

EVALUATING AND REFINING THE CNCPS FEED LIBRARY USING COMMERCIAL LABORATORY FEED DATABASES

R.J. Higgs, L.E. Chase, D.A. Ross, and M.E. Van Amburgh
Department of Animal Science
Cornell University

INTRODUCTION

Globally, food production systems are under pressure to reduce the impact they have on the environment and manage feed costs. The Cornell Net Carbohydrate and Protein System (CNCPS) is a nutritional model that enables the formulation of diets that closely match animal requirements. The model relies on empirical estimations of carbohydrate and protein degradation and passage rates to predict the extent of ruminal fermentation, microbial growth, and the absorption of metabolizable energy and protein through the digestive tract (Fox et al., 2004). The most recent version of the CNCPS (Tylutki et al., 2008; Van Amburgh et al., 2010) provides a framework for precision feeding where diets can be formulated to minimize nutrient excretion to the environment. Robust inputs are critical to any model simulation, but are particularly important when practicing precision feeding. The objective of this study was to evaluate the CNCPS feed library against commercial laboratory data, and update the library as required. The CNCPS feed library consists of approximately 800 ingredients including forages, concentrates, vitamins, minerals and commercial products and serves as the reference database for describing the chemical composition of a diet. A multi-step approach was used to evaluate, refine and standardize the chemical composition of the feeds in the feed library. The approach was designed to combine current feed library information with new information and predict uncertain values.

MATERIALS AND METHODS

A spreadsheet was constructed in Microsoft Excel that enabled each component of each feed to be evaluated against current data and updated where required. The variables of importance were those routinely analyzed by commercial labs and required by the CNCPS for simulation. These include: Dry matter (DM), crude protein (CP), soluble protein (SP), ammonia, protein insoluble in acid detergent (ADIP), protein insoluble in neutral detergent (NDIP), acetic acid, propionic acid, butyric acid, lactic acid, organic acids, sugar, starch, acid detergent fiber (ADF), neutral detergent fiber (NDF), lignin, ash, ether extract (EE) and soluble fiber. Fractionation of components within the framework of the CNCPS are described by Tylutki et al. (2008). Individual amino acids, fatty acids, minerals, vitamins and digestion rates included in the CNCPS feed library were not evaluated in this project. To complete the analysis, datasets were provided by two commercial laboratories (Cumberland Valley Analytical Services Inc, Maugansville, MD, USA and Dairy One Cooperative Inc, Ithaca, NY, USA). The compiled dataset included 90 different ingredients and >100,000 individual samples. Additional means and standard deviations of individual feeds were sourced from the

laboratory websites. The online resource for both labs includes >10 years of data and an extensive collection of different ingredients. Each feed was evaluated for internal consistency, and consistency against laboratory data. Internal consistency required each feed to adhere to the fractionation scheme described by Tylutki et al. (2008) and summarized in Table 1.

Table 1. Equations used by the CNCPS to calculate carbohydrate and protein fractions

Variables ^a	Description	Equations ^b	
CHO _j	Carbohydrate	$100 - CP_j - EE_j - Ash_j$	(1)
CC _j	CHO C fraction (Lignin × 2.4)	$(NDF_j \times Lignin_j \times 2.4) / 100$	(2)
CB3 _j	CHO B3 fraction (available NDF)	$NDF_j - CC_j$	(3)
NFC _j	Non-fiber CHO	$CHO_j - NDF_j$	(4)
CB2 _j	CHO B2 fraction (soluble fiber)	$NFC_j - CA1_j - CA2_j - CA3_j - CA4_j - CB1_j$	(5)
CA1 _j	CHO A1 fraction	$Acetate_j + Propionate_j + Butyrate_j$	(6)
CA2 _j	CHO A2 fraction	$Lactate_j$	(7)
CA3 _j	CHO A3 fraction	$Organic\ acids_j$	(8)
CA4 _j	CHO A4 fraction	$Sugars_j$	(9)
CB1 _j	CHO B1 fraction	$Starch_j$	(10)
PA1 _j ^c	Protein A1 fraction (Ammonia)	$Ammonia_j \times (SP_j/100) \times (CP_j/100)$	(11)
PA2 _j	Protein A2 fraction (Soluble true protein)	$SP_j \times CP_j / 100 - PA1_j$	(12)
PB1 _j	Protein B1 fraction (Moderately degradable protein)	$CP_j - (PA1_j - PA2_j - PB2_j - PC_j)$	(13)
PB2 _j	Protein B2 fraction (Slowly degraded protein, bound in NDF)	$(NDIP_j - ADIP_j) \times CP_j / 100$	(14)
PC _j	Protein C fraction (Unavailable protein)	$ADIP_j \times CP_j / 100$	(15)

