Methodology for splitting nitrogen between livestock dung and urine

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Contents

Abbreviations and glossary

AIC	Akaike's Information Criteria
AIM	Agricultural Inventory Model
BIC	Bayesian Information Criteria
CCC	Concordance correlation coefficient analysis
CT	Condensed tannins
DM	Dry matter
DMI	Dry matter intake (kg/d)
$DMI_{\%LW}$	Dry matter intake expressed as a percentage of liveweight
DOMD	Digestible organic matter in the dry matter (g/kg)
EF	Emission factor(s)
FN	Faecal nitrogen excreted, (g/d)
$FN_{\%exN}$	Faecal nitrogen expressed as percentage of total excreta N (g/100 g)
$FN_{\%Ni}$	Faecal nitrogen expressed as percentage of nitrogen intake (g/100 g)
GHG	Greenhouse gas(es)
LW	Liveweight (kg)
ME	Metabolisable energy (MJ/kg dry matter)
$ME_{LW0.75}$	Metabolisable energy intake per unit of metabolic weight ($LW^{0.75}$) (MJ/kg)
MPI	Ministry for Primary Industries
MSPE	Mean square prediction error
N	Nitrogen
N:ME	Ratio of N to ME in the diet (g/MJ ME)
N_{diet}	Concentration of N in the dietary dry matter (in this report: g/100 g DM)
Ni	Nitrogen intake (g/day)
Ni_{LW}	Nitrogen intake per unit of liveweight (g/kg)
$Ni_{LW0.75}$	Nitrogen intake per unit of metabolic weight ($BW^{0.75}$) (g/kg)
OM	Organic matter
OMD	Organic matter digestibility
r^2	Coefficient of determination of a regression
RMSPE	Root mean square prediction error, calculated as the square root of MSPE.
RPE	Relative prediction error: RMSPE expressed as a percentage of the mean of the observed values
RSR	Ratio RMSPE to standard deviation (of observed values)
UN	Urinary nitrogen excreted (g/day)
$UN_{\%exN}$	Urinary nitrogen expressed as percentage of total excreta N (g/100 g)
$UN_{\%Ni}$	Faecal nitrogen expressed as percentage of nitrogen intake (g/100 g)

1. Executive Summary

A database of nitrogen (**N**) measurements has been created from studies of cattle (beef and dairy), sheep and deer where intakes and partition of N have been collated. The data have been used to assess the current equation used in the New Zealand greenhouse gas (**GHG**) inventory model to estimate the partitioning of excreta N into urine and faeces (dung). The database was also used to develop alternative equations. Each observation recorded in the database represented an experimental mean from published science articles, client reports and post-graduate theses in which cattle, sheep and deer were offered forage-based rations.

On average, forage comprised 80% of the rations for beef cattle, sheep and deer and 76% for dairy cattle. A total of 448 observations were evaluated: 67 from beef cattle, 182 from dairy cattle, 46 from deer and 153 from sheep. Fresh grasses and legumes dominated 228 diets and 184 were dominated by conserved grasses, legumes and maize silage. All datasets included measures of dietary N intake, N excreted and metabolisable energy (**ME**) were available or could be derived from 312 of the records.

A first objective was to evaluate the predictive performance of the models developed by Luo and Kelliher (2010) (currently used in the inventory model) and Thomson and Muir (2016) against observations in the database. The model of Luo and Kelliher (2010) predicts the percentage of urine N in total excreta N while the model of Thomson and Muir (2016) predicts the amount of urine N excreted. Overall, the prediction of the proportion of urine N in total excreta N was achieved with smaller relative prediction error than the prediction of urinary N excretion. The equation of Luo and Kelliher (2010) could be considered adequate for beef cattle and sheep because of the relatively small mean bias and prediction error, but the model was less adequate for predictions related to dairy cattle and deer. The model of Thomson and Muir (2016) had a large proportion of random error and was moderately accurate for dairy cattle, but had large slope and mean biases when predicting beef cattle data and sheep data, respectively. Overall, the prediction of the amount of N excreted in urine was made with moderate to high precision, which supports the statement by Thomson and Muir (2016) that a model based on Ni provides “stronger” relationships with urinary N excretion. The main conclusion from this part of the study was that neither model performed consistently, in terms of accuracy and precision, across the livestock classes under study.

A second objective consisted in the development of alternative equations with improved predictive ability that could be implemented in the inventory model. These focused on 5 dependent variables associated with N intake, N in urine and faeces and the partition of

N between urine and faeces, and 15 independent variables defined by linear and quadratic terms of N, ME and liveweight and their derived ratios. Analyses were undertaken for individual livestock classes (beef, dairy, sheep and deer) and with all data combined.

Linear regression analysis identified the sets of dietary and animal variables that explained as much of the variation in N excretion as possible. An important finding was that having more than three independent variables in a model resulted in little additional benefit in terms of accounting for variation in the data. The models identified using the linear regression with up to three variables were then evaluated using a cross-validation approach to determine their predictive ability. This resulted in a selection of models which were parameterised using 80% of the observations (training dataset), with random stratification according to the number of observations per livestock class.

The parameterised models were then assessed by comparing their predictions for the remaining 20% of the observations (evaluation dataset) that were not included in the model development. A further selection was based on predictive ability, mean square prediction error, the root mean square prediction error and its decomposition in mean bias, slope bias and random error and concordance correlation coefficients.

Equations were parameterised to fit one of three alternatives:

Alternative 1: the current approach of using a single equation in AIM to estimate the proportion of urinary N in excreta ($UN_{\%exN}$) for the four livestock classes of interest is retained. Equations 1 and 2 (below) can be considered as suitable alternatives to the current equation in AIM because of their smaller bias (-0.4 to 3.1 depending on livestock class, compared with 0.2 to 6.9 for the current equation). Their relative prediction error is 4.0 to 11.3% of the observed mean vs. 7.9 to 11.7% of the current equation, their concordance coefficient is improved (0.28 to 0.74 vs. 0.27 to 0.67) and random error contributes a larger proportion to the error, as opposed to systematic biases. Because the equations have regressors currently used in AIM, they can be implemented readily into the inventory model.

$$UN_{\%exN} = 25.060 + (N_{diet} \times 12.441) \qquad \text{(Eq. 1)}$$

and

$$UN_{\%exN} = 26.573 + (N_{diet} \times 12.972) + (DMI \times 0.321) \qquad \text{(Eq. 2)}$$

where N_{diet} is the N concentration in the feed dry matter (g/100 g DM) and DMI is the dry matter intake (kg/d) of the animal.

Alternative 2: the approach used in AIM to predict the proportion of urinary N in total excreta N is retained, but livestock class-specific equations are introduced.

The following equations are proposed for each of the livestock classes of interest: Equation 2 for beef cattle, Equation 3 for dairy cattle, Equation 4 for deer and Equation 5 for sheep:

$$UN_{\%exN} = 26.573 + (N_{diet} \times 12.972) + (DMI \times 0.321) \quad \text{(Eq. 2)}$$

$$UN_{\%exN} = 24.527 + (N_{diet} \times 22.676) + (ME_{LW0.75} \times -9.206) + [(N{:}ME)^2 \times -2.116] \quad \text{(Eq. 3)}$$

$$UN_{\%exN} = 5.699 + (N_{diet} \times 28.151) + (N{:}ME \times -7.823) \quad \text{(Eq.4)}$$

$$UN_{\%exN} = 29.539 + (N_{diet} \times 11.980) \quad \text{(Eq. 5)}$$

where N_{diet} and DMI are as defined above, and $ME_{LW0.75}$ is the ME intake per kg of metabolic liveweight, and N:ME and N:ME are the ratio of N and ME in the diet (g N/MJ ME per kg DM).

These equations improved predictions for dairy cattle, deer and sheep by further reducing the mean bias of the prediction and generally increasing precision (r^2 values of 0.43 to 0.74 vs. 0.27 to 0.74 of Equations 1 and 4).

Alternative 3: Rather than predicting the proportion of urine N in total excreta N, equations to predict faecal N excretion were developed. The prediction of faecal N is proposed as an alternative because it is less prone to measurement errors than urinary N during N balance studies.

Equation 6 is proposed to predict FN from beef cattle, dairy cattle and deer; while Equation 7 is proposed for sheep:

$$FN = -4.623 + (N_{diet} \times 1.970) + (DMI \times 7.890) \quad \text{(Eq. 6)}$$

$$FN = 2.230 + (Ni \times 0.299) + [(N_{diet})^2 \times - 0.237] \quad \text{(Eq. 7)}$$

where N_{diet} is as described above and Ni is the N intake per animal (g/d). The prediction error obtained from these equation is similar to those that can be achieved by using Equations 1-5 for cattle (~15% of the mean of observations) but for sheep and deer the relative prediction error increases to ~30%. The models to predict FN had acceptable accuracy (concordance coefficients ranging from 0.72 to 0.94) and precision (r^2 values ranging from 0.57 to 0.96). These two equations were better than published prediction equations because they had less bias and larger proportion of random error in their predictions. Equations 6 and 7 are functions of independent variables as used in the inventory model and therefore could be readily implemented in AIM.

We recommend equations are used to predict the amount of FN directly from DMI, N concentration and intake and these be implemented in the inventory model as an alternative to the current equation that predicts the proportion of urine N in total excreta N. The estimation of the amount of UN can then be calculated by difference from the amount of total N in excreta to then calculate the GHG emissions from urine N deposition in agricultural soils.

2. Background

The Agricultural Inventory Model (**AIM**) (Pickering and Wear, 2013) is used to estimate GHG emissions from the agricultural sector. Calculation of nitrous oxide emissions are based on the amount of nitrogen (**N**) excreted by ruminants to the environment in the form of urine and faeces (dung). Emission factors (**EF**) are then applied to estimate the amount of nitrous oxide that is emitted from each form of excreta. The AIM estimates the amount of excreta N as the difference between the N intake (**Ni**) by the animals and the amount of N used for productive purposes (milk, live weight gain, wool growth for sheep and velvet growth for deer).

The N in excreta (g/d) is then partitioned into urine N (**UN:** g/d) and faecal N (**FN:** g/d) using the equation developed by Luo and Kelliher (2010):

$$UN_{\%exN} = 33.5 + (N_{diet} \times 10.5)$$

which includes the N concentration (**N_{diet}**) in in the feed of dry matter (**DM**) as the independent variable (also described here in as predictor, regressor or explanatory variable). Their equation predicts the percentage of excreted N accounted for by UN, with FN then calculated by difference from excreta N. This equation was reviewed by Thomson and Muir (2016), who recommended the development of alternative equations to estimate the amount (g/d) of UN directly from Ni, rather than the relative contribution of UN to total excreta N (**$UN_{\%exN}$**) as a function of N_{diet}:

$$UN = -2.84 + (Ni \times 0.453)$$

The ***first objective*** of this project was to evaluate the approaches proposed by Luo and Kelliher (2010) and Thomson and Muir (2016), supported by a the development of an expanded database from studies reporting the partitioning of N between product, urine and faeces in four ruminant livestock classes (beef cattle, dairy cattle, sheep and deer). A ***second objective*** was to use the enlarged database to generate a model with improved predictive ability to be used in AIM.

Vibart et al. (2009) reported that, while N_{diet} and Ni are the main drivers for N partitioning in lactating dairy cows, predictive models that include other aspects of feed quality, such as fermentable carbohydrates and/or fibre, accounted for a greater proportion of variance in regressions models to predict N partitioning. This has a sound biological base because the type of dietary carbohydrate affects microbial growth in the rumen and this affects N partitioning to production, faeces and urine (Kebreab et al., 2001). We acknowledge that the AIM does not describe feed in terms of carbohydrate type and concentrations, but inputs do include metabolisable energy (**ME**) of the feed. The ME content is itself a function of the chemical composition of the feed (AFRC, 1993; NRC, 2001; CSIRO, 2007) and we hypothesise that inclusion of ME in the equations will better predict the partitioning of excreta N between urine and dung.

3. Methods

The relationships between the concentration in the diet of N (N_{diet}: g/100 g dry matter: DM), metabolisable energy (ME: MJ/kg DM) and daily intake of N (Ni; g/d) were evaluated with regard to excretion of urinary N (UN; g/d) and faecal N (FN; g/d). As part of the evaluation, UN and FN were also expressed as a percentage of Ni ($UN_{\%Ni}$ and $FN_{\%Ni}$) and also the percentage of UN in total excreta N ($UN_{\%exN}$; %). Relationships were explored using data from experiments in which the partitioning of N has been measured. The percentage of FN in total excreta N ($FN_{\%exN}$) was not modelled because it is calculated by subtracting the $UN_{\%exN}$ value from 100.

3.1 Data

Data from nitrogen balance studies with dairy cattle, beef cattle, sheep and deer were collected from the literature. In the case of dairy cattle, a previously assembled database (Vibart et al., 2009) was used and supplemented with additional information. However, data for the other livestock classes were collected directly from the literature. Data provided by the Ministry for Primary Industries (**MPI**) collated as part of a previous project (Thomson and Muir, 2016) was not used directly because there was insufficient description of bibliographic variables, dietary ME and liveweight (**LW**) of the experimental animals. Each observation in the database represented an experimental mean from a published scientific journal, supplemented with data from client reports and post-graduate theses where appropriate.

Data from studies used in previous reports to develop or evaluate predictive equations (e.g. Luo and Kelliher, 2010; Thomson and Muir, 2016) were included as appropriate. Overall, 343 experimental means that had not been included in previous reports (56, 102, 46 and 139 for beef, dairy, deer and sheep, respectively) were obtained. In addition, the database included 33 means used by Luo and Kelliher (2010) of which 11 and 22 were for beef and dairy cattle respectively. The database also included 58 and 14 experimental means (dairy cattle and sheep, respectively) that were part of the additional observations included in the report of Thomson and Muir (2016). It should be noted that not all the experimental means included in previous reports have been considered in this study, due to the application of selection criteria for inclusion of studies as described below.

3.1.1 Criteria for inclusion of data

Data from selected publications and reports were included in the database according to the following criteria:

Methodological considerations in animal studies. Studies were included in the database if they reported actual measurements for dry matter intake (**DMI**) and results from N balance studies in which total or partial collection of urine and dung were performed. Studies in which DMI was estimated from pre- and post-grazing residuals or back-calculated from energy requirements were not included. Similarly, studies in which UN was estimated (e.g. using creatinine concentrations) from spot-samples were not included. In addition to the urinary and faecal N excretion, data on N retention were also recorded. For the purposes of this study, N partitioning in an animal was calculated on a daily basis. The daily Ni in the studies included in the database was partitioned into UN and FN, which were added up to calculate total N in excreta. In lactating animals, milk N data was also included in the database. When N retention in body weight gain was not reported, it was assumed to be equal to the Ni minus the sum of N in excreta (and milk for lactating animals). No other data on N losses (e.g. dermal scuff) or sinks (wool or velvet) were considered in the calculations.

Diet type. Because the diets consumed by ruminants in New Zealand are predominantly based on forages, the database was collated using reports in which forages represented a majority of the ration used. Initially, it was intended to only have studies in which fresh grasses were fed as the experimental diet, as previously done for dairy cattle (e.g. Vibart et al., 2009). However, the number of observations in the database was too small for some of the ruminant classes under study. Therefore, the definition of forage was expanded to also include conserved forages (hay and silage) and their derivatives (e.g. dry grass pellets). Data from studies in which forages other than grasses, such as legumes, herbs and forage crops were also included. While there is a plethora of studies presenting N balances, particularly for dairy cattle, studies in which large amounts of supplements are fed to increase the amount rumen undegradable protein in the diet were not included. They were excluded because such diets were not representative of the dietary conditions commonly used in New Zealand pastoral systems. Also, data from studies in which tropical and subtropical grasses (C4 grasses) were fed were not included in the database, because they were not considered to be representative of the diets fed to ruminant livestock in New Zealand.

Animal species, breeds and physiological stage. For cattle, only data from studies using *Bos taurus* cattle were included in the database. For sheep, only data from fleeced sheep were included in the database. Because of the paucity of data on deer studies, a wider range of species was allowed in the database, including observations from red deer and elk (*Cervus elaphus*), Sika deer (*C. nippon*), and Rusa deer (*C. timorensis*). The database included a range of different animal types within each of the four livestock classes, ranging from growing ruminants to adults. Data collated from dairy cattle included both lactating and non-lactating cows, but the bigger proportion of the data for dairy cattle comprised lactating cows.

After all the criteria above were applied, a database comprising 448 experimental means from 105 studies was used for the development of models. Table 1 summarises the studies for each livestock class, and the explanation of the basis for categorisation is given below. The list of references included in the database is presented in Appendix 1.

3.1.2 Database construction

In the database, rations were arbitrarily classified into the following categories (Table 1): fresh perennial ryegrass, other grasses (fresh), fresh legume, condensed tannin (**CT**)-containing legume, concentrate (grains and industrial by-products), conserved grass (either hay, silage or dried and pelleted), rations based on maize silage, conserved legumes (hay, silage or dried and pelleted) and “other” diets (tree leaves, forest by-product silages, among others). If a ration contained more than one of the feedstuffs listed above, the classification was based on the largest contribution to the total ration. For example, a treatment with 20% lucerne silage, 40% maize silage, 35% concentrates and 5% pre-mixes was classified as “maize silage”.

Table 1. Number of observations (experimental means) in the database according to livestock class and type of diet.

Main ration component[1]	Beef	Dairy	Deer	Sheep	Total per ration
Fresh perennial ryegrass	11	79	0	46	136
Other fresh grass	17	15	10	6	48
Fresh legume	0	1	3	33	37
Fresh CT[2]-legume	0	3	0	4	7
Concentrate	0	3	1	5	9
Conserved grass	20	67	10	29	126
Maize silage	16	7	3	1	27
Conserved legume	1	7	12	11	31
Other diet	2	0	7	18	27
Total per livestock class	67	182	46	153	
Grand total					**448**

[1] See text for explanation of main dietary component description.

[2] Condensed tannin

Dietary characteristics. For most references, the reported dietary composition was transcribed into the database. If any of the variables of interest were not explicitly reported, the following calculations and assumptions were made:

a) if dietary N concentration was not reported, it was calculated from Ni (g/d) and DMI (kg/d) as:

N concentration (g per 100 g DM) = (Ni/DMI)/10

b) if dietary ME content was not reported, it was estimated from the digestible organic matter in the dry matter (**DOMD:** g/kg) using the equation from the AFRC (1993)

ME (MJ per kg DM) = 0.0157 × DOMD

The DOMD was in turn calculated from reported organic matter digestibility (**OMD:** g/kg) and the organic matter (**OM:** g/kg) concentration in dry matter as:

DOMD (g per kg DM) = OMD × (OM/1000)

If OM was not reported, it was calculated by difference from ash (g/kg DM):

OM (g/kg DM) = 1000 - ash

If a study reported DOM but not OM or ash, the mean value for ash across the database (91 g/kg DM) was imputed.

In addition to the dietary variables obtained from the literature contributing to the database, additional explanatory variables were calculated from the dataset. These included the ratio of N relative to dietary ME (**N:ME**: g N/MJ ME), and expression of Ni relative to animal LW (Ni/kg LW and Ni/kg $LW^{0.75}$) and DMI (kg/d and expressed as percentage of LW). Also, nonlinear relationships were examined by calculating quadratic terms of the explanatory variables in the datasets

3.2 Development of models

The development of models involved a series of steps to determine which variables listed in Table 2 were included as predictors for the variables of interest, using simple correlation and regression analysis.

Table 2. Dependent variables and independent variables (regressors) included in the development of models.

