A GENERALIZED MODEL FOR DESCRIBING FIBER DYNAMICS IN THE RUMINANT GASTROINTESTINAL TRACT. 3. ESTIMATING DIGESTION-RELATED KINETIC PARAMETERS

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Summary

A generalized compartmental model of digestion based on gamma time dependency of lag phenomena (G_NG_1) was applied to estimate kinetic parameters of forage digestion in ruminants. Overall qualities of fit of four possible versions of the model for N compartments varying from one to four were evaluated. Parameter estimates were affected by forage quality, particularly the indigestible fraction and the fractional degradation rate. The relationship between time dependency and quality deserves further investigation. Nevertheless, the model had a high goodness-of-fit and comparable estimates could be obtained for comparison purposes with single pool models.

Introduction

The digesta stratification in the ruminoreticulum of forage-fed ruminants occurs whenever environmental and animal characteristics do not constrain intake to a selective eating behavior for a diet rich in neutral detergent solubles (Van Soest, 1996). Hence, domestic ruminants that depend on roughage resources have heterogeneous pools (Vieira et al., 2007a). Events related to the dynamic nature of fibrous digesta particles were discussed in a companion report (Vieira et al., 2007b).

Systems dynamics has evolved in parallel to computational resources; consequently complexity of natural phenomena can be conceptualized and simulated more reliably. Transfer mechanisms between system variables and interchange flows can be modeled by accommodating delays. In ruminant nutrition, pioneering studies in this field (Blaxter et al., 1956; Matis, 1972; Pond et al., 1988; Van Milgen et al., 1991) provided a theoretical description of the biological processes involved. In this report, we presented a quantitative description of events related to digestion kinetics in the ruminoreticulum.

Experimental Procedures

The theoretical basis of the degradation model is outlined as follows. When a large fibrous particle enters the rumen several processes must occur prior to its digestion (Vieira et al., 2007b). These processes are aggregated and represented by a single kinetic rate named k_a, assumed gamma distributed over time ($\Gamma(N_a, \lambda_a, t)$) with parameters $\lambda_a \in \Re^+$, $N_a \in \Im^+$, and $E(k_a) = \bar{k}_a = \hat{\lambda}_a / N_a$ under the assumption of steady-state. The newly ingested particle could be schematically divided into three conceptual compartments: an unavailable (U_d) and an available (A_d) potentially digestible and an indigestible (I) fractions. Deserve prominence, however, the fact that both U_d and A_d are physically the same entity, but divided schematically to represent lag transfer phenomena that promote the gradual availability of U_d into A_d. In advance, the latter is degraded by microbial enzymes following first-order kinetics as shown in Figure 1.

Although treated separately, the processes described by the kinetic rate k_a (Figure 1) are part of the processes represented by the k_r parameter described by Vieira et al. (2007b), and it is assumed that $k_a > k_r$. The rates k_a and k_d could be estimated by fitting the generalized compartmental model (G_NG_1, of Eq. 1) to fiber degradation profiles obtained from *in situ* or *in vitro* studies.

$$\begin{cases} R(t) = U_d(0)\left\{\delta^{N_a}\exp(-k_d t) + \exp(-\lambda_a t)\left[\sum_{i=0}^{N_a-1}\left(1-\delta^{N_a-i}\right)\gamma_i\right]\right\} + I(0) \\ \delta = \dfrac{\lambda_a}{\lambda_a - k_d} \text{ and } \gamma_i = (\lambda_a t)^i / i! \end{cases}$$

(Eq. 1)

The Eq. 1 is a transition function that represents the amount of residual feedstuff matter after *in situ* or *in vitro* incubation. It is analogous to the transition function presented by Pond et al. (1988), who described the total dose of a marker remaining in a system of two sequential compartments when a gamma time dependency is included.

Comparable results to first-order models could be obtained numerically from the first and second derivatives of Eq. 1:

$$\frac{dR(t)}{dt} = -U_d(0)\left\{\delta^{N_a} k_d \exp(-k_d t) + \lambda_a \exp(-\lambda_a t)\left[\left(1-\delta^{N_a}\right) + \varphi\right]\right\}$$

(Eq. 2)

$$\varphi = \sum_{i=0}^{N_a-1}\left\{\left(1-\delta^{N_a-1-i}\right)\gamma_i\left[\frac{\lambda_a t}{(i+1)} - 1\right]\right\}$$