^a Subscript *j* means for the *j*th feed in the library.

^b NDF = Neutral detergent fiber (g/kg DM); ADF = Acid detergent fiber (g/kg DM); Lignin (% NDF); CP = Crude protein (g/kg DM); SP = Soluble protein (% CP); EE = Ether extract.

^c Previous versions of the CNCPS feed library use NPN for the PA1 fraction. This has been replaced with ammonia.

Eq. (1) provides the relationship between carbohydrates (CHO), CP, EE and Ash. CHO is decomposed by Eq. (4) and (5) to NDF, acetate, propionate, butyrate, lactate, organic acids, sugar, starch and soluble fiber. From Eq. (1), (4) and (5), equation 16 can be derived.

$$100 = CP_j + EE_j + Ash_j + NDF_j + Acetate_j + Propionate_j + Butyrate_j + Lactate_j + Organics_j + Sugars_j + Starch_j + Soluble\ fiber_j \quad (16)$$

Soluble fiber (CB2) is calculated in the CNCPS by difference (Eq. 5). This means any error in the estimation of the CA1, CA2, CA3, CA4 or CB1 fractions will result in an over- or under-estimation of soluble fiber. Also, error in the estimation of CP, EE, Ash or NDF will cause error in soluble fiber through the calculation of CHO (Eq. (1)) and the subsequent calculation of non-fiber carbohydrates (NFC; Eq. (4)). Overestimation of components in Eq. (16) can cause a situation where soluble fiber is forced to 0 and the sum of the equation is greater than 100 % DM which is chemically impossible. Feeds that didn't adhere to the assumptions of Eq. (16) were updated. Evaluation against laboratory data compared each individual feed in the feed library to the mean and SD of the corresponding feed in the online databases available by the commercial labs. Each component within each feed was required to fall within 1 SD of the mean value from the laboratory dataset, or the entire feed would be updated. The calculation procedure consisted of four steps:

Step 1 – Setting Descriptive Values

Chemical components used to differentiate different forms of the same feed were fixed. The CNCPS has multiple options for many of the feeds in the feed library to give users the flexibility to pick the feed that best matches what they are feeding on the farm. For example, the feed library has 24 different options for processed corn silage which are differentiated on the basis of DM and NDF. Therefore, in this example, DM and NDF were maintained as they were in the original library while other components were re-calculated.

Step 2 – Simple Linear Regression

In the second step, the dataset provided was used to establish relationships using linear regression ($Y = A + BX_1 + CX_2 + DX_3$). Regression was used if components could be robustly predicted by other components within a feed ($R^2 > 0.65$). Most commonly, ADF was predicted from NDF and lignin, however, corn silage starch was also able to be predicted by NDF and CP. Regression equations were calculated using SAS (2010) and are in Table 2.