Variable type	Abbreviation	Units
Dependent variables		
Urine N	UN	g N/d
UN relative to excreta N	UN%exN	%
UN relative to N intake	UN%Ni	%
Faecal N	FN	g N/d
FN relative to N intake	FN%Ni	%
Independent variables		
N concentration in the diet	N_{diet}	% of DM
N intake (Ni: g/d)	Ni	g/d
Metabolisable energy (ME) content of the diet	ME	MJ/kg DM
DMI	DMI	kg/d
DMI relative to body weight (LW)	DMI%LW	%
Ratio of N to ME in the diet	N:ME	g N/MJ ME
Ni per kg of LWNi_LW: g/kg LW)	Ni_{LW}	g N/kg LW
Ni per kg of metabolic weight ($LW^{0.75}$)	$Ni_{LW}0.75$	g N/kg $LW^{0.75}$
ME per kg of metabolic weight ($LW^{0.75}$)	$ME_{LW}0.75$	MJ ME/kg $LW^{0.75}$
N concentration quadratic	N_{diet}^2	$\%^2$
Ni quadratic	Ni^2	$(g/d)^2$
ME quadratic	ME^2	$(MJ/kg\ DM)^2$
Ni:ME quadratic	$N:ME^2$	$(g/MJ)^2$
Ni:LW quadratic	Ni_{LW}^2	$(g/kg)^2$
Ni:metabolic weight quadratic	Ni_{LW}^2	$(g/kg)^2$

Then, model structures were identified and parameterised to generate predictive equations. After models were parameterised, an evaluation was performed and recommendation on models made. The steps are summarised in Figure 1.

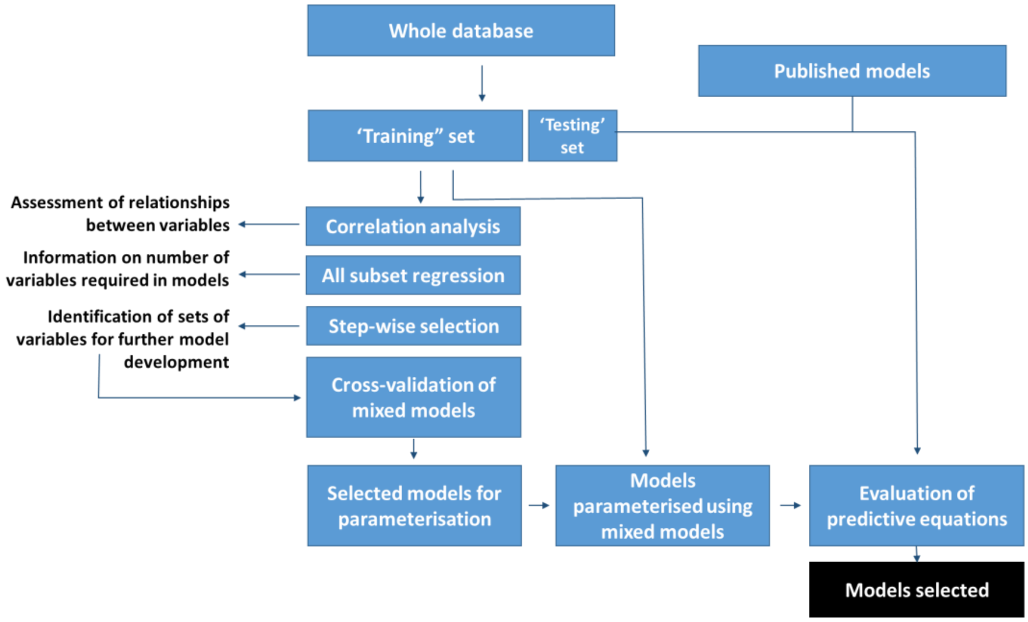

Figure 1. Diagram of steps used to develop and evaluate equations in this project.

3.2.1 Exploration of relationships between variables of interest and independent variables

Initial assessment of the relationships between variables was done by calculating pair-wise correlations between the variables in Table 2, using the CORR procedure in SAS v. 9.4 (SAS Institute Inc., 2012).

A second exploratory stage performed an “all subsets” regression analysis with the REG procedure (SAS Institute Inc., 2012). This used the coefficient of determination (**r^2**) as the criteria for model selection to understand the fit of the models in relation to the number of independent variables in the model. This was followed by a selection of single and multiple regression models using a step-wise selection of regression with probabilities of 0.05 and 0.01 for entry and to stay (respectively) in the model (REG procedure in SAS). The step-wise regression approach helped to inform the models that were further developed using mixed-model methodology.

3.2.2 Cross-validation modelling to select final model structures

In order to select the best mixed models for each dependent variable, a Monte-Carlo k-fold cross-validation approach was implemented. Because the number of observations was small for some of the livestock classes under study, a five-fold cross validation enabled the assessment of the ability of the models to predict observations not used to build the model (Slaets et al., 2014). Briefly, the data set was randomly divided into 5 parts (folds), stratified per livestock class (i.e. each fold contained a similar proportion of observations for each class as the whole database). Then, different mixed models were built using observations from 4 of the folds, while the 5th fold was used to assess the predictions of the model. The five-fold sets were generated using the SURVEYSELECT procedure in SAS, replicated 50 times. Predictions from the 50 replicates generated with four fifths of the data were used to predict the values of the one fifth that was left out. Then, an r^2 value of the cross-validation was generated across all the replicates to identify the best model structure to build the predictive equations for the variables of interest.

3.2.3 Development of predictive equations

Three different types of predictive models were developed:

1) A ‘universal’ model for each variable of interest, using the information from the four different livestock classes,

2) A model using all data, but with the inclusion of livestock class as a model term effect, allowing to the generation of class-specific parameters while still utilising the information from all classes, and

3) Livestock class-specific models using observations from each of the livestock classes separately.

In contrast to Luo and Kelliher (2010) and Thomson and Muir (2016), who reported only the fit (r^2) of the regression equation as a measurement of adequacy of the model, we developed models with a subset of observations and evaluated them against observations not used for the parameterisation.

Table 3. Description of the dataset used for model training.

Main ration component	**Beef**	**Dairy**	**Deer**	**Sheep**
Fresh perennial ryegrass	11	60	0	39
Other fresh grass	13	11	9	5
Fresh legume	0	0	3	25
Fresh CT[1]-legume	0	3	0	3
Concentrate	0	2	1	5
Conserved grass	16	58	6	23
Maize silage	11	7	3	1
Conserved legume	1	5	9	10
Other diet	2	0	6	12

[1]Condensed tannin

Two data subsets were created for model development (training: 80% of the observations: Table 3) and evaluation (20% of the observations: Table 4), using similar procedures to generate the datasets (i.e. stratified according to livestock class) as described above for the cross-validation (i.e. SURVEYSELECT in SAS). The models were developed using data from references previously reported by Luo and Kelliher (2010) and Thomson and Muir (2016) as well as the new observations collected in this project.

Table 4. Description of database for model evaluation.

Main ration component	**Beef**	**Dairy**	**Deer**	**Sheep**
Fresh perennial ryegrass	0	17	0	5
Other fresh grass	3	4	0	1
Fresh legume	0	1	0	8
Fresh CT[1]-legume	0	0	0	1
Concentrate	0	1	0	0
Conserved grass	3	6	2	6
Maize silage	5	0	0	0
Conserved legume	0	2	2	1
Other diet	0	0	1	6

[1]Condensed tannin

The final predictive models were developed as mixed models, considering the independent variables as fixed effects, with random slopes included in the model, using the study as a subject (St-Pierre, 2001). While the regression analysis describes the general response across studies, the mixed models account for random study effects allowing the estimation of parameters that capture both the between- and within-studies information (St-Pierre, 2001). Random intercepts were also included in the models, but their inclusion did not improve the model fit (based on Akaike's and Bayesian Information Criteria: **AIC** and **BIC**, respectively) and therefore not included in the final model parameterisation. An unstructured variance-covariance matrix was deemed to be the best fit for the data, also based on AIC and BIC values.

3.3 Evaluation of models

To fulfil the first objective, the predictions generated by the equations of Luo and Kelliher (2010) for estimating the percentage of excreta N accounted for by UN:

$UN_{\%exN} = 33.5 + (N \times 10.5)$

and Thomson and Muir (2016) for estimating UN output (g/d):

$UN = -2.84 + (Ni \times 0.453)$

were evaluated using the observations from the dataset described in Table 3.

Following these evaluations, models developed using the training dataset were also evaluated for their predictive ability against the observations in the evaluation dataset. In addition, some published animal class-specific equations (Patra, 2010; Stergiadis et al., 2015; Schuba et al., 2017) and also others compiled and reported by Johnson et al. (2016) were also evaluated against this dataset.

Predicted values from each of the models were compared to the observed (experimental mean) values using regression analysis, concordance correlation coefficient (**CCC**) analysis (Lin, 1989) and error decomposition analysis (Bibby and Toutenburg, 1977). For the latter, the mean square prediction error (**MSPE**), the root mean square prediction error (**RMSPE**: to bring the MSPE to the same units as the observed values) were calculated and then the error was partitioned into mean bias (the degree at which a model under- or over-predicts the mean of the observations), slope bias (the degree at which a model is appropriate across the range of observations) and random error (random dispersion around the line of the regression observed vs. predicted).

To allow comparisons of models, the RMSPE was expressed as a percentage of the observed mean (relative prediction error: **RPE**). Values of RPE less than 10% indicate that the model predictions are good and values between 10-25% are acceptable, according to the guidelines quoted by Johnson et al. (2016). In terms of the error partitioning, a robust model should have small biases, with most of the errors in prediction being random (>90%). The accuracy of the model was assessed *via* the CCC. The CCC measures the degree of agreement between two variables, in similar fashion to the coefficient of determination (r^2) of a regression. The r^2 value is an indication of precision (i.e. how close the individual predicted values are to each other), while the CCC statistic provides an indication of how close a predicted value is to the observed value (i.e. the ideal being the slope of the regression observed vs. predicted being 1; Tedeschi, 2006). The closer the CCC is to 1, the better. Finally, the RMSPE to standard deviation of observed values ratio (**RSR**) was calculated to compare the magnitude of the error associated to the model predictions with the inherent variability in observed values. With this statistic, values closer to zero are considered better than values greater than one (Moriasi et al., 2007). For RSR, values <0.5 indicate very good, and <0.75 good predictive ability of the model, whereas values >1 suggest that the model predictions have uncertainty greater than the variation in the variable that is being predicted. All the above model evaluations were conducted in SAS.

4. Results and Discussion

4.1 Database features

4.1.1 Dietary characteristics

The summary statistics (minimum, maximum and mean) for all dependent and independent variables are presented in Appendix 2 for beef, dairy, deer, sheep and all livestock classes combined. Appendix 3 presents the summary for the diet types listed in Table 1.

Dietary N concentrations in the database ranged from 0.8 to 5.0% of DM and ME was reported to range from 5.6 to 13.7 MJ/kg DM. The range was similar across diets for different livestock classes (Table 5 and Figure 2), but the mean ME value in rations for dairy cattle was greater than for other classes. The diets for beef cattle and deer had, on average, lower N content than the diets for sheep and dairy cattle. No other dietary components have been included in this study as potential explanatory variables for N partitioning in excreta, because the AIM only includes N and ME for the diets consumed by New Zealand ruminants (Pickering and Wear, 2013).

Table 5. Summary of nitrogen (N_{diet}, g/100 g DM) and metabolisable energy (ME) concentrations (MJ/kg DM) from rations included in the database, according to livestock class.

Livestock class	Variable	Mean	Minimum	Maximum	Number of records
All	N_{diet}	2.6	0.8	5.0	448
	ME	10.3	5.6	13.7	312
Beef cattle	N_{diet}	2.1	0.8	4.5	67
	ME	9.9	7.3	12.5	41
Dairy cattle	N_{diet}	2.8	1.2	4.5	182
	ME	11.1	8.6	13.7	136
Deer	N_{diet}	2.2	0.9	4.7	46
	ME	8.8	5.6	11.2	14
Sheep	N_{diet}	2.6	0.8	5.0	153
	ME	9.7	5.6	12.7	121

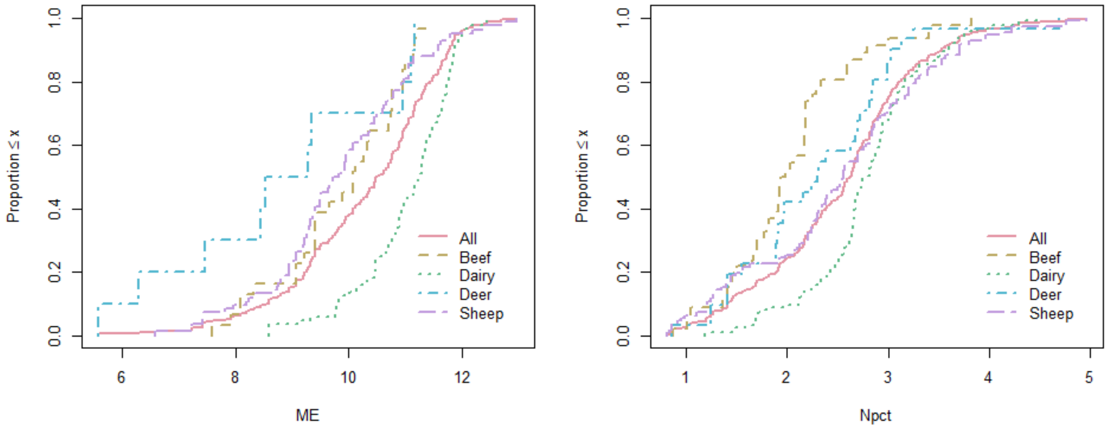

Figure 2. Cumulative distribution of the content of metabolisable energy (ME) and nitrogen (N_{diet}: g/100 g DM) from rations included in the database, according to livestock class.

Overall, forage comprised over 80% of the DM of the diets in the dataset, with exception of dairy cattle (76% of the diet as forage). The legumes (both CT-containing and non-CT containing) contained, on average, between 1.2 and 1.6 times the concentration of N in the DM, compared to grasses, with concentrate-based diets and ‘other’ diets falling in between. Conserved forages contained less N than fresh forage, both for legumes and grasses. Perennial ryegrass diets contained more N and ME than other temperate grasses included in the database. Maize silage and grasses other than ryegrass had comparable N and ME concentrations (Table 6 and Figure 3).

Table 6. Summary of nitrogen (N_{diet}, g/100 g DM) and metabolisable concentrations (MJ/kg DM) from diets included in the database, according to diet type.

Main ration component	Variable	Mean	Minimum	Maximum	Number of records
Fresh perennial ryegrass	N_{diet}	2.8	0.8	4.5	136
	ME	11.1	8.6	13.7	99
Other fresh grass	N_{diet}	2.2	0.8	4.7	48
	ME	9.8	7.3	12.5	28
Fresh legume	N_{diet}	3.3	2.4	4.8	37
	ME	9.6	7.8	12.3	32
Fresh CT-legume	N_{diet}	3.5	2.7	3.8	7
	ME	10.8	9.9	12.0	7
Concentrate	N_{diet}	2.5	2.2	3.1	9
	ME	10.4	8.5	11.8	5
Conserved grass	N_{diet}	2.3	0.9	3.3	126
	ME	10.0	6.8	12.1	77
Maize silage	N_{diet}	2.2	1.0	3.7	27
	ME	10.8	9.9	11.4	21
Conserved legume	N_{diet}	2.7	2.0	3.6	31
	ME	9.2	5.6	11.1	23
Other diet	N_{diet}	2.5	1.9	5.0	27
	ME	10.1	7.5	12.7	20

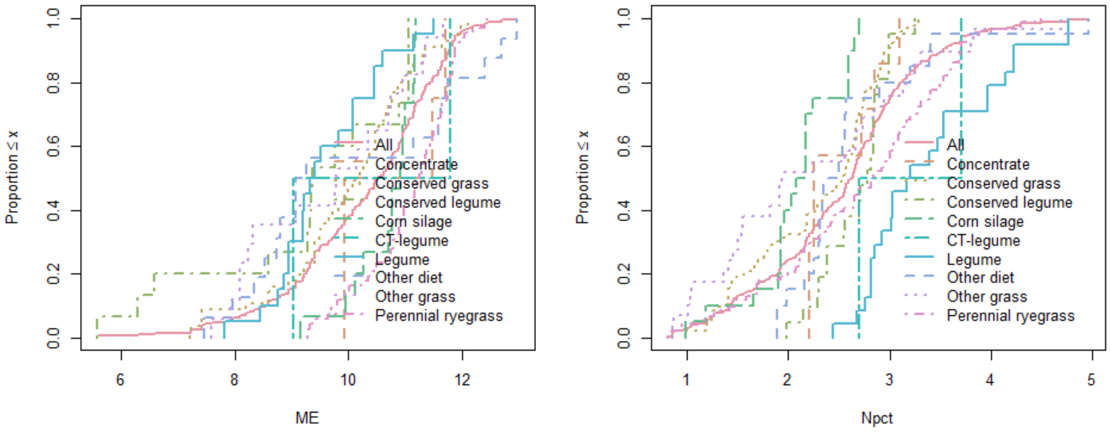

Figure 3. Cumulative distribution of the content of metabolisable energy (ME) and nitrogen (N_{diet}: g/100 g DM) from rations included in the database, according to diet type.

4.1.2 N excreta characteristics

As expected, the absolute amounts of N excreted are greater for larger and more productive animals (Appendix 2). The mean percentage of N that is excreted in urine varies from 48.8% in deer to 61.5% in sheep, but the extremes by animal group in the data set (Table 7) are 12.5% (deer) to 84.8% in sheep. Deer have lower values for $UN_{\%exN}$, as indicated in Figure 3, and lower dietary N concentrations (Table 3). When expressed in terms of dietary N intake, means for animal groups for the percentage of dietary N intake that is excreted in urine ($UN_{\%Ni}$) are similar for cattle and deer (40.3-42.5%) and higher for sheep (53.4%) and extremes by animal group for $UN_{\%Ni}$ range from 8.4 (deer) to 82.8 (sheep).

Table 7. Mean, minimum and maximum values of the variables describing partitioning of nitrogen in the excreta of beef cattle, dairy cattle, deer and sheep from the database collated.

Livestock class	**Variable**	**Mean**	**Minimum**	**Maximum**	***Number of records***
Beef cattle	$UN_{\%exN}$	54.5	30.8	75.0	67
	$FN_{\%exN}$	45.5	25.0	69.2	67
	$FN_{\%Ni}$	34.4	15.2	63.1	67
	$UN_{\%Ni}$	42.5	21.4	66.4	67
Dairy cattle	$UN_{\%exN}$	57.2	32.5	76.6	182
	$FN_{\%exN}$	42.8	23.4	67.5	182
	$FN_{\%Ni}$	30.2	18.7	55.8	180
	$UN_{\%Ni}$	41.2	17.9	62.3	180
Deer	$UN_{\%exN}$	48.8	12.5	70.5	29
	$FN_{\%exN}$	51.2	29.5	87.5	29
	$FN_{\%Ni}$	43.3	12.0	96.6	46
	$UN_{\%Ni}$	40.3	8.4	60.7	29
Sheep	$UN_{\%exN}$	61.5	26.0	84.8	140
	$FN_{\%exN}$	38.5	15.2	74.0	140
	$FN_{\%Ni}$	35.8	13.5	92.7	153
	$UN_{\%Ni}$	53.4	20.0	82.8	140
Overall	$UN_{\%exN}$	57.6	12.5	84.8	418
	$FN_{\%exN}$	42.4	15.2	87.5	418
	$FN_{\%Ni}$	34.1	12.0	96.6	446
	$UN_{\%Ni}$	45.4	8.4	82.8	416

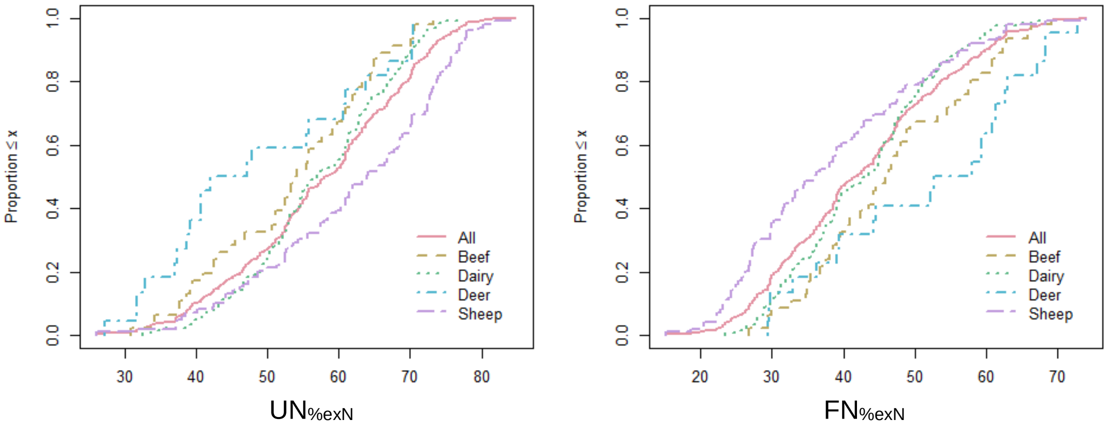

Figure 4. Cumulative distribution of the partition of nitrogen excretion into urinary N ($UN_{\%exN}$) and faecal N ($FN_{\%exN}$), according to livestock class. Partition is expressed as g per 100 g of manure N.

