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# Evaluation of the National Research Council (2001) dairy model and derivation of new prediction equations. 1. Digestibility of fiber, fat, protein, and nonfiber carbohydrate

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## Evaluation of the National Research Council (2001) dairy model and derivation of new prediction equations. 1. Digestibility of fiber, fat, protein, and nonfiber carbohydrate<sup>1</sup>

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### ABSTRACT

Evaluation of ration balancing systems such as the National Research Council (NRC) *Nutrient Requirements* series is important for improving predictions of animal nutrient requirements and advancing feeding strategies. This work used a literature data set ( $n = 550$ ) to evaluate predictions of total-tract digested neutral detergent fiber (NDF), fatty acid (FA), crude protein (CP), and nonfiber carbohydrate (NFC) estimated by the NRC (2001) dairy model. Mean biases suggested that the NRC (2001) lactating cow model overestimated true FA and CP digestibility by 26 and 7%, respectively, and under-predicted NDF digestibility by 16%. All NRC (2001) estimates had notable mean and slope biases and large root mean squared prediction error (RMSPE), and concordance (CCC) ranged from poor to good. Predicting NDF digestibility with independent equations for legumes, corn silage, other

forages, and nonforage feeds improved CCC (0.85 vs. 0.76) compared with the re-derived NRC (2001) equation form (NRC equation with parameter estimates re-derived against this data set). Separate FA digestion coefficients were derived for different fat supplements (animal fats, oils, and other fat types) and for the basal diet. This equation returned improved (from 0.76 to 0.94) CCC compared with the re-derived NRC (2001) equation form. Unique CP digestibility equations were derived for forages, animal protein feeds, plant protein feeds, and other feeds, which improved CCC compared with the re-derived NRC (2001) equation form (0.74 to 0.85). New NFC digestibility coefficients were derived for grain-specific starch digestibilities, with residual organic matter assumed to be 98% digestible. A Monte Carlo cross-validation was performed to evaluate repeatability of model fit. In this procedure, data were randomly subsetted 500 times into derivation (60%) and evaluation (40%) data sets, and equations were derived using the derivation data and then evaluated against the independent evaluation data. Models derived with random study effects demonstrated poor repeatability of fit in independent evaluation. Similar equations derived without random study effects showed improved fit against independent data and little evidence of biased parameter estimates associated with failure to include study effects. The equations derived in this analysis provide interesting insight into how NDF, starch, FA, and CP digestibilities are affected by intake, feed type, and diet composition.

**Key words:** National Research Council (2001) dairy model, total-tract digestibility, model evaluation

### INTRODUCTION

Ration evaluation programs and the equations that comprise them such as those proposed by the National

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Research Council (NRC) are an essential component of animal nutrition research, education, and extension in the United States and throughout the world, where these ration evaluation systems are employed. To ensure that these ration balancing systems meet their objectives, it is necessary to evaluate them extensively against published data. Although the NRC (2001) dairy model was quantitatively evaluated before publication, the extent of the evaluations was limited and largely restricted to protein supply and milk yield (NRC, 2001; St-Pierre, 2003).

The energy and protein fractionation schemes used within the NRC (2001) dairy model are process-based, but the processes are described primarily by empirical equations that predict energy and N fluxes through the dairy cow. The energy fractionation scheme relies heavily on the estimation of nutrient digestibility within different feed classifications (NRC, 2001). Errors for predicting TDN and digestible energy (DE) within the NRC (2001) model might be a result of either poorly characterized feed composition or poorly parameterized equations for determining nutrient digestibilities. The relative contributions of these sources of error is currently unknown, and future efforts in model refinement might be misdirected without assessment of these error sources.

The objectives of this work were to use a literature data set of apparent total-tract digestibility of NDF, fatty acids (FA), CP, OM, and starch to evaluate the nutrient digestibility estimates provided by the NRC (2001) dairy model and to derive new equations, when necessary. The NRC (2001) predictions of true total-tract digestibilities were evaluated by adjusting apparent FA and N digestibilities to a true basis based on estimated endogenous contributions. We hypothesized (1) that NRC (2001) digestible nutrient predictions would have poor fit when compared with measured data, and (2) that model accuracy and precision would be improved by deriving new equation forms. The effects of these adjustments on RUP and RDP estimates and predicted milk yield are detailed in a companion paper (White et al., 2017).

## MATERIALS AND METHODS

The analysis conducted in this study is described here as a series of steps, including (1) data collection; (2) correcting mis-specified ingredients; (3) evaluating the NRC (2001) model; (4) deriving new models; and (5) cross-validating new models. The objective of this work is not to define the superiority of new equations compared with the NRC (2001) model. Direct comparison of these models is essentially infeasible because the

new equations were derived and evaluated against the same data set. The primary purpose of deriving new equations was to identify which variables helped to reduce mean and slope biases and improve fit against independent data when predicting nutrient digestibility.

### Data Collection

Data were collected from the original set of papers used to evaluate the NRC (2001) dairy model. This collection of papers was updated with more recent work published between the early 2000s until mid-2015. Data from lactating and nonlactating cattle were used, and an exhaustive listing of studies in the data set is presented in Supplemental File S1 (<https://doi.org/10.3168/jds.2015-10800>). Studies were included in the data set if they presented a numerical measurement of duodenal or omasal N flows or apparent total-tract digestibility measurements. Studies were excluded if they failed to report feed ingredients used and their inclusion rates. The final data set contained usable data from 550 treatment means from 147 studies. The number of treatments used for model derivation was nutrient specific because not all studies reported all response variables (some studies only reported total-tract digestibility of NDF and starch but not CP and FA). The summary statistics for the resulting data set are included in Table 1, and a copy of the data can be downloaded from the National Animal Nutrition Program (2015) website.

Because measured digestibility data from total-tract digestibility experiments were the only data used, the equations in this study reflect prediction of digested material, rather than potentially digestible material. Throughout the paper, the terms “digested” and “digestibility” are used to refer to the actually digested material or reported apparent total-tract digestibility.

### Evaluating and Correcting Ingredient Biases

Most studies reported the inclusion rates of the ingredients used in diets (Table 1); however, few studies reported nutrient composition of all ingredients. When ingredient nutrient composition data were available, they were used to calculate dietary nutrient provision. When ingredient-level data were not available, data were populated from the NRC (2001) feed table. In most cases, FA, NDF, ADF, DM, and CP of diets were reported. When the measured dietary nutrient compositions were compared with the predicted dietary nutrient compositions (calculated from ingredient inclusion levels and tabular feed composition), mean and slope

**Table 1.** A summary of the data contained in the data set

Variable <sup>1</sup>	n <sup>2</sup>	Mean	SD	Minimum	Maximum
DMI, kg/d	550	19.7	3.92	5.8	30.4
DMIMBW, kg/kg <sup>0.75</sup>	550	0.16	0.03	0.05	0.25
BW, kg	457	598	58.5	464	788
DIM, d	401	106	58.5	0	323
Milk, kg/d	456	29.0	7.7	0	47.0
Milk lactose, %	209	4.78	0.17	4.07	5.09
Milk protein, %	408	3.14	0.24	2.59	3.90
Milk fat, %	408	3.59	0.50	2.11	4.86
Nutrient composition of the total diet, % of DM					
DM	332	60.2	15.0	15.7	93.0
Ash	91	7.2	1.1	5.3	11.7
CP	497	17.1	1.9	10.3	24.6
NDF	431	32.5	5.8	17.6	50.9
ADF	366	19.4	4.4	8.8	34.3
NFC	28	38.5	3.1	30.6	45.5
Starch	242	28.1	9.2	0.4	47.9
FA	132	5.0	2.5	1.6	18.2
Ether extract	46	5.8	2.3	2.2	19.2
Apparent total-tract nutrient digestibility, %					
NDF	337	50.4	10.8	19.5	84.0
FA	55	71.5	9.5	40.2	93.1
CP	399	67.5	5.4	40.3	86.6
Starch	190	92.1	6.6	68.5	99.7
Feed type inclusion					
Treatments with:	n <sup>2</sup>	Treatments with:		n <sup>2</sup>	
Grass	350	Other wet forage <sup>3</sup>	34		
Legumes	182	Other dry forage <sup>3</sup>	29		
Corn silage	299	Plant protein	474		
Oil	55	By-product feeds	229		
Prilled fat	29	Energy sources (grain)	520		
Fatty acids	35	Animal protein	160		
Animal fat or tallow	47	Vitamin/minerals	508		
Vegetable oil	12	Corn gluten feed	8		
Other fat	4	Distillers grains	55		
Wheat middlings	15	Soyhulls	15		
Beet pulp	42				

<sup>1</sup>Dry matter intake per unit of metabolic BW (DMIMBW).

<sup>2</sup>n indicates number of treatments with feed type reported.

<sup>3</sup>Other forages included small grain crop forage.

biases were evident. To minimize errors associated with ingredient mis-specification, the correction approach presented in Hanigan et al. (2013) was applied. Briefly, study-level residuals for each nutrient were calculated

and added back to each treatment feed composition after weighting by feed nutrient composition and inclusion rate. The results of this adjustment are detailed in Table 2.

**Table 2.** A summary of bias adjustments applied to predicted dietary nutrients by study

Item	NDF	Fattt acids	CP	Starch	ADF
No. of treatments	366	132	497	242	431
Mean residual, <sup>1</sup> % of DM	2.1	-0.3	-0.2	-2.8	0.4
Minimum residual, % of DM	-18.9	-14.1	-8.2	-16.9	-14.7
Maximum residual, % of DM	20.5	13.1	6.2	12.4	21.8
RMSE, % of mean	17.3	63.1	11.4	23.9	23.2
Bias-adjusted RMSE, <sup>2</sup> % of mean	13.1	51.8	9.4	19.1	17.2
Error reduction, %	24.3	17.9	17.6	20.1	25.9

<sup>1</sup>Residuals were calculated as observed – predicted.

<sup>2</sup>Root mean squared error (RMSE) of calculated and reported diet nutrient composition after applying study-level residual adjustments as described in Hanigan et al. (2013).

### Calculating NRC Predictions

The model equations used in the NRC (2001) dairy model code, available as a text file on the compact disk distributed with the publication, and the equations listed in the NRC (2001) publication were used to reconstruct the model in SAS (version 9.3; SAS Institute, 2005) and R (version 3.1.0; R Core Team, 2014). Both versions were tested to ensure that they replicated the NRC (2001) software outputs for a wide variety of diets using feeds from each feed classification and calculating requirements for lactating and nonlactating cows. Both outputs [net energy (NE)- and MP-allowable milk and gain] and intermediate variables (TDN, discounted TDN, microbial N, NE supply and requirements, MP supply and requirements, RDP supply and requirements, and RUP supply and requirements) were evaluated for accuracy. The NRC (2001) program used for this was that distributed on the National Animal Nutrition Program (2015) website (<https://nanp-nrsp-9.org/nrc-dairy-model/>), which has been updated to remove coding errors in the passage rate (Kp) equation present in the original program.

The SAS program was used to predict nutrient supply and NE- and MP-allowable milk yields for each treatment within the data set. Many studies did not report all animal performance data required as inputs to the NRC (2001) model. When treatment-specific data were not available for an input, reference input data [averages from the unadjusted data set or NRC (2001) software default values] were used. These were age = 50 mo, BW = 598 kg, milk fat = 3.59%, lactose = 4.78%, milk true protein = 3.14%, mature BW = 680 kg, age at first calving = 24 mo, daily BW gain = 0 kg/d, and calf birth weight = 45 kg. Although calf birth weight, mature BW, age at first calving, BW gain, and age were not reported in most studies, 83% of treatments reported BW and 74% reported milk fat and true protein. Values were applied irrespective of breed used in the study because many studies that failed to report milk production or composition also failed to provide detailed animal descriptions. Any potential introduced errors associated with failing to represent cow breed are likely accounted for in the models that included random study effects but not by those that included only fixed effects. The summary statistics in Table 1 include only treatments for which these default values were not used.