(Eq. 3)

$$\frac{d^2R(t)}{dt^2} = U_d(0)\left\{\delta^{N_a} k_d^2 \exp(-k_d t) + \lambda_a^2 \exp(-\lambda_a t)\left[\left(1-\delta^{N_a}\right) + \left(1-\delta^{N_a-1}\right)(\lambda_a t - 2) + v\psi\right]\right\}$$

(Eq. 4)

$$\psi = \sum_{i=0}^{N_a-2}\left\{\left(1-\delta^{N_a-2-i}\right)\gamma_i\left[\frac{(\lambda t)^2}{(i+2)(i+1)} - 2\frac{\lambda t}{(i+1)} + 1\right]\right\}$$

(Eq. 5)

In which δ and γ_i are auxiliary terms defined in Eq. 1. The auxiliary variables φ and ψ were employed to simplify mathematical description. The comparable first-order digestion rate or fractional specific digestion first-order rate (k_f) could be defined as follows.

$$k_f = -\frac{dR(t_i)/dt}{U_d(0)}$$

(Eq.6)

being t_i the abscissa coordinate at the inflection point. By its turn, t_i could be estimated numerically or graphically by solving for the roots of t_i that satisfies Eq. 7.

$$\frac{d^2R(t_i)}{dt^2} = 0 \qquad \text{(Eq. 7)}$$

To demonstrate the flexibility of the model to fit degradation profiles, *in vitro* incubations of two grasses (orchardgrass, *Dactylis glomerata*, and timothy, *Phleum pretense*) and two legumes (alfalfa, *Medicago sativa*, and red clover, *Trifolium pretense*) were gathered from Mertens (1973). The chemical composition in terms of crude protein (CP), neutral detergent fiber (NDF), sulfuric acid lignin (H_2SO_4 Lignin), insoluble nitrogen in neutral (NDIN) and acid (ADIN) detergents, neutral detergent insoluble ash (NDIA), ash and silica (SiO_2) were reported (Table 1). Forages were chosen according to three levels (low, medium, and high) of sulfuric acid lignin content in the DM to account for quality variability. A total of 12 degradation profiles were analyzed by fitting the general compartmental model of digestion (Eq. 1) by using the Marquardt algorithm of the NLIN procedure of SAS (SAS Inst. Inc., Cary, NC). A description of SAS routines could be found in the Appendix. The quality of fit criterion was subjectively based on the minimum sum of squares of error (SSE), or whether a minimum was not reached, a minimum of 10% reduction in SSE of the preceding $G_{N-1}G1$ should be obtained after fitting the G_NG_1 model for N varying from two to four.

Results and Discussion

With the exception of alfalfa, observed trends in CP along with the H_2SO_4 Lignin content in NDF were indicative of the forage quality variability (Table 1). Incrustation of cell wall by lignin also lowers nitrogen availability as revealed by the ratio of acid detergent insoluble nitrogen to the total nitrogen content (Table 1).

A recently ingested particle is not readily available for microbial breakdown. Hydration, solubilization of digestion inhibitors, and accessibility and colonization of feed particles by rumen microbes are events that have to occur prior to digestion itself. These processes transform the unavailable potentially digestible large particle entity (U_d, Figure 1) into a form prone to be digested, an available entity of the same large particle named A_d (Figure 1). It is reasonable to expect that chemical composition and ultra-structural characteristics of forage tissues (Akin, 1979; Wilson, 1993), probably constrain the transfer mechanisms and delays the rate of availability of the substrate to be digested (Ellis et al., 2005). Additionally, a discrete lag time (τ) could be incorporated in the model described by Eq. 1 so that its effect on order of time dependency could be evaluated, i.e. the quality of fit of higher order models corrected for a discrete lag (substitute t in Eq. 1 by $t - \tau$).

It should be recognized, however, that the processes associated to the forage tissues disruption during ingestive mastication as described by Pond et al. (1984), could not be simulated by using the *in vitro* incubation because of the required fine grinding of forage samples. Nevertheless, all *in vivo* digestion estimates are expected to be higher than those estimated with techniques based on an unconstrained particle size (Huhtanen et al., 2007).

The difference in quality was also demonstrated by the increased percentage of estimated indigestible NDF and the trends of the k_d estimates in becoming lower as quality decreases, irrespective of model used and forage evaluated (Tables 2 and 3). Nevertheless λ_a estimates did not share a regular trend pattern with respect to quality and further investigations with a larger data set are necessary.

