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1 Simulation of timothy nutritive value : A comparison of three process-based models

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16 Abstract

Different forage grass models are used to simulate forage yield and nutritive attributes, but 17 18 these models are seldom compared, particularly those for timothy (Phleum pratense L.), a 19 widely grown forage grass species in agricultural regions with a cold temperate climate. We 20 compared the models BASGRA, CATIMO and STICS for their predictions of timothy crude 21 protein (CP) concentration, neutral detergent fibre (NDF) concentration and NDF digestibility 22 (dNDF), three important forage nutritive attributes. Data on CP and NDF concentrations, and dNDF and the associated weather and soil data for seven cultivars, taken from eight field 23 24 experiments in Canada, Finland, Norway, and Sweden, were divided into calibration and validation datasets. Model parameters were estimated for each cultivar separately (cultivar-25 26 specific calibration) and for all cultivars together (generic calibration), using different methods 27 for the three models. Normalized root mean square error (RMSE) in prediction of CP 28 concentration varied between 16 and 26 % for BASGRA, 45 and 101 % for CATIMO and 27 and 45 % for STICS across the two calibration methods and the calibration and validation datasets. 29 Normalised RMSE in prediction of NDF concentration varied between 8 and 13 % for BASGRA, 30 31 14 and 21 % for CATIMO and 8 and 12 % for STICS, while for dNDF it varied between 7 and 22 % for BASGRA, 7 and 38 % for CATIMO and 5 and 6 % for STICS. Cultivar-specific calibration 32 33 improved the performance of CATIMO and STICS, but not BASGRA, compared with generic calibration. The prediction accuracy for NDF concentration and dNDF with the three models 34 was within the same range or better than that for forage dry matter (DM) yield of timothy. 35 36 Overall, the three models performed well in predicting some nutritive attributes and yield in 37 Northern Europe and Canada, but improvements are required, particularly to increase the prediction accuracy of CP concentration. 38

39 Key words: BASGRA, CATIMO, crude protein, fibre, forage grass, grassland, NDF, dNDF, STICS

41 1. Introduction

Forage grasses serve as the main source of energy and nutrients for ruminant livestock, 42 including dairy cows, beef cattle, sheep and goats, in many regions of the world (Fulkerson et 43 44 al., 2007; Thornton, 2010). Hence, management for optimal energy and nutrient content in 45 forage crops is crucial to these animals. Feed evaluation for ruminants usually takes into 46 account the digestibility and protein concentration of the forage (Bruinenberg et al., 2002). 47 Because the cell contents are almost totally digestible, the concentration of cell walls is crucial to the nutritive value of forages (Buxton, 1996). Typically measured indicators of forage 48 nutritive value are the concentration and digestibility of neutral detergent fibre (NDF) and the 49 crude protein (CP) concentration. The development of stem and inflorescence on 50 51 reproductive tillers generally lowers the nutritive value of the forage, because these plant parts are less digestible than leaves (Chapman et al., 2014; Elgersma and Søegaard, 2018). 52 However, as the forage grass sward grows and develops more reproductive tillers, the total 53 aboveground biomass also increases causing a negative relationship between nutritive value 54 and dry matter yield (Wilkinson and Rinne, 2018). 55

In Northern Europe and Canada, perennial forage grasses grown for intensive dairy production 56 57 are usually cut and harvested 2-3 times per growing season and conserved as silage (Höglind et al., 2005; Casler and Kallenbach, 2007; Jing et al., 2012). Timothy (Phleum pratense L.) is 58 one of the most widely used forage grass species in cold-temperate regions of the world 59 (Wilkinson and Rinne, 2018), where it is grown under a wide range of climate, soil and 60 management conditions. This species exhibits slower development, expressed as growing 61 degree-days from the start of the growing season until the start of anthesis, than many other 62 cold temperate forage grasses (Pontes et al., 2007). Comparisons with other forage grasses in 63

the same environment also show that timothy has high (Pontes et al., 2007) to intermediate 64 65 (Jensen et al., 2016) CP concentration and digestibility. The DM yield and nutritive value of the timothy vary with growing conditions and management practices, such as cutting and 66 fertilisation regimes (Bélanger et al., 2001). In addition, the relationship between 67 68 development, growth and nutritive value varies between timothy cultivars (Jokela et al., 2015). Length of the growing season, temperature and precipitation patterns during the 69 growing season and conditions in the previous winter are particularly important for growth, 70 71 yield development and management of this species.