### Evaluating Prediction Errors

The NRC (2001) nutrient supply model predicted total-tract digestibility of NFC, NDF, FA, and CP and

integrated them to estimate TDN and DE. Predicted TDN and dietary crude fat concentration are used to discount energy derived from the diet as a function of multiples of maintenance. Discounted DE is summed across feedstuffs and converted to ME and NE in a feed-type-specific manner. Although numerous assessments of the NRC (2001) model have been conducted (Seo et al., 2006; Lanzas et al., 2007; Krizsan et al., 2010), few have explicitly addressed the hierarchical structure inherent in the calculation method. To more precisely evaluate the NRC (2001) model predictions, we assert that one must begin with evaluating predictions of nutrient digestibility and subsequently evaluate predicted protein flows from the rumen before finally addressing milk yield predictions. Only when following this sequence can one assign downstream prediction errors to the proper source. Ideally, one would also evaluate DE, ME, and NE estimates; however, minimal additional data have been collected to evaluate conversions to DE to ME and ME to NE since NRC (2001).

Model predictions of digestible nutrients (NDF, CP, and FA) were evaluated in comparison to apparent total-tract nutrient digestibility reported in the data set and adjusted to a true basis. The NRC (2001) predicted digested nutrients as a percent of dietary DM; therefore, a series of transformations were used to match the NRC (2001) predicted digestibility with measured digestibility adjusted to a true basis. The general system fit for each nutrient was

$$TTDC_{nut,f,t,s} = f(\mathbf{x}), \quad [1]$$

$$TTDP_{nut,t,s} = \sum_{f=i}^k TTDC_{nut,f,t,s} \times C_{nut,f,t,s}, \quad [2]$$

$$TTDF_{nut,t,s} = \frac{TTDP_{nut,t,s}}{100} \times DMI_{t,s}, \quad [3]$$

where  $TTDC_{nut,f,t,s}$  was the NRC (2001) predicted total-tract digestibility coefficient of a nutrient ( $nut$ ) within a feed in a treatment ( $t$ ) within study ( $s$ ) expressed as a proportion of the nutrient intake;  $\mathbf{x}$  was a vector of parameters for the NRC (2001) equations;  $TTDP_{nut,t,s}$  was the nutrient digestibility expressed as a percentage of DMI;  $C_{nut,f,t,s}$  is the concentration of nutrient ( $nut$ ) in feed ( $f$ ) in treatment ( $t$ ) within study ( $s$ );  $TTDF_{nut,t,s}$  was the digested nutrient intake (kg or g/d);  $DMI_{t,s}$  was the DMI within treatment ( $t$ ) within study ( $s$ ); and  $k$  was the number of feeds within a treatment.

Because variables were often specific to a certain level of aggregation (feed, treatment, study), subscripts

were used throughout to denote the appropriate level for which a variable held unique values. Variables with subscript  $f$  were sourced from the NRC (2001) feed table because they held a specific value for each feed that did not vary with treatment or study. Variables with subscript  $f,t,s$  varied with feed, treatment, and study. The subscript  $t,s$  represented values that were aggregated over feeds within a dietary treatment (e.g.,  $DMI_{t,s}$ ) or otherwise did not vary at the feed level (e.g.,  $BW_{t,s}$ ). For ease of reading, the *nut* subscript is dropped for concentration variables used in the paper and the nutrient is identified as the main abbreviation.

Digestibility of nutrients generally decreases with increasing intake and thus is typically scaled per multiple of maintenance (Moe, 1981; VandeHaar, 1998; Huhtanen et al., 2009). In the NRC (2001) model, this decrease in digestibility was accounted for in the calculation of TDN (above  $1\times$  maintenance) and DE, rather than in the calculation of specific digestible nutrients. As a result, to properly evaluate the digestibility predictions within the model, one should use the calculated TDN discount to correct nutrient digestibilities before comparing with observed data. This adjustment assumed that the NRC (2001) digestibility discount applied equally across all nutrients. Because the NRC (2001) discount variable is dependent on dietary FA percent, common application of the discount variable across specific nutrient digestibilities (FA, NDF, CP, and NFC) may misrepresent some intended variable discount for FA. Because no specific FA discount was defined in the NRC (2001), the best alternative was to assume a common application of the discount across nutrients. When used, the NRC (2001) estimate of the digestibility discount was always calculated from the NRC (2001) estimate of TDN and not from any updated digestibility equations derived herein. This was done to ensure a more valid evaluation of the NRC (2001) calculation structure.

This common, diet-level digestibility discount may misrepresent effects of diet characteristics on digestibility of particular nutrients. Thus, when new parameter values were derived, nutrient-specific discounts were identified and used. These nutrient-specific discounts were estimated as proportional to DMI per unit of metabolic BW [ $DMIMBW$ , (kg/d)/kg of  $BW^{0.75}$ ] to avoid the circular calculation problem inherent in the calculation of multiples of maintenance. Because these discounts were applied at the nutrient digestibility level, further adjustments when aggregating digestibilities to calculate energy intake were not required. Again, this was only pertinent to equations that were re-derived. The original NRC (2001) calculations were as described by the NRC (2001).

Prediction errors in the NRC (2001) calculations were assessed using root mean squared error of prediction as a percentage of the mean observed value (**RMSPE**), mean and slope biases as a percentage of the mean squared error (**MSE**; Bibby and Toutenburg, 1978), and concordance correlation coefficients (**CCC**; Lin, 1989). Because the models derived herein were evaluated against the same data used for derivation, they were assessed using the root mean squared error as a percentage of the mean observed value (**RMSE**), mean and slope bias as a percentage of MSE, and CCC. Although calculated in the same way, RMSPE and RMSE should be interpreted differently as the former reflects evaluation of a prediction against independent data, whereas the latter reflects evaluation of a prediction against data used for derivation.

### Model-Fitting Procedure

Two model-fitting procedures were used to solve for parameter estimates: nonlinear mixed-effects regression (**NLME**) or nonlinear least squares regression (**NLS**). For the models estimated with NLME, fixed effects varied by equation and are detailed in the subsequent sections. A random intercept effect for study was used to adjust the predicted digestibility coefficient at a diet level (analogous to an intercept in Eq. [2]). Variance inflation parameters were calculated from the variance-covariance matrix of each model to evaluate the degree of parameter correlation. Variance inflation factors for intercept-like coefficients were allowed to vary  $>10$  because intercepts implicitly co-vary with slopes. All slope-like coefficients were restricted to a variance inflation factor of  $\leq 10$ . For models estimated with NLS, parameters varied with equation functional form. Because NLME models were derived with what is considered to be a statistically superior approach, they are presented in entirety and only the NLS model with the best fit for each response variable is presented in the main text. Other NLS models are included in Supplemental File S2 (<https://doi.org/10.3168/jds.2015-10800>).

The parameter estimates used in the NRC (2001) equations predicting  $TTDC_{nut,f,t,s}$  were re-derived, and the new coefficients were used to predict  $TTDP_{nut,t,s}$  and  $TTDF_{nut,t,s}$ . Additionally, alternative equation forms were fitted to the data and compared with the NRC (2001) equation with the re-derived parameter estimates. Our alternative equation forms were derived from all data. Direct comparison of these equations to the original NRC (2001) equations is inappropriate primarily because it is unknown which data in this set were used to derive the NRC (2001) equations. It would have been possible to subset the data into pre-2001

and post-2001; however, this would have reduced the variation in the explanatory variables available in the derivation data set and precluded opportunities to define relationships with nutrient digestibility. Splitting data in model derivation exercises is discouraged for this reason (Seni and Elder, 2010). To more appropriately compare equations, the re-derived NRC (2001) equation was compared directly to replacement equations using the corrected Akaike Information Criterion (AICc; Hurvich and Tsai, 1993). Mean and slope bias, RMSE, and CCC were also compared.

Replacement equations included (1) a 1- or 2-parameter model representing the most parsimonious approach (predicting digestibility as a percentage of the nutrient content); (2) a higher-order equation designed to replicate known biological phenomena based on significance of parameters and relationships revealed through stepwise, backward elimination, regression; and (3) a feed type-specific equation from which digestibility was predicted differently for different feed classifications. Derivation of models defined by (2) and (3) above are described in detail in subsequent sections. The first 2 model types applied an intake discount at the diet level, whereas the third type applied a discount specific to different feed types.

### Cross-Validation and Comparison of Model-Fitting Strategies

We utilized a Monte-Carlo cross-validation approach to assess how each model would perform on an independent data set (Seni and Elder, 2010). For this analysis, data were randomly divided into 2 groups. The first data group (60% of treatments) was used to derive new parameter estimates for the equation form. Then, the remaining 40% of treatments that were not used in derivation was used to independently evaluate the model. This data splitting, model derivation, and model evaluation was repeated 500 times to more closely approximate an exhaustive cross-validation. The average and standard deviation of the RMSPE, mean and slope bias as a percentage of MSPE, and CCC from the 500 independent evaluations were calculated and used as a measure of the repeatability of the equation form's ability to explain the biological relationships inherent in the data. Because many of the mixed effects models had extremely poor fit against independent data, NLS models were derived and evaluated in an identical manner. These NLS models are listed in Supplemental File S2 (<https://doi.org/10.3168/jds.2015-10800>), and the NLS model with best fit is reported in the main manu-

script text for comparison with the NLME functions. The NLS and NLME models were compared in terms of their ability to predict nutrient digestibilities of the independent data sets in the cross-validation.

### Addressing Prediction Biases

**Digestible NDF.** The NRC (2001) predicts total-tract digestible NDF intake ( $TTDF_{NDF,f,t,s}$ ; % of DM) based on NDF (% of DM), NDF insoluble protein (NDFIP; % of DM), and lignin (% of DM) concentrations in feed:

$$TTDP_{NDF,t,s} = \sum_{f=k}^l 0.750 \times \left[ (NDF_{f,t,s} - NDFIP_f) - Lignin_f \right] \times \left[ 1 - \left( \frac{Lignin_f}{NDF_{f,t,s} - NDFIP_f} \right)^{0.667} \right],$$

$$TTDF_{NDF,t,s} = \frac{TTDP_{NDF,t,s}}{100} \times DMI_{t,s} \times Discount_{t,s},$$
[4]

where  $Discount_{t,s}$  was the NRC (2001) digestibility discount applied at the diet level. Although NDF concentrations were adjusted based on study reported NDF content, NDFIP and lignin were rarely reported in studies and were estimated based on NRC (2001) feed library values. As such, NDFIP estimates were most reflective of NDFIP measured with sodium sulfite as the NRC (2001) feed library used these values. The digestion coefficient in the NDF equation was re-derived to provide more appropriate comparison between the NRC (2001) equation structure and the newly derived equation forms for  $TTDF_{NDF,f,t,s}$  prediction. When re-derived, a new diet-level discount proportional to DMIMBW was included instead.

$$TTDP_{NDF,t,s} = \sum_{f=k}^l a \times \left[ (NDF_{f,t,s} - NDFIP_f) - Lignin_f \right] \times \left[ 1 - \left( \frac{Lignin_f}{NDF_{f,t,s} - NDFIP_f} \right)^{0.667} \right],$$

$$TTDF_{NDF,t,s} = \frac{TTDP_{NDF,t,s}}{100} \times DMI_{t,s} \times (1 - b \times DMIMBW_{t,s}),$$
[5]

where  $a$  and  $b$  were derived during fitting. A series of additional equations were also evaluated to predict

$TTDF_{NDF,f,t,s}$  including a simple average prediction of NDF digestibility:

$$\begin{aligned}
 TTDC_{NDF,f,t,s} &= a, \\
 TTDP_{NDF,t,s} &= \sum_{f=k}^l TTDC_{NDF,f,t,s} \times NDF_{f,t,s}, \\
 TTDF_{NDF,t,s} &= \frac{TTDP_{NDF,t,s}}{100} \times DMI_{t,s} \\
 &\quad \times (1 + b \times DMIMBW_{t,s} + c \times DietStarch),
 \end{aligned}
 \tag{6}$$

where  $a$ ,  $b$ , and  $c$  were derived during fitting and *DietStarch* is dietary starch percent (% of DM). An equation considering interactions among nutrients was also tested:

$$\begin{aligned}
 TTDC_{NDF,f,t,s} &= a + b \times NDFIP_f + c \times Lignin_f + d \times ADF_f \\
 &\quad + e \times CP_f, \\
 TTDP_{NDF,t,s} &= \sum_{f=k}^l TTDC_{NDF,f,t,s} \times NDF_{f,t,s}, \\
 TTDF_{NDF,t,s} &= \frac{TTDP_{NDF,t,s}}{100} \times DMI_{t,s} \\
 &\quad \times (1 + f \times DMIMBW_{t,s} + g \times DietStarch_{t,s}),
 \end{aligned}
 \tag{7}$$

where  $a$  through  $g$  were derived during fitting,  $ADF_f$  is dietary ADF (% of DM), and  $CP_f$  is dietary CP (% of DM).