Models chosen to represent degradation profiles according to the established criteria varied according to the order of gamma time dependency. As an additional criterion, whenever the estimates of parameter λ_a approached k_d, the goodness-of-fit was considered inappropriate and higher order models were further evaluated according to the previously established SSR criteria. For Orchardgrass of low, medium and high H_2SO_4 Lignin in the DM, selected models were G_3G_1, G_2G_1 and G_2G_1, respectively. The respective choices regarding the same quality classes for timothy grass were G_2G_1, G_2G_1 and G_3G_1 (Table 2). Models chosen to represent alfalfa profiles were G_1G_1, G_3G_1 and G_2G_1, and just one version of the model (G_2G_1) was selected to describe degradation kinetics of the three quality classes of red clover. Here, there was no apparent relationship between order of time dependency and quality, with the exception of the timothy grass. The expected k_a values, i.e. $\overline{k}_a$ estimates for each chosen model within each forage and quality

class were presented graphically. No apparent relationship could be inferred; nevertheless, a more detailed investigation is needed because systematic reductions in $\overline{k}_a$ between the low and high lignin content in forages are likely (Figure 2).

The most striking characteristics that reflected quality were the indigestible fraction and the first order degradation rate, which varied systematically (Tables 2 and 3 and Figure 3). The U_d fraction consequently was also affected, since it is calculated by the difference between the observed residue at t = 0 and the estimate of the indigestible fraction. Nutritionists should be aware that considerable biases could be impinged to the truly indigestible fraction by short term incubations such as those used in the present study (Van Soest et al., 2005; Ellis et al., 2005).

The ideal indigestible entity of large particles (I, Figure 1) can not be digested by rumen microbes. On the other hand, U_d becomes available to be degraded after completion of the events described by k_a as above mentioned. The digestion processes promoted by microbial enzymes are kinetically described by the rate k_d, assumed to be exponentially distributed over time (first-order). As the ageing chain of processes related to the transfer of particles from the large particles pool into the pool of small particles succeeds, the indigestible entity and the available potentially degradable fraction (A_d) remnants constitute the fibrous mass of small particles, i.e. U_d was completely transformed into A_d (Figure 1). Since events that occur prior to digestion represented by k_a occurred in the raft, the kinetic forces of first-order digestion and escape of particles are the remaining actions concurring to the clearance of small particles from the ruminoreticulum (Vieira et al., 2007b).

There are considerable empirical evidences that the indigestible entity is not accurately estimated by short fermentation times. Biases could be reduced by fitting models that account for heterogeneous potentially digestible fiber fractions or a gamma mixture of exponentials (Van Soest et al., 2005; Ellis et al., 2005). Henceforth, if long *in vitro* incubation times could not be performed due to medium limitations in maintaining microbial numbers and good anaerobic conditions, or if particle losses with the *in situ* technique either hamper accurate measurements of long incubation times, then perhaps the combined powers of concepts that leads to the construction of Eq. 1 with those that leads to models that account for heterogeneous pools may be useful to produce estimates of the indigestible entity. As a corollary, heterogeneous potentially digestible fractions and its dynamic lags and degradation rates could be more properly estimated as well. However, such estimates need to be evaluated in terms of relevant scientific and economical variables of the ruminant production system.

Implications

The generalized compartmental model (G_NG_1) of digestion could be used to estimate parameters related to time degradation profiles. The model presented an overall good quality of fit and adherence to time profiles. Further studies are required to the estimation of heterogeneous potentially degradable fractions and accurate estimates of the indigestible fiber. These estimates could be applied to simulate the dynamic behavior of the fiber in the gastrointestinal tract of ruminants, but evaluations of predictions based on such estimates are still required.

Literature Cited

Akin, D.E. 1979. Microscopic evaluation of forage digestion by rumen microorganisms – A review. J.Anim. Sci., 48:701-710.

Allen, M.S., Mertens, D.R. Evaluating constraints on fiber digestion by rumen microbes. J. Nutr., 118:261-270.

Blaxter, K.L., Graham, McC., Wainman, F.W. 1956. Some observations on the digestibility of food by sheep, and on related problems. Brit. J. Nutr., 10:69-91.

Ellis, W.C., Mahlooji, M., Matis, J.H. 2005. Models for estimating parameters of neutral detergent fiber digestion by ruminal microorganisms. J. Anim. Sci., 83:1591-1601.

Ellis, W.C., Matis, J.H., Hill, T.H., Murphy, M.R. 1994. Methodology for estimating digestion and passage kinetics of forages. In: Fahey Jr., G.C. (Ed.) Forage Quality, Evaluation and Utilization. American Societies of Agronomy, Madison, p.682-756.