Although most diets resulted in similar distribution of N between urine and faeces ($UN_{\%exN}$ and $FN_{\%exN}$ values), the legume diets were associated with lower values of $FN_{\%exN}$ (and correspondingly greater values of $UN_{\%exN}$) values as shown by the cumulative distributions in Figure 5.

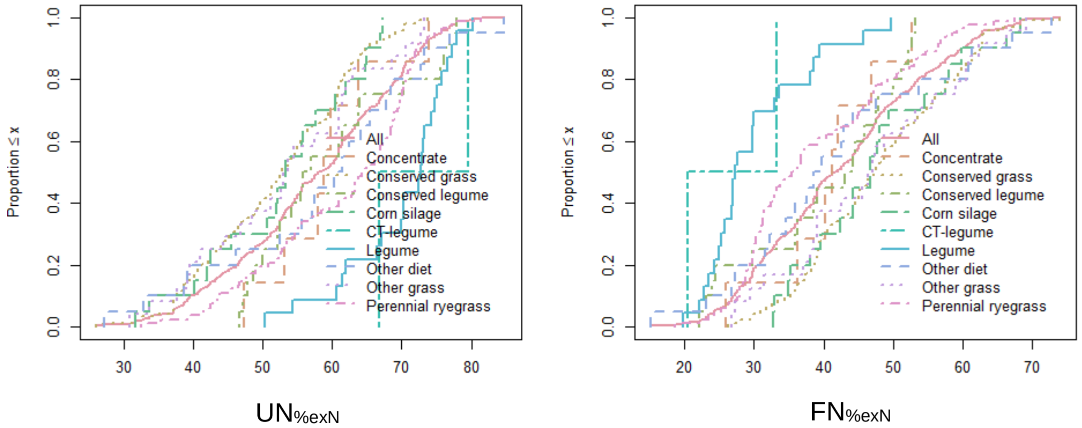

Figure 5. Cumulative distribution of the partition of nitrogen excretion into urinary N ($UN_{\%exN}$) and faecal N ($FN_{\%exN}$), according to diet type. Partition is expressed as g per 100 g of manure N.

4.1.3 Estimation of ME from DOMD

Because not all publications reported ME, the estimation of this variable from DOMD is a key assumption underpinning the model development. A regression analysis was performed on the subset of observations for which both ME and DOMD were reported to assess the agreement between ME estimated from DOMD and reported ME. Although the r^2 of the regression is modest (0.66), a slope of 1.00 (s.e. 0.08) and an intercept not significantly different from zero (0.32: p=0.69) provide confidence that the DOMD estimate is a good representation of the reported ME of the diets (Figure 6).

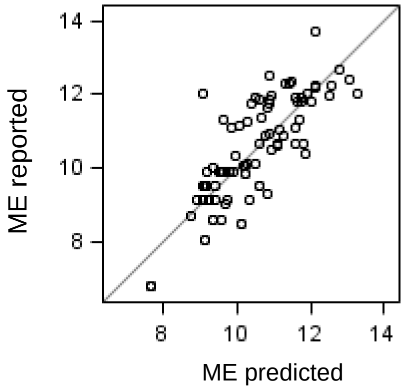

Figure 6. Scatterplot of predicted metabolisable energy (ME: using the equation from AFRC (1993) to estimate ME from digestible organic matter in the dry matter: DOMD) against the ME value reported. ME: MJ/kd dietary dry matter. Data from studies that reported both ME and DOMD.

4.2 Objective 1: Evaluation of models from previous reports

A direct comparison of the approaches suggested in previous reports is constrained by the fact that the equations of Luo and Kelliher (2010) and Thomson and Muir (2016) estimate different variables ($UN_{\%exN}$ and UN, respectively). Further, their estimates apply to a different range of livestock classes (the latter report does not include deer as part of the livestock classes).

In general, the prediction of $UN_{\%exN}$ using the equation of Luo and Kelliher (2010) has smaller relative prediction error (RMSPE is 12.3 to 31.1 percent of the mean) than UN (RMSPE 26.3 to 46.1 of the mean) predicted from the equation of Thomson and Muir (2016). The prediction of $UN_{\%exN}$ from the equation by Luo and Kelliher (2010) can be considered suitable for beef and sheep because of the small bias and RMSPE, the large proportion of random error and CCC values greater than 0.7. However, this model has large mean bias (~40% of the error) and only moderate CCC (~0.4) for sheep and dairy.

The model of Thomson and Muir (2016) has a large proportion of random error for dairy cattle (~90% of the RMSPE) and CCC is ~0.7, both of which could be considered adequate, but it overestimated the mean of observations by ~8%. For beef cattle, this model had large slope bias (~30% of the RMSPE) while the prediction for sheep was characterised by a large mean bias (70% of the RMSPE).

Overall, the prediction of UN from the Thomson and Muir (2016) model has moderate to high precision (r^2 values of 0.60 to 89), which supports their statement that a model based on Ni provides “stronger” relationships with UN excretion than a model based on N_{diet}. The model of Luo and Kelliher (2010) had r^2 values between 0.42 and 0.63. The difference in dispersion of the data between the 2 variables is apparent in the scatterplots shown in Figure 7 and 8, particularly for the combined data (panels 7a and 8a) and beef cattle (panels 7b and 8b).

These 2 models were developed using combined data from different livestock classes to parameterise one predictive equation. Without debating the merit of predicting $UN_{\%exN}$ or UN, the evaluation of these 2 equations indicates that a single equation for combined data cannot predict either $UN_{\%exN}$ or UN with the same degree of accuracy and precision for all the livestock classes.

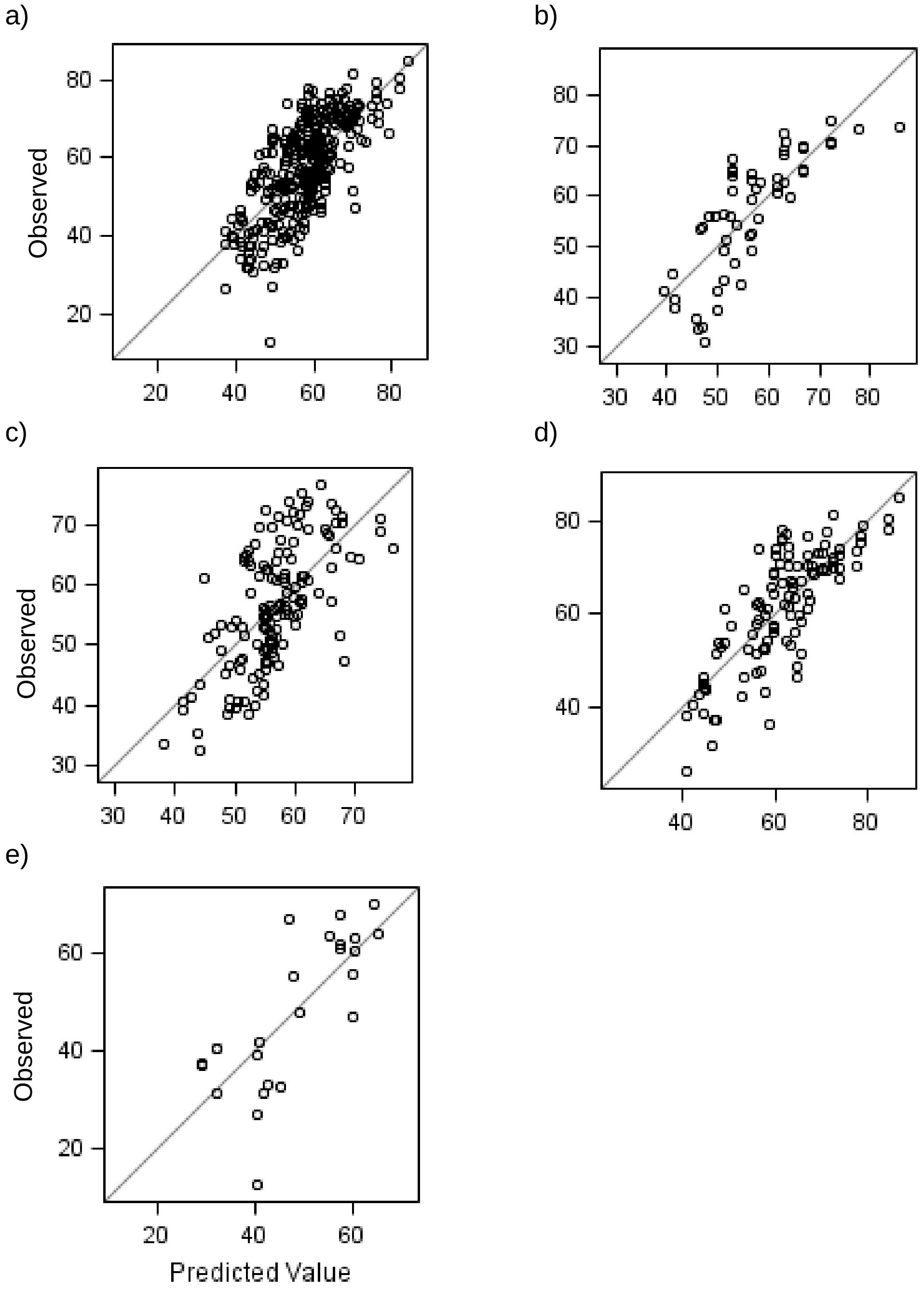

Figure 7. Scatter plots of values for the percentage of excreta nitrogen (N) accounted for by urine N ($UN_{\%exN}$) predicted from the equation of Luo and Kelliher (2010) versus the observed values for a) all livestock classes, b) beef cattle, c) dairy cattle, d) sheep and e) deer. The line represents perfect agreement (observed=predicted).

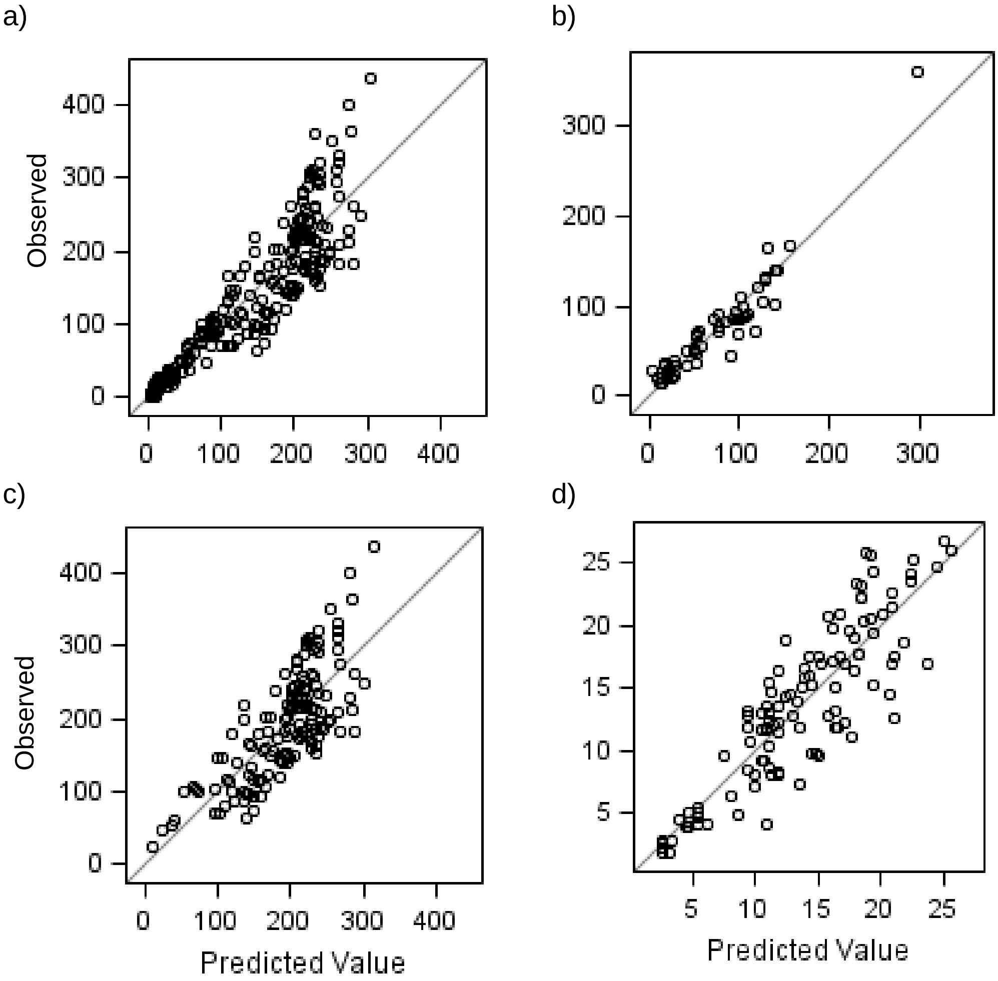

Figure 8. Scatter plots of values for the amount of urinary nitrogen (UN) excreted predicted from the equation of Thomson and Muir (2016) versus the observed values for a) all livestock classes, b) beef cattle, c) dairy cattle and d) sheep. The line represents perfect agreement (observed=predicted).

Table 8. Evaluation of the equations of Luo and Kelliher (2010) and Thomson and Muir (2016) to predict the percentage of urine nitrogen (N) in N excreted ($UN_{\%exN}$) and urine N (UN), respectively. Evaluation was conducted using the root mean square prediction error (RMSPE) and its decomposition (mean bias, slope bias and random error), the concordance correlation coefficient (CCC) and the RMSPE to standard deviation of the observations ratio (RSR). RPE is the relative prediction error (RMSPE expressed as a percentage of the mean of observed values and r^2 value is the coefficient of determination of the regression between observed and predicted values.

Model and variable predicted	**Livestock class**	**Mean observed**	**Mean predicted**	**Bias**	**MSPE**	**RPE**	**Mean bias (% RMSPE)**	**Slope bias (% RMSPE)**	**Random error (% RMSPE)**	**RMSPE**	**CCC**	**SRS**	**r^2**	**slope y=x**
Model from Luo & Kelliher (2010) for $UN_{\%exN}$														
$UN_{\%exN}$	Beef	56.5	56.5	0.0	55.3	13.2	0.0	5.9	94.1	7.4	0.72	0.62	0.63	1.24
$UN_{\%exN}$	Dairy	56.6	62.8	6.2	97.1	17.4	39.1	0.3	60.5	9.9	0.44	0.98	0.42	1.09
$UN_{\%exN}$	Deer	47.7	56.6	9.9	219.2	31.1	44.3	3.6	46.5	14.8	0.42	0.95	0.56	1.68
$UN_{\%exN}$	Sheep	61.5	60.7	0.5	57.5	12.3	0.4	0.0	98.9	7.6	0.76	0.61	0.63	1.07
Model from Thomson and Muir (2016) for UN														
UN	Beef	74.6	72.5	-2.1	480.6	29.4	0.9	31.3	67.8	21.9	0.90	0.39	0.89	1.31
UN	Dairy	192.5	208.4	15.9	2568.9	26.3	9.8	0.3	89.9	50.7	0.72	0.67	0.60	1.05
UN	Sheep	13.5	7.6	-5.2	38.8	46.1	70.3	2.4	25.1	6.2	0.56	0.96	0.77	1.20

4.3 Objective 2. Development of alternative models using the database collated

4.3.1 Initial exploration of the relationships between variables

Examination of the r^2 values from the all subsets regression analysis indicated that, with exception of $UN_{\%Ni}$ (percentage of N intake excreted in urine), a single variable tended to explain a large proportion of the variation in the dependent variables.

The plot of r^2 values against the number of independent variables (Figure 9) used in the multiple regression indicate that regression models with absolute amounts as dependent variables (e.g. UN and FN) have greater precision as defined by the larger r^2 values (>0.85) compared to regression models for relative amounts (e.g. $UN_{\%exN}$, $FN_{\%Ni}$ and $UN_{\%Ni}$), which had r^2 values between 0.35 and 0.65) as shown in Figure 9. This is in agreement with previous reports of prediction for both absolute and relative excretion of N (Dong et al., 2014; Stergiadis et al., 2015). Thomson and Muir (2016) also reported greater r^2 values for a regression equation using Ni to predict UN (absolute amount: g/d) compared to the regressions developed to predict UN relative to the total amount of N in excreta. When the data were analysed for each livestock class, a similar pattern was observed, but there were differences in the r^2 values differed for each of the dependent variables (FN, UN, $FN_{\%Ni}$, $UN_{\%Ni}$, $UN_{\%exN}$ for the different livestock classes (Appendix 4.).

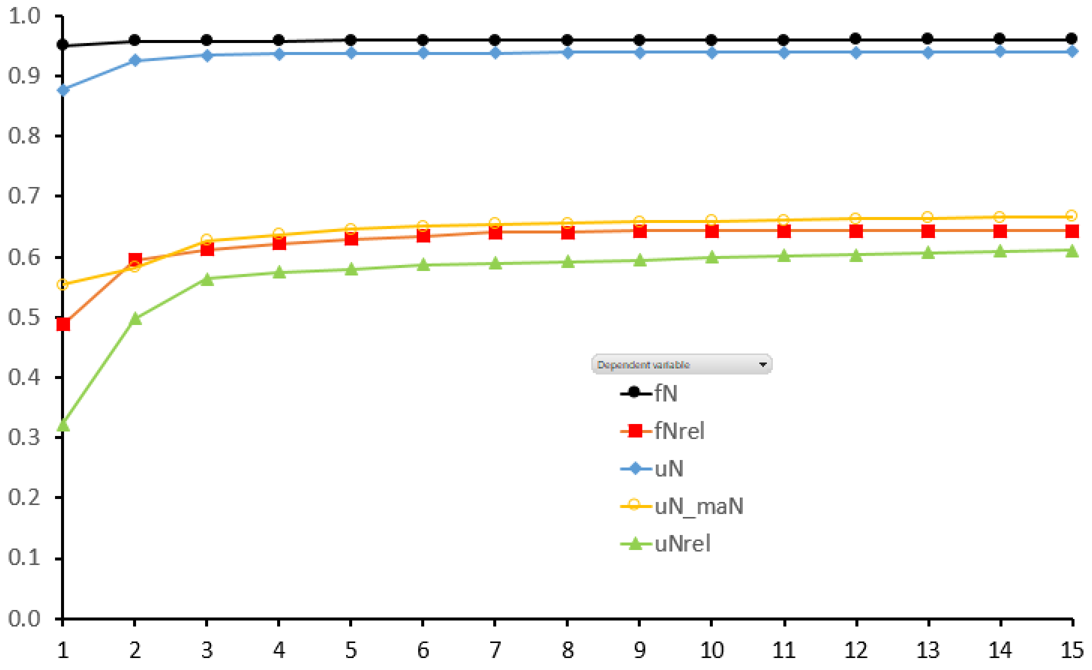

Figure 9. Coefficient of determination (r^2) of linear models as a function of the number of independent variables in the model (variables from Table 2).

Figure 9 also indicates that including a second and third explanatory variable increased the proportion of the variation explained by the model, but inclusion of four or more variables resulted only in small additional gains. Therefore, a relative simple equation with up to three independent variables appears to be sufficient to predict N excretion from the ruminants studied here.