The parameters in Eq. [7] were those revealed as significant from a stepwise regression that originally contained NDF,  $NDF^2$ ,  $NDFIP$ ,  $NDFIP^2$ , Lignin,  $Lignin^2$ , ADF,  $ADF^2$ , and CP. Both Eq. [6] and [7] also included a diet-level digestibility discount that was derived based on DMIMBW and dietary starch percentage (*DietStarch*; % of DM). A feed-type-specific prediction was also derived:

$$TTDC_{NDF,f,t,s} = \begin{cases} \text{if Forage} = \text{"Legume"} \text{ then :} \\ \left( a + b \times \frac{Lignin_f}{ADF_{f,t,s}} \right) \times [1 + (c \times DMIMBW_{t,s})] \\ \text{if Forage} = \text{"CornSilage"} \text{ then :} \\ \left( d + e \times \frac{Lignin_f}{ADF_{f,t,s}} \right) \times [1 + (c \times DMIMBW_{t,s})] \\ \text{if Forage} = \text{"Grass"} \text{ then :} \\ (f + g \times DietNDF_{t,s}) \times [1 + (c \times DMIMBW_{t,s})] \\ \text{if Forage} = \text{"Other Dry Forage"} \text{ then :} \\ (h) \times [1 + (c \times DMIMBW_{t,s})] \\ \text{if Forage} = \text{"Other Wet Forage"} \text{ then :} \\ (i) \times [1 + (c \times DMIMBW_{t,s})] \\ \text{if Feed} = \text{"GlutenFeed"} \text{ then :} \\ (j) \times [1 + (k \times DMIMBW_{t,s})] \\ \text{if Feed} = \text{"Distillers"} \text{ then :} \\ (l) \times [1 + (k \times DMIMBW_{t,s})] \\ \text{if Feed} = \text{"Soyhulls"} \text{ then :} \\ (m) \times [1 + (k \times DMIMBW_{t,s})] \\ \text{if Feed} = \text{"WheatMidds"} \text{ then :} \\ (n) \times [1 + (k \times DMIMBW_{t,s})] \\ \text{if Feed} = \text{"BeetPulp"} \text{ then :} \\ (o) \times [1 + (k \times DMIMBW_{t,s})] \\ \text{else :} \\ (p + q \times DietNDF) \times [1 + (k \times DMIMBW_{t,s})] \end{cases}$$

$$\begin{aligned}
 TTDP_{NDF,t,s} &= \sum_{f=k}^l TTDC_{NDF,f,t,s} \times NDF_{f,t,s}, \\
 TTDF_{NDF,t,s} &= \frac{TTDP_{NDF,t,s}}{100} \times DMI_{t,s},
 \end{aligned}
 \tag{8}$$

where  $a$  through  $q$  were derived during fitting,  $DietNDF_{t,s}$  is dietary NDF percent (% of DM), and feeds were classified by forage as legumes (those reported as legume or mostly legume forage), corn silage (feeds reported to be corn silage of any maturity or variety), grasses, other wet forage, and other dry forages. Unique digestion coefficients for high-fiber byproduct feeds were also fit [corn gluten feeds (*Gluten Feed*), distillers grains (*Distillers*), soy hulls (*Soyhulls*), wheat middlings (*WheatMidds*), beet pulp (*BeetPulp*)]. Equation [8] was derived in a stepwise manner with terms for ADF, lignin, NDF, CP, DM, ash, DMIMBW, and starch for each feed type included in the initial equations. Dietary CP, FA, and starch were also tested.

The analogous NLS equations are presented in Supplemental File S2 (<https://doi.org/10.3168/jds.2015-10800>). The best NLS model, as defined by numerical

improvement in RMSPE, mean and slope bias, and CCC from cross-validation was

$$\begin{aligned}
 TTDC_{NDF,f,t,s} &= \begin{cases} \text{if Forage} = \text{"Legume"} \text{ then :} \\ \left( a \times \frac{ADF}{NDF} \right) \\ \times \left( 1 - (b + c \times DietStarch_{t,s}) \times \frac{DMI_{t,s}}{MBW_{t,s}} \right) \\ \text{if Forage} = \text{"CornSilage"} \text{ then :} \\ \left( d \times \frac{ADF}{NDF} \right) \\ \times \left( 1 - (b + c \times DietStarch_{t,s}) \times \frac{DMI_{t,s}}{MBW_{t,s}} \right) \\ \text{if Forage} = \text{"OtherForage"} \text{ then :} \\ (e + f \times DietNDF) \\ \times \left( 1 - (b + c \times DietStarch_{t,s}) \times \frac{DMI_{t,s}}{MBW_{t,s}} \right) \\ \text{else :} \\ (g) \times \left( 1 - (h + c \times DietStarch_{t,s}) \times \frac{DMI_{t,s}}{MBW_{t,s}} \right) \end{cases} \\
 TTDP_{NDF,t,s} &= \sum_{f=k}^l TTDC_{NDF,f,t,s} \times NDF_{f,t,s}, \\
 TTDF_{NDF,t,s} &= \frac{TTDP_{NDF,t,s}}{100} \times DMI_{t,s},
 \end{aligned} \tag{9}$$

where *a* through *h* were derived during fitting, *ADF/NDF* is the ADF to NDF ratio in a feed (%/%), *DietStarch<sub>t,s</sub>* is the dietary starch concentration (% of DM), and *DietNDF<sub>t,s</sub>* is dietary NDF percent (% of DM).

**Digestible FA.** Within the NRC (2001) dairy model, true total-tract digested FA is predicted as

$$\begin{aligned}
 TTDC_{FA,f,t,s} &= DC_{FA,f}, \\
 TTDP_{FA,t,s} &= \sum_{f=k}^l \begin{cases} \text{if Category}_f = \text{"Fat"} \ \& \ \text{Class}_f = \text{"Fat"} \\ 1 + [(FA_{f,t,s} - 1) \times TTDC_{FA,f,t,s}] \\ \text{else, if Category}_f = \text{"Fat"} \ \& \ \text{Class}_f \neq \text{"Fat"} \\ FA_{f,t,s} \times TTDC_{FA,f,t,s} \\ \text{else,} \\ FA_{f,t,s} - 1 \end{cases} \\
 TTDF_{FA,t,s} &= \frac{TTDP_{FA,t,s}}{100} \times DMI_{t,s} \times Discount_{t,s}.
 \end{aligned} \tag{10}$$

Energy equation classes (*Class*) specified feeds as fat (e.g., lard, tallow, oil), fatty acid, forage, concentrate, and vitamin/mineral. Dietary FA digestibility coefficients (*DC<sub>Fat</sub>*, %) and dietary FA concentration (*FA<sub>f,t,s</sub>*; % of DM) of specific feeds were sourced from the NRC (2001) feed table. The apparent total-tract FA digestibility measurements collected from the literature were adjusted for endogenous FA production to yield estimates of true FA digestibility. Endogenous FA yield was estimated at 2.0 g/kg of DMI as described in Supplemental File S3 (<https://doi.org/10.3168/jds.2015-10800>).

Because the digestibility coefficients (DC) for fat are derived at the ingredient level, an attempt was made to bias adjust the derived values from Eq. [10] to yield estimates of digestibility that better aligned with the observed values:

$$\begin{aligned}
 TTDC_{FA,f,t,s} &= DC_{FA,f}, \\
 TTDP_{FA,t,s} &= \sum_{f=k}^l \begin{cases} \text{if Category}_f = \text{"Fat"} \ \& \ \text{Class}_f = \text{"Fat"} \\ a \times \left\{ 1 + [(FA_{f,t,s} - 1) \times TTDC_{FA,f,t,s}] \right\} \\ \text{else, if Category}_f = \text{"Fat"} \\ \ \& \ \text{Class}_f \neq \text{"Fat"} \\ b \times FA_{f,t,s} \times TTDC_{FA,f,t,s} \\ \text{else,} \\ c \times (FA_{f,t,s} - 1) \end{cases} \\
 TTDF_{FA,t,s} &= \frac{TTDP_{FA,t,s}}{100} \times DMI_{t,s} \times \left( 1 - d \times DMIMBW_{t,s} \right),
 \end{aligned} \tag{11}$$

where *a*, *b*, *c*, and *d* were estimated during fitting and *DC<sub>fat,f</sub>* was a digestion coefficient sourced from the NRC (2001) feed library. Fit statistics of the resulting predictions of total-tract FA digestibility were compared with fit statistics from digestibility predicted by the original model. A series of additional methods of calculating FA digestibility were compiled based on residuals of the NRC (2001) *TTDF<sub>FA,f,t,s</sub>* prediction:

$$\begin{aligned}
 TTDC_{FA,f,t,s} &= a, \\
 TTDP_{FA,t,s} &= \sum_{f=k}^l TTDC_{FA,f,t,s} \times FA_{f,t,s}, \\
 TTDF_{FA,t,s} &= \frac{TTDP_{FA,t,s}}{100} \times DMI_{t,s} \times \left( 1 - b \times DMIMBW_{t,s} \right),
 \end{aligned} \tag{12}$$

where  $a$  and  $b$  were estimated during fitting.

An additional equation was derived that considered interactions with other chemical components of the diet:

$$\begin{aligned}
 TTDC_{FA,f,t,s} &= a + b \times FA_{f,t,s} + c \times Lignin_{t,s} + d \times CP_{f,t,s}, \\
 TTDP_{FA,t,s} &= \sum_{f=k}^l TTDC_{FA,f,t,s} \times FA_{f,t,s}, \\
 TTDF_{FA,t,s} &= \frac{TTDP_{FA,t,s}}{100} \times DMI_{t,s} \times (1 - e \times DMIMBW_{t,s}),
 \end{aligned}
 \tag{13}$$

where  $a$  through  $e$  were estimated during model derivation. Although additional explanatory variables were tested (DM, CP, NDF, ADF, ash), FA digestibility was best associated with lignin, ADF, CP, and FA percentage and DMI. To better account for the effect of different fat sources on FA digestibility, a feed-type-specific equation was also derived:

$$TTDC_{FA,f,t,s} = \begin{cases} \text{if Fat Category}_f = \text{"Animal Fat" or} \\ \text{"Hydrogenated Tallow"} \\ (a + b \times DietFA) \times (1 - c \times DMIMBW_{t,s}) \\ \text{else, if Fat Category}_f = \text{"Vegetable Oil"} \\ (1 - c \times DMIMBW_{t,s}) \\ \text{else, if Fat Category}_f = \text{"Other Fat"} \\ (d + b \times DietFA) \times (1 - c \times DMIMBW_{t,s}) \\ \text{else, if Feed Type}_f = \text{"Forage"} \\ (e + f \times DietFA) \times (1 - g \times DMIMBW_{t,s}) \\ \text{else, if Feed Type}_f = \text{"Grain"} \\ (h + f \times DietFA) \times (1 - g \times DMIMBW_{t,s}) \\ \text{else, if Feed Type}_f = \text{"Byproduct"} \\ (i + f \times DietFA) \times (1 - g \times DMIMBW_{t,s}) \\ \text{else,} \\ (f \times DietFA) \times (1 - g \times DMIMBW_{t,s}) \end{cases}$$

$$\begin{aligned}
 TTDP_{FA,t,s} &= \sum_{f=k}^l TTDC_{FA,f,t,s} \times FA_{f,t,s}, \\
 TTDF_{FA,t,s} &= \frac{TTDP_{FA,t,s}}{100} \times DMI_{t,s},
 \end{aligned}
 \tag{14}$$

where  $a$  through  $g$  were estimated during model derivation. In a deviation from the NRC (2001) approach, supplemental fat sources were split into categories that seemed to better reflect natural variation among sources as supported by analyses of residuals. These included animal fat, hydrogenated tallow, vegetable oil, and other fat supplements. Fatty acid digestibility in the basal diet was predicted as a function of CP and FA percentage and total dietary FA percentage ( $DietFA_{t,s}$ ).