Step 3 – Matrix Regression

In the third step, factors that couldn't be predicted using standard linear regression were calculated using a matrix of regression coefficients derived from data generated using a Monte Carlo simulation (Law and Kelton, 2000). The Monte Carlo simulation was completed using @Risk version 5.7 (Palisade Corporation, Ithaca, NY, USA). To complete the analysis, probability density functions were fit to each chemical component of each feed using the data provided by the commercial labs and the distribution fitting function in @Risk (Palisade, 2010a). Distributions were ranked on how well they fit the input data using the Chi-Squared goodness of fit statistic. Equiprobable bins were used to adjust bin size in the Chi-Square calculation to contain an equal amount of probability

(Law and Kelton, 2000). The distribution with the lowest Chi-Square was assigned to each component.

Table 2. Predicting chemical components of feeds using simple and multiple linear regression ($Y = A + BX_1 + CX_2 + DX_3$)^a

Feed name	Y	X ₁	X ₂	X ₃	A	B	C	D	RMSE ^b	R ²
Barley silage	ADF	NDF	Lignin		-7.15	0.69	0.50		1.53	0.90
Corn Silage	ADF	NDF			-3.67	0.68			1.28	0.89
	Starch	NDF	CP		96.18	-1.18	1.62		2.60	0.87
Fresh grass (High NDF)	ADF	NDF	Lignin	CP	0.47	0.54	0.75	0.27	2.54	0.67
Fresh grass (Low NDF)	ADF	NDF	Lignin	CP	5.84	0.45	0.51	0.17	2.11	0.83
Fresh legume	ADF	NDF	Lignin		-6.31	0.69	0.52		1.53	0.88
Grass hay	ADF	NDF			3.57	0.57			3.21	0.69
Grass silage	ADF	NDF	Lignin		-0.25	0.57	0.47		1.79	0.85
High moisture ear corn	ADF	NDF	Lignin		-2.04	0.45	0.34		0.61	0.97
High moisture shell corn	ADF	NDF	Lignin		-1.73	0.49	0.05		0.45	0.85
Legume hay	ADF	NDF			3.33	0.72			1.10	0.91
Legume silage	ADF	NDF	Lignin		-7.11	0.75	0.50		1.79	0.83
Mixed hay	ADF	NDF	Lignin		-5.65	0.61	0.82		2.07	0.83
Mixed silage	ADF	NDF	Lignin		-2.89	0.59	0.62		1.45	0.86
Oat hay	ADF	NDF	Lignin		-4.48	0.62	0.73		1.66	0.77
Oat silage	ADF	NDF	Lignin		-1.18	0.60	0.48		1.60	0.83
Sorghum silage	ADF	NDF	Lignin		-2.91	0.63	0.41		1.70	0.87
Sorghum sudan silage	ADF	NDF	Lignin		-6.70	0.69	0.45		1.68	0.83
Straw	ADF	NDF	Lignin		-11.86	0.74	0.87		2.97	0.81
Triticale silage	ADF	NDF	Lignin		-2.94	0.61	0.65		1.78	0.83
Wheat hay	ADF	NDF	Lignin		3.26	0.52	0.49		1.78	0.74
Wheat silage	ADF	NDF	Lignin		1.10	0.56	0.49		1.60	0.83

^a NDF = Neutral detergent fiber (g/kg DM); ADF = Acid detergent fiber (g/kg DM); CP = Crude protein (g/kg DM); Lignin (% NDF).

^b RMSE = Root mean square error.

Components within each feed were then correlated to each other using laboratory data and the define correlation function in @Risk (Palisade, 2010a). If components were not correlated, they would change randomly relative to each other during the Monte Carlo simulation. Correlating the components meant that for each iteration, components changed in tandem relative to each other with the magnitude of the change depending

on the assigned correlation coefficient (Law and Kelton, 2000). Spearman rank order correlations were used which determine the rank of a component relative to another by its position within the min-max range of possible values. Rank correlations can range between -1 and 1 with a value of 1 meaning components are 100% positively correlated, -1 meaning components are 100% negatively correlated and 0 meaning there is no relationship between components (Law and Kelton, 2000).