From this initial analysis, it can be concluded that even if more data becomes available, it is unlikely that models of increasing complexity will result in increased precision of the prediction, unless variables other than ME and N content are used in AIM to describe the diets eaten by ruminants. Therefore, only models with up to three explanatory variables were further explored using mixed model regression methodology using the MIXED procedure in (SAS Institute Inc., 2012), using the sets of explanatory variables identified by the correlation and linear regression analysis.

When linear regressions models were built using a step-wise approach to variable selection, N_{diet} (N concentration in the diet eaten) was the single variable that explained a largest proportion of the variation in the dataset for dependent variables expressed as relative amounts (e.g. $UN_{\%exN}$, $UN_{\%Ni}$). This is to be expected because the concentration of N in the feed will affect the proportion of excreted in urine and is in agreement with the reports of Ledgard et al. (2003) and Luo and Kelliher (2010) who developed the current equation used in the AIM using N_{diet} as the single predictor. However, dietary N_{diet} does not indicate the amount of N excreted, because absolute excretion is a reflection of intake, and it is an important driver of GHG emissions and N leachate (Ledgard et al., 2009). The dependent variables expressed as absolute amounts (FN, UN; g/d), were best predicted by Ni as suggested by Thomson and Muir (2016).

Additional variables (from Table 2) selected for further development of models created from data for all livestock classes included DMI (kg/d and expressed as percentage of LW), ME intake per kg metabolic LW (MJ ME per $kg^{0.75}$), the squared term of N intake per kg of metabolic LW (g/kg), and the square term of the ratio of N to ME in the ration. When data for individual classes were used for model development, other variables in addition to N_{diet} and Ni were included as follows: N:ME ratio, quadratic forms of Ni and the N:ME ratio (for beef cattle); N intake per kg metabolic LW, DMI as percentage of LW and the quadratic form of N concentration in the diet (for dairy cattle); and N:ME ratio in linear and quadratic form and the quadratic for of N concentration in the diet (for sheep).

The regressions identified using the step-wise approach for variable selection were then progressed to model selection using mixed models and cross-validation approaches. The rationale behind the cross-validation is to identify the best model structures across a number (50 replicates) of models in which different sets of observations are used to develop and to evaluate the model. In this way, not only the amount of variance explained by an equation is considered, but also how well such equation predicts values outside the data used for its parameterisation.

4.3.2 Cross-validation results using linear mixed models

The results of the cross validation of models are presented in Figures 10 and 11 for the 5 dependent variables considered above (FN, UN, $FN_{\%Ni}$, $UN_{\%Ni}$, $UN_{\%exN}$). The r^2 value across the 50 replicates represents the level of agreement between the predictions from models created including a particular set of one, two or three explanatory variables and the observations left out of the dataset when building the model. In these histograms, gaps in the plot for a combination of livestock class and model indicates that the parameterisation did not converge into a solution or that a particular model structure was not used for that class.

In general, the results of the cross-validation show that nitrogen intake (Ni) is a better predictor of the amount of UN and FN (g/d), while N concentration in the feed (N_{diet}) is a better predictor of the excretion of N in relative terms ($UN_{\%exN}$, $UN_{\%Ni}$ and $FN_{\%Ni}$).

A second feature of the graphs is that the inclusion of more independent variables in the equations does not necessarily result in greater r^2 in the cross-validation set. This contrasts with the linear regression analysis (Figure 9) and could be related to the smaller number of observations available to estimate parameters for variables such as ME or LW (Appendix 2.) when mixed models were used. The difference between the r^2 of the regressions (Figure 9) and the r^2 of the cross-validation can also be explained by the fact that a model that explains most of the variation in a particular dataset may not necessarily be the best model to predict new observations. This is because models of increasing complexity have additional variables that, when included in the model, reduce the ‘noise’ inherent in the training dataset, but may not add value to explaining the underlying relationship between dependent and independent variables for new observations.

A third feature emerging from the cross-validation analysis is that for most of the variables under study, there will be marked differences in the predictive ability of models for different livestock classes, particularly for prediction of relative excretion ($UN_{\%exN}$, $UN_{\%Ni}$ and $FN_{\%Ni}$) which supports the finding from the evaluation of the models by Luo and Kelliher (2010) described in section 4.2. Models to predict partitioning of excreta from deer consistently featured lower cross-validation r^2 values than those models for other species, probably because there were fewer observations from deer studies. However, the number of observations for a livestock class is not always responsible for lower r^2 values, as exemplified by the consistently lower r^2 values from models for sheep, compared to beef cattle, despite the larger number of observations for the former.

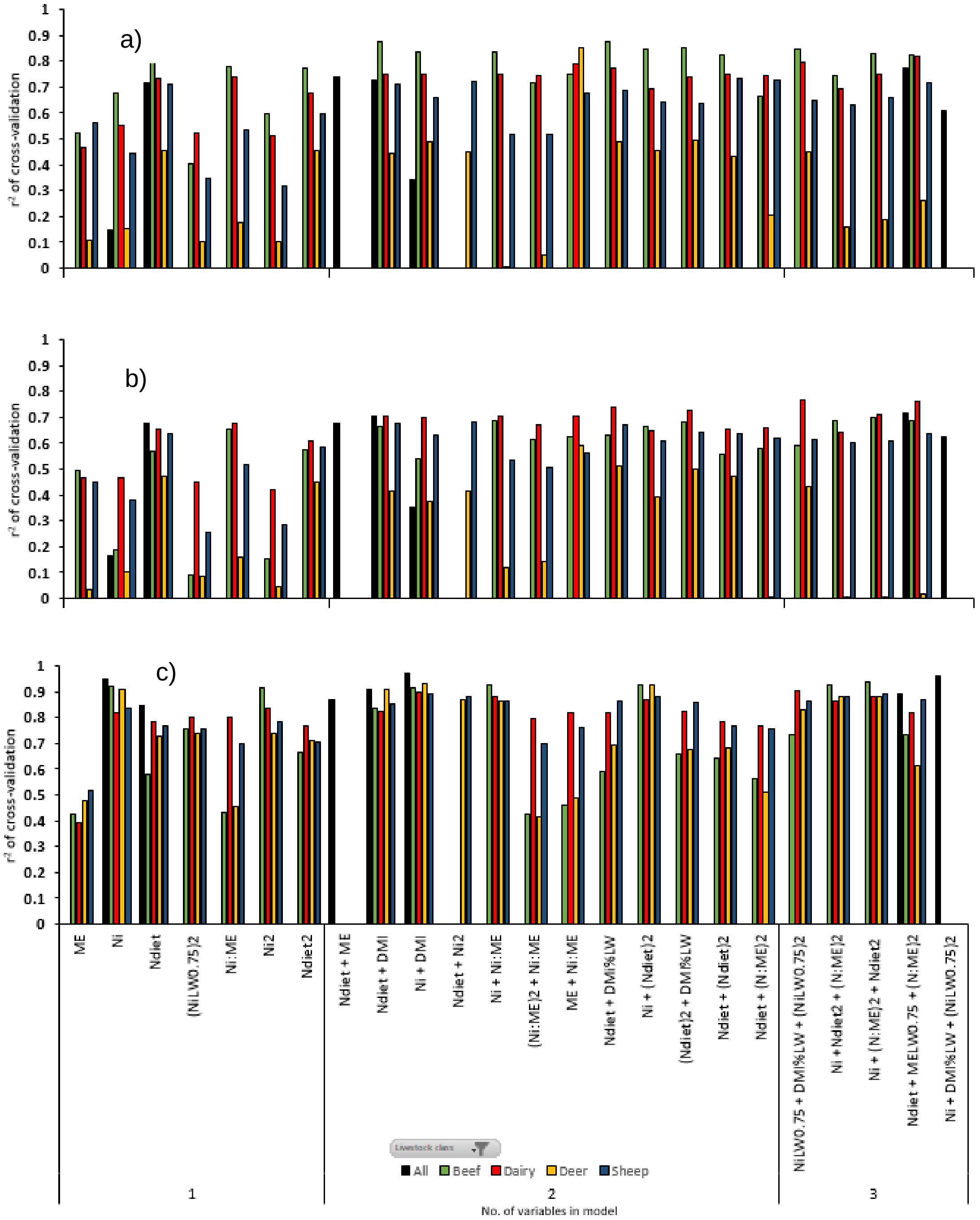

Figure 10. Coefficient of determination of the cross-validation of mixed regression models, using a 5-fold cross-validation with 50 replicates for urine N variables. The greater the bar, the better the model created with 80% of the data predicted values in the 20% of data left out in each replicate. Histograms included models created with data from all livestock classes (All) or class-specific models for a) urinary nitrogen (N) excretion expressed as a percentage of manure N excretion: UN$_{\%exN}$;, b) urinary N excretion expressed as percentage of N intake: UN$_{\%Ni}$ and c) urinary N excretion in grams per day. The histograms are for models that included 1, 2 or 3 explanatory variables.

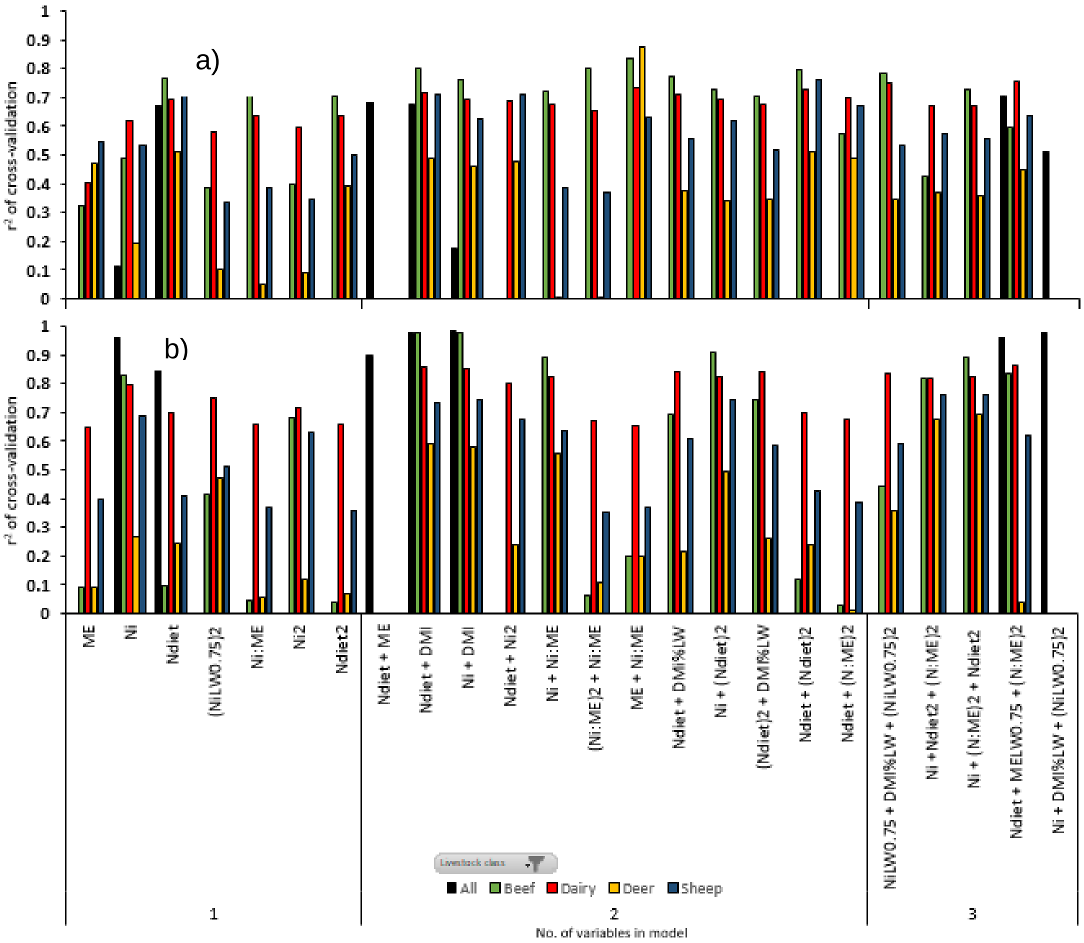

Figure 11. Coefficient of determination of the cross-validation of mixed regression models, using a 5-fold cross-validation with 50 replicates for faecal N variables. The greater the bar, the better the model created with 80% of the data predicted values in the 20% of data left out in each replicate. HIstograms included models created with data from all livestock classes (All) or class-specific models for a) faecal N excretion expressed as percentage of N intake: $FN_{\%Ni}$ and b) faecal N excretion in grams per day. The histograms are for models that included 1, 2 or 3 explanatory variables.

Based on the results of the cross-validation, a number of model structures were selected to generate predictive equations for the dependent variables (FN, UN, $FN_{\%Ni}$, $UN_{\%Ni}$ and $UN_{\%exN}$) based on all data and for each livestock class (Table 9). Models were chosen when there was a high r^2 from cross-validation. When several models had similar r^2 values, the model with the lower mean absolute error of the prediction was selected. These models were parameterised using the dataset summarised in Table 3, using the mixed model approach described in the methods.

Table 9. Models selected for development of predictive equations using the dataset for model development described in Table 3. The selection is based on the cross-validation modelling.

Dependent variables and model code	**Data used to develop model**	**Variables in model**
$UN_{\%exN}$		
1.01.01	All[1]	N_{diet}
1.01.02		N_{diet} + $ME_{LW}0.75$ + $(N{:}ME)^2$
1.01.03		N_{diet} + DMI
2.01.01	Beef	N_{diet} + $DMI_{\%LW}$
2.01.02		N_{diet}
2.01.03		N_{diet} + DMI
3.01.01	Dairy	N_{diet} + $ME_{LW}0.75$ + $(Ni{:}ME)^2$
3.01.02		N_{diet}
3.01.03		ME + N:ME
4.01.01	Deer	ME + N:ME
4.01.02		N_{diet} + N:ME
4.01.03		N_{diet}
5.01.01	Sheep	N_{diet} + $(N_{diet})^2$
5.01.02		N_{diet}
$UN_{\%Ni}$		
1.02.01	All	N_{diet}
1.02.02		N_{diet} + $ME_{LW}0.75$ + $(Ni{:}ME)^2$
2.02.01	Beef	Ni + NI:ME + $(N_{diet})^2$
3.02.01	Dairy	$Ni_{LW}0.75$ + $DMI_{\%LW}$ + $(Ni_{LW}0.75)^2$
4.02.01	Deer	ME + Ni:ME
5.02.01	Sheep	Ni + $(N_{diet})^2$
5.02.02		N_{diet} + $ME_{LW}0.75$ + $(Ni{:}ME)^2$
UN		
1.03.01	All	Ni
1.03.02		Ni + $Ni_{LW}0.75$ + $DMI_{\%LW}$
1.03.03		N_{diet} + DMI
2.03.01	Beef	Ni
2.03.02		Ni + $(N_{diet})^2$
2.03.03		Ni + DMI
3.03.01	Dairy	$Ni_{LW}0.75$ + $DMI_{\%LW}$ + $(Ni_{LW}0.75)^2$
3.03.02		Ni + $(N_{diet})^2$
3.03.03		Ni + DMI
4.03.01	Deer	Ni
4.03.02		Ni + DMI
5.03.01	Sheep	Ni + $(N_{diet})^2$
5.03.02		Ni + NI:ME + $(N_{diet})^2$
5.03.03		Ni + DMI

Dependent variables and model code	Data used to develop model	Variables in model
$FN_{\%Ni}$		
1.04.01	All	N_{diet}
1.04.02		$N_{diet} + ME_{LW}0.75 + (Ni:ME)^2$
2.04.01	Beef	$ME + Ni:ME$
3.04.01	Dairy	$N_{diet} + ME_{LW}0.75 + (Ni:ME)^2$
4.04.01	Deer	$ME + N:ME$
5.04.01	Sheep	$N_{diet} + (N_{diet})^2$
FN		
1.05.01	All	Ni
1.05.02		$Ni + DMI_{\%LW} + (Ni_{LW}0.75)^2$
1.05.03		$N_{diet} + DMI$
2.05.01	Beef	$Ni + (N_{diet})^2$
2.05.02		Ni + DMI
3.05.01	Dairy	$N_{diet} + ME_{LW}0.75 + (Ni:ME)^2$
3.05.02		Ni + DMI
4.05.01	Deer	$Ni + NI:ME + (N_{diet})^2$
4.05.02		Ni + DMI
5.05.01	Sheep	$Ni + (N_{diet})^2$
5.05.02		Ni + DMI

[1] Equations developed using data from all livestock classes included models with and without livestock class as term in the model. Model naming convention is dataset.variable.model number, where dataset 1 is all species, 2 is beef cattle, 3 is dairy cattle, 4 is deer and 5 is sheep; variable 1 is $UN_{\%exN}$; 2 is $UN_{\%Ni}$, 3 is UN, 4 is $FN_{\%Ni}$ and 5 is FN.

4.4 New equations developed using the training dataset

The following models were not further advanced because they contained non-significant slope parameters: models: 2.01.03, 3.01.03 ($UN_{\%exN}$), 1.02.01 with species effect, 1.02.02, 1.02.02 with species effect, 2.02.01, 3.02.01 (for $UN_{\%Ni}$); 1.03.02 with species effect, 2.03.02, 2.03.03, 3.03.01, 5.03.02 (UN); 1.04.02, 1.04.02 with species effect, 3.04.01 ($FN_{\%Ni}$) and 1.05.02 with species effect, 1.05.03 with species effect, 2.05.02 and 4.05.02 (FN).

4.4.1 Evaluation of models developed using the evaluation dataset

The analysis of the predictive ability of each of the models developed is presented in Tables A5.1 to A.5.5 in Appendix 5. Although some models were developed using data from all livestock classes, these models were evaluated both against the aggregated data and also against data each of the classes. This comparison is an important consideration in this study, because a 'universal' model may have different predictive ability for each of the livestock classes under study, as demonstrated in section 4.2.

In general, the RPE values indicate that $UN_{\%exN}$ is the variable that can be estimated with the smallest prediction error (approx. 15% of the observed mean), and this trend is observed regardless of whether models were developed using all data or from data for each livestock class separately. The models developed using all data tended to give poorer predictions for deer (UN, FN and $FN_{\%Ni}$) and sheep (UN, FN and $UN_{\%Ni}$). For these combinations of variables and species, the relative prediction error was between 32 to 63% of the mean of the observed values. Therefore, if a similar level of precision is desired for such variables, the use of species-specific models is essential.

In general, the models developed exhibited small mean and slope bias when evaluated against new data. Some of the models developed using data from all livestock classes had a large proportion of the prediction (~80%) being random, with exception of beef (UN and FN). While the use of class-specific data resulted in models with small biases for dairy cattle and sheep, the use of beef cattle and deer data did not lead to marked improvement in bias reduction relative to the 'universal models' based on all data.

Overall, the models developed using the combined data from all species had moderate to good accuracy, as indicated by CCC values of 0.6 to 0.7 for most variables. Relative to the equations generated using all data, improvements in accuracy were achieved for most variables when class-specific models were developed for dairy cattle, deer and sheep. Finally, the equations developed had prediction errors that was 0.6 to 0.8 of the standard deviation of the observations. This means that the error in the predictions is well within the variability on observed values.

The comparison of the models developed in this project against those obtained from the literature (Patra, 2010; Higgs et al., 2012; Dong et al., 2014; Stergiadis et al., 2015; Johnson et al., 2016) is also favourable. Most of the published models tested resulted in predictions with greater biases, greater RPE and lower CCC. In the case of models reported by Schuba et al. (2017), the predictions were poor, which could be due to an error in the parameters reported in the manuscript (Jan Schuba, pers. comm.). The predictions for dairy cattle from the model presented by Stergiadis et al. (2015) were also poor. In this case, the most likely explanation is that the models in that publication were developed to predict N partitioning from dry cows fed at maintenance intakes, which had much smaller N intakes (0.4 to 2.2 g/kg $LW^{0.75}$) compared to the values in the current dataset for dairy cattle (0.9 to 6.1 g/kg $LW^{0.75}$). The models proposed by Dong et al. (2014) were generated from studies that used diets typical of feedlots in North America (high proportion of processed cereal grains) and that could explain their poorer performance predicting N excretion from forage based diets. If the diet type underlying the model development is the reason for the discrepancy between the models of Dong et al. (2014)

and the ones developed as part of this project, it validates our criteria for selection of studies to predict diets representative of New Zealand conditions.