The analogous NLS equations are presented in Supplemental File S2 (<https://doi.org/10.3168/jds.2015-10800>). The best NLS model was

$$TTDC_{FA,f,t,s} = \begin{cases} \text{if Fat Category}_f = \text{"Animal Fat" or} \\ \text{"Hydrogenated Tallow"} \\ (a) \times \left(1 - b \times \frac{DMI_{t,s}}{MBW_{t,s}}\right) \\ \text{else, if Fat Category}_f = \text{"Vegetable Oil"} \\ (c) \times \left(1 - b \times \frac{DMI_{t,s}}{MBW_{t,s}}\right) \\ \text{else, if Fat Category}_f = \text{"Other Fat"} \\ (d) \times \left(1 - b \times \frac{DMI_{t,s}}{MBW_{t,s}}\right) \\ \text{else,} \\ (e \times DM_{f,t,s} + f \times CP_{f,t,s} + g \times FA_{t,s} \\ + h \times DietFA_{t,s}) \end{cases}$$

$$\begin{aligned}
 TTDP_{FA,t,s} &= \sum_{f=k}^l TTDC_{FA,f,t,s} \times FA_{f,t,s}, \\
 TTDF_{FA,t,s} &= \frac{TTDP_{FA,t,s}}{100} \times DMI_{t,s},
 \end{aligned}
 \tag{15}$$

where  $a$  through  $h$  were derived during model fitting.

**Digestible CP.** True total-tract CP digestibility ( $TTDC_{CP,f,t,s}$ , % of DM) was used in TDN predictions in the NRC (2001). True CP digestibility was calculated from apparent CP digestibility reported in the studies assuming endogenous CP flow was 3% of DMI (Swanson, 1982). The NRC (2001) equation for predicting CP digestion is

$$TTDP_{CP,t,s} = \begin{cases} \text{if } CP_{f,t,s} > 0 \text{ \& } Class_f = \text{"Wet" or "Dry"} \\ \quad e^{-1.2 \times \frac{ADFIP_f}{CP_{f,t,s}}} \times CP_{f,t,s} \\ \text{else, if } CP_{f,t,s} > 0 \text{ \& } Class_f = \text{"Animal"} \\ \quad 1.0 \times CP_{f,t,s} \\ \text{else,} \\ \quad \left[ 1 - \left( 0.40 \times \frac{ADFIP_f}{CP_{f,t,s}} \right) \right] \times CP_{f,t,s} \end{cases}$$

$$TTDF_{CP,t,s} = \frac{TTDP_{CP,t,s}}{100} \times DMI_{t,s} \times Discount_{t,s}, \quad [16]$$

where acid detergent insoluble protein (**ADFIP**; % of DM), CP (% of DM), and feed class were from the NRC (2001) feed tables. New parameter estimates for Eq. [16] were fit to the available data and a new discount was derived, assuming any digestibility depression was proportional to DMIMBW:

$$TTDP_{CP,t,s} = \sum_{f=k}^l \begin{cases} \text{if } CP_{f,t,s} > 0 \text{ \& } Class_f = \text{"Wet" or "Dry"} \\ \quad \left( a \times \frac{ADFIP_f}{CP_{f,t,s}} \right) \times CP_{f,t,s} \\ \text{else, if } CP_{f,t,s} > 0 \text{ \& } Class_f = \text{"Animal"} \\ \quad b \times CP_{f,t,s} \\ \text{else,} \\ \quad \left[ 1 - \left( c \times \frac{ADFIP_f}{CP_{f,t,s}} \right) \right] \times CP_{f,t,s} \end{cases}$$

$$TTDF_{CP,t,s} = \frac{TTDP_{CP,t,s}}{100} \times DMI_{t,s} \times (1 + d \times DMIMBW_{t,s}), \quad [17]$$

where *a* through *d* were fit during model derivation.

True total-tract CP digestibility was also derived using a series of additional CP models including a simple common digestibility coefficient (Eq. [18]).

$$TTDC_{CP,f,t,s} = a,$$

$$TTDP_{CP,t,s} = \sum_{f=k}^l TTDC_{CP,f,t,s} \times CP_{f,t,s},$$

$$TTDF_{CP,t,s} = \frac{TTDP_{CP,t,s}}{100} \times DMI_{t,s} \times (1 + b \times DMIMBW_{t,s}), \quad [18]$$

where *a* and *b* were fit during model derivation.

An equation was also derived through stepwise regression and the final model included ADF (% of DM), ADFIP (% of DM), and NDF (% of DM) effects on CP digestibility:

$$TTDC_{CP,f,t,s} = a + b \times ADF_{f,t,s} + c \times ADFIP_f + d \times NDFIP_f,$$

$$TTDP_{CP,t,s} = \sum_{f=k}^l TTDC_{CP,f,t,s} \times CP_{f,t,s},$$

$$TTDF_{CP,t,s} = \frac{TTDP_{CP,t,s}}{100} \times DMI_{t,s}, \quad [19]$$

where *a* through *d* were estimated during model fitting.

An additional feed-type-specific equation was derived in a stepwise manner that included ADF, ADFIP (% of DM), NDFIP (% of DM), and DMIMBW (kg/kg) as explanatory variables for each feed type:

$$TTDC_{CP,f,t,s} = \begin{cases} \text{if } ForageType_f \neq \text{"Concentrate"} \\ \quad (a + b \times ADFIP_{f,t,s} + c \times CP_{f,t,s}) \\ \quad \times (1 + d \times DMIMBW_{t,s}) \\ \text{else, if } Class_f = \text{"Animal"} \\ \quad (e) \\ \text{else, if } Class_f = \text{"Plant"} \\ \quad (f + g \times ADF_{f,t,s}) \\ \text{else,} \\ \quad (h + i \times NDFIP_{f,t,s} + j \times CP_{f,t,s}) \\ \quad \times (1 + k \times DMIMBW_{t,s}) \end{cases}$$

$$TTDP_{CP,t,s} = \sum_{f=k}^l TTDC_{CP,f,t,s} \times CP_{f,t,s},$$

$$TTDF_{CP,f,t,s} = \frac{TTDP_{CP,t,s}}{100} \times DMI_{t,s}. \quad [20]$$

The analogous NLS equations are presented in Supplemental File S2 (<https://doi.org/10.3168/jds.2015-10800>). The best NLS model was

$$\begin{aligned}
 TTDC_{CP,f,t,s} &= \begin{cases} \text{if } ForageType_f \neq \text{"Concentrate"} \\ (a + b \times ADF_{f,t,s} + c \times CP_{f,t,s} + d \times DietCP_{t,s}) \\ \text{else, if } Class_f = \text{"Animal"} \\ (e) \\ \text{else, if } Class_f = \text{"Plant"} \\ (f + g \times ADF_{f,t,s} + h \times ADFIP_{f,t,s} \\ + i \times NDFIP_{f,t,s}) \times \left(1 - j \times \frac{DMI_{t,s}}{MBW_{t,s}}\right) \\ \text{else,} \\ (k + l \times DietCP_{t,s}) \end{cases} \\
 TTDP_{CP,t,s} &= \sum_{f=k}^l TTDC_{CP,f,t,s} \times CP_{f,t,s}, \\
 TTDF_{CP,f,t,s} &= \frac{TTDP_{CP,t,s}}{100} \times DMI_{t,s},
 \end{aligned} \tag{21}$$

where *a* through *l* were estimated during model fitting and *DietCP* was dietary CP percentage (% of DM).

**Digestible NFC.** The NRC (2001) approach assumed NFC, as calculated by difference, was 98% digestible and was discounted with increasing DMI. The data collected in this study had no direct reports of NFC digestibility to evaluate this estimate against; however, several studies reported starch digestibility. Starch (St) digestibility was predicted assuming a constant digestion coefficient (Eq. [22]). The digestibility discount with increasing DMI also dropped from the starch function:

$$\begin{aligned}
 TTDC_{St,f,t,s} &= a, \\
 TTDP_{St,t,s} &= \sum_{f=k}^l TTDC_{St,f,t,s} \times Starch_{f,t,s}, \\
 TTDF_{St,t,s} &= \frac{TTDP_{St,t,s}}{100} \times DMI_{t,s},
 \end{aligned} \tag{22}$$

where *a* was fit during the model derivation process.

A more complicated equation was derived using stepwise regression:

$$\begin{aligned}
 TTDC_{St,f,t,s} &= a + b \times Ash_f + c \times Starch_{f,t,s}, \\
 TTDP_{St,t,s} &= \sum_{f=k}^l TTDC_{St,f,t,s} \times Starch_{f,t,s}, \\
 TTDF_{St,t,s} &= \frac{TTDP_{St,t,s}}{100} \times DMI_{t,s} \times (1 + d \times DMIMBW_{t,s}),
 \end{aligned} \tag{23}$$

where *a* through *e* were fit during model derivation.

Unique digestibility coefficients for different grain sources, forage and other feeds could also be identified:

$$\begin{aligned}
 TTDC_{St,f,t,s} &= \begin{cases} \text{if } Feed = \text{"Dry Ground Corn"} \text{ then :} \\ a \\ \text{else, if } Feed = \text{"Steam Flaked Corn"} \text{ then :} \\ b \\ \text{else, if } Feed = \text{"High Moisture Corn"} \text{ then :} \\ c \\ \text{else, if } Feed = \text{"Barley"} \text{ then :} \\ d \\ \text{else, if } Feed = \text{"Other Gain"} \text{ then :} \\ e \\ \text{else, if } Feed \text{ Type} = \text{"Forage"} \text{ then :} \\ f + g \times DM_{f,t,s} \\ \text{else,} \\ h \end{cases} \\
 TTDP_{St,t,s} &= \sum_{f=k}^l TTDC_{St,f,t,s} \times Starch_{f,t,s}, \\
 TTDF_{St,t,s} &= \frac{TTDP_{St,t,s}}{100} \times DMI_{t,s},
 \end{aligned} \tag{24}$$

where *a* through *h* were fit during model derivation.

The ideal NLS starch digestibility function was very similar:

$$\begin{aligned}
 TTDC_{St,f,t,s} &= \begin{cases} \text{if } Feed = \text{"Dry Ground Corn"} \text{ then :} \\ a \\ \text{else, if } Feed = \text{"Steam Flaked Corn"} \text{ then :} \\ b \\ \text{else, if } Feed = \text{"High Moisture Corn"} \text{ then :} \\ c \\ \text{else, if } Feed = \text{"Barley"} \text{ then :} \\ d \\ \text{else, if } Feed = \text{"Other Gain"} \text{ then :} \\ e \\ \text{else, if } Feed \text{ Type} = \text{"Forage"} \text{ then :} \\ f + g \times ADF_{f,t,s} + h \times NDF_{f,t,s} \\ \text{else,} \\ i \end{cases} \\
 TTDP_{St,t,s} &= \sum_{f=k}^l TTDC_{St,f,t,s} \times Starch_{f,t,s}, \\
 TTDF_{St,t,s} &= \frac{TTDP_{St,t,s}}{100} \times DMI_{t,s},
 \end{aligned} \tag{25}$$

where *a* through *i* were fit during model derivation.

Because total-tract digested NFC could not be reliably estimated, the NRC (2001) assumption of 98% digestibility was applied to all residual OM (**rOM**). A weighted average of this digestible and  $TTDP_{St,t,s}$  was used to calculate total-tract NFC digestibility for use in downstream calculations of microbial N and milk yield.

**Calculation of TDN.** To evaluate the practicality of the functions selected for TDN calculation, the equations were used to predict TDN for a series of scenarios differing in DMI level, fat type, forage type, and protein supplement type. The contributions of digested CP, NDF, starch, rOM, and FA to TDN were evaluated in addition to the dietary TDN.

## RESULTS AND DISCUSSION

### Digestible NDF

Total-tract digested NDF (kg/d) was compared with measurements from the 337 treatments in the data set reporting digested NDF (Table 3). The NRC (2001) under-predicted NDF digested by 0.56 kg (16% of mean observed NDF digested); this mean bias represented 24% of MSPE. The slope bias was minor (1.8% of MSPE). The RMSPE was high (39% of mean observed digested NDF), suggesting that alternative equations likely exist that could account for more of the variation. Digested nutrient composition is an important component of predicting energy supplied by the diet (NRC, 2001), and NDF digestibility is negatively correlated with feeding level, affects rumen health, and alters energy partitioning toward milk production (Chalupa et al., 1986; Weiss, 1998; Oba and Allen, 1999). Thus, an accurate calculation of NDF digestibility is an important component in the NRC (2001) model and dairy cattle feeding.