Huhtanen, P., Asikainen, U., Arkkila, M., Jaakkola, S. 2007. Cell wall digestion and passage kinetics estimated by marker and in situ methods or by rumen evacuations in cattle fed hay 2 or 18 times daily. Anim. Feed Sci. and Technol., 133:206-227.

Matis, J.H. 1972. Gamma time-dependency in Blaxter's compartmental model. *Biometrics*, 28(2):597-602.

Mertens, D.R. 1973. Application of theoretical mathematical models to cell wall digestion and forage intake in ruminants. Cornell University, 217p. (Thesis).

Pond, D.P., Ellis, W.C., Akin, D.E. 1984. Ingestive mastication and fragmentation of forages. J. Anim. Sci., 58:1567-1574.

Pond, D.P., Ellis, W.C., Matis, J.H., Ferreiro, H.M., Sutton, J.D. 1988. Compartmental models for estimating attributes of digesta flow in cattle. Brit. J. Nutr., 60:571-595.

Van Milgen, J., Murphy, M.R., Berger, L.L. 1991. A compartmental model to analyze ruminal digestion. J. Dairy Sci., 74:2515-2529.

Van Soest, P.J. 1996. Allometry and ecology of feeding behavior and digestive capacity in herbivores: a review. Zoo Biol., 15:455-479.

Van Soest, P.J., Van Amburgh, M.E., Robertson, J.B., Knaus, W.F. Validation of the 2.4 times lignin factor for ultimate extent of NDF digestion, and curve peeling rate of fermentation curves into pools. Proceedings of the 67th Cornell Nutrition Conference, pp.139-149.

Vieira, R.A.M., Tedeschi, L.O., Cannas, A. 2007a. A generalized model for describing fiber dynamics in the ruminant gastrointestinal tract. 1. The heterogeneity of the pool of fiber particles in the ruminoreticulum. Beef Cattle Res. Texas, Vieira, R.A.M., Tedeschi, L.O., Cannas, A. 2007b. A generalized model for describing fiber dynamics in the ruminant gastrointestinal tract. 2. Accounting for heterogeneous pools in the ruminoreticulum. Beef Cattle Res. Texas.

Wilson, J.R. 1993. Organization of forage plant tissues. In: Jung, H.G., Buxton, D.R., Hatfield, R.D., Mertens, D.R. (Eds.) *Forage cell wall structure and digestibility*. Madison: American Society of Agronomy, Inc., Crop Science Society of America, Inc., Soil Science Society of America, Inc., 1993, p.1-32.

Table 1. Chemical composition[1,2] of orchard grass (*Dactylis glomerata*), timothy grass (*Phleum pretense*), alfalfa (*Medicago sativa*), and red clover (*Trifolium pretense*) used to generate time degradation profiles[3], distributed according to the H_2SO_4 Lignin content in the dry matter

Forage[4]	CP	NDF	H_2SO_4 Lignin	Lignin (%NDF[5])	NDIN	ADIN	$\frac{\text{ADIN}}{\text{NC}}$ (%NC[6])	NDIA	Ash	SiO_2
Orchardgrass										
Low	27.7	48.2	2.1	4.36	1.76	0.11	2.48	3.4	NR	2.3
Medium	8.4	68.5	4.3	6.28	0.56	0.12	8.93	0.8	6.4	0.8
High	6.8	78.0	6.6	8.46	0.41	0.12	11.03	1.1	NR	0.4
Timothy										
Low	23.9	47.6	2.4	5.04	1.17	0.08	2.09	1.3	NR	0.8
Medium	14.3	62.4	4.2	6.73	0.77	0.14	6.12	0.9	6.2	0.7
High	10.8	68.2	6.0	8.80	0.78	0.23	13.31	0.9	5.8	1.2
Alfalfa										
Low	25.0	31.5	5.0	15.87	NR	NR	–	2.2	12.4	1.5
Medium	19.3	47.2	7.3	15.47	0.54	0.22	7.12	1.1	7.9	0.6
High	16.4	50.8	8.1	15.94	0.34	0.21	8.00	0.5	9.2	0.1
Red clover										
Low	14.4	58.3	4.0	6.86	1.14	0.17	7.38	0.9	8.0	1.0
Medium	13.7	69.4	5.5	7.93	1.25	0.26	11.86	1.5	7.8	1.4
High	10.9	66.1	7.8	11.80	0.84	0.33	18.92	1.1	5.6	1.2

[1]Expressed in % of the dry matter unless otherwise specified.