4.5 Alternative equations for inclusion in AIM

In the following section, we present three different alternatives to estimate the partition of N in excreta. For each of the alternatives, the equations proposed were selected based on the evaluation of the models' predictive performance (Tables in Appendix 5). The selection of models was based on identification of models with small bias and RMSPE, and greater proportion of random error, CCC and r^2 of the regression between predicted and observed values using the results from the evaluation dataset[1]. Where models of different complexity had similar predictive ability, the simpler model of a group was chosen.

The three scenarios presented are offered to suit different levels of integration in AIM:

Alternative 1. An improved equation for the current AIM framework, namely, a single equation that predicts $UN_{\%exN}$ for all four livestock classes (beef, dairy, deer and sheep).

Alternative 2. A selection of models that best predict $UN_{\%exN}$ for each of the four livestock classes.

Alternative 3. An alternative to predict absolute amounts of FN, rather than the relative contribution of UN to total N in excreta.

4.5.1 Alternative 1: one equation in AIM for all livestock classes.

Two equations are presented as alternatives to improve the predictions of N partitioning within AIM while maintaining the model algorithms largely unchanged. The equations are presented with the standard error of the estimate as subscript in brackets. Unless specified, the probability of the parameters being zero is less than 0.05.

The models selected as alternatives to the current equation to predict the proportion of excreta N as urine are model 1.01.01 and 1.01.03 (Table 9):

$$UN_{\%exN} = 25.060_{(1.759)} + (N_{diet} \times 12.441_{(0.751)}) \qquad \text{(Eq. 1)}$$

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[1] We acknowledge that the evaluation set is smal for some livestock classes, but when the models listed were evaluated with the commonly used approach of using the same dataset for training and evaluation, the results suggested that the models chosen were suitable to predict both within and outside the training dataset (Appendix 6).

and

$$UN_{\%exN} = 26.573_{(1.762)} + (N_{diet} \times 12.972_{(0.740)}) + (DMI \times 0.321_{(0.093)}) \qquad \text{(Eq. 2)}$$

where N_{diet} is the concentration of N in the diet (g/100g DM) and DMI is the amount of feed eaten by the animal (kg DM/d).

Compared to more complex models (e.g. 1.01.02), these two equations had good distribution of random error (>76%) for all livestock classes, smaller bias and RMSPE, but were outperformed by model Model 1.01.02 in terms of precision (i.e. they had slightly lower r^2 values for the regression of observed vs. predicted values) (Table 10).

Equations 1 and 2 outperformed the current equation in AIM by having smaller mean bias (-3.1 to 3.7 vs. 0.02 to 6.9 for the different classes) and, overall, a greater proportion of random error (40 to 99% vs. 24 to 90.1 for the different classes). For beef cattle, the improvement is particularly noticeable with the RMSPE from the 2 proposed alternatives (~5%) being less than half of the value from the model of Luo and Kelliher (2010).

These 2 models also outperformed published models to predict excretion from beef cattle (Dong et al., 2014) and dairy cattle (Stergiadis et al., 2015) by having smaller bias, greater proportion of random error and smaller RMSPE (Appendix 5).

4.5.2 Alternative 2: one equation in AIM for each livestock class

While the equations proposed in the previous section have a better predictive performance than the current equation used in AIM, the RPE for deer is larger (~19%) than for the other livestock classes (~12%) while predictions for beef cattle have larger mean bias (~16% of the RMSPE) than those of the other classes (~5% of the RMSPE). The use of class-specific equations is a means to achieving similar levels of precision and accuracy for the prediction of N excreta across the four livestock classes (Table 11).

4.5.2.1 Equation for prediction of $UN_{\%exN}$ from beef cattle

Despite its larger proportional mean bias relative to other classes, the model 1.01.03 (Equation 2) was the best model identified for this livestock class. As discussed before, this model outperformed the current equation in AIM and published models to predict portioning of N excreta from beef cattle (Dong et al., 2014)

$$UN_{\%exN} = 26.573_{(1.762)} + (N_{diet} \times 12.972_{(0.740)}) + (DMI \times 0.321_{(0.093)}) \qquad \text{(Eq. 2)}$$

4.5.2.2 Equation for prediction of $UN_{\%exN}$ from dairy cattle

For dairy cattle, model 3.01.01 based on the dairy cattle data only, including ME intake per unit of metabolic LW and the ratio of Ni to ME in addition to the N concentration in the feed, resulted in slightly smaller relative prediction error (11.6% vs 12.1 to 12.6%) and slightly better precision (r^2, 0.43 vs. 0.33 to 0.35) and accuracy (CCC: 0.64 vs. 0.55) than the equations presented for this livestock class in the previous section.

$UN_{\%exN} = 24.527_{(4.659)} + (N_{diet} \times 22.676_{(3.417)} + (ME_{LW0.75} \times -9.206_{(2.444)} + [(Ni:ME)^2 \times -2.116_{(0.734)}]$ (Eq. 3).

where N_{diet} is N concentration in the diet as explained above, $ME_{LW0.75}$ is the ME intake (MJ per kg of $LW^{0.75}$) and Ni:ME is the ratio of N in the feed to ME intake (g N/MJ ME per kg DM.).

4.5.2.1 Equation for prediction of $UN_{\%exN}$ from deer

A model incorporating the ratio of N:ME in the diet in addition to the N concentration of the feed (4.01.02) generated using only deer data is proposed because of its greater accuracy and precision, as denoted by its smaller RPE (15% vs. ~19%) and greater CCC (0.67 vs. 0.38) and r^2 (0.53 vs. 0.27) than the single equation for all classes:

$UN_{\%exN} = 5.699_{(21.058)} + (N_{diet} \times 28.151_{(9.666)}) + (N:ME \times -7.823_{(3.938)})$ (Eq. 4)

where N:ME is the ratio of N to ME (g N/MJ ME per kg of feed DM).

Although model 4.01.01, also generated from deer-specific data, had an even lower RMSPE than the proposed deer-specific equation, it was not recommended here because of the large proportion of error contributed by mean bias (~50%). However, equation 4 has the drawback of large standard error of the parameters, with the p-values for the intercept being 0.80 (i.e. not significantly different than zero) and for the Ni:ME 0.09.

4.5.2.2 Equation for prediction of $UN_{\%exN}$ from sheep

For sheep, model 1.01.03, including DMI (kg/d) in addition to the concentration of N in the diet (N_{diet} g/100 g DM) and generated from data for all the livestock classes is proposed as an alternative to the current equation in AIM because it predicts with slightly smaller RMPSE (8.1 vs. ~8.5) and slope bias (1.2 vs.9.4% of RMSPE) and slightly greater CCC (0.73 vs. 0.67) compared to the equation of Luo and Kelliher (2010), although with a slightly greater mean bias.

$UN_{\%exN} = 26.573_{(1.762)} + (N_{diet} \times 12.972_{(0.740)}) + (DMI \times -0.321_{(0.093)})$ (Eq. 2)

Table 10. Comparison of the predictive performance of models developed in this project with the current equation in AIM (Luo and Kelliher, 2010) to predict the percentage of urinary nitrogen (N) in excreta ($UN_{\%exN}$). Evaluation was conducted using the root mean square prediction error (RMSPE) and its decomposition (mean bias, slope bias and random error), the concordance correlation coefficient (CCC) and the RMSPE to standard deviation of the observations ratio (RSR). Codes for model developed in this project are in Table 9. RPE is the relative prediction error (RMSPE expressed as a percentage of the mean of observed values and r_2 value is the coefficient of determination of the regression between observed and predicted values.

						Error partitioning (% RMSPE)						
Model and livestock class	**Mean observed**	**Mean predicted**	**Bias**	**RMSPE**	**RPE**	**Mean bias**	**Slope bias**	**Random error**	**CCC**	**SRS**	**r2**	**slope y=x**
1.01.01 (**Equation 1**)												
Beef	45.3	47.3	1.9	4.43	9.8	19.1	2.2	78.8	0.78	0.62	0.67	0.90
Dairy	61.2	61.3	0.2	7.39	12.1	0.0	2.5	97.4	0.54	0.82	0.33	0.81
Deer	58.3	58.9	0.6	11.01	18.9	0.3	1.1	98.7	0.38	0.77	0.27	1.21
Sheep	61.7	58.7	-3.1	8.75	14.2	12.2	2.1	85.7	0.69	0.67	0.60	1.15
1.01.03 (**Equation 2**)												
Beef	45.3	47.2	1.8	4.00	8.8	21.1	2.2	76.8	0.83	0.56	0.74	0.91
Dairy	61.2	58.8	-2.4	7.70	12.6	9.8	3.7	86.5	0.55	0.85	0.35	0.78
Deer	58.3	61.4	3.1	11.34	19.5	7.2	0.9	91.9	0.38	0.79	0.28	1.19
Sheep	61.7	61.3	-0.4	8.12	13.2	0.3	1.2	98.5	0.73	0.62	0.60	1.10
Luo and Kelliher (2010)												
Beef	45.3	52.2	6.9	7.96	17.6	75.4	0.2	24.4	0.50	1.11	0.67	1.06
Dairy	61.2	64.1	2.9	7.86	12.9	13.9	0.1	86.1	0.47	0.87	0.33	0.96
Deer	58.3	62.0	3.7	11.73	20.1	10.1	2.9	87.0	0.32	0.82	0.27	1.43
Sheep	61.7	61.9	0.2	8.52	13.8	0.0	9.4	90.6	0.67	0.65	0.60	1.36

Table 11. Predictive performance of livestock class-specific models proposed to predict the percentage of urinary nitrogen (N) in excreta ($UN_{\%exN}$). Evaluation was conducted using the root mean square prediction error (RMSPE) and its decomposition (mean bias, slope bias and random error), the concordance correlation coefficient (CCC) and the RMSPE to standard deviation of the observations ratio (RSR). Codes for model developed in this project are in Table 9. RPE is the relative prediction error (RMSPE expressed as a percentage of the mean of observed values and r_2 value is the coefficient of determination of the regression between observed and predicted values.

						Error partitioning (% RMSPE)						
Model and livestock class	**Mean observed**	**Mean predicted**	**Bias**	**RMSPE**	**RPE**	**Mean bias**	**Slope bias**	**Random error**	**CCC**	**SRS**	**r^2**	**slope y=x**
1.01.03 (**Equation 2**)												
Beef	45.3	47.2	1.8	4.0	8.8	21.1	2.2	76.8	0.83	0.56	0.74	0.91
Sheep	61.7	61.3	-0.4	8.1	13.2	0.3	1.2	98.5	0.73	0.62	0.60	1.10
3.01.01 (**Equation 3**)												
Dairy	61.1	59.7	-1.4	7.1	11.7	3.6	4.5	91.9	0.64	0.79	0.43	0.80
4.01.02 (**Equation 4**)												
Deer	58.3	59.7	1.4	9.0	15.3	2.4	0.2	97.4	0.67	0.62	0.53	1.05
5.01.02 (**Equation 5**)												
Sheep	61.7	61.9	0.2	8.3	13.4	0.0	3.7	96.3	0.71	0.63	0.60	1.19

A second option for this livestock class is an equation that has the same structure to Equation 1, but parameterised using only data from sheep studies (model 5.01.02). This option (Equation 5) maintains some of the advantages listed for Equation 2 in terms of RMSPE, CCC and random error, while also matching the performance of the model of Luo and Kelliher (2010) with regards to mean bias (<0.1 % of RMSPE).

$$UN_{\%exN} = 29.539_{(2.479)} + (N_{diet} \times 11.980_{(1.032)}) \qquad \text{(Eq. 5)}$$

4.5.3 Alternative 3: predicting faecal nitrogen in AIM instead of the prediction of the proportion of urine in excreta

The equations presented in Sections 4.5.1 and 4.5.2 above represent an improvement for predicting the percentage of excreta N accounted for by urine. However, we suggest the partitioning of excreta N into urine and faeces should be based on an estimate of FN with UN calculated by difference. This will provide both the distribution of N between urine and faeces, and the amount of N in each excreta type, which then can be used to estimate GHG (and nitrate leaching) because they are primarily affected by the amount of UN deposited in the soil (Selbie et al., 2015).

The rationale for our suggestion of predicting N is based on the methodological aspects of N balance studies in ruminants and errors associated with the measurement of UN. A nitrogen balance requires measurement of the amounts of N eaten, the amounts of faeces and urine produced and their N concentration and the amount of N in milk. The difference between inputs (feed) and outputs (milk, faeces and urine) is often deemed to be the amount of N retained in tissues (N retention, in LW gain, wool, etc). However, several authors have suggested that many reported values for N retention (based on N balance studies) are too high to be explained by gains in LW (Higgs et al., 2012; Moate et al., 2017). MacRae et al. (1993) provided evidence that N balance over-estimate N retention when compared to measurements of tissue accretion using tracer amino acids.

While experimental error in measuring inputs (feed) and outputs (faeces and urine) all contribute to the error in estimated N retention, overestimation of N retention is primarily due to N losses from urine, leading to underestimation of urine N (Spek et al., 2013). This is because urinary N can be volatilised and lost as ammonia, with losses which can be as high as 100 g/day from lactating dairy cows (Spek et al., 2013). In N balance studies, it is common practice to acidify the urine collected to pH < 4, but variation in procedures, the amounts of acid and urine, efficacy of mixing and also the efficacy of ventilation systems in animal facilities all contribute to variation in the accuracy of urinary N measurements.

Correction of urinary N excretion values for lactating animals can be done by subtracting FN and milk N from Ni, assuming no retention in body tissues. For growing animals, determining of urine N would require measuring the rates of LW gain, and while the amount of N in gain is a small proportion of Ni, LW gain cannot be measuring accurately when animals are maintained indoors during N balance studies. Corrections to the amounts of UN amounts were not undertaken in this project, but should be considered in a separate project. Spek et al. (2013) reported that correcting UN by assuming zero N retained could result in a trade-off between precision and accuracy of a model.

In their analysis of models to predict UN and FN, Johnson et al. (2016) also indicated that UN is the form of N excretion that is predicted with most bias, citing similar methodological issues as the ones above, which supports our statement that predicting FN is a sensible approach to be considered in AIM. Therefore, we propose that FN is predicted within AIM as a preferred approach because the data used to generate predictive equations is less impacted by experimental and methodological errors. Also, because of the explanation above, the models for predicting UN or $UN_{\%Ni}$ were not further explored as alternatives.

4.5.3.1 Equations for prediction of faecal N excretion for beef, dairy and deer

In general, the models for predicting FN from beef cattle had relatively large proportion of mean and slope bias contributing to the error. Despite of this, an equation generated from all data (model 1.05.03 in Table 9) still yielded smaller bias and RPE than any of the published models evaluated for data from this livestock class.

$$FN = -4.623_{(1.730)} + (N_{diet} \times 1.970_{(0.627)}) + (DMI \times 7.890_{(0.199)}) \qquad \text{(Eq. 6)}$$

where N_{diet} is the concentration of N in the diet (g/100 g DM) and DMI is the feed intake by an animal (kg DM/d).

The RPE for equation 6 (14.4 and 15.1% of the observed mean for beef and dairy cattle, respectively) is comparable to the RPE for models to predict $UN_{\%exN}$ presented in the sections 4.5.1 and 4.5.2 above. Also, the RPE is much lower than those obtained from published equations (23 to 52%: Table 12). However, if the prediction of FN is implemented in AIM, further evaluation and fine-tuning of this equation as more beef cattle data becomes available would be recommended.

For dairy cattle, Equation 6 had a large proportion of random error (~90%), a slightly greater CCC and slightly smaller RPE than model 3.05.01, which is far more complex.

For deer, this model outperformed those developed with deer-specific data, resulting in smaller RPE and greater CCC and r^2 and by having a larger proportion of random error (79%) than the next best model (4.05.02 with 70%).

For Equation 6, the selection of DMI and N_{diet} as separate inputs, instead of their combined function (i.e. Ni) has a biological basis because DMI is directly related to the endogenous faecal losses (NRC, 2001). These losses have been postulated to be constant across species, even those with different digestion types (e.g. hindgut vs. foregut fermenters: Richard et al., 2017), providing a justification for the use of a common equation across livestock classes. The integration of DMI in the equation to predict FN is also in agreement with a number of models that have been developed and include DMI as an explanatory variable (e.g. see Johnson et al., 2016).

4.5.3.1 Equation for prediction of faecal N excretion for sheep

Sheep was the only livestock class for which an equation developed from class-specific data (model 5.05.01 from Table 9) had better predictive performance than the Equation 6 presented above.

$$FN = 2.230_{(0.299)} + (Ni \times 0.299_{(0.023)}) + [(N_{diet}^{2}) \times - 0.237_{(0.042)}] \qquad \text{(Eq. 7)}$$

where Ni is the intake of N (g/d) and N_{diet}^2 is the quadratic form of the concentration of N in the feed dry matter (g/100g DM).

Table 12 presents the predictive performance of the model proposed against alternative models available in the literature.

Relative to Eq. 6, Equation 7 had slightly greater proportion of random error and CCC and slightly smaller RPE and r^2. Schuba et al. (2017) also reported a model to predict FN as a function of Ni, but their model had parameters that were not significantly different from zero. Other published models to predict FN in sheep have also included Ni alone and Ni and N_{diet} as predictors (Patra, 2010), supporting our findings. Compared to published models (Patra, 2010; Schuba et al., 2017), Equation 7 resulted in predictions with smaller bias (RPE 28% vs. > 45%) and better distribution of the prediction error (86% of error being random vs. <76%), although it is noted that the parameters of the models reported by Schuba et al. (2017) may contain an error (J. Schuba, pers. comm.).

Because in AIM the amount of total N excreta is known, the prediction of FN is compatible with the model's structure. By subtracting FN from total N excreta, then it is possible to estimate UN to then calculated nitrous oxide emissions from urine patches in agricultural soils.

Table 12. Evaluation of proposed models to predict faecal nitrogen (N) output (g/d) using the root mean square prediction error (RMSPE) and its decomposition (mean bias, slope bias and random error), the concordance correlation coefficient (CCC) and the RMSPE to standard deviation of the observations ratio (RSR). See footnote for codes for models from the literature. RPE is the relative prediction error (RMSPE expressed as a percentage of the mean of observed values), r^2 value is the coefficient of determination of the regression between observed and predicted values, with slope y=x.