Re-derivation of the base digestibility coefficient in the existing NRC (2001) equation (Eq. [5]; Table 3) returned an RMSE of 20% and CCC of 0.79; mean and slope bias were minimal ( $\geq 1\%$  MSE). The parsimonious approach (Eq. [6]; Table 3) reduced RMSE (to 18%), and mean and slope biases were, again,  $\leq 1\%$  MSE. Both the CCC (0.82) and the AICc (929) were marginally improved compared with the re-derived NRC (2001) equation. Conceptually, NDF digestibility should be related to the proportion of indigestible material within NDF because indigestible lignin-hemicellulose complexes tie up digestible hemicellulose and cellulose in close proximity (Van Soest, 1994). Including NDFIP was originally done to correct the equation proposed by Conrad et al. (1984) for the proportion of NDF that is not cellulose, hemicellulose, or lignin (Weiss et al., 1992). The Conrad et al. (1984) model was driven by the concept that NDF digestibility is proportional

to the percentage of the surface area of feed particles that is not lignin. However, AICc supports the use of a simple average compared with the NRC (2001) equation form (Table 3).

Equation [7] was constructed as a more flexible, empirical representation of NDF digestibility. All parameter estimates were significant (Table 3), but the RMSE and CCC were only slightly improved to 17% and 0.84. Mean and slope biases were still negligible ( $\leq 1\%$  MSE). Comparison based on AICc supported the use of Eq. [7] over Eq. [6] or [5] as the best NLME equation tested. The digested NDF equation was able to detect significant relationships with feed ADF (Table 3; Eq. [7], *d*), CP (Table 3; Eq. [7], *e*), NDFIP (Table 3; Eq. [7], *b*) and lignin (Table 3; Eq. [7], *c*), and was discounted at a dietary level by DMIMBW (Table 3; Eq. [7], *f*) and dietary starch concentration (Table 3; Eq. [7], *g*). The discount based on DMIMBW and starch suggests an interaction between starch and DMI that results in a curvilinear reduction in NDF digestibility with increasing starch intake; however, correlations in the explanatory variables make this equation difficult to interpret definitively. Although the equation is a very different form from the NRC (2001), it importantly retains the ability to explain relationships among ADF, lignin, and NDF digestibility (Jung et al., 1997; Traxler et al., 1998) with the added benefit of considering starch feeding level.

The interactions between dietary starch percentage and DMI with respect to discounting NDF warrant further investigation. Decades of work studying associative effects suggest that starch percent should be antagonistic to NDF digestibility (Ferraretto et al., 2013). Increasing starch percent decreases DMI when fill is not restricting (Allen and Bradford, 2012). As such, the starch interaction with intake may be compensating for this relationship (i.e., the reduction in DMI causes a slight increase in digestibility, whereas the increase in starch causes a reduction). The covariation among these parameters makes individual interpretation difficult and future experimentation focused specifically on starch/intake interactions will be required to properly parameterize models describing this response surface.

Residuals analysis indicated that additional progress could be made in predicting NDF digestibility by fitting the regression coefficients of Eq. [7] within feed type. This was done using NLME in Eq. [8] and using NLS in Eq. [9]. Because of the differing fitting methods, it is difficult to objectively compare Eq. [7], [8], and [9] using any metrics except those derived through cross-validation. Minimal difference in fit was observed between Eq. [7] and [8], suggesting that the addition of so many parameters in Eq. [8] was not justified by a corresponding improvement in fit.

**NDF Digestibility Cross-Validation and Model Selection**

The results of cross-validation are presented in Table 3. In general, the fits of newly derived equations against independent data sets were very precise. Although Eq. [5] had higher CCC than the other NLME equations, it also had a slight slope bias, whereas the other NLME equations (Eq. [6] and Eq. [7]) showed negligible slope bias (3.5 vs.  $\leq 1.0$ ). Considering the margin of error around the fit statistics, Eq. [9] performed substantially better than all NLME models and thus was used for

downstream calculation of TDN. As described in the Comparison of Fixed- and Mixed-Effects Models section, this presents some practical concerns about external application of these equations.

The equations derived here demonstrate that future NDF digestibility predictions should continue to account for feed chemical factors related to digestibility. The newly derived alternative equations had improved fit compared with the re-derived NRC (2001) equation. However, some important physiological relationships could not be represented with the available data set. As such, future efforts to quantify NDF digestibility should

**Table 3.** Parameter estimates and overall model fitness for NRC (2001) and selected new equations for predicting NDF digested (n = 337)

Item <sup>1</sup>	NRC	Eq. [5]	Eq. [6]	Eq. [7]	Eq. [8]	Eq. [9]
Parameter <sup>2</sup>						
<i>a</i>		1.34 (<0.001)	0.624 (<0.001)	0.295 (0.017)	1.96 (<0.001)	1.07 (<0.001)
<i>b</i>		2.26 (<0.001)	-4.15 (<0.001)	-0.0400 (0.002)	-4.45 (0.012)	2.02 (<0.001)
<i>c</i>			0.0173 (<0.001)	-0.0237 (0.007)	-2.82 (<0.001)	-5.74 × 10 <sup>-4</sup> (0.025)
<i>d</i>				0.00569 (0.055)	1.62 (<0.001)	1.05 (<0.001)
<i>e</i>				0.0208 (<0.001)	-6.05 (0.079)	0.400 (0.009)
<i>f</i>				4.53 (<0.001)	1.70 (<0.001)	0.0115 (<0.001)
<i>g</i>				2.16 (<0.001)	-0.0182 (0.004)	1.06 (<0.001)
<i>h</i>					0.908 (<0.001)	0.0390 (<0.001)
<i>i</i>					0.936 (<0.001)	
<i>j</i>					1.65 (0.024)	
<i>k</i>					0.764 (0.034)	
<i>l</i>					0.850 (<0.001)	
<i>m</i>					-2.90 (0.029)	
<i>n</i>					2.25 (0.002)	
<i>o</i>					-4.27 (<0.001)	
<i>p</i>					4.36 (0.001)	
<i>q</i>					-0.103 (0.001)	
<i>r</i>					-5.90 (<0.001)	
Fitting method <sup>3</sup>		ME	ME	ME	ME	FE
Mean random effect		0.094	-4.8 × 10 <sup>-8</sup>	-0.0039	-0.0087	NA <sup>4</sup>
Observed mean, kg/d	3.45	3.45	3.45	3.45	3.45	3.45
Predicted mean, kg/d	2.89	3.39	3.42	3.42	3.43	3.45
RMSE or RMSPE, % of mean	39	20	18	17	16	23
Mean bias, % of MSE or MSPE	24	<1.0	<1.0	<1.0	<1.0	<1.0
Slope bias, % of MSE or MSPE	1.8	1.0	<1.0	<1.0	<1.0	<1.0
RMSPE/SD or RMSE/SD	1.01	0.61	0.54	0.52	0.50	0.70
CCC	0.35	0.79	0.82	0.84	0.85	0.65
AICc		988	929	910	910	824
σ <sub>s</sub>		1.14	1.08	1.04	1.01	
σ <sub>e</sub>		0.77	0.70	0.67	0.64	
Unadjusted RMSE		29	27	28	29	
Unadjusted CCC		0.44	0.40	0.36	0.31	
Monte Carlo cross-validation <sup>5</sup>						
RMSE, % of mean		29 ± 1.2	29 ± 1.6	29 ± 1.3	31 ± 1.9	25 ± 1.2
Mean bias, % of MSE		<1.0 ± 0.3	<1.0 ± 0.2	<1.0 ± 0.4	<1.0 ± 1.0	1.1 ± 1.7
Slope bias, % of MSE		3.5 ± 1.0	<1.0 ± 0.3	<1.0 ± 0.7	4.3 ± 4.2	2.6 ± 2.6
CCC		0.43 ± 0.04	0.31 ± 0.08	0.30 ± 0.08	0.22 ± 0.11	0.60 ± 0.03

<sup>1</sup>Model evaluation criteria included root mean squared prediction error as a percent of observed mean (RMSPE), mean and slope bias as a percent of mean squared prediction error (MSPE), RMSPE as a fraction of observed standard deviation (RMSPE/SD), and concordance correlation coefficient (CCC) for the NRC (2001). Evaluation criteria for derived equations included root mean squared prediction error (RMSE), mean and slope bias as a percent of mean squared error (MSE), RMSE as a fraction of observed standard deviation (RMSE/SD), CCC, corrected Akaike information criterion (AICc), variance from study (σ<sub>s</sub>) and residual error (σ<sub>e</sub>), and RMSE and CCC unadjusted for study effects.

<sup>2</sup>Parameter names are as referenced in each equation, and parameter estimates are presented with significance values in parentheses.

<sup>3</sup>Fitting method indicates whether models were fit with mixed effect regression (ME) or nonlinear least squares (FE).

<sup>4</sup>NA = not applicable.

<sup>5</sup>Cross-validation (±SD of the output variable) was performed using 500 iterations of a repeated random sampling approach, in which 60% of the data was used for derivation and 40% used as an independent evaluation.

focus on improved representation of the relationships between forage type, DMI, ruminal passage rate (Kp), and potentially digestible fiber (Oba and Allen, 1999; Mertens, 2005); moreover, more thoroughly accounting for negative associative effects on NDF digestibility (Laplace et al., 1989; Sarwar et al., 1991; Niderkorn and Baumont, 2009) might greatly enhance model capacity.

### Digestible FA

Predicted FA digestibility in the NRC (2001) model is a function of 3 feed-type-specific digestion coefficients. Calculating FA digestibility in that manner results in a RMSPE of 36% with mean (70% of MSPE) and slope (7.6% of MSPE) biases (Table 4). On average, FA digested was overestimated by 202 g/d (26.0% of mean digested FA reported). This is a considerable overestimation that would contribute to energy-allowable milk prediction errors.

Re-deriving parameters within the existing system (Table 4; Eq. [11]) and incorporating a new, nutrient-specific digestibility returned low mean (1.3% of MSE) and slope (2.8% of MSE) biases, RMSE (22%), and moderate CCC (0.76; Table 4). In comparison to the re-derived NRC (2001) equation, a simple average digestibility had marginally increased RMSE (23%), mean (1.5% of MSE), and slope (3.8% of MSE) bias and reduced CCC (0.74); however, comparison based on AICc supported use of Eq. [12] over Eq. [11]. Intercept FA digestibility was 106% (Eq. [12], *a*), and digestibility decreased sharply with increasing DMIMBW (Eq. [12], *b*). At the mean DMI in the data set, FA digestibility was predicted to be 69% by Eq. [12].

Previous work has demonstrated that FA digestibility differs by fat type (Jenkins and Palmquist, 1984; Doreau and Ferlay, 1994; Schmidely et al., 2008). In a stepwise regression against available chemical composition data, FA digestibility was found to be affected by dietary concentrations of FA (% of DM), lignin (% of DM), and CP (% of DM). An additional discount for DMIMBW was also significant. These relationships between FA digestibility and feed chemical composition returned negligible mean and slope biases ( $\leq 1\%$  MSE; Table 4) from the prediction and improved RMSE to 19%. The CCC and AICc also supported use of Eq. [13] over Eq. [11] or [12].

Equations [14] and [15] were derived to better account for differences in digested FA across feed types. Equation [14] improved RMSE to 12% and the CCC to 0.94 (Table 4). Equation [15] also showed improvement with RMSPE of 10% and CCC of 0.95 (Table 4); however, direct comparison of Eq. [14] and [15] is difficult because they were derived with different fitting methods. As expected (Sackmann et al., 2003; Benchaar

et al., 2006; Reveneau et al., 2012), Eq. [14] and [15] estimated that vegetable oils and hydrogenated tallow would be more digestible than other fat types (e.g., fish oils).