Once the probability density functions had been fit to each component, and components within each feed correlated, a Monte Carlo simulation was performed with 30,000 iterations. Various sampling techniques are available in @Risk to draw the sample from the probability density function (Palisade, 2010a). The Latin Hypercube technique was used which divides the distribution into intervals of equal probability and then randomly takes a sample from each interval forcing the simulation to represent the whole distribution (Shapiro, 2003). The raw data from the simulation was then used to construct a matrix of regression estimates in the arrangement shown in Figure 1 and according to the general form $Y_{ij} = A + BX$ where Y is the response variable and column vector for the i th component in the j th feed with n entries, A is the intercept arranged in an $n \times p$ matrix, B is the predictor variable arranged in an $n \times p$ matrix and X is the regression coefficient and row vector for the i th component with n entries. In this arrangement $Y_n = X_n$ and, therefore, $A_{np} = 0$ and $B_{np} = 1$. For example, if Y_1 was the response variable CP, then the predictor variable X_1 would also be CP and the relationship would have an intercept of 0 and slope of 1. Therefore, equations where $Y_n = X_n$ were excluded from the matrix.

$$Y = \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix} \quad A = \begin{pmatrix} A_{11} & \dots & A_{1p} \\ A_{21} & \dots & A_{2p} \\ \vdots & \ddots & \vdots \\ A_{n1} & \dots & A_{np} \end{pmatrix}, \quad B = \begin{pmatrix} B_{11} & \dots & B_{1p} \\ B_{21} & \dots & B_{2p} \\ \vdots & \ddots & \vdots \\ B_{n1} & \dots & B_{np} \end{pmatrix}, \quad X = \begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ X_n \end{pmatrix}$$

Figure 1: Arrangement of regression coefficients in matrix form used to predict feed components.

The weighted mean of response variables were calculated across each row of the matrix. The coefficients used to correlate each probability density function for the Monte Carlo simulation were normalized to sum to 1 and then used as weights (W) in the weighted mean, i.e.

$$\sum_{i=1}^n W_i = 1 \quad \text{and, therefore,} \quad \bar{Y} = \sum_{i=1}^n W_i X_i.$$

Using correlation coefficients as weights meant components within a specific feed that were more highly correlated had more influence on the mean and *vice versa*.

Components calculated using this method varied depending on the data available for a specific feed. To avoid confounding, components within a feed that were calculated by

the matrix were not used as predictor variables for other components in the matrix. Therefore, the number of components calculated using the matrix was limited to avoid running out of predictor variables. Typically, nitrogenous components (SP, Ammonia, NDIP, ADIP) not calculated in the preceding steps and not factors in Eq. (16) were calculated in this step.

Step 4 – Optimize to a Final Solution

Lastly, components that were not assigned values in any of the preceding steps were calculated using an optimization. RISKOptimizer version 5.7 (Palisade Corporation, Ithaca, NY, USA) was used to perform the optimization which uses a genetic algorithm and Monte Carlo simulation to find solutions when there is uncertainty around the values (Palisade, 2010b). Minimum and maximum boundaries for each component within a feed were set to constrain the optimizer to a likely range of values. The data used to calculate the range in each component was taken from the databases available online from the laboratories. Each range was calculated as the mean plus or minus the standard deviation of each component multiplied by global coefficient that was adjusted in order to allow the optimizer to converge. Typically the coefficient used was between 0.5 and 1.5 meaning the range for each component was the mean plus or minus 0.5 to 1.5 times the standard deviation of each component.