72 Process-based simulation models for forage grass (e.g. Bonesmo and Belanger, 2002a; Wu et al., 2007; Köchy, 2008; Chang et al., 2013; Jégo et al., 2013; Vital et al., 2013; Höglind et al., 73 74 2016) seek to represent the physiological processes behind sward growth and development. 75 However, the representation of processes such as water and nutrient uptake, carbon (C) assimilation and carbohydrate allocation and transfer between plant compartments varies 76 between models (Kipling et al., 2016; Sándor et al., 2017). Previous studies showed different 77 responses in gross primary production (Sándor et al., 2016), biomass (Hurtado-Uria et al., 78 2013; Sándor et al., 2017; Ehrhardt et al., 2018) and N₂O emissions (Ehrhardt et al., 2018) for 79 80 different grassland models when compared under various environmental conditions. As for 81 timothy, Korhonen et al. (2018) compared three models for their ability to predict DM yield in 82 Northern Europe and Canada. However, to our knowledge, there are no other published comparisons of the ability of forage grass models to predict nutritive value. 83

The underlying processes explaining the yield and nutritive value in forage grasses are arguably more complex than those explaining only DM production. In particular, as pointed out by Virkajärvi et al. (manuscript under preparation), models of forage grasses differ

considerably in how they handle plant processes related to plant N requirements and cell wall formation and content. A comparison of the ability of forage grass models to predict nutritive value in field experiments could provide knowledge about the utility of these models under different weather, soil, cutting and fertiliser management conditions. Such knowledge could help select prediction models for different conditions, in quantifying uncertainty in model predictions under different conditions, and in identifying potential improvements in the representation of physiological processes in different models.

In this study, the ability of three simulation models (BASGRA, CATIMO and STICS) to predict three key nutritive attributes [CP concentration, NDF concentration and the digestibility of NDF (dNDF)] in timothy in a wide range of environments representing the main regions where timothy is grown in the northern hemisphere was compared. In addition, we tested two different calibration strategies: generic and cultivar-specific.

99

100 2. Materials and methods

101 2.1. Model descriptions

The BASGRA, CATIMO, and STICS models simulate the growth and the development of the primary growth of timothy and its first regrowth as a function of the weather, soil conditions, and management practices, with a daily time step. In all three models, accumulation of biomass is based on the concept of radiation use efficiency where intercepted solar radiation is converted into biomass.

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108 2.1.1. BASGRA

The Basic Grassland (BASGRA) model (Höglind et al., 2016) is a further development of the 109 110 LINGRA model, which was initially developed to simulate perennial ryegrass (Schapendonk et 111 al., 1998) and later adapted to timothy (Höglind et al., 2001). In BASGRA, the plant is divided into stem, leaf, stubble, root and reserve compartments. The model is based on the source-112 113 sink concept. The source tissue, with net export of photosynthetic assimilates, consists of developed leaves, other photosynthetic tissues and carbohydrate reserves. The sink tissue, 114 with net import of photosynthetic assimilates, comprises newly developed plant parts and 115 116 roots. Sward development is driven by air temperature and day length. Carbohydrate reserves are used for producing new leaf tissue at the start of the growing season or after defoliation 117 when there is little source tissue. Equations to simulate soil and plant N and forage nutritive 118 119 value have recently been developed (Höglind et al., manuscript under preparation). The soil is 120 described as one single homogeneous layer. Plant-available water in the soil is set as the difference between the water content at field capacity and the water content at wilting point. 121 122 The soil water content is affected by infiltration, soil surface evaporation and run-off, water 123 uptake by plants and percolation of water above field capacity, simulated using the tipping-124 bucket method. Soil C is divided into three pools with different residence times, i.e. litter, soil organic matter with a fast decomposition rate and soil organic matter with a slow 125 126 decomposition rate. Soil N is divided into four pools: similar litter and soil organic matter pools as used for C, plus a pool of mineral N. Nitrogen can flow between these pools through 127 128 decomposition, mineralisation and immobilisation processes, which are all affected by soil 129 temperature. Nitrogen is added to the litter pool by shoot senescence, while root senescence 130 adds N to the fast-decomposing soil organic pool. Decomposition of organic N adds to the soil 131 mineral N pool, which is depleted by leaching, emissions of nitrous oxide and nitrogen oxide, and plant N uptake. Nitrogen leaching is driven by the rate of water drainage which, in turn, 132

is affected by soil hydraulic properties and infiltration, transpiration and evaporation.
Nitrogen emissions increase with availability of mineral N. The soil N functions are obtained
from the forest model BASFOR (Van Oijen et al., 2005).