### FA Digestibility Cross-Validation and Model Selection

The results of the cross-validation of FA digestibility are reported in Table 4. Fatty acid digestibility had the smallest available data set and, as a result, the fits obtained from cross-validation differed notably from those evaluated against the entire data set. Although Eq. [14] was an obvious choice among NLME models when evaluated against the full data set, it suffered during cross-validation with a mean RMSPE of 52% of the observed mean. The re-derived NRC (2001) equation also returned poor fit (RMSPE 84% of observed mean). Much like the NDF data, the NLS model (Eq. [15]) returned improved fit in cross-validation compared with the other model forms and therefore this model was used in downstream estimates of TDN. As described in the Comparison of Fixed- and Mixed-Effects Models section, this presents some practical concerns that should be considered if these models are used outside the derivation database.

Although the models here provide an opportunity to detect differences in FA digestion related to fat type, additional work is needed to define the digestibility of individual FA and the effect of FA profiles on total-tract digestion, energy availability, and milk FA profiles (Glasser et al., 2008a). Thorough meta-analysis of FA digestibility is warranted to better understand what components of forages and byproduct feeds co-vary with digestibility of FA, especially on 18C (Glasser et al., 2008b) and with increasing inclusion of fats that contain 18:0 (Boerman et al., 2015).

### Digestible CP

The NRC (2001) model predicts CP digestibility as a function of ADFIP and CP. Historical estimates of true CP digestibility range from 90 to 100% (Weiss et al., 1992). The mean true total-tract CP digestibility in this data set, after correction for endogenous N losses, was 86.4%. The NRC (2001) predicted CP digestibility with an RMSPE of 15% and a CCC of 0.79 but overestimated digestible CP flows by 31 g/d (7% of mean CP digested). This mean bias accounted for 18% of MSPE (Table 5). A slope bias (17% MSPE) was also apparent, indicating that the discount for ADFIP as a proportion of CP was insufficient to replicate the measured behavior of CP digestibility. Re-deriving coefficients for the current calculation scheme and adding a digest-

**Table 4.** Parameter estimates and overall model fitness for NRC (2001) and selected new equations for predicting fatty acid digested (n = 55)

Item <sup>1</sup>	NRC	Eq. [11]	Eq. [12]	Eq. [13]	Eq. [14]	Eq. [15]
Parameter <sup>2</sup>						
<i>a</i>		1.36 (0.011)	1.76 (<0.001)	3.45 (<0.001)	-0.426 (0.015)	1.36 (<0.001)
<i>b</i>		1.52 (0.095)	3.57 (<0.001)	-0.0305 (<0.001)	0.150 (<0.001)	4.26 (<0.001)
<i>c</i>		1.79 (<0.001)		-0.0498 (0.133)	6.60 (<0.001)	1.09 (0.002)
<i>d</i>		3.42 (<0.001)		-0.0577 (0.002)	7.71 (<0.001)	0.841 (0.111)
<i>e</i>				2.69 (<0.001)	2.05 (<0.001)	0.0111 (<0.001)
<i>f</i>					2.79 (<0.001)	-0.0177 (<0.001)
<i>g</i>					2.44 (0.003)	-0.0197 (<0.001)
<i>h</i>					6.40 (0.009)	0.104 (<0.001)
<i>i</i>					0.0443 (0.056)	
Fitting method <sup>3</sup>		ME	ME	ME	ME	FE
Mean random effect		0.0273	<0.0001	-0.0170	0.00888	
Observed mean, kg/d	776	776	779	779	776	776
Predicted mean, kg/d	978	732	730	743	750	776
RMSE or RMSPE, % of mean	36	22	23	19	12	10
Mean bias, % of MSE or MSPE	70	1.3	1.5	<1.0	<1.0	<1.0
Slope bias, % of MSE or MSPE	7.6	2.8	3.8	<1.0	<1.0	<1.0
RMSPE/SD or RMSE/SD	2.1	0.69	0.87	0.87	0.44	0.37
CCC	0.63	0.76	0.74	0.82	0.94	0.95
AICc		782	777	766	733	646
$\sigma_s$		355	330	300	255	
$\sigma_e$		188	195	159	100	
Unadjusted RMSE		33	34	31	55	
Unadjusted CCC		0.31	0.33	0.30	-0.61	
Monte Carlo cross-validation <sup>4</sup>						
RMSE, % of mean		84 ± 9	32 ± 6	34 ± 4	52 ± 6	11 ± 2.9
Mean bias, % of MSE		88 ± 2	6 ± 10	3 ± 5	4 ± 7	13 ± 10
Slope bias, % of MSE		1 ± 3	15 ± 10	14 ± 3	72 ± 16	12 ± 11
CCC		0.07 ± 0.03	0.33 ± 0.12	0.04 ± 0.14	0.04 ± 0.26	0.90 ± 0.06

<sup>1</sup>Model evaluation criteria included root mean squared prediction error as a percent of observed mean (RMSPE), mean and slope bias as a percent of mean squared prediction error (MSPE), RMSPE as a fraction of observed standard deviation (RMSPE/SD), and concordance correlation coefficient (CCC) for the NRC (2001). Evaluation criteria for derived equations included root mean squared prediction error (RMSE), mean and slope bias as a percent of mean squared error (MSE), RMSE as a fraction of observed standard deviation (RMSE/SD), CCC, corrected Akaike information criterion (AICc), variance from study ( $\sigma_s$ ) and residual error ( $\sigma_e$ ), and RMSE and CCC unadjusted for study effects.

<sup>2</sup>Parameter names are as referenced in each equation, and parameter estimates are presented with significance values in parentheses.

<sup>3</sup>Fitting method indicated whether models were fit with mixed effect regression (ME) or nonlinear least squares (FE).

<sup>4</sup>Cross-validation ( $\pm$ SD of the output variable) was performed using 500 iterations of a repeated random sampling approach, in which 60% of the data was used for derivation and 40% used as an independent evaluation.

ibility discount for feeding level returned an RMSE of 16% and a CCC of 0.74. Although the absolute fit was lower than expected, the equation had reduced mean (1.5% of MSE) and slope bias (7.7% of MSE; Table 5). Although the fit statistics for the reparametrized NRC (2001) equation suggest a good fit, a simple single coefficient equation (Eq. [18]) yielded an equally good fit. Thus, there were no clear advantages to the NRC (2001) equation structure.

Derivation of a digestibility coefficient dependent on interacting feed chemical components yielded significant parameter estimates for NDF, ADFIP, fat, and

lignin (Table 5; Eq. [19]). The slope bias was marginally reduced in Eq. [19] compared with the re-derived NRC (2001) equation (5.4 vs 7.7% of MSE); similarly, the RMSE and CCC improved only slightly (15 vs. 16% and 0.78 vs. 0.75; Table 5). Comparison based on AICc also favored Eq. [19] compared with Eq. [17]. Associative effects of different nutrients in dairy cattle diets have been well studied (Niderkorn and Baumont, 2009; Nousiainen et al., 2009), and protein digestibility, forage maturity, and ruminally available CP are correlated (Van Vuuren et al., 1991; Getachew et al., 2004). Equation [19] contained significant parameter estimates for

**Table 5.** Parameter estimates and overall model fitness for NRC (2001) and selected new equations for predicting total-tract CP digested ( $n = 399$ )

Item <sup>1</sup>	NRC	Eq. [17]	Eq. [18]	Eq. [19]	Eq. [20]	Eq. [21]
Parameter <sup>2</sup>						
<i>a</i>		-5.89 (<0.001)	1.80 (<0.001)	1.47 (<0.001)	3.57 (<0.001)	1.44 (<0.001)
<i>b</i>		1.67 (<0.001)	-3.15 (<0.001)	0.0251 (<0.001)	-0.241 (0.108)	0.0119 (<0.001)
<i>c</i>		-2.29 (0.258)		-0.256 (<0.001)	-2.06 (0.001)	-0.141 (<0.001)
<i>d</i>		-3.06 (<0.001)		0.0264 (0.046)	0.229 (0.028)	-0.0232 (<0.001)
<i>e</i>				-0.0745 (0.009)	0.354 (<0.001)	0.678 (<0.001)
<i>f</i>				-3.10 (<0.001)	0.0104 (0.025)	0.291 (<0.001)
<i>g</i>					4.49 (<0.001)	0.00627 (0.001)
<i>h</i>					-0.329 (<0.001)	-0.0603 (<0.001)
<i>i</i>					-4.19 (<0.001)	0.00630 (<0.001)
<i>j</i>					-0.0984 (<0.001)	7.26 (0.027)
<i>k</i>					-0.00486 (0.058)	0.520 (<0.001)
<i>l</i>						0.0825 (0.020)
Fitting method <sup>3</sup>		ME	ME	ME	ME	FE
Mean random effect		5.74	$10.0 \times 10^{-7}$	0.403	0.227	NA <sup>4</sup>
Observed mean, kg/d	456	456	456	456	456	456
Predicted mean, kg/d	487	447	449	450	453	456
RMSE or RMSPE, % of mean	15	16	16	15	12	10
Mean bias, % of MSE or MSPE	18	1.5	1.1	<1.0	<1.0	<1.0
Slope bias, % of MSE or MSPE	17	7.7	6.9	5.4	1.1	<1.0
RMSPE/SD or RMSE/SD	0.70	0.70	0.67	0.64	0.52	0.43
CCC	0.79	0.74	0.75	0.78	0.85	0.89
AICc		4,888	4,868	4,850	4,725	4,200
$\sigma_s$		108	166	113	166	
$\sigma_e$		84	81	78	63	
Unadjusted RMSE		21	22	23	24	
Unadjusted CCC		0.46	0.40	0.34	0.17	
Monte Carlo cross-validation <sup>5</sup>						
RMSPE, % of mean		23 ± 0.98	24 ± 1.0	25 ± 1.1	24 ± 1.5	11 ± 0.5
Mean bias, % of MSE		<1.0 ± 0.9	<1.0 ± 0.6	<1.0 ± 0.5	<1.0 ± 0.8	<1.0 ± 0.8
Slope bias, % of MSE		17 ± 2	11 ± 3	15 ± 4	18 ± 4	0.33 ± 0.4
CCC		0.37 ± 0.05	0.30 ± 0.06	0.24 ± 0.06	0.15 ± 0.10	0.89 ± 0.01

<sup>1</sup>Model evaluation criteria included root mean squared prediction error as a percent of observed mean (RMSPE), mean and slope bias as a percent of mean squared prediction error (MSPE), RMSPE as a fraction of observed standard deviation (RMSPE/SD), and concordance correlation coefficient (CCC) for the NRC (2001). Evaluation criteria for derived equations included root mean squared prediction error (RMSE), mean and slope bias as a percent of mean squared error (MSE), RMSE as a fraction of observed standard deviation (RMSE/SD), CCC, corrected Akaike information criterion (AICc), variance from study ( $\sigma_s$ ) and residual error ( $\sigma_e$ ), and RMSE and CCC unadjusted for study effects.

<sup>2</sup>Parameter names are as referenced in each equation, and parameter estimates are presented with significance values in parentheses.

<sup>3</sup>Fitting method indicated whether models were fit with mixed effect regression (ME) or nonlinear least squares (FE).

<sup>4</sup>NA = not applicable.

<sup>5</sup>Cross-validation ( $\pm$ SD of the output variable) was performed using 500 iterations of a repeated random sampling approach, in which 60% of the data was used for derivation and 40% used as an independent evaluation.

NDF (% of DM), FA (% DM), ADFIP (% of DM), and lignin (% of DM), suggesting it may have sufficient capacity to explain some of these associative effects.

The relationships among ADF, NDFIP, ADFIP, and CP digestibility differed by feed type (Table 5; Eq. [20] and [21]). Of the newly derived NLME equations, Eq. [20] returned the lowest RMSE (12%), highest CCC (0.85), and most favorable AICc (4,725; Table 5). However, comparison of AICc between Eq. [20] and [21] strongly favored the equation fit using NLS (Eq. [21]). In both Eq. [20] and [21], lack of significance eliminated NDF and lignin from the equation for forage  $TTDC'_{CP,f,t,s}$ , suggesting that relationships between forage quality and CP digestibility are better explained by ADFIP and CP than by lignin or NDF. Digestibility of animal protein feeds was much higher in Eq.

[21] than in Eq. [20] (68 vs. 23%) and, given the NRC (2001) estimate, this higher digestibility was expected. Because the DMIMBW coefficient dropped from most CP digestibility models in the stepwise regression procedure, discounting digestibility of CP based on intake appeared less important than discounting digestibility of other feed components and forages.