Model	Data used	Livestock class	Mean observed	Mean predicted	Bias	RPE	Mean bias (%RMSPE)	Slope bias (%RMSPE)	Random error (%RMSPE)	RMSPE	CCC	SRS	r^2	slope y=x
Mod1.05.03 (**Eq. 6**)	All	Beef	58.0	61.8	3.9	14.4	21.1	37.7	41.2	8.4	0.94	0.31	0.96	1.26
ModJohnson41	Beef	Beef	58.0	51.2	-6.8	23.2	25.3	6.9	67.8	13.4	0.84	0.50	0.82	1.18
ModJohnson42	Beef	Beef	58.0	46.5	-11.5	37.4	28.2	45.8	26.0	21.7	0.47	0.80	0.82	2.69
ModJohnson43	Beef	Beef	58.0	43.9	-14.1	49.4	24.2	2.4	73.3	28.6	0.07	1.06	0.10	2.23
ModJohnson44	Beef	Beef	58.0	39.9	-18.1	52.7	35.1	0.6	64.2	30.6	0.09	1.13	0.10	1.43
ModJohnson45	Beef	Beef	58.0	44.6	-13.3	36.4	39.9	32.7	27.4	21.1	0.55	0.78	0.82	2.07
ModSchuba2b	Beef	Beef	58.0	392.2	334.2	614.4	88.0	11.9	0.1	356.2	0.06	13.16	0.82	0.16
Mod1.05.03 (**Eq. 6**)	All	Dairy	137.2	139.3	2.1	15.1	1.0	9.2	89.8	20.7	0.75	0.68	0.57	0.78
ModHiggsFN5	Dairy	Dairy	137.2	174.4	37.3	32.5	70.0	12.7	17.3	44.5	0.49	1.46	0.62	0.60
ModJohnson11	Dairy	Dairy	137.2	158.4	21.2	23.7	42.2	20.4	37.4	32.6	0.61	1.07	0.56	0.60
ModJohnson13	Dairy	Dairy	137.2	158.5	21.4	21.7	51.4	0.4	48.2	29.8	0.54	0.98	0.52	0.92
ModJohnson14	Dairy	Dairy	137.2	145.4	8.2	18.7	10.1	29.7	60.2	25.7	0.71	0.84	0.56	0.61
ModJohnson15	Dairy	Dairy	137.2	147.9	10.8	17.5	20.0	19.7	60.3	24.0	0.74	0.79	0.61	0.69
ModJohnson16	Dairy	Dairy	137.2	151.7	14.5	19.7	28.5	13.1	58.3	27.1	0.65	0.89	0.52	0.69
Mod1.05.03 (**Eq. 6**)	All	Deer	13.1	12.0	-1.1	22.2	13.5	7.7	78.9	2.9	0.79	0.51	0.74	1.23
Mod5.05.01 (**Eq. 7**)	Sheep	Sheep	8.4	8.2	-0.2	28.0	0.9	12.8	86.3	2.4	0.72	0.61	0.67	1.37
ModPatra3a	Sheep	Sheep	9.3	12.3	3.1	44.6	54.5	0.0	45.4	4.1	0.46	1.07	0.49	1.03
ModSchuba2c	Sheep	Sheep	8.4	54.0	45.5	552.2	95.4	4.3	0.3	46.6	0.03	12.03	0.54	0.22

‘ModJohnsonsonXX’ are models reported by Johnson et al. (2016), using the model notation as reported in the publication; ‘ModPatraXx’ are models reported by Patra (2010), named after the table number in which the model was reported; ‘ModSchubaXx’ are models reported by Schuba et al. (2017), named after the table number in which the model was reported. “ModHiggs’ is the model reported by Higgs et al. (2012) as reported in the publication.

4.6 Implications of the implementation of the equations developed into the New Zealand inventory

Three alternative scenarios have been developed, based on either $UN_{\%exN}$ for all or individual livestock classes or the prediction of FN enabling the calculation of UN. The implications of these alternative equations for use in AIM to calculate the GHG emissions are two-fold.

Firstly, the implementation of a new equation requires suitable representation of the independent variables in the model. Although some models have been developed using dietary compositions variables such as neutral detergent fibre, ash and rumen degradable protein (Higgs et al., 2012; Johnson et al., 2016), we have limited this study to the variables that are currently used in AIM. In terms of implementation, Equations 1, 2 and 5 would be the most expeditious way to introduce an improvement in the inventory predictions compared to the use of the current equation. Equations 3 and 4 require reliable estimates of LW of the animals and ME of the diet. If these variables are not adequately estimated, there is a risk that predictions will then lack in accuracy. Investigating the quality of these driver variables (LW, ME, N_{diet}) within the AIM is beyond the scope of this project.

Table 13. Calculation of the impact on the predictions of nitrous oxide (N_2O) and total greenhouse gases (GHG: expresed as CO_2-equivalents: CO_2-e) emissions in the Agricultural Inventory Model (AIM) resulting from alternative equations developed in this project. Data used for the calculations corresponds to the 2015 inventory values and alternatives detailed in Section 4.5, and includes a correction for excreta N for sheep introduced in 2017 (M. Rollo, pers. comm.).

	BAU[1]	**Alternative 1**	**Alternative 2**	**Alternative 3**
Equation	Luo and Kelliher (2010)	Eq. 1 (all classes)	Eq. 2 (beef cattle) Eq. 3 (dairy cattle) Eq. 4 (deer) Eq. 5 (sheep)	Eq. 6 (beef, dairy and deer) Eq. 7 (sheep)
Independent variables	N_{diet} = 3.7	N_{diet} = 3.7	N_{diet} = 3.7 ME = 11.46 (dairy) 10.53 (deer) LW = 448 (dairy) DMI = 7.5 (beef)	N_{diet} = 3.7 DMI =10.7 (dairy) 7.5 (beef) 1.6 (sheep) 2.9 (deer)
Predicted variable and values	$UN_{\%exN}$ 72.4% (all livestock classes)	$UN_{\%exN}$ 71.1% (all livestock classes)	$UN_{\%exN}$ 74.8% (dairy) 77.0% (beef) 73.9% (sheep) 82.4% (deer)	FN 87 g/d (dairy) 61 g/d (beef) 17 g/d (sheep) 26 g/d (deer)
Total N_2O (kT)	29.36	29.53	30.24	29.32
Δ (% relative to BAU)	0	- 0.8 %	+ 1.6 %	- 1.5 %

[1] BAU: business as usual, current equation in AIM.

Δ: change

The second implication of the use of new equations is the actual effect that the new equation will have on the prediction of GHG emissions (nitrous oxide in this case), when integrated in the AIM. The effect of introducing changes in the equations for each scenario is presented in presented in Table 13.

The estimation of FN presented in Table 13 equate to N digestibility values of 0.72 to 0.78, which are close to estimated values reported for pasture by Waghorn et al. (2007) (0.60 to 0.82), considering that a pasture with 3.7% N would be expected to be in the upper range in quality.

The results presented in Table 13 indicate that the equations proposed are readily implementable in AIM and that changes to the equation would result in very small changes in the overall nitrous oxide emissions from agricultural soils in the inventory (from -0.7 to + 1.6%), which are likely to fall within the margin of error of the inventory. It is noted that the changes recommended are based on the analysis of predictive quality of different equations from an expanded dataset and best-practice approaches for model evaluation (Tedeschi, 2006). The use of such principles in the selection of equations will help to increase the confidence in the predictions of AIM. The changes in emissions presented in Table 13 are for indicative purposes only and are secondary to the robustness of the evaluation of equations presented in this report.

Improvements in inputs, especially N concentrations of the diet, are essential to provide more accurate estimates in N excreta and then the value of calculating amounts of FN and deriving UN will become apparent to enable a defensible calculation of GHG from agricultural soils. This is because the use of a single value to describe the N content of the feed may be inconsistent with values reported for diets for different livestock classes (e.g. Figure 2).

5. Conclusions and Recommendations

The evaluation of the current equation for *partitioning of excreta* N in the AIM (Luo and Kelliher) show the predictions from this equation have a systematic bias for at least 3 out of the 4 livestock classes under study, with over prediction of observed values collated from the literature. Using the same dataset, the equation proposed by Thomson and Muir (2016) to predict the *amount of urinary N* also was biased, slightly over predicting data for dairy cattle and under predicting for beef cattle (slightly) and sheep (markedly).

Because neither equation had good predictive performance across the four livestock classes of interest, new equations with improved predictive performance (compared to these two models and published models) were developed. These new models were characterised by smaller biases, greater proportion of random error in the prediction and accuracy, and generally greater precision. The evaluation of the models presented here were performed using a dataset which included observations not used in the model development. This is a different approach to those used in previous reports and published journal articles, where the adequacy of the model has been evaluated by comparing the predictions of models against data used in their parameterisation. We acknowledge that the evaluation dataset is small for beef cattle and deer and future evaluation of the equations proposed here would be advisable.

While the equations proposed to predict the percentage of UN in excreta N are an improvement over the *status quo* in terms of accuracy and precision, errors in the measurement of UN excretion, even with total collection methods, has resulted in our recommendation that the AIM structure is modified to predict FN, and this will enable a more robust estimation of UN. Such change would be readily implementable and would contribute to increasing the confidence of the estimates for excreta N in the national inventory.

Recommendation 1.

That the AIM is updated with equations 6 and 7 generated in this project to predict FN (g/d) instead of predicting the proportion of UN in excreta.

$FN = -4.623 + (N_{diet} \times 1.970) + (DMI \times 7.890)$ (Eq. 6)

$FN = 2.230 + (Ni \times 0.299) + [(N_{diet}^2) \times - 0.237]$ (Eq. 7)

Recommendation 2.

If Recommendation 1 is not implemented, that livestock class-specific equations (equations 2-5 generated in this project) are introduced in AIM to predict the proportion of UN in excreta.

$UN_{\%exN} = 26.573 + (N_{diet} \times 12.972) + (DMI \times 0.321)$ (Eq. 2)

$UN_{\%exN} = 24.527 + (N_{diet} \times 22.676) + (ME_{LW0.75} \times -9.206) + [(N:ME)^2 \times -2.116]$ (Eq. 3)

$UN_{\%exN} = 5.699 + (N_{diet} \times 28.151) + (N:ME \times -7.823)$ (Eq.4)

$UN_{\%exN} = 29.539 + (N_{diet} \times 11.98)$ (Eq. 5)

Recommendation 3.

If recommendations 1 and 2 are not implemented, and the use of a single equation is preferred, that equation 1 generated in this project replaces the equation by Luo and Kelliher (2010).

$$UN_{\%exN} = 25.060 + (N_{diet} \times 12.441) \quad \text{(Eq. 1)}$$

Recommendation 4.

If recommendations 2 or 3 are adopted, or the *status quo* retained, then a review should be commissioned to determine the impact of correction of underestimated values of UN excretion on the equations used in AIM.

Recommendation 5.

Although not part of the scope of this project, we recommend that N_{diet} values, upon which the AIM is based, is improved by incorporating representative and readily available data for the concentration of N in diets consumed by New Zealand ruminants on a monthly basis (e.g. Wilson et al., 1995; Litherland and Lambert, 2007).

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8. Appendices

Appendix 1. List of references used in the project.

List of references included in the database.

Ref. No.	Author and year of publication	Livestock class	Reference	Number of means included
1	Archibeque et al. (2001)	Beef	J. Anim. Sci. 79:1937-1943	4
2	Archibeque et al. (2002)	Beef	J. Anim. Sci. 80:1344-1351	2
3	Betteridge et al. (1986)	Beef	J. Agric. Sci. 106:393-404	11
4	Browne et al. (2005)	Beef	Anim. Feed.Sci. Tech. 119:55-68	4
5	Drewnoski and Poore (2012)	Beef	J. Anim. Sci. 90:881-891	3
6	Estermann et al. (2002)	Beef	J. Anim. Sci. 80:1124-1134	9
7	Fiems et al. (1997)	Beef	J. Anim. Phys. Anim. Nutr. 77:1-9	8
8	Rouzbehan et al. (1996)	Beef	Anim. Feed Sci. Tech. 62:151-162	4
9	Shreck et al. (2017)	Beef	J. Anim. Sci. 95:2133-2143	2
10	Taylor-Edwards et al. (2009)	Beef	J. Anim. Sci. 87:209-221	2
11	Terada et al. (1998)	Beef	Anim. Sci Technol. 69:697-701	2
12	Waggoner et al. (2009)	Beef	J. Anim. Sci. 87:681-692	1
13	Wei et al. (2016)	Beef	Arch. Anim. Nutr. 70:416-423	4
14	Wickersham et al. (2008b)	Beef	J. Anim. Sci. 86:3089-3099	5
15	Wickersham et al. (2008a)	Beef	J. Anim. Sci. 86:3079-3088	4
		Beef Total		**65**
16	Arndt et al. (2015)	Dairy	J. Dairy Sci. 98:418-430	4
17	Astigarraga et al. (2002)	Dairy	Anim. Res. 51:279-293	3
18	Aston et al. (1998)	Dairy	Anim. Sci. 67:17-26	3
19	Bargo et al. (2002)	Dairy	J. Dairy Sci. 85:1777-1792	4
20	Bertilsson et al. (2017)	Dairy	J. Dairy Sci. 100:7990-8003	8
21	Brookes (1984)	Dairy	NZ J. Agric. Res. 27:491-493	2
22	Burke et al. (2008)	Dairy	Livestock Sci. 114:325-335	5
23	Carruthers and Neil (1997)	Dairy	NZ J. Agric. Res. 40:513-521	4
24	Carruthers et al. (1997)	Dairy	Anim. Sci. 64:393-402	6
25	Castillo et al. (2001a)	Dairy	J. Anim. Sci. 79:240-246	4
26	Castillo et al. (2001b)	Dairy	J. Anim. Sci. 79:247-253	5
27	Cheng et al. (2011)	Dairy	J. Dairy Sci. 94:2031-2041	9
28	Cheng et al. (2014)	Dairy	Anim. Prod. Sci. 54:1651-1656	2
29	Delagarde et al. (1997)	Dairy	Anim. Feed Sci. Tech. 66:165-180	2
30	Estermann et al. (2001)	Dairy	Anim. Res. 50:477-493	4
31	Higgs et al. (2013)	Dairy	J. Dairy Sci. 96:3857-3866	2
32	Stergiadis et al. (2015)	Dairy	J. Dairy Sci. 99:8111-8120	3
33	Jonker et al. (2002)	Dairy	J. Appl. Anim. Res. 21:81-92	3

Ref. No.	Author and year of publication	Livestock class	Reference	Number of means included
34	Keady and Murphy (1998)	Dairy	Anim. Sci. 66:9-20	4
35	Keady et al. (1998)	Dairy	Anim. Sci. 66:21-33	3
36	Kebreab et al. (2000)	Dairy	J. Dairy Sci. 83:1274-1285	17
37	Kolver et al. (1998)	Dairy	J. Dairy Sci. 81:2017-2028	2
38	Mackle et al. (1996)	Dairy	NZ J. Agric. Res. 39:341-356	4
39	(Miller et al.)	Dairy	Proc. Br. Soc. Anim. Sci. 1999:208	2
40	(Miller et al.)	Dairy	Proc. 6th Res. Conf. Br. Grassl. Soc.	2
41	Miller et al. (2001)	Dairy	Grass Forage Sci. 56:383-394	2
42	Moate et al. (2017)	Dairy	Anim. Prod. Sci. 57:1520-1524	8
43	Moorby and Theobald (1999)	Dairy	J. Dairy Sci. 82:2440-2442	2
44	Moorby et al. (2006)	Dairy	Grass Forage Sci. 61:52-59	2
45	Moorby et al. (2000)	Dairy	J. Dairy Sci. 83:1795-1805	9
46	Mulligan et al. (2004)	Dairy	J. Dairy Sci. 87:3451-3460	5
47	Ohtani et al. (2001)	Dairy	Anim. Sci. J. 72:239-246	3
48	Pacheco et al. (2003)	Dairy	Br. J. Nutr. 90:271-281	2
49	Petit and Tremblay (1995)	Dairy	J. Dairy Sci. 78:342-352	5
50	Peyraud et al. (1997)	Dairy	Anim. Feed Sci. Technol. 64:155-171	2
51	Rearte et al. (2003)	Dairy	Trop. Subtrop. Agroecosyst. 3:251-254	2
52	Reynolds et al. (2001)	Dairy	J. Dairy Sci. 84:2250-2259	2
53	Ruiz et al. (2001)	Dairy	J. Dairy Sci. 84:1717-1727	1
54	Sánchez-Chopa et al. (2016)	Dairy	Anim. Prod. Sci. 56:2039-2046	2
55	Tas et al. (2006)	Dairy	Livestock Sci. 100:159–168	12
56	Valk (1994)	Dairy	Livestock Prod. Sci. 40:241-250	1
57	Van Vuuren et al. (1993)	Dairy	J. Dairy Sci. 76:2982-2993	2
58	Whelan et al. (2011)	Dairy	J. Dairy Sci. 94:5080-5089	2
59	Whelan et al. (2012)	Dairy	J. Dairy Sci. 95:4468-4477	3
60	Woodward et al. (2009)	Dairy	Proc. NZSAP 69:179-183	4
61	Woodward et al. (2012)	Dairy	AADS 2012 464-464	2
62	Zanton and Heinrichs (2009)	Dairy	J. Dairy Sci. 92:2078-2094	4
		Dairy Total		**184**
63	Freudenberger et al. (1994)	Deer	Br. J. Nutr. 71:489-499	3
64	Jeon et al. (2003)	Deer	Asian Aust. J. Anim. Sci. 16:702-705	3
65	Kim et al. (1996)	Deer	Anim. Feed Sci. Tech. 61:351-359	5
66	Moon et al. (2004)	Deer	Asian Aust. J. Anim. Sci. 17:80-85	4
67	Mould and Robbins (1981)	Deer	J Wildl. Manage. 45:323-334	13
68	Puttoo and Dryden (1998)	Deer	Anim. Prod. Australia 1.15	4
		Deer Total		**32**
69	Barry et al. (1986)	Sheep	Br. J. Nutr. 55:123-127	1

Ref. No.	Author and year of publication	Livestock class	Reference	Number of means included
70	Bermingham (2004)	Sheep	Thesis	2
71	Bremmers et al. (1988)	Sheep	NZ J. Agric. Res. 31:1-7	4
72	Cheng et al. (2013)	Sheep	Animal 7-8:1274-1279	3
73	Dellow et al. (1988)	Sheep	Proc. NZSAP 48:253-255	2
74	Dias (2010)	Sheep	Thesis	16
75	Domingue et al. (1991)	Sheep	NZ J. Agric. Res. 34:45-53	4
76	Hoskin et al. (2002)	Sheep	Proc. NZSAP 62:72-76	1
77	Jonker et al. (2015)	Sheep	Proc. NZSAP 75:74-78	6
78	Joyce et al. (1972)	Sheep	Proc. NZSAP 32:54-63	10
79	Luo et al. (2015)	Sheep	Animal 9:534-543	4
80	Maas et al. (2001)	Sheep	J. Anim. Sci. 79:1052-1058	2
81	Maloiy and Kay (1971)	Sheep	Quart. J. Exp. Physiol 56:257-266	10
82	Masuko et al. (1997)	Sheep	Grasslands Sci. 43:32-36	12
83	McCutcheon et al. (1987)	Sheep	Aust. J. Agric. Res. 38:917-926	2
84	Min et al. (2002)	Sheep	Can. J. Microbiol. 48:911-921	2
85	Mouro et al. (2007)	Sheep	R. Brasil. Zootec. 36:489-498	4
86	Nolan and Stachiw (1979)	Sheep	Br. J. Nutr. 42:63-80	4
87	Offer et al. (1978)	Sheep	Br. J. Nutr. 40:35-44	7
88	Pinares-Patino et al. (2003)	Sheep	J. Agric. Sci. 140:215-226	2
89	Rattray and Joyce (1969)	Sheep	Proc. NZSAP 29:102-113	6
90	Recavarren and Milano (2014)	Sheep	J. Anim. Phys. Anim. Nutr. 98:1047-1053	4
91	Simpson (2000)	Sheep	Thesis	4
92	(Sun et al., 2016)	Sheep	Client report	6
93	Sun et al. (1994)	Sheep	Aust. J. Agric. Res. 45: 339-354	4
94	Sun et al. (2013)	Sheep	MPI SLMACC report	4
95	Thomson (1987)	Sheep	Thesis	2
96	Ulyatt et al. (1984)	Sheep	J. Agric. Sci. 102:645-657	4
97	van der Walt et al. (1999)	Sheep	S. Afr. J. Anim. Sci. 29:105-119	4
98	Van Emon et al. (2017)	Sheep	Small Rum. Res. 150:118-125	3
99	Vercoe et al. (1962)	Sheep	J. Agric. Sci. 59:343-348	13
100	Vranic et al. (2007)	Sheep	Agric. Food Sci. 16:17-24	4
101	Vranić et al. (2009)	Sheep	Asian Aust. J. Anim. Sci. 22:225-231	3
102	Yu et al. (2001)	Sheep	Anim. Feed Sci. Tech. 93:71-91	5
103	Zhao et al. (2017)	Sheep	J. Anim. Sci. 95:3762-3771	3
		Sheep Total		**167**
		Grand Total		**448**

Appendix 2. Summary statistics per livestock class.

Summary statistics (per livestock class) of the whole database compiled for this study.