The second constraint applied to the optimization was the relationship described by Eq. (16). Components included in the optimization were, therefore, adjusted within the calculated range to the most likely values in which Eq. (16) summed to 100 % DM. The optimization step was completed last in the calculation process to ‘fit’ the components within each feed together within the described constraints. The process was dynamic in that the values calculated in the optimization fed back into the matrix and regression calculations described above. Typically, the optimizer had to be run numerous times before it would converge and stabilize. If insufficient data was available to perform any of the calculation steps described above, current CNCPS library values were retained. The approach was not acceptable for many proprietary feeds due to a lack of a robust database of chemical components or the functional nature of some ingredients beyond the nutrient content. Current library values were retained in these circumstances. Approximately 75% of the feeds in the feed library were updated and 25% remained unchanged. Those remaining unchanged were primarily minerals and vitamins along with unusual feeds with little information within the databases. Examples of updates made to selected feeds are in Table 3.

RESULTS AND DISCUSSION

Obtaining useful outputs from biological models is very dependent on the quality of the information being used to perform a simulation (Haefner, 2005). The CNCPS feed library provides the platform for inputting dietary information into the CNCPS and contains information not routinely available from commercial labs such as AA profiles, fatty acid profiles, digestion rates and intestinal digestibility's (Tylutki et al., 2008). The feed library also provides commonly analyzed fractions that can be used as they are, or

updated by the user. Correct estimation of these chemical components is critical in enabling the CNCPS to best predict the ME, MP and other specific nutrients available from a given ration (Lanzas et al., 2007a; Lanzas et al., 2007b; Offner and Sauvant, 2004). Although laboratory analysis of each feed used in a ration will provide the most accurate representation of a diet, in some situations this isn't possible and feed library values have to be relied on. In other situations, feed compositions are very consistent meaning library values provide a reasonable estimation without laboratory analysis. For these reasons, the feed library was reviewed and updated.

The process of evaluating and updating the feed library was designed specifically to pool data from various sources and combine it to estimate likely values. Many external factors affect the nutrient composition of feeds both pre- and post-harvest. When considering forages, pre-harvest environmental factors such as temperature, light intensity, nitrogen availability, water and predation impact quality and composition (Van Soest et al., 1978). Post-harvest, management factors such as packing density, particle size, silo type, silo filling rate and the way in which the face of the silo is managed can impact ADF, NSC, ADIN, SP, ammonia, pH, surface temperature and aerobic instability (Ruppel et al., 1995). Furthermore, biological processes during ensiling such as plant respiration, plant enzymatic activity, clostridial activity and aerobic microbial activity will impact levels of rapidly fermentable CHO, AA, NPN and can lead to heating and Maillard reactions (Muck, 1988). Analytically, elevated levels of ADIN are indicative that Maillard reactions have occurred and are common in many heat dried feeds and fermented feeds where excessive heating occurred (Van Soest and Mason, 1991). Although the dataset used in this analysis encompassed a large number of samples from a wide range of situations, information on environmental and management factors implicit in the composition of an individual sample were not available. Given the importance of external factors on the composition of different feeds, the process used in this project was not sensitive enough to accurately predict the composition of feeds on a sample by sample basis. However, it was capable of producing estimated compositions under average conditions in an efficient and repeatable manner which was useful for reviewing and updating a large database such as the CNCPS feed library.

Chemical components and fractionation of feeds in the updated library were maintained in the format described by Tylutki et al. (2008) with the exception of the protein A1 fraction. Previously this has been classified as non-protein nitrogen (NPN) which is measured as the nitrogen passing into the filtrate after precipitation with protein specific reagent (tungstic or trichloroacetic acid; Licitra et al., 1996). The protein A1 fraction is typically assumed to be completely degraded in the rumen (Lanzas et al., 2007b). However, small peptides and free AA not precipitated by this method are still metabolically relevant to the animal if they escape rumen degradation and flow through to the small intestine (Givens and Rulquin, 2004). Choi et al. (2002) suggested 10% of the AA flowing through to the small intestine originated from dietary NPN sources which under the current system are unaccounted for. Likewise, Velle et al. (1997) infused free AA into the rumen at various rates and showed up to 20% could escape degradation and flow through to the small intestine which is in agreement with data from Volden et al. (1998). Van Amburgh et al. (2010) suggested it may be more appropriate to redefine

the protein A1 pool from NPN as described by Licitra et al. (1996) to ammonia. This would shift small peptides and free AA currently associated with the A1 pool into the A2 pool where they could contribute to MP supply. Ammonia has the advantage of being easily measured and available from most commercial laboratories. Therefore, the NPN pool in previous feed libraries has been updated to ammonia in the current version. This represents an initial step in a process aimed at improving MP and AA predictions in the CNCPS.