### CP Digestibility Cross-Validation and Model Selection

The results of the cross-validation of CP digestibility models are included in Table 5. In general, the fits of the CP digestibility equations were extremely precise (SD of RMSPE were <2%; Table 5). The re-derived NRC (2001) equation had the most accurate and pre-

cise fit among all NLME models in the cross-validation (Table 5); however, it also had a large slope bias (17% of MSPE). The simple average model (Eq. [16]) had similar fit to the re-derived NRC (2001) model but returned a lower (11% of MSPE) slope bias. However, much like the other response variables, the NLS equation fit substantially better during cross-validation than any NLME function (RMSPE 11%, slope bias <1% MSPE) and thus was used for downstream calculation of TDN.

### **Digestible Starch**

Starch digestibility was predicted with notable precision and accuracy (Table 6), perhaps reflecting the high extent of digestion and thus small errors of prediction. The average starch digestibility was 92.1%, and digestibility was affected by feed ash (Table 6; Eq. [23], *b*) and starch (Table 6; Eq. [23], *c*). Grain-specific differences in starch digestibility could also be identified (Eq. [24] and [25]). In the NLME model (Eq. [24]), barley and other small grains were predicted to have higher starch digestibility than corn. High-moisture corn had higher digestibility than ground or steam-flaked corn but lower digestibility than small grains. In the NLS model (Eq. [25]), corn grain and small grains had the highest predicted starch digestibility, followed by high-moisture corn, barley, and other non-grain starch sources. The differences in starch digestibility among model fitting approaches highlight some instability in these models which may impair application in an external context.

### **Starch Digestibility Cross-Validation and Model Selection**

The results of cross validating the starch digestibility equations are reported in Table 6. The simple average model of starch digestibility had the lowest RMSPE (24% of observed mean) and highest CCC (0.57) of any NLME model when evaluated using cross-validation. Although Eq. [24] had the most favorable RMSE, CCC, and AICc against the full data set, it returned the least favorable results in cross-validation. Much like the other nutrients, the NLS model (Eq. [25]) had the most favorable performance in cross-validation and therefore was used for downstream calculation.

Total-tract digestibilities of nonstarch NFC (rOM) were not reported in the studies used. An attempt to derive rOM digestibilities gave a value of 6.8% (data not shown). This value is too low for a fraction that contains what are considered to be the most digestible carbohydrates, despite inclusion of materials such as tannins that are indigestible. Explanations of the error include differing composition of NFC in feed and feces and that fecal CP is likely not 16% N (Van Soest,

1994). Accordingly, the NRC (2001) estimate of 98% digestibility for NFC was applied to rOM when calculating TDN.

### **Comparison of Fixed- and Mixed-Effect Models**

The RMSPE, mean and slope bias, and CCC from cross-validation are listed in the individual nutrient tables (Tables 3, 4, 5, and 6), and the RMSPE and CCC from cross validating the additional NLS models are included in Supplemental File S2 (tables; <https://doi.org/10.3168/jds.2015-10800>). When mixed-effect regression equations were evaluated in a cross-validation, CCC was poor (<0.50), and slope bias was generally increased in comparison to the fit against all data (Tables 3 through 6). In contrast, when equations of similar form were derived using NLS and evaluated in a cross-validation, this dramatic shift in fit statistics did not occur (see tables in Supplemental File S3).

Because the cross-validation repeatedly evaluated model performance against independent data, the NLME and NLS model-fitting approaches can be directly compared with these statistics. If NLME models were truly superior to the NLS models, this superiority should have been apparent in the cross-validation. The equations compared have different parameter estimates when a random study effect was included, so a direct comparison of the specific model pairings is imperfect. The differing significance of variables was expected because NLME models were designed to prevent falsely specifying slopes truly caused by variance attributable to study. However, if this misspecification of slopes occurred during fitting, one would expect that the equation would perform poorly when evaluated against independent data, which was not the case for the NLS models. Collectively, this comparison suggests that, in this study, the models derived in the absence of study effects have more accurate predictive power.

However, the superior performance of the NLS equations is somewhat problematic for the application of these equations outside their current context. The purpose of a mixed-effect model is to account for between-study differences that could falsely affect slopes, thus resulting in more robust models that can be applied across wider data sets. In this case, our NLME models worked well against the derivation data (as evidenced by low RMSPE and high CCC) but poorly in the cross-validation, suggesting that models derived using this approach did not perform well against independent data, on average. The NLS models that included no study effects did perform well in the cross-validation; however, these models have no statistical safeguards to prevent falsely partitioning slope that should be attributable to methodological or other study-related dif-

ferences into biologically relevant parameters. As such, application of these models outside their current context should be done with care and future work should focus on testing these models against broader data sets.

### Predicting TDN

The NLS models were used for TDN prediction. Model predictions of TDN were calculated using the equations identified in each above section and by assuming that rOM was 98% digestible. A series of scenarios were used to evaluate TDN predictions (Figure 1). Scenarios 1 through 4 represent the effects of increasing level of DMI. A linear regression of these TDN predictions suggests that each 1-kg change in DMI reduced TDN by 1.7 percentage units. This discount is much larger than the discount used in the NRC (2001). It is highly likely that the discount here represents an over-estimate of a true digestibility discount because the models used often had few other explanatory variables, meaning that some variance that should be at-

tributable to dietary chemical composition or that feed selection was likely partitioned into the intake effect. The model detected only slight differences in FA digestibility of tallow compared with oil (scenario 5 vs. 6; Figure 1), which reflected the differing digestibility of these feed types as predicted by the model. The model predicted that TDN should increase when grass forage is replaced with alfalfa (scenario 7 vs. 8; Figure 1). Additionally, predicted TDN decreased when fishmeal was substituted for soybean meal (scenario 9 vs. 10; Figure 1). Aside from the over-responsiveness to intake (1.7 percentage unit decrease in TDN per kg of DMI), the predicted TDN agreed well with responses that would be expected from different diet types.

### CONCLUSIONS

Mean and slope biases were evident in the NRC (2001) modeled estimates of nutrient digestibility. The relationships between feed chemical composition and NDF digestibility differed by feed class, and unique

**Table 6.** Parameter estimates and overall model fitness for selected new equations for predicting starch digested (n = 190)

Item <sup>1</sup>	Eq. [22]	Eq. [23]	Eq. [24]	Eq. [25]
Parameter <sup>2</sup>				
<i>a</i>	0.785 (<0.001)	1.40 (<0.001)	0.495 (<0.001)	0.926 (<0.001)
<i>b</i>		0.0930 (0.002)	0.447 (<0.001)	0.972 (<0.001)
<i>c</i>		-0.0128 (0.012)	0.571 (<0.001)	0.894 (<0.001)
<i>d</i>		1.92 (<0.001)	0.706 (<0.001)	0.853 (<0.001)
<i>e</i>			0.686 (<0.001)	0.988 (<0.001)
<i>f</i>			0.690 (<0.001)	0.894 (<0.001)
<i>g</i>			0.00960 (<0.001)	0.00869 (0.008)
<i>h</i>			0.757 (<0.001)	-0.00475 (<0.001)
<i>i</i>				0.905 (<0.001)
Fitting method <sup>3</sup>	ME	ME	ME	FE
Mean random effect	-1.3 × 10 <sup>-7</sup>	0.0049	4.9 × 10 <sup>-6</sup>	
Observed mean, g/d	5.8	5.8	5.8	6.78
Predicted mean, g/d	5.7	5.8	5.8	6.78
RMSE, % of mean	16	12.7	14	5.84
Mean bias, % of MSE	<1.0	<1.0	<1.0	<1.0
Slope bias, % of MSE	<1.0	<1.0	<1.0	<1.0
RMSE/SD	0.48	0.34	0.42	0.175
CCC	0.87	0.91	0.90	0.96
AICc	650	595	631	208.2
σ <sub>s</sub>	1.87	1.77	1.88	
σ <sub>e</sub>	1.06	0.86	0.93	
Unadjusted RMSE	23	30	28	
Unadjusted CCC	0.63	0.28	0.40	
Monte Carlo cross-validation <sup>4</sup>				
RMSPE, % of mean	24 ± 1.9	31 ± 2.6	29 ± 3.6	17 ± 1.8
Mean bias, % of MSE	6.8 ± 9.8	4.8 ± 6.5	4.9 ± 7.8	2.9 ± 3.1
Slope bias, % of MSE	11 ± 6.0	3.3 ± 4.3	3.7 ± 4.5	3.8 ± 3.6
CCC	0.57 ± 0.04	0.19 ± 0.10	0.38 ± 0.09	0.82 ± 0.03

<sup>1</sup>Evaluation criteria for derived equations included root mean squared prediction error (RMSE), mean and slope bias as a percent of mean squared error (MSE), RMSPE as a fraction of observed standard deviation (RMSE/SD), CCC, corrected Akaike information criterion (AICc), variance from study (σ<sub>s</sub>) and residual error (σ<sub>e</sub>), and RMSE and CCC unadjusted for study effects.

<sup>2</sup>Parameter names are as referenced in each equation, and parameter estimates are presented with significance values parenthetically.

<sup>3</sup>Fitting method indicated whether models were fit with mixed effect regression (ME) or nonlinear least squares (FE).

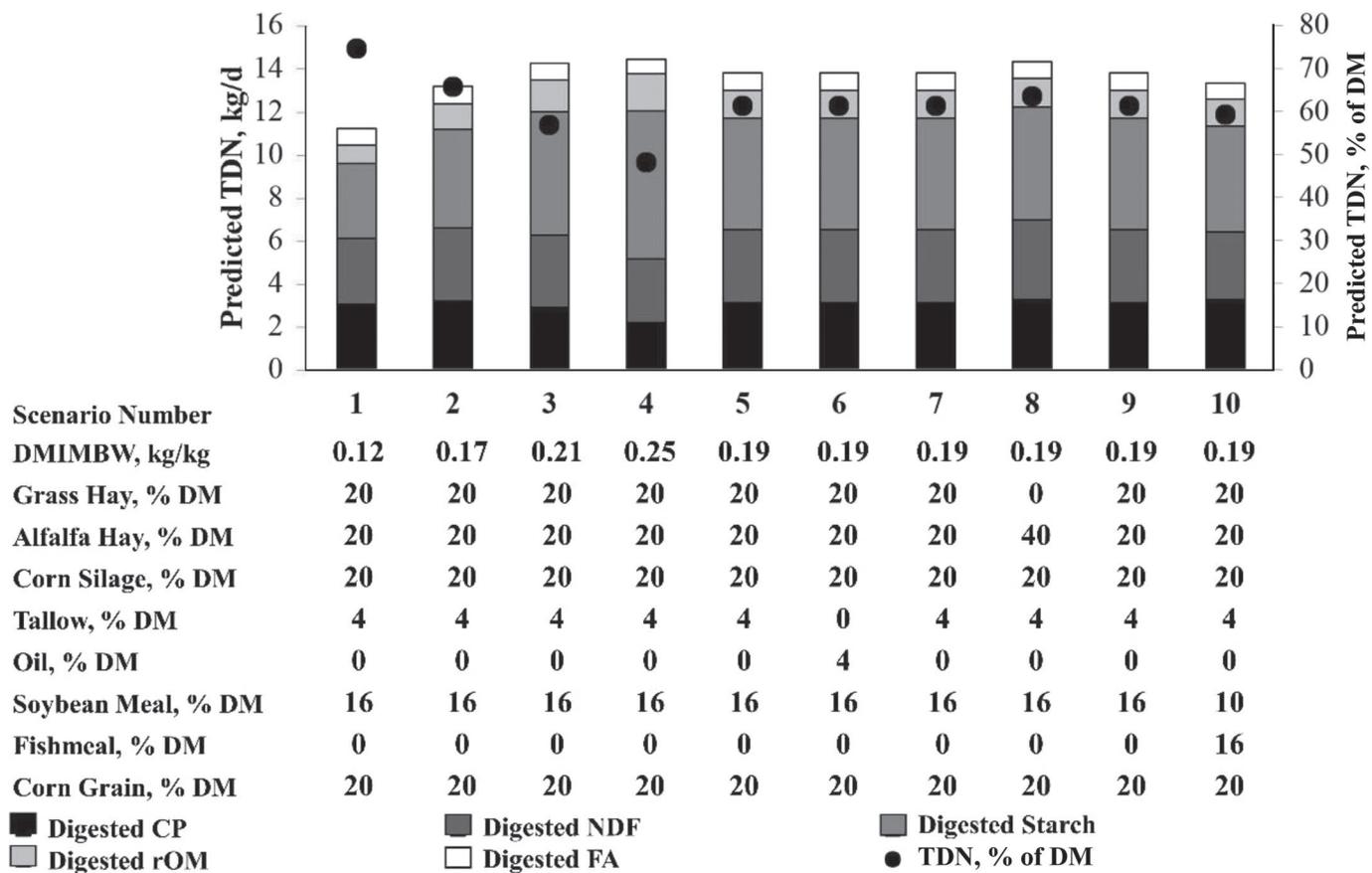
<sup>4</sup>Cross-validation (±SD of the output variable) was performed using 500 iterations of a repeated random sampling approach, in which 60% of the data was used for derivation and 40% used as an independent evaluation.