[2]Acronyms are crude protein (CP), neutral detergent fiber (NDF), sulfuric acid lignin (H_2SO_4 Lignin), insoluble nitrogen in neutral (NDIN) and acid (ADIN) detergents, neutral detergent insoluble ash (NDIA), ash and silica (SiO_2), and when a value was not reported, NR was displayed.

[3]Data obtained from Mertens (1973).

[4]Divided according to the H_2SO_4 Lignin in the dry matter.

[5]H_2SO_4 Lignin in the NDF.

[6]Percentage of the nitrogen content (NC), i.e. CP/6.25.

Table 2. Parameters estimates (± asymptotic standard errors) and sum of squares of error (SSE[1]) after fitting a generalized compartmental model (G_NG_1) to *in vitro* degradation profiles of orchard and timothy grasses

Forage[2]	Parameter[3]	G_1G_1	G_2G_1	G_3G_1	G_4G_1
Orchardgrass					
	SSE	132.1 (100%)	90.8 (69%)	77.8 (59%)	72.0 (54%)
	U_d (%NDF)	86.95	86.90	86.99	87.09
Low	I (%NDF)	13.15 ± 1.31	13.10 ± 1.26	13.01 ± 1.31	12.91 ± 1.35
	λ_a (1/h)	0.4182 ± 0.1345	0.9282 ± 0.2055	1.4789 ± 0.3074	2.0553 ± 0.4177
	k_d (1/h)	0.1155 ± 0.0157	0.1114 ± 0.0107	0.1089 ± 0.0098	0.1073 ± 0.0093
	SSE	593.1 (100%)	417.3 (70%)	372.7 (63%)	361.4 (61%)
	U_d (%NDF)	63.60	63.66	63.69	63.72
Medium	I (%NDF)	36.40 ± 2.46	36.34 ± 1.90	36.31 ± 1.75	36.28 ± 1.69
	λ_a (1/h)	0.1072 ± 0.1220	0.2858 ± 0.0747	0.4441 ± 0.0894	0.5988 ± 0.1076
	k_d (1/h)	0.0748 ± 0.0709	0.0625 ± 0.0126	0.0610 ± 0.0097	0.0605 ± 0.0087
	SSE	181.2 (100%)	178.7 (99%)	189.2 (104%)	196.4 (108%)
	U_d (%NDF)	48.20	48.20	48.20	48.20
High	I (%NDF)	51.80 ± 1.11	51.80 ± 0.89	51.80 ± 0.80	51.80 ± 0.78
	λ_a (1/h)	0.3070 ± 0.1011	0.6301 ± 0.1309	0.9558 ± 0.1660	1.2832 ± 0.2029
	k_d (1/h)	0.0489 ± 0.0055	0.0486 ± 0.0037	0.0485 ± 0.0032	0.0484 ± 0.0029
Timothy					
	SSE	71.3 (100%)	55.8 (78%)	70.6 (99%)	84.0 (118%)
	U_d (%NDF)	86.95	87.12	87.25	87.34
Low	I (%NDF)	13.05 ± 0.74	12.88 ± 0.65	12.75 ± 0.74	12.66 ± 0.78
	λ_a (1/h)	0.1828 ± 1329	0.5968 ± 0.0598	0.9852 ± 0.0930	1.3732 ± 0.1319
	k_d (1/h)	0.1828 ± 1329	0.1287 ± 0.0084	0.1221 ± 0.0073	0.1193 ± 0.0072
	SSE	171.5 (100%)	122.7 (72%)	123.3 (72%)	131.0 (76%)
	U_d (%NDF)	74.00	74.07	74.14	74.17
Medium	I (%NDF)	26.00 ± 1.06	25.93 ± 0.86	25.86 ± 0.86	25.83 ± 0.89
	λ_a (1/h)	0.2932 ± 0.0819	0.6583 ± 0.0999	1.0282 ± 0.1372	1.4051 ± 0.1819
	k_d (1/h)	0.0931 ± 0.0123	0.0890 ± 0.0064	0.0875 ± 0.0056	0.0866 ± 0.0054
	SSE	231.5 (100%)	123.8 (53%)	96.4 (42%)	87.4 (38%)
	U_d (%NDF)	65.59	65.71	65.74	65.80
High	I (%NDF)	34.41 ± 1.39	34.29 ± 0.96	34.26 ± 0.83	34.20 ± 0.80
	λ_a (1/h)	0.1905 ± 0.0670	0.4399 ± 0.0680	0.6838 ± 0.0812	0.9288 ± 0.0976
	k_d (1/h)	0.0704 ± 0.0139	0.0660 ± 0.0056	0.0649 ± 0.0043	0.0642 ± 0.0038

[1]Values within parenthesis are percentages (%) in relation to the SSE estimate after fitting the G1G1 model.
[2]Divided according to the sulfuric acid lignin (Lignin H_2SO_4) content in the dry matter.
[3]Parameter U doest not present an SE estimate because it was indirectly estimated from R(0) – I for each profile.