CONCLUSION

Chemical components of feeds in the CNCPS feed library have been evaluated and refined using a multi-step process designed to pool data from various sources and optimize feeds to be both internally consistent, and consistent with current laboratory data. When using the CNCPS to formulate rations, the variation associated with environmental and management factors, both pre- and post-harvest, should not be overlooked as they can have marked effects on the composition of a feed. Regular laboratory analysis of samples taken on-farm, therefore, remains the recommended approach to characterizing the components in a ration. However, updates to CNCPS feed library provide a database of ingredients that are consistent with current laboratory data and can be used as a platform to, both formulate rations and improve the biology within the model.

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Table 3. Examples of the changes made to the chemical composition of feeds during the editing process.

Component ^a	Alfalfa Hay 20		Alfalfa Silage		Corn Silage		Blood Meal		Corn Grain		Soybean Meal	
	Old	New	Old	New	Old	New	Old	New	Old	New	Old	New
CP	20.0	20.0	20.0	20.0	9.5	9.5	93.0	93.0	9.0	9.0	51.5	51.5
SP %CP	40.0	42.6	60.0	60.0	58.0	55.7	3.7	11.5	19.0	20.2	20.0	20.0
NPN/Ammonia % SP ^b	40.0	0.0	65.0	13.9	65.0	13.4	10.0	0.0	39.0	0.0	12.0	0.0
ADIP %CP	6.0	7.1	12.0	7.2	7.0	8.4	1.0	1.0	5.0	5.5	2.0	1.8
NDIP %CP	16.0	16.9	18.0	14.4	16.0	15.3	40.6	2.8	10.0	13.2	3.1	2.0
Acetic acid	0.0	0.0	1.7	1.7	1.7	1.7	0.0	0.0	0.0	0.0	0.0	0.0
Propionic acid	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Butyric acid	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Lactic acid	0.0	0.0	5.0	5.0	4.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0
Other organic acids	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Sugar	9.7	9.0	3.7	3.7	1.4	1.4	0.0	0.0	1.5	1.6	10.9	10.9
Starch	1.6	1.6	1.6	1.6	28.7	23.1	0.0	0.0	74.8	74.8	2.2	1.9
Soluble fiber	17.9	17.4	18.7	14.5	0.0	4.0	2.6	0.0	0.8	0.0	14.1	16.2
ADF	32.0	32.0	36.0	31.5	30.0	29.7	0.1	0.1	4.0	3.6	6.0	6.8
NDF	40.0	40.0	40.0	40.0	49.0	49.0	37.8	2.8	9.0	9.0	10.0	10.0
Lignin % NDF	17.0	16.8	17.0	17.1	10.0	7.2	0.0	1.0	2.2	13.5	2.5	8.5
Ash	8.0	9.1	8.0	9.0	4.0	4.0	2.4	2.2	1.6	1.6	6.7	6.7
EE	3.0	2.8	4.4	4.4	3.2	3.2	2.0	2.0	4.2	4.0	2.8	2.8
NFC	29.0	28.0	27.6	26.6	34.3	34.3	-35.2	0.0	76.2	76.4	29.0	29.0
Eq. (16)	103.2	100.0	103.1	100.0	101.5	100.0	137.7	100.0	100.9	100.0	98.2	100.0

^a Expressed as % DM unless stated otherwise.

^b Changed from NPN to Ammonia in the new library.

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