equations were identified for forage (legume, corn silage, and other forage) and non-forage NDF. Future work on NDF digestibility should focus on understanding how DMI, ruminal passage rates, dietary CP, and starch percentages affect NDF digestibility. Digestibility of FA differed by feed type. These feed-type differences likely are a result of differing FA profiles within feed types, and future work evaluating FA digestibility should focus on understanding how specific FA digestibilities are affected by dietary components. Digestibility of CP was also unique to different feed classes, including forages, animal proteins, plant proteins, and other feeds. NRC (2001) assumed a constant, diet-level TDN discount; however, we found that digestibility discounts were specific to nutrients and feed-types. Future work should more thoroughly investigate opportunities to account for the relationships among DMI and nutrient digestibilities. Finally, although it is recommended to use a random study effect when fitting models derived from literature data, cross-validation of models fit with and without study effects showed improved fit of models

derived with fixed-effects only. Although these models may have mis-specified slope estimates and should be applied externally with great care, it appeared that they predicted digestibility within this data set with greater precision and accuracy than those models derived with study effects.

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**Figure 1.** Predicted TDN (kg/d and % of DM) for 10 scenarios as estimated by the adjusted equations derived herein. Predicted nutrient [fatty acid (FA); residual OM (rOM); starch; NDF; CP) contributions to TDN (kg/d) are indicated by colored bar sections. Predicted TDN (% of DM) is mapped to the right y-axis and is represented by the black circles. Scenario details, including DMI per unit of metabolic BW (DMIMBW) within the range of intakes in the data set and feedstuff inclusion rates (% DM), are listed in tabular format under each bar.

## REFERENCES

- Allen, M. S., and B. J. Bradford. 2012. Control of food intake by metabolism of fuels: A comparison across species. *Proc. Nutr. Soc.* 71:401–409.
- Benchaar, C., H. Petit, R. Berthiaume, T. Whyte, and P. Chouinard. 2006. Effects of addition of essential oils and monensin premix on digestion, ruminal fermentation, milk production, and milk composition in dairy cows. *J. Dairy Sci.* 89:4352–4364.
- Bibby, J., and H. Toutenburg. 1978. Improved estimation and prediction. *Z. Angew. Math. Mech.* 58:45–49.
- Boerman, J. P., J. Firkins, N. St-Pierre, and A. Lock. 2015. Intestinal digestibility of long-chain fatty acids in lactating dairy cows: A meta-analysis and meta-regression. *J. Dairy Sci.* 98:8889–8903.
- Chalupa, W., B. Vecchiarelli, A. E. Elser, D. Kronfeld, D. Sklan, and D. L. Palmquist. 1986. Ruminal fermentation in vivo as influenced by long-chain fatty acids. *J. Dairy Sci.* 69:1293–1301.
- Conrad, H., W. Weiss, W. Odwongo, and W. Shockey. 1984. Estimating net energy lactation from components of cell solubles and cell walls. *J. Dairy Sci.* 67:427–436.
- Doreau, M., and A. Ferlay. 1994. Digestion and utilisation of fatty acids by ruminants. *Anim. Feed Sci. Technol.* 45:379–396.
- Ferraretto, L. F., P. Crump, and R. Shaver. 2013. Effect of cereal grain type and corn grain harvesting and processing methods on intake, digestion, and milk production by dairy cows through a meta-analysis. *J. Dairy Sci.* 96:533–550.
- Getachew, G., P. Robinson, E. DePeters, and S. Taylor. 2004. Relationships between chemical composition, dry matter degradation and in vitro gas production of several ruminant feeds. *Anim. Feed Sci. Technol.* 111:57–71.
- Glasser, F., A. Ferlay, M. Doreau, P. Schmidely, D. Sauvant, and Y. Chilliard. 2008a. Long-chain fatty acid metabolism in dairy cows: A meta-analysis of milk fatty acid yield in relation to duodenal flows and de novo synthesis. *J. Dairy Sci.* 91:2771–2785.
- Glasser, F., P. Schmidely, D. Sauvant, and M. Doreau. 2008b. Digestion of fatty acids in ruminants: A meta-analysis of flows and variation factors: 2. C18 fatty acids. *Animal* 2:691–704.
- Hanigan, M. D., J. Appuhamy, and P. Gregorini. 2013. Revised digestive parameter estimates for the Molly cow model. *J. Dairy Sci.* 96:3867–3885.
- Huhtanen, P., M. Rinne, and J. Nousiainen. 2009. A meta-analysis of feed digestion in dairy cows. 2. The effects of feeding level and diet composition on digestibility. *J. Dairy Sci.* 92:5031–5042.
- Hurvich, C. M., and C. L. Tsai. 1993. A corrected Akaike information criterion for vector autoregressive model selection. *J. Time Ser. Anal.* 14:271–279.
- Jenkins, T. C., and D. Palmquist. 1984. Effect of fatty acids or calcium soaps on rumen and total nutrient digestibility of dairy rations. *J. Dairy Sci.* 67:978–986.
- Jung, H. G., D. Mertens, and A. Payne. 1997. Correlation of acid detergent lignin and Klason lignin with digestibility of forage dry matter and neutral detergent fiber. *J. Dairy Sci.* 80:1622–1628.
- Krizsan, S. J., S. Ahvenjarvi, and P. Huhtanen. 2010. A meta-analysis of passage rate estimated by rumen evacuation with cattle and evaluation of passage rate prediction models. *J. Dairy Sci.* 93:5890–5901.
- Lanzas, C., L. O. Tedeschi, S. Seo, and D. G. Fox. 2007. Evaluation of protein fractionation systems used in formulating rations for dairy cattle. *J. Dairy Sci.* 90:507–521.
- Laplace, J. P., B. Darcy-Vrillon, J. Perez, Y. Henry, S. Giger, and D. Sauvant. 1989. Associative effects between two fibre sources on ileal and overall digestibilities of amino acids, energy and cell-wall components in growing pigs. *Br. J. Nutr.* 61:75–87.
- Lin, L. I. 1989. A concordance correlation coefficient to evaluate reproducibility. *Biometrics* 45:255–268.
- Mertens, D. 2005. Rate and extent of digestion. Pages 13–47 in *Quantitative Aspects of Ruminant Digestion and Metabolism*. CABI, Wallingford, UK.
- Moe, P. W. 1981. Energy metabolism of dairy cattle. *J. Dairy Sci.* 64:1120–1139.
- National Animal Nutrition Program. 2015. Dairy–NRC Dairy (2001). Accessed May 18, 2015. <https://nanp-nrsp-9.org/perf/search/?animal=all&dataset=all&table=Studies&column=Year&comparator=exact&value=>.
- Niderkorn, V., and R. Baumont. 2009. Associative effects between forages on feed intake and digestion in ruminants. *Animal* 3:951–960.
- Nousiainen, J., M. Rinne, and P. Huhtanen. 2009. A meta-analysis of feed digestion in dairy cows. 1. The effects of forage and concentrate factors on total diet digestibility. *J. Dairy Sci.* 92:5019–5030.
- NRC. 2001. *Nutrient Requirements of Dairy Cattle*. 7th ed. National Academies Press, Washington, DC.
- Oba, M., and M. Allen. 1999. Evaluation of the importance of the digestibility of neutral detergent fiber from forage: effects on dry matter intake and milk yield of dairy cows. *J. Dairy Sci.* 82:589–596.
- R Core Team. 2014. *R: A language and environment for statistical computing*. R Foundation for Statistical Computing, Vienna, Austria. <http://www.R-project.org/>.
- Reveneau, C., C. Ribeiro, M. Eastridge, and J. Firkins. 2012. Interaction of unsaturated fat or coconut oil with monensin in lactating dairy cows fed 12 times daily. II. Fatty acid flow to the omasum and milk fatty acid profile. *J. Dairy Sci.* 95:2061–2069.
- Sackmann, J. R., S. Duckett, M. Gillis, C. Realini, A. Parks, and R. Eggelston. 2003. Effects of forage and sunflower oil levels on ruminal biohydrogenation of fatty acids and conjugated linoleic acid formation in beef steers fed finishing diets. *J. Anim. Sci.* 81:3174–3181.
- Sarwar, M., J. Firkins, and M. Eastridge. 1991. Effect of replacing neutral detergent fiber of forage with soyhulls and corn gluten feed for dairy heifers. *J. Dairy Sci.* 74:1006–1017.
- SAS Institute. 2005. *SAS User's Guide*. Version 9.2. SAS Institute Inc., Cary, NC.
- Schmidely, P., F. Glasser, M. Doreau, and D. Sauvant. 2008. Digestion of fatty acids in ruminants: a meta-analysis of flows and variation factors. 1. Total fatty acids. *Animal* 2:677–690.
- Seni, G., and J. F. Elder. 2010. Synthesis lectures on data mining and knowledge discovery. Pages 21–38 in *Model Complexity, Model Selection and Regularization*. R. Grossman, ed. Morgan & Claypool, San Rafael, CA.
- Seo, S., L. Tedeschi, C. Schwab, B. Garthwaite, and D. Fox. 2006. Evaluation of the passage rate equations in the 2001 Dairy NRC Model. *J. Dairy Sci.* 89:2327–2342.
- St-Pierre, N. R. 2003. Reassessment of biases in predicted nitrogen flows to the duodenum by NRC 2001. *J. Dairy Sci.* 86:344–350.
- Swanson, E. W. 1982. Estimation of metabolic protein requirements to cover unavoidable losses of endogenous nitrogen in maintenance of cattle. Pages 183–197 in *Proc. Protein Requirements for Cattle*. Division of Agriculture, Oklahoma State University, Stillwater.
- Traxler, M. J., D. G. Fox, P. J. Van Soest, A. N. Pell, C. E. Lascano, D. P. Lanna, J. E. Moore, R. P. Lana, M. Velez, and A. Flores. 1998. Predicting forage indigestible NDF from lignin concentration. *J. Anim. Sci.* 76:1469–1480.
- Van Soest, P. J. 1994. *Nutritional Ecology of the Ruminant*. Cornell University Press, Ithaca, NY.
- Van Vuuren, A., S. Tamminga, and R. Ketelaar. 1991. In sacco degradation of organic matter and crude protein of fresh grass (*Lolium perenne*) in the rumen of grazing dairy cows. *J. Agric. Sci.* 116:429–436.
- VandeHaar, M. J. 1998. Efficiency of nutrient use and relationship to profitability on dairy farms. *J. Dairy Sci.* 81:272–282.
- Weiss, W. P. 1998. Estimating the available energy content of feeds for dairy cattle. *J. Dairy Sci.* 81:830–839.
- Weiss, W. P., H. Conrad, and N. S. Pierre. 1992. A theoretically-based model for predicting total digestible nutrient values of forages and concentrates. *Anim. Feed Sci. Technol.* 39:95–110.
- White, R. R., Y. Roman-Garcia, J. Firkins, M. J. Vandehaar, T. McGill, R. Garnett, and M. D. Hanigan. 2017. Evaluation of the National Research Council (2001) dairy model and derivation of new prediction equations: 2. Rumen degradable and undegradable protein. *J. Dairy Sci.* 100:3611–3627. <https://doi.org/10.3168/jds.2015-10801>.