Table 3. Parameters estimates (± asymptotic standard errors) and sum of squares of error (SSE[1]) after fitting a generalized compartmental model (G_NG_1) to *in vitro* degradation profiles of alfalfa and red clover

Forage[2]	Parameter[3]	G_1G_1	G_2G_1	G_3G_1	G_4G_1
Alfalfa					
	SSE	17.2 (100%)	22.4 (131%)	25.8 (150%)	27.4 (160%)
	U_d (%NDF)	59.22	59.35	59.41	59.48
Low	I (%NDF)	40.78 ± 0.52	40.65 ± 0.65	40.59 ± 0.65	40.52 ± 0.65
	λ_a (1/h)	0.4159 ± 0.0852	1.0060 ± 0.1661	1.6370 ± 0.2697	2.2795 ± 0.3740
	k_d (1/h)	0.1242 ± 0.0113	0.1159 ± 0.0081	0.1127 ± 0.0076	0.1111 ± 0.0074
	SSE	97.4 (100%)	50.6 (52%)	38.4 (39%)	33.4 (34%)
	U_d (%NDF)	47.76	47.72	47.81	47.85
Medium	I (%NDF)	52.24 ± 1.02	52.28 ± 0.88	52.19 ± 0.74	52.15 ± 0.69
	λ_a (1/h)	0.1081 ± 719	0.3182 ± 0.0613	0.5148 ± 0.0694	0.7090 ± 0.0814
	k_d (1/h)	0.1081 ± 719	0.0812 ± 0.0124	0.0770 ± 0.0079	0.0752 ± 0.0065
	SSE	27.1 (100%)	34.1 (126%)	42.0 (155%)	47.4 (175%)
	U_d (%NDF)	39.77	40.02	40.18	40.23
High	I (%NDF)	60.23 ± 0.46	59.98 ± 0.63	59.82 ± 0.67	59.77 ± 0.71
	λ_a (1/h)	0.1216 ± 637	0.4326 ± 0.0730	0.7114 ± 0.1177	1.0016 ± 0.1645
	k_d (1/h)	0.1216 ± 637	0.0812 ± 0.0088	0.0764 ± 0.0074	0.0744 ± 0.0069
Red Clover					
	SSE	238.2 (100%)	123.6 (52%)	108.0 (45%)	110.6 (46%)
	U_d (%NDF)	77.83	77.94	78.09	78.17
Low	I (%NDF)	22.17 ± 1.46	22.06 ± 1.09	21.91 ± 0.98	21.83 ± 1.01
	λ_a (1/h)	0.1123 ± 1219	0.3483 ± 0.0521	0.5551 ± 0.0636	0.7622 ± 0.0809
	k_d (1/h)	0.1123 ± 1219	0.0809 ± 0.0089	0.0777 ± 0.0064	0.0761 ± 0.0057
	SSE	194.0 (100%)	80.1 (41%)	76.2 (39%)	87.0 (45%)
	U_d (%NDF)	72.78	72.58	72.81	72.94
Medium	I (%NDF)	27.22 ± 1.25	27.42 ± 0.89	27.19 ± 0.85	27.06 ± 0.89
	λ_a (1/h)	0.0918 ± 798	0.2675 ± 0.0299	0.4358 ± 0.0377	0.6008 ± 0.0506
	k_d (1/h)	0.0918 ± 798	0.0696 ± 0.0066	0.0655 ± 0.0047	0.0638 ± 0.0044
	SSe	412.8 (100%)	371.0 (90%)	357.8 (87%)	353.8 (86%)
	U_d (%NDF)	59.32	60.20	60.37	60.43
High	I (%NDF)	40.68 ± 3.06	39.80 ± 2.71	39.63 ± 2.61	39.57 ± 2.54
	λ_a (1/h)	0.0992 ± 0.0817	0.2897 ± 0.0888	0.4572 ± 0.1191	0.6211 ± 0.1503
	k_d (1/h)	0.0548 ± 0.0348	0.0438 ± 0.0092	0.0426 ± 0.0076	0.0421 ± 0.0071

[1]Values within parenthesis are percentages (%) in relation to the SSE estimate after fitting the G1G1 model.
[2]Divided according to the sulfuric acid lignin (Lignin H_2SO_4) content in the dry matter.
[3]Parameter U doest not present an SE estimate because it was indirectly estimated from R(0) – I for each profile.

