertalanffy function when MSE parameter was taken into consideration whereas the best model for vetch hay was the Von Bertalanffy and Orskov functions when R^2_{adj} parameter was taken into consideration. The best model for the gas production of wheat straw is the Orskov, Menke and Von Bertalanffy functions when MSE parameter was taken into consideration whereas the best model for the wheat straw was the Von Bertalanffy function when the R^2_{adj} parameter was taken into consideration. The best model for the gas production of wheat grain is the Orskov and Von Bertalanffy functions when DW parameter was taken into consideration. On the other hand, the best model for the gas production of vetch hay and wheat straw is the Orskov and Menke functions when DW parameter was taken into consideration.

The adjusted coefficient of determination is preferred to R^2 for models that involve different numbers of parameters. A model with large R^2_{adj} is more favorable. Due to its structure, the R^2_{adj} criterion results in the same conclusion as the MSE criterion (Costello, 1994). The Durbin-Watson (DW) statistic is widely employed to determine for the presence of 1st-order autocorrelation in the errors. In the presence of positive autocorrelation, Durbin-Watson statistic will be near zero when successive errors are close to each other. On the other hand, in the presence of negative autocorrelation, Durbin-Watson statistic is very close to four when successive errors are far from each other (Silvestre *et al.*, 2006).

In Table 3, there is no 1st order auto-correlation in errors of wheat grain and vetch hay estimated by four models used in the current study therefore, the four models can be used to fit the individual gas production data measured in different time intervals. Von Bertalanffy function is not suggested to fit the gas production data since, there is negative autocorrelation in errors of wheat straw. Distributions of residual estimated from the differences between measured individual gas production and estimated gas production using Orskov, Menke, Von Bertalanffy and France models are shown in Fig. 4. Although, the Von Bertalanffy function is very successful in the prediction of gas production initial

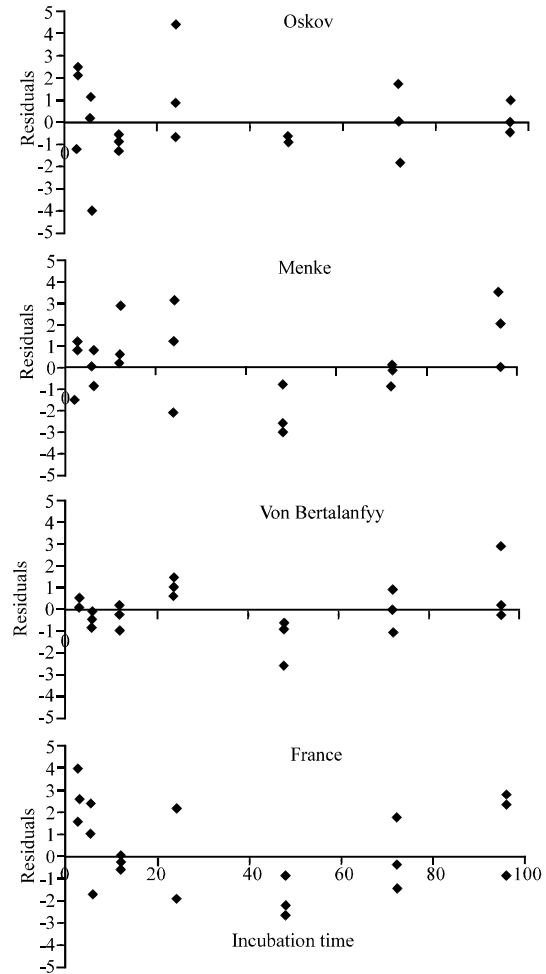


Fig. 4: Distribution of residual estimated from the differences between measured individual gas production and estimated gas production using Orskov, Menke and Von Bertalanffy and France models

phase, the Orskov, Menke and France models failed in prediction of gas production during the initials phase. These results are in agreement with finding of Noguera *et al.* (2004) who found that the France and Orskov models underestimated the production of gas during the initial phase. The results also is in agreement with finding of Posada and Noguera (2007) who found that logistic model had greater residuals and greater tendency to overestimate and to underestimate the time course gas production when compared with France model.

CONCLUSION

There is no perfect model to fit all gas production data obtained from different forages, there is little to

choose model. Therefore, choice of best model should be made on the basis of fitting criteria and feedstuffs since goodness of fit of model is depended on feedstuffs tested and fitting criteria.

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