Livestock class	Variable	Mean	Minimum	Maximum	No. of records
Beef	N_{diet}	2.1	0.8	4.5	67
	ME	9.8	7.3	11.4	41
	% forage	80.1	0.0	100.0	67
	LW	369.5	153.0	631.6	67
	DMI	7.3	1.6	16.2	67
	$DMI_{\%LW}$	2.0	1.0	3.3	67
	Ni	160.1	38.5	544.0	67
	Ni_{LW}	0.4	0.1	1.1	67
	Ni_MetLW	1.9	0.6	4.5	67
	UN	69.2	13.7	361.0	67
	FN	50.8	14.9	150.0	67
	$UN_{\%exN}$	54.5	30.8	75.0	67
	$FN_{\%exN}$	45.5	25.0	69.2	67
Dairy	N_{diet}	2.8	1.2	4.5	182
	ME	11.0	8.6	12.4	136
	% forage	76.3	34.6	100.0	182
	LW	575.7	160.9	727.0	160
	DMI	17.1	4.7	24.8	182
	$DMI_{\%LW}$	3.0	1.6	4.1	160
	Ni	471.6	84.8	726.0	182
	Ni_{LW}	0.8	0.2	1.3	160
	Ni_MetLW	4.1	0.9	6.1	160
	UN	197.3	24.1	437.0	182
	FN	138.8	45.2	223.9	182
	$UN_{\%exN}$	57.2	32.5	76.6	182
	$FN_{\%exN}$	42.8	23.4	67.5	182
Deer	N_{diet}	2.2	0.9	4.7	46
	ME	8.8	5.6	11.2	14
	% forage	87.6	53.2	100.0	46
	LW	56.9	32.0	109.7	33
	DMI	1.7	0.7	4.6	46
	$DMI_{\%LW}$	2.3	1.5	3.4	33
	Ni	38.2	12.4	143.4	46
	Ni_{LW}	0.5	0.2	0.9	33
	Ni_MetLW	1.4	0.6	3.0	33
	UN	14.0	2.0	51.9	29
	FN	14.4	4.7	47.2	46
	$UN_{\%exN}$	48.8	12.5	70.5	29
	$FN_{\%exN}$	51.2	29.5	87.5	29

Livestock class	Variable	Mean	Minimum	Maximum	No. of records
Sheep	N_{diet}	2.6	0.8	5.0	153
	ME	9.8	5.6	13.2	121
	% forage	85.4	0.0	100.0	153
	LW	39.9	20.2	63.1	123
	DMI	0.9	0.3	1.5	153
	$DMI_{\%LW}$	2.5	0.9	4.2	123
	Ni	23.4	3.4	45.1	153
	Ni_{LW}	0.7	0.2	1.6	123
	Ni_MetLW	1.6	0.4	3.3	123
	UN	13.6	1.7	26.8	140
	FN	7.6	2.9	22.1	153
	$UN_{\%exN}$	61.5	26.0	84.8	140
	$FN_{\%exN}$	38.5	15.2	74.0	140
Overall	N_{diet}	2.6	0.8	5.0	448
	ME	10.3	5.6	13.2	312
	% forage	81.1	0.0	100.0	448
	LW	322.9	20.2	727.0	383
	DMI	8.5	0.3	24.8	448
	$DMI_{\%LW}$	2.6	0.9	4.2	383
	Ni	227.4	3.4	726.0	448
	Ni_{LW}	0.7	0.1	1.6	383
	Ni_MetLW	2.7	0.4	6.1	383
	UN	102.5	1.7	437.0	418
	FN	68.0	2.9	223.9	448
	$UN_{\%exN}$	57.6	12.5	84.8	418
	$FN_{\%exN}$	42.4	15.2	87.5	418

Appendix 3. Summary statistics per diet type.

Summary statistics of the database (per diet type) compiled for this study and used in the development of predictive equations for N in excreta.

Diet	Variable	Mean	Minimum	Maximum	No. of records
Fresh perennial ryegrass	Npct	2.8	0.8	4.5	136
	ME	11.1	9.3	12.4	99
	Forage (% of diet)	89.8	49.4	100.0	136
Other fresh grass	Npct	2.2	0.8	4.7	48
	ME	9.8	7.3	12.4	28
	Forage (% of diet)	90.9	36.9	100.0	48
Fresh Legume	Npct	3.3	2.4	4.8	37
	ME	9.5	7.8	11.5	32
	Forage (% of diet)	98.0	57.1	100.0	37
Fresh CT[1]-legume	Npct	3.5	2.7	3.8	7
	ME	10.5	9.0	11.8	7
	Forage (% of diet)	100.0	100.0	100.0	7
Concentrate	Npct	2.5	2.2	3.1	9
	ME	11.0	9.9	11.8	5
	Forage (% of diet)	19.8	0.0	61.7	9
Conserved grass	Npct	2.3	0.9	3.3	126
	ME	9.9	7.2	12.1	77
	Forage (% of diet)	74.7	40.0	100.0	126
Maize silage	Npct	2.2	1.0	3.7	27
	ME	10.6	9.2	11.2	21
	Forage (% of diet)	59.1	46.0	100.0	27
Conserved legume	Npct	2.7	2.0	3.6	31
	ME	9.2	5.6	11.1	23
	Forage (% of diet)	91.3	55.0	100.0	31
Other diet	Npct	2.5	1.9	5.0	27
	ME	10.3	7.5	13.2	20
	Forage (% of diet)	53.2	0.0	100.0	27

[1] Condensed tannins

Appendix 4. All subset regression per livestock class.

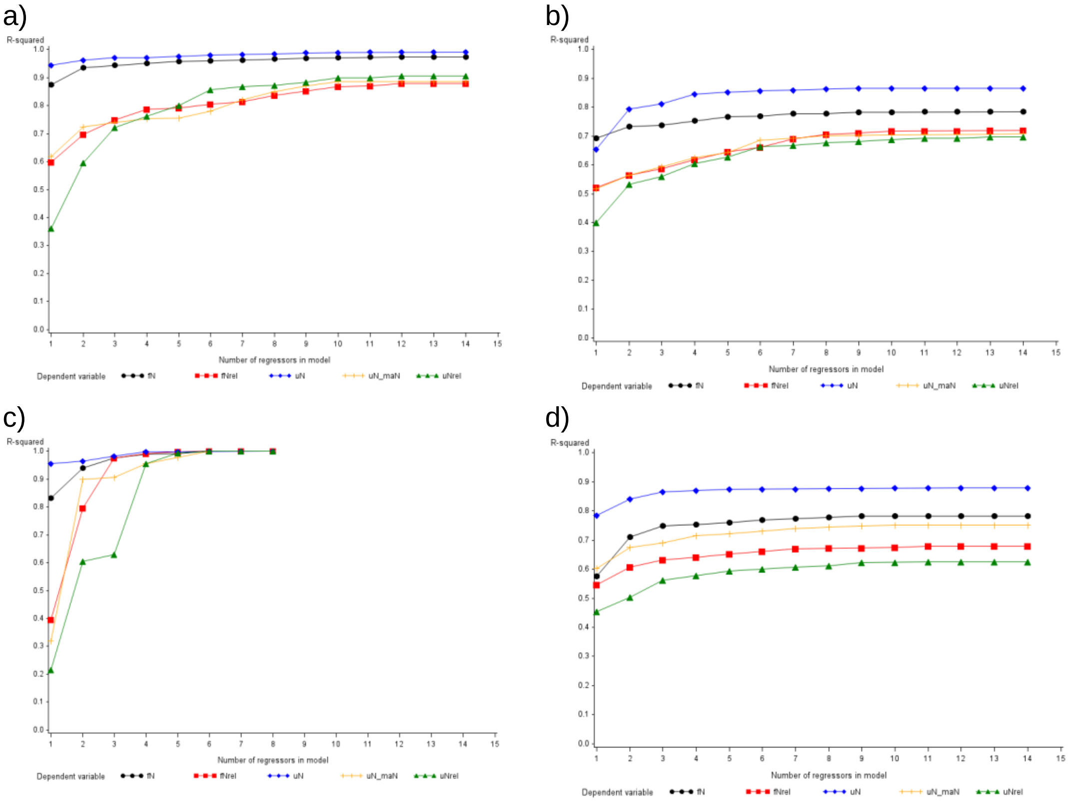

Figure A4.1. Coefficients of determination (r2) for the all subset regressions for a) beef cattle, b) dairy cattle, c) deer and d) sheep. x axis is the number of independent variables in the model and y axis is the r^2 *value is the best fit for a particular number of independent variables.*

Appendix 5. Evaluation of models using the evaluation dataset.

Table A5.1. Evaluation of models to predict urinary nitrogen (N) as a proportion of total manure N ($UN_{\%exN}$*) using the root mean square prediction error (RMSPE) and its decomposition (mean bias, slope bias and random error), the concordance correlation coefficient (CCC) and the RMSPE to standard deviation of the observations ratio (RSR). Codes for model developed in this project are in Table 9. See footnote for codes for models from the literature. RPE is the relative prediction error (RMSPE expressed as a percentage of the mean of observed values and* r^2 *value is the coefficient of determination of the regression between observed and predicted values.*

Model	Data used	Livestock class	Mean observed	Mean predicted	Bias	RPE	Mean bias (% RMSPE)	Slope bias (% RMSPE)	Random error (% RMSPE)	RMSPE	CCC	RSR	r^2
Mod1.01.01	All	Beef	45.3	47.3	1.9	9.8	19.1	2.2	78.8	4.43	0.78	0.62	0.67
	All	Dairy	61.2	61.3	0.2	12.1	0.0	2.5	97.4	7.39	0.54	0.82	0.33
	All	Deer	58.3	58.9	0.6	18.9	0.3	1.1	98.7	11.01	0.38	0.77	0.27
	All	Sheep	61.7	58.7	-3.1	14.2	12.2	2.1	85.7	8.75	0.69	0.67	0.60
Mod1.01.01sp[1]	All	Beef	45.3	50.0	4.7	14.0	55.9	5.5	38.6	6.3	0.67	0.88	0.67
	All	Dairy	61.2	58.5	-2.7	12.9	11.8	2.7	85.4	7.9	0.52	0.87	0.33
	All	Deer	58.3	59.6	1.3	19.4	1.3	5.5	93.2	11.3	0.49	0.79	0.27
	All	Sheep	61.7	61.5	-0.2	13.4	0.1	3.3	96.6	8.2	0.71	0.63	0.60
Mod1.01.02	All	Beef	45.3	49.1	3.7	11.8	48.5	12.0	39.5	5.4	0.77	0.75	0.76
	All	Dairy	61.1	59.2	-1.9	11.9	6.9	2.3	90.8	7.3	0.60	0.80	0.41
	All	Deer	58.3	61.3	3.0	17.0	9.3	44.3	46.3	9.9	0.49	0.69	0.72
	All	Sheep	59.0	59.5	0.5	12.1	0.4	18.3	81.3	7.2	0.78	0.55	0.75
Mod1.01.02sp	All	Beef	45.3	50.0	4.7	13.4	59.6	12.3	28.1	6.1	0.74	0.85	0.78
	All	Dairy	61.1	59.4	-1.7	11.7	5.7	4.0	90.3	7.2	0.63	0.79	0.43
	All	Deer	58.3	59.6	1.3	16.5	1.9	0.3	97.8	9.6	0.63	0.67	0.45
	All	Sheep	59.0	58.9	-0.1	12.1	0.0	21.4	78.6	7.1	0.78	0.55	0.76
Mod1.01.03	All	Beef	45.3	47.2	1.8	8.8	21.1	2.2	76.8	4.0	0.83	0.56	0.74
	All	Dairy	61.2	58.8	-2.4	12.6	9.8	3.7	86.5	7.7	0.55	0.85	0.35
	All	Deer	58.3	61.4	3.1	19.5	7.2	0.9	91.9	11.3	0.38	0.79	0.28
	All	Sheep	61.7	61.3	-0.4	13.2	0.3	1.2	98.5	8.1	0.73	0.62	0.60
Mod2.01.01	Beef	Beef	45.3	49.4	4.1	12.7	49.5	18.8	31.7	5.8	0.76	0.81	0.77
Mod2.01.02	Beef	Beef	45.3	49.9	4.6	14.1	50.5	11.7	37.8	6.4	0.69	0.89	0.67
Mod3.01.01	Dairy	Dairy	61.1	59.7	-1.4	11.7	3.6	4.5	91.9	7.1	0.64	0.79	0.43

Model	Data used	Livestock class	Mean observed	Mean predicted	Bias	RPE	Mean bias (% RMSPE)	Slope bias (% RMSPE)	Random error (% RMSPE)	RMSPE	CCC	RSR	r^2
Mod3.01.02	Dairy	Dairy	61.2	58.5	-2.7	12.9	11.4	2.9	85.7	7.9	0.52	0.87	0.33
Mod4.01.01	Deer	Deer	58.3	62.2	3.9	8.9	55.6	2.2	42.3	5.2	0.93	0.36	0.93
Mod4.01.02	Deer	Deer	58.3	59.7	1.4	15.3	2.4	0.2	97.4	9.0	0.67	0.62	0.53
Mod4.01.03	Deer	Deer	58.3	55.6	-2.7	19.5	5.6	1.5	92.9	11.4	0.46	0.79	0.27
Mod5.01.01	Sheep	Sheep	61.7	62.4	0.7	13.3	0.6	4.8	94.6	8.2	0.71	0.63	0.61
Mod5.01.02	Sheep	Sheep	61.7	61.9	0.2	13.4	0.0	3.7	96.3	8.3	0.71	0.63	0.60
Mod 5 Dong	Beef	Beef	45.3	50.6	5.3	14.7	64.2	0.7	35.0	6.6	0.57	0.93	0.67
Mod 6 Dong	Beef	Beef	45.3	54.6	9.3	26.2	61.5	8.6	29.9	11.9	0.15	1.66	0.10
Mod Luo	Beef	Beef	45.3	52.2	6.9	17.6	75.4	0.2	24.4	8.0	0.50	1.11	0.67
	All	Dairy	61.2	64.1	2.9	12.9	13.9	0.1	86.1	7.9	0.47	0.87	0.33
	All	Deer	58.3	62.0	3.7	20.1	10.1	2.9	87.0	11.7	0.32	0.82	0.27
	All	Sheep	61.7	61.9	0.2	13.8	0.0	9.4	90.6	8.5	0.67	0.65	0.60
ModSterg3a	Dairy	Dairy	61.2	7.6	-53.6	88.7	97.5	0.7	1.8	54.3	0.00	5.99	0.33
ModSterg3b	Dairy	Dairy	61.2	75.9	14.7	26.8	80.0	1.2	18.9	16.4	0.13	1.81	0.36
ModSterg3g	Dairy	Dairy	61.2	78.5	17.3	31.6	80.2	1.1	18.7	19.3	0.08	2.13	0.12
ModSterg3j	Dairy	Dairy	61.1	108.9	47.8	80.5	94.5	2.5	3.0	49.2	0.03	5.43	0.12
ModSterg3k	Dairy	Dairy	61.1	-16.7	-77.8	155.0	67.5	31.7	0.8	94.7	-0.03	10.45	0.09

[1] Models with ‘sp’ suffix are the same as the ‘universal’ models, but species-specific parameters have been generated by including species in the model.
‘Mod Luo’: current model in the AIM, from Luo and Kelliher (2010).
‘ModSterg*Xx*’ are models reported by Stergiadis et al. (2015), using the model notation as reported in the publication.

Table A5.2. Evaluation of models to predict urinary nitrogen (N) as a proportion of N intake ($UN_{\%Ni}$) using the root mean square prediction error (RMSPE) and its decomposition (mean bias, slope bias and random error), the concordance correlation coefficient (CCC) and the RMSPE to standard deviation of the observations ratio (RSR). Codes for model developed in this project are in Table 9. See footnote for codes for models from the literature. RPE is the relative prediction error (RMSPE expressed as a percentage of the mean of observed values and r^2 value is the coefficient of determination of the regression between observed and predicted values.

Model	Data used	Livestock class	Mean observed	Mean predicted	Bias	RPE	Mean bias (% RMSPE)	Slope bias (% RMSPE)	Random error (% RMSPE)	RMSPE	CCC	RSR	r^2
Mod1.02.01	All	Beef	35.7	36.8	1.1	20.7	2.1	25.3	72.6	7.4	0.21	1.09	0.05
	All	Dairy	44.7	48.3	3.7	21.4	14.6	0.2	85.2	9.6	0.35	0.94	0.22
	All	Deer	48.7	46.3	-2.4	21.5	5.2	0.2	94.6	10.5	0.30	0.82	0.20
	All	Sheep	53.0	46.1	-6.9	22.6	33.0	21.2	45.8	12.0	0.56	0.78	0.71
Mod4.02.01	Deer	Deer	48.7	46.5	-2.2	20.5	4.9	43.1	52.0	10.0	0.73	0.78	0.60
Mod5.02.01	Sheep	Sheep	53.0	52.8	-0.2	15.9	0.1	24.2	75.8	8.4	0.77	0.55	0.76
Mod5.02.02	Sheep	Sheep	50.0	51.2	1.3	16.8	2.3	21.3	76.4	8.4	0.76	0.55	0.75
ModSterg4a	Dairy	Dairy	44.7	25.8	-18.9	46.7	82.1	0.0	17.9	20.9	0.09	2.05	0.22
ModSterg4d	Dairy	Dairy	44.7	31.0	-13.7	37.8	65.8	2.0	32.2	16.9	0.10	1.66	0.09

‘ModStergXx’ are models reported by Stergiadis et al. (2015), using the model notation as reported in the publication.