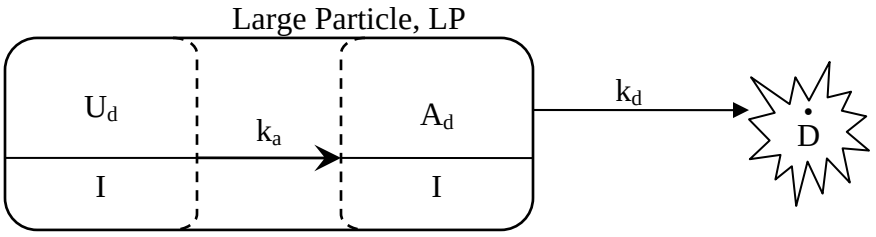

Figure 1. Schematic representation of the kinetic processes suffered by large particles in the rumen mat. Adapted from Allen and Mertens (1988). See details in the text and in a companion report (Vieira et al., 2007b).

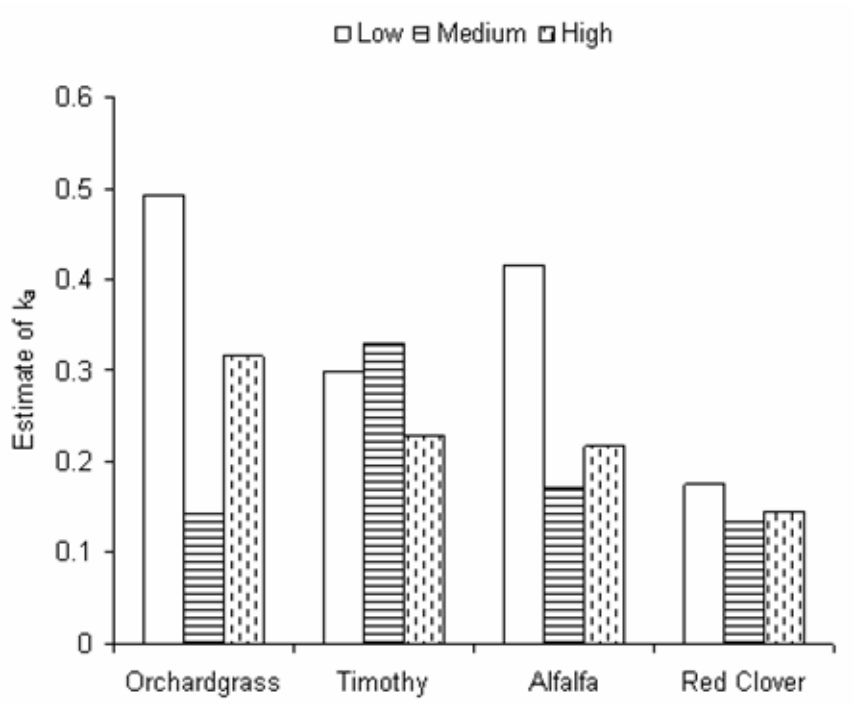

Figure 2. Estimates of $\bar{k}_a$ ($\hat{\lambda}_a / N_a$) for each forage and class of quality (low, medium and high lignin content in the dry matter), according to the quality of fit criteria for choosing a specific version of the generalized compartmental model.

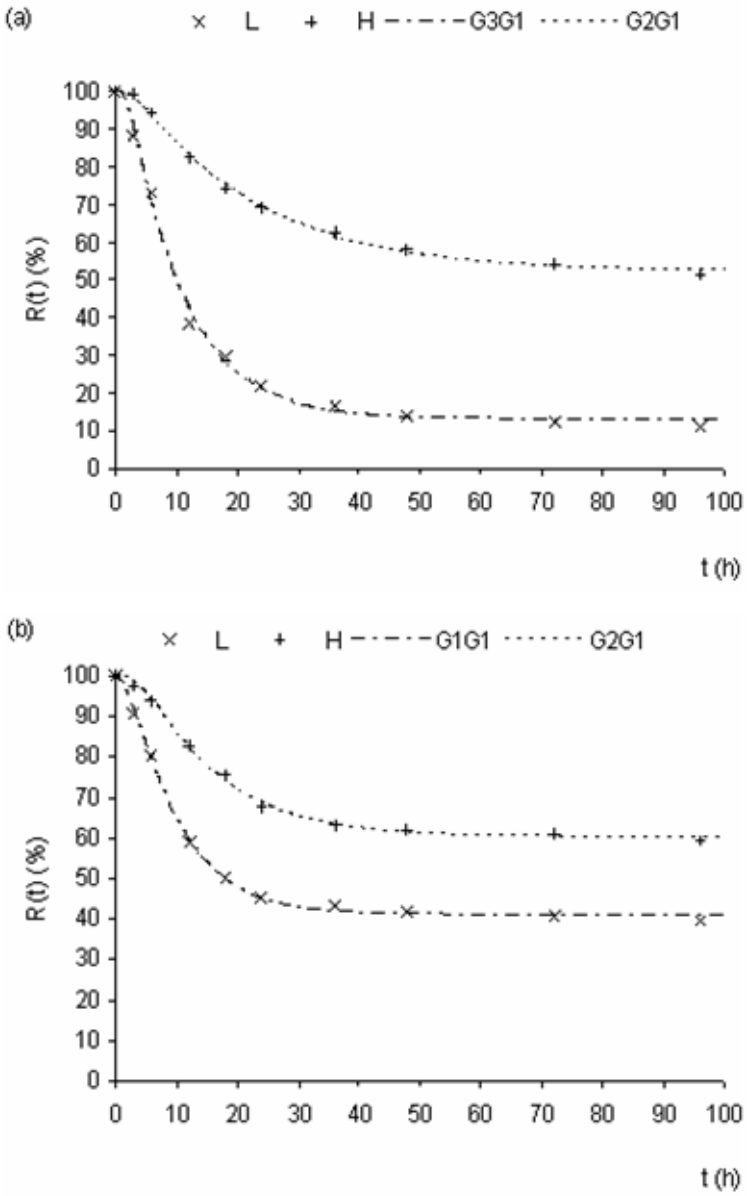

Figure 3. Degradation profiles of orchard grass (a) and alfalfa (b). Letters L and H are related to low and high sulfuric acid lignin in the dry matter. The lines - – - – and - - - - represent the resultant fitted generalized compartmental model G_NG_1 to data.

APPENDIX

A.1) SAS procedures for NLIN fitting of G1G1 model:

```
proc nlin best=5 method=marquardt;
parms
i=10 to 150 by 2
l=.01 to 1 by .05   (obs.: l = represents lambda)
k=.001 to .2 by .005;
bounds 0<k, 0<l, 0<i;
z=l/(l-k);
e1=exp(-k*t);
u=l*t;
e2=exp(-u);
model Y=(266.6-i)*(z*e1+e2*(1-z))+i;
output out=g1g1 h=ha r=aresid student=rsa;
run;
proc print;
data g1g1;
run;
```

A.2) SAS procedures for NLIN fitting of G2G1 model (see and repeat abbreviations in G1G1):

```
proc nlin best=5 method=marquardt;
parms
i=10 to 150 by 2
l=.01 to 1 by .05
k=.001 to .2 by .005;
bounds 0<k, 0<l, 0<i;
model Y=(306.8-i)*(z**2*e1+e2*((1-z**2)+(1-z)*u))+i;
output out=g2g1 h=hc r=cresid student=rsc;
run;
proc print;
data g2g1;
run;
```

A.3) SAS procedures for NLIN fitting of G3G1 model (see and repeat abbreviations in G1G1):

```
proc nlin best=5 method=marquardt;
parms
i=10 to 150 by 2
l=.01 to 1 by .05
k=.001 to .2 by .005;
bounds 0<k, 0<l, 0<i;
model Y=(304.5-i)*(z**3*e1+e2*((1-z**3)+(1-z**2)*u+(1-
z)*u**2/2))+i;
output out=g3g1 h=hb r=bresid student=rsb;
run;
proc print;
data g3g1;
run;
```

A.4) SAS procedures for NLIN fitting of G4G1 model (see and repeat abbreviations in G1G1):

```
proc nlin best=5 method=marquardt;
parms
i=10 to 150 by 2
l=.01 to 1 by .05
k=.001 to .2 by .005;
bounds 0<k, 0<l, 0<i;
model Y=(266.6-i)*(z**4*e1+e2*((1-z**4)+(1-z**3)*u+(1-
z**2)*u**2/2+(1-z)*u**3/6))+i;
output out=g4g1 h=ha r=aresid student=rsa;
run;
proc print;
data g4g1;
run;
```