Table A5.3. Evaluation of models to predict urinary nitrogen (N) output (g/d) using the root mean square prediction error (RMSPE) and its decomposition (mean bias, slope bias and random error), the concordance correlation coefficient (CCC) and the RMSPE to standard deviation of the observations ratio (RSR). Codes for model developed in this project are in Table 9. See footnote for codes for models from the literature. RPE is the relative prediction error (RMSPE expressed as a percentage of the mean of observed values and r^2 *value is the coefficient of determination of the regression between observed and predicted values.*

Model	**Data used**	**Livestock class**	**Mean observed**	**Mean predicted**	**Bias**	**RPE**	**Mean bias (% RMSPE)**	**Slope bias (% RMSPE)**	**Random error (% RMSPE)**	**RMSPE**	**CCC**	**RSR**	**r^2**
Mod1.03.01	All	Beef	49.5	60.9	11.4	29.7	60.1	3.1	36.8	14.7	0.83	0.62	0.84
	All	Dairy	226.7	211.1	-15.6	24.1	8.2	0.2	91.6	54.6	0.60	0.75	0.47
	All	Deer	19.2	17.5	-1.8	24.0	14.6	13.0	72.4	4.6	0.86	0.43	0.83
	All	Sheep	13.8	12.0	-1.8	29.2	19.9	0.1	79.9	4.0	0.56	0.81	0.45
Mod1.03.01sp[1]	All	Beef	49.5	64.5	14.9	40.2	56.3	23.6	20.1	19.9	0.77	0.84	0.84
	All	Dairy	226.7	212.1	-14.6	24.1	7.1	1.4	91.4	54.7	0.65	0.75	0.47
	All	Deer	19.2	18.9	-0.4	21.5	0.9	8.9	90.2	4.1	0.91	0.38	0.83
	All	Sheep	13.8	14.5	0.7	28.0	3.4	9.9	86.6	3.9	0.66	0.78	0.45
Mod1.03.02	All	Beef	49.5	54.7	5.1	16.4	40.2	0.7	59.1	8.1	0.94	0.34	0.92
	All	Dairy	225.3	216.8	-8.5	22.2	2.8	0.4	96.8	50.1	0.70	0.69	0.54
	All	Deer	19.2	19.9	0.6	25.8	1.6	44.7	53.8	5.0	0.90	0.46	0.86
	All	Sheep	13.8	12.2	-1.5	33.7	10.9	47.7	41.4	4.6	0.76	0.94	0.68
Mod1.03.03	All	Beef	49.5	61.8	12.3	36.6	45.8	26.2	28.0	18.1	0.79	0.76	0.82
	All	Dairy	226.7	182.7	-44.0	32.7	35.2	0.6	64.2	74.2	0.33	1.02	0.31
	All	Deer	19.2	43.6	24.4	135.7	87.1	12.8	0.2	26.1	0.39	2.43	0.99
	All	Sheep	13.8	39.6	25.8	242.2	59.5	39.8	0.7	33.4	0.15	6.75	0.67
Mod1.03.03sp	All	Beef	49.5	80.1	30.6	81.5	57.3	32.7	10.0	40.4	0.50	1.70	0.68
	All	Dairy	226.7	203.0	-23.7	24.1	18.8	0.0	81.2	54.7	0.65	0.75	0.53
	All	Deer	19.2	19.7	0.5	23.5	1.0	1.6	97.4	4.5	0.88	0.42	0.79
	All	Sheep	13.8	14.5	0.7	20.5	6.4	2.1	91.5	2.8	0.79	0.57	0.69
Mod2.03.01	Beef	Beef	49.5	62.9	13.4	36.1	56.2	18.9	24.9	17.9	0.80	0.75	0.84
Mod3.03.02	Dairy	Dairy	226.7	212.3	-14.4	20.7	9.4	0.0	90.5	47.0	0.74	0.65	0.61
Mod3.03.03	Dairy	Dairy	226.7	217.8	-8.9	18.2	4.6	0.0	95.4	41.3	0.80	0.57	0.68
Mod4.03.01	Deer	Deer	19.2	18.6	-0.6	21.5	2.2	7.7	90.1	4.1	0.91	0.38	0.83

Model	**Data used**	**Livestock class**	**Mean observed**	**Mean predicted**	**Bias**	**RPE**	**Mean bias (% RMSPE)**	**Slope bias (% RMSPE)**	**Random error (% RMSPE)**	**RMSPE**	**CCC**	**RSR**	**r^2**
Mod4.03.02	Deer	Deer	19.2	18.9	-0.3	16.5	0.9	15.2	83.9	3.2	0.95	0.30	0.91
Mod5.03.01	Sheep	Sheep	13.8	14.3	0.5	17.0	5.4	0.1	94.5	2.3	0.87	0.47	0.78
Mod5.03.03	Sheep	Sheep	13.8	14.2	0.4	16.8	2.3	3.0	94.7	2.3	0.88	0.47	0.78
ModJohnson1	Dairy	Dairy	226.7	180.5	-46.2	31.2	42.7	2.7	54.6	70.7	0.43	0.97	0.47
ModJohnson3	Dairy	Dairy	226.7	202.5	-24.2	30.0	12.7	18.9	68.5	67.9	0.59	0.93	0.38
ModJohnson4	Dairy	Dairy	226.7	216.0	-10.7	26.4	3.2	20.3	76.5	59.8	0.68	0.82	0.47
ModJohnson5	Dairy	Dairy	226.7	226.4	-0.3	18.0	0.0	3.3	96.7	40.7	0.83	0.56	0.69
ModJohnson6	Dairy	Dairy	226.7	231.3	4.6	18.8	1.2	3.1	95.7	42.6	0.81	0.59	0.66
ModJohnson8	Dairy	Dairy	226.7	212.3	-14.4	24.1	7.0	1.3	91.7	54.6	0.58	0.75	0.47
ModJohnson9	Dairy	Dairy	226.7	-447.5	-674.2	300.8	97.8	1.2	1.1	681.9	0.01	9.37	0.03
ModJohnson34	Beef	Beef	49.5	65.2	15.6	36.6	74.5	1.3	24.3	18.1	0.76	0.76	0.84
ModJohnson35	Beef	Beef	49.5	51.0	1.5	26.0	1.4	71.9	26.8	12.9	0.89	0.54	0.91
ModJohnson36	Beef	Beef	49.5	55.7	6.2	22.5	30.9	32.2	36.8	11.2	0.91	0.47	0.91
ModJohnson37	Beef	Beef	49.5	59.5	10.0	34.7	33.8	39.2	27.0	17.2	0.82	0.72	0.84
ModJohnson38	Beef	Beef	49.5	44.4	-5.2	29.9	12.2	0.2	87.6	14.8	0.75	0.63	0.62
ModJohnson39	Beef	Beef	49.5	45.3	-4.2	29.4	8.4	0.6	91.1	14.5	0.76	0.61	0.62
ModJohnson40	Beef	Beef	49.5	59.4	9.8	31.2	40.4	26.3	33.3	15.5	0.84	0.65	0.84
ModPatra3b	Sheep	Sheep	13.8	7.4	-6.4	55.6	69.1	6.5	24.4	7.7	0.18	1.55	0.49
ModSchuba2d	Dairy	Dairy	226.7	919.3	692.6	308.6	98.0	1.4	0.6	699.6	0.03	9.61	0.47
Modschuba2f	Sheep	Sheep	13.8	34.9	21.1	157.3	94.8	2.4	2.7	21.7	0.09	4.39	0.45
ModSterg7a	Dairy	Dairy	226.7	318.0	91.3	47.3	72.7	3.4	23.8	107.1	0.38	1.47	0.47
ModSterg7f	Dairy	Dairy	225.3	9.3	-216.0	100.9	90.3	0.0	9.7	227.3	0.01	3.12	0.04
ModThomson		Beef	49.5	62.4	12.9	33.1	62.0	8.3	29.6	16.4	0.81	0.69	0.84
		Dairy	226.7	226.3	-0.4	23.1	0.0	0.1	99.9	52.3	0.64	0.72	0.47
		Sheep	13.8	9.0	-4.8	43.3	63.6	0.1	36.3	6.0	0.39	1.21	0.45

[1] Models with ‘sp’ suffix are the same as the ‘universal’ models, but species-specific parameters have been generated by including species in the model.
‘ModJohnsonXX’ are models reported by Johnson et al. (2016), using the model notation as reported in the publication.
‘ModPatraXx’ are models reported by Patra (2010), named after the table number in which the model was reported.
‘ModSchubaXx’ are models reported by Schuba et al. (), named after the table number in which the model was reported.

‘ModStergXx’ are models reported by Stergiadis et al. (2015), using the model notation as reported in the publication.
‘ModThomson’ is the model reported by Thomson and Muir (2016).

Table A5.4. Evaluation of models to predict faecal nitrogen (N) as a proportion of N intake ($FN_{\%Ni}$) using the root mean square prediction error (RMSPE) and its decomposition (mean bias, slope bias and random error), the concordance correlation coefficient (CCC) and the RMSPE to standard deviation of the observations ratio (RSR). Codes for model developed in this project are in Table 9. See footnote for codes for models from the literature. RPE is the relative prediction error (RMSPE expressed as a percentage of the mean of observed values and r^2 value is the coefficient of determination of the regression between observed and predicted values.

Model	**Data used**	**Livestock class**	**Mean observed**	**Mean predicted**	**Bias**	**RPE**	**Mean bias (% RMSPE)**	**Slope bias (% RMSPE)**	**Random error (% RMSPE)**	**RMSPE**	**CCC**	**RSR**	**r^2**
Mod1.04.01	All	Beef	41.5	43.8	2.2	12.3	19.4	4.0	76.6	5.1	0.80	0.55	0.75
	All	Dairy	27.8	28.8	1.0	20.7	3.1	40.2	56.7	5.7	0.56	1.06	0.34
	All	Deer	35.0	31.4	-3.7	33.1	10.0	0.1	89.9	11.6	0.36	0.82	0.24
	All	Sheep	32.1	31.6	-0.5	26.6	0.3	13.0	86.8	8.5	0.61	0.84	0.37
Mod1.04.01sp[1]	All	Beef	41.5	37.9	-3.6	14.5	35.6	9.2	55.1	6.0	0.72	0.65	0.75
	All	Dairy	27.8	29.2	1.4	16.6	9.5	3.1	87.4	4.6	0.53	0.86	0.34
	All	Deer	35.0	34.9	-0.2	31.8	0.0	3.0	97.0	11.2	0.45	0.79	0.24
	All	Sheep	32.1	33.7	1.6	27.0	3.6	12.2	84.3	8.7	0.60	0.85	0.37
Mod1.04.03	All	Beef	41.5	43.9	2.4	13.7	17.5	30.2	52.3	5.7	0.84	0.61	0.78
	All	Dairy	27.8	29.5	1.7	15.4	16.4	0.9	82.7	4.3	0.61	0.80	0.46
	All	Deer	35.0	30.8	-4.3	33.9	13.0	14.7	72.3	11.9	0.25	0.84	0.36
	All	Sheep	32.1	32.1	0.1	24.8	0.0	1.1	98.9	7.9	0.58	0.78	0.38
Mod2.04.01	Beef	Beef	41.5	41.3	-0.2	11.7	0.1	26.6	73.3	4.9	0.87	0.52	0.78
Mod2.04.02	Beef	Beef	41.5	37.4	-4.1	14.2	47.9	0.5	51.6	5.9	0.77	0.64	0.77
Mod3.04.02	Dairy	Dairy	27.8	29.5	1.7	15.8	15.6	0.1	84.3	4.4	0.54	0.81	0.42
Mod4.04.01	Deer	Deer	35.0	29.0	-6.1	22.9	57.1	11.8	31.2	8.0	0.86	0.57	0.87
Mod4.04.02	Deer	Deer	35.0	35.2	0.2	30.6	0.0	0.1	99.9	10.7	0.43	0.76	0.28
Mod5.04.01	Sheep	Sheep	32.1	32.4	0.3	25.4	0.1	6.3	93.6	8.1	0.61	0.80	0.38
Mod5.04.02	Sheep	Sheep	32.1	33.0	0.9	25.0	1.3	1.5	97.2	8.0	0.58	0.78	0.38

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[1] Models with ‘sp’ suffix are the same as the ‘universal’ models, but species-specific parameters have been generated by including species in the model.

Table A5.5. Evaluation of models to predict faecal nitrogen (N) output (g/d) using the root mean square prediction error (RMSPE) and its decomposition (mean bias, slope bias and random error), the concordance correlation coefficient (CCC) and the RMSPE to standard deviation of the observations ratio (RSR). Codes for model developed in this project are in Table 9. See footnote for codes for models from the literature. RPE is the relative prediction error (RMSPE expressed as a percentage of the mean of observed values and r^2 value is the coefficient of determination of the regression between observed and predicted values.

Model	Data used	Livestock class	Mean observed	Mean predicted	Bias	RPE	Mean bias (% RMSPE)	Slope bias (% RMSPE)	Random error (% RMSPE)	RMSPE	CCC	RSR	r^2
Mod1.05.01	All	Beef	58.0	44.9	-13.1	31.9	50.1	14.0	35.9	18.5	0.70	0.68	0.82
	All	Dairy	137.2	150.6	13.4	19.7	24.4	17.0	58.5	27.0	0.66	0.89	0.52
	All	Deer	13.1	14.3	1.3	26.0	14.1	7.6	78.2	3.4	0.79	0.60	0.65
	All	Sheep	8.4	10.5	2.0	39.6	37.2	3.2	59.6	3.3	0.53	0.86	0.54
Mod1.05.01sp[1]	All	Beef	58.0	48.4	-9.6	27.3	36.6	14.4	49.0	15.8	0.77	0.58	0.82
	All	Dairy	137.2	143.9	6.7	15.9	9.5	0.1	90.4	21.8	0.67	0.72	0.52
	All	Deer	13.1	14.7	1.6	28.3	19.3	14.7	66.0	3.7	0.62	0.65	0.65
	All	Sheep	8.4	8.1	-0.3	33.0	1.3	13.0	85.6	2.8	0.56	0.72	0.54
Mod1.05.02	All	Beef	58.0	51.4	-6.6	21.1	28.7	25.3	45.9	12.3	0.86	0.45	0.90
	All	Dairy	136.7	144.1	7.4	16.1	11.3	6.6	82.0	22.0	0.73	0.72	0.57
	All	Deer	13.1	12.5	-0.6	22.8	3.7	81.5	14.8	3.0	0.72	0.52	0.95
	All	Sheep	9.3	10.1	0.8	38.7	4.9	14.4	80.7	3.6	0.55	0.93	0.31
Mod1.05.03	All	Beef	58.0	61.8	3.9	14.4	21.1	37.7	41.2	8.4	0.94	0.31	0.96
	All	Dairy	137.2	139.3	2.1	15.1	1.0	9.2	89.8	20.7	0.75	0.68	0.57
	All	Deer	13.1	12.0	-1.1	22.2	13.5	7.7	78.9	2.9	0.79	0.51	0.74
	All	Sheep	8.4	8.7	0.3	28.6	1.1	24.3	74.7	2.4	0.69	0.62	0.70
Mod2.05.01	Beef	Beef	58.0	51.8	-6.2	21.3	25.2	67.2	7.6	12.3	0.84	0.46	0.98
Mod3.05.01	Dairy	Dairy	136.7	137.2	0.5	15.7	0.1	0.7	99.3	21.5	0.68	0.71	0.50
Mod3.05.02	Dairy	Dairy	137.2	144.4	7.2	14.7	12.8	3.0	84.2	20.2	0.76	0.66	0.62
Mod4.05.01	Deer	Deer	13.1	11.1	-2.0	28.4	27.6	0.2	72.2	3.7	0.70	0.65	0.61
Mod5.05.01	Sheep	Sheep	8.4	8.2	-0.2	28.0	0.9	12.8	86.3	2.4	0.72	0.61	0.67
Mod5.05.02	Sheep	Sheep	8.4	8.3	-0.2	27.0	0.6	23.0	76.4	2.3	0.73	0.59	0.73
ModHiggsFN5	Dairy	Dairy	137.2	174.4	37.3	32.5	70.0	12.7	17.3	44.5	0.49	1.46	0.62
ModJohnson11	Dairy	Dairy	137.2	158.4	21.2	23.7	42.2	20.4	37.4	32.6	0.61	1.07	0.56

ModJohnson13	Dairy	Dairy	137.2	158.5	21.4	21.7	51.4	0.4	48.2	29.8	0.54	0.98	0.52
ModJohnson14	Dairy	Dairy	137.2	145.4	8.2	18.7	10.1	29.7	60.2	25.7	0.71	0.84	0.56
ModJohnson15	Dairy	Dairy	137.2	147.9	10.8	17.5	20.0	19.7	60.3	24.0	0.74	0.79	0.61
ModJohnson16	Dairy	Dairy	137.2	151.7	14.5	19.7	28.5	13.1	58.3	27.1	0.65	0.89	0.52
ModJohnson41	Beef	Beef	58.0	51.2	-6.8	23.2	25.3	6.9	67.8	13.4	0.84	0.50	0.82
ModJohnson42	Beef	Beef	58.0	46.5	-11.5	37.4	28.2	45.8	26.0	21.7	0.47	0.80	0.82
ModJohnson43	Beef	Beef	58.0	43.9	-14.1	49.4	24.2	2.4	73.3	28.6	0.07	1.06	0.10
ModJohnson44	Beef	Beef	58.0	39.9	-18.1	52.7	35.1	0.6	64.2	30.6	0.09	1.13	0.10
ModJohnson45	Beef	Beef	58.0	44.6	-13.3	36.4	39.9	32.7	27.4	21.1	0.55	0.78	0.82
ModPatra3a	Sheep	Sheep	9.3	12.3	3.1	44.6	54.5	0.0	45.4	4.1	0.46	1.07	0.49
ModSchuba2b	Beef	Beef	58.0	392.2	334.2	614.4	88.0	11.9	0.1	356.2	0.06	13.16	0.82
ModSchuba2c	Sheep	Sheep	8.4	54.0	45.5	552.2	95.4	4.3	0.3	46.6	0.03	12.03	0.54

[1] Models with ‘sp’ suffix are the same as the ‘universal’ models, but species-specific parameters have been generated by including species in the model.
‘ModJohnsonsonXX’ are models reported by Johnson et al. (2016), using the model notation as reported in the publication.
‘ModPatraXx’ are models reported by Patra (2010), named after the table number in which the model was reported.
‘ModSchubaXx’ are models reported by Schuba et al. (2017), named after the table number in which the model was reported.
‘ModStergXx’ are models reported by Stergiadis et al. (2015), using the model notation as reported in the publication.

Appendix 6. Evaluation of models proposed using the training dataset.

Table A6.1. Evaluation of models developed using the training dataset. Models listed are those proposed as alternatives to predict the percentage of urinary nitrogen in total excreta ($UN_{\%exN}$) and faecal nitrogen output (FN) in AIM. Evaluation was done using the root mean square prediction error (RMSPE) and its decomposition (mean bias, slope bias and random error), the concordance correlation coefficient (CCC) and the RMSPE to standard deviation of the observations ratio (RSR). RPE is the relative prediction error (RMSPE expressed as a percentage of the mean of observed values and r^2 value is the coefficient of determination of the regression between observed and predicted values. Slope y=x is the slope of the regression observed=predicted.

Model	**Data used**	**Livestock class**	**Mean observed**	**Mean predicted**	**Bias**	**RPE**	**Mean bias (% RMPSE)**	**Slope bias (% RMSPE)**	**Random error (% RMSPE)**	**RMSPE**	**CCC**	**SRS**	**r^2**	**slope y=x**
$UN_{\%exN}$ models														
Mod 1.01.01 **(Eq. 1)**	All	All	57.6	57.0	0.2	14.9	0.1	2.3	99.3	8.6	0.69	0.70	0.51	0.93
	All	Beef	56.5	52.4	-4.2	14.8	25.2	0.2	74.6	8.4	0.71	0.70	0.63	1.04
	All	Dairy	56.6	59.7	3.1	14.7	14.3	0.4	85.3	8.3	0.57	0.82	0.42	0.92
	All	Deer	47.7	52.4	5.9	25.4	23.4	1.0	69.7	12.1	0.56	0.78	0.56	1.42
	All	Sheep	61.5	57.2	-2.7	13.1	11.0	5.3	87.3	8.1	0.77	0.65	0.63	0.90
Mod 1.01.03 **(Eq. 2)**	All	All	57.6	57.2	0.3	14.5	0.1	2.7	98.7	8.3	0.72	0.68	0.54	0.91
	All	Beef	56.5	52.7	-3.8	14.8	21.1	0.1	78.8	8.4	0.72	0.70	0.61	0.98
	All	Dairy	56.6	57.3	0.7	13.6	0.8	1.4	97.8	7.7	0.62	0.76	0.43	0.88
	All	Deer	47.7	54.5	8.2	27.9	37.7	0.4	57.5	13.3	0.52	0.86	0.57	1.38
	All	Sheep	61.5	59.8	0.0	12.5	0.0	9.3	96.2	7.7	0.79	0.62	0.63	0.87
Mod 3.01.01 **(Eq. 3)**	Dairy	Dairy	58.4	57.8	-0.5	12.2	0.6	0.8	98.6	7.1	0.72	0.71	0.59	1.08
Mod 4.01.02 **(Eq. 4)**	Deer	Deer	56.5	56.5	0.0	12.2	0.0	0.0	100.0	6.9	0.77	0.45	0.62	1.00
Mod 5.01.02 **(Eq. 5)**	Sheep	Sheep	61.5	60.5	0.6	12.3	0.5	3.5	98.8	7.6	0.78	0.61	0.63	0.94
FN models														
Mod 1.05.03 **(Eq. 6)**	All	All	67.9	67.2	-0.8	24.4	0.2	1.3	98.5	16.5	0.97	0.25	0.94	1.03
	All	Beef	49.9	56.7	6.8	23.9	32.5	1.3	66.2	12.0	0.87	0.48	0.85	1.06
	All	Dairy	139.0	134.8	-4.2	17.8	2.9	0.1	97.0	24.7	0.72	0.67	0.56	0.97
	All	Deer	15.1	13.8	-1.3	36.6	5.4	1.4	93.2	5.5	0.78	0.61	0.64	0.92
Mod 5.05.01 **(Eq. 7)**	Sheep	Sheep	7.4	7.3	-0.1	25.0	0.1	0.6	99.3	1.9	0.81	0.55	0.69	1.06