136

137 Sub-optimal plant N status affects the shoot C sink strength and thus shoot growth. Tillering rate also depends on the plant N status. Plant N availability is the sum of soil N that is available 138 for plant uptake and plant N that is available for remobilisation within the above-ground plant 139 parts. The latter is the amount of N above an optimal N concentration profile that follows the 140 light extinction profile from the top to the bottom of the canopy, which is allocated to growing 141 142 plant tissue. Consequently, the optimal N concentration decreases as more light is 143 extinguished through the canopy as it grows. The nitrogen-carbon ratio in the roots is constant. The plant CP concentration is the N concentration multiplied by 6.25. The fraction 144 of cell walls in the biomass, as expressed by the NDF concentration, is allowed to differ 145 146 between leaves and stems, and increases with phenological stage (Bélanger and McQueen, 147 1999; Nordheim-Viken et al., 2009), but is not directly affected by temperature or N 148 concentration. The digestibility of the cell wall (dNDF) of both leaves and stems decreases with phenological stage (Bélanger and McQueen, 1999; Nordheim-Viken et al., 2009). The 149 150 digestible fraction of the cell wall is assumed to be the same in all plant components. In stubble, the cell wall fraction is set at 100%, whereas there is no cell wall fraction in the 151 152 reserves. The digestibility of the cell content is set at 100%.

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154 2.1.2. CATIMO

The Canadian Timothy Model (CATIMO) was developed to simulate the growth of timothy, 155 including N processes (Bonesmo and Bélanger, 2002a) and fibre concentration and 156 157 digestibility (Bonesmo and Bélanger, 2002b). The model allocates biomass into green leaves, stems and roots. Similarly to BASGRA, a portion of the biomass that is allocated to the above-158 159 ground compartments is allocated to reserves, which is used to form new tissue after defoliation or winter. The light-driven biomass growth is decreased under sub-optimal soil 160 water, plant N, photosynthetically active radiation (PAR) and temperature conditions. The 161 potential radiation use efficiency, which determines growth when there are no limiting 162 factors, is constant throughout the growing season. The soil hydraulic properties and C and N 163 content are simulated in one homogeneous layer. The N stress is estimated from an index of 164 165 N nutrition that is calculated as the ratio of N concentration to the critical N concentration for a given biomass (Bélanger and Gastal, 2000). Plant N uptake is determined by crop demand 166 and soil N supply. The soil N supply is estimated from soil mineral N content and N 167 mineralisation. The N demand is defined as the difference between actual and maximum N 168 169 concentration, with the latter decreasing with increasing sward biomass using an N dilution 170 curve. The plant CP concentration is calculated by multiplying the N concentration by 6.25. For simulation of forage digestibility, the sward is considered to consist of green leaves, dead 171 172 leaves and stems including leaf sheaths, each with their own NDF concentration and digestibility. The dry matter (DM) digestibility of the sward is calculated by combining the DM 173 digestibility of green leaves, dead leaves, and stems with their respective weight. The DM 174 digestibility of the cellular content of green leaves and stems is set at 0.98 g g⁻¹ DM. Dead 175 leaves are assumed to have a NDF concentration of 1.0 g g⁻¹ DM, with a DM digestibility of 176 0.70 g g⁻¹ DM. The NDF concentration of green leaves and stems is obtained by integrating the 177 proportion of the respective daily growth rates partitioned to cell wall, the daily rates of 178

179 conversion of cellular contents into cell wall and the daily death rate of leaves. The dNDF of 180 green leaves and stems is determined from an initial maximum value and a daily rate of 181 decrease related to daily mean temperature. Both temperature and N stress are taken into 182 account in simulation of the NDF concentration and dNDF of green leaves and stems.

183

184 2.1.3. STICS

185 The multidisciplinary simulator for standard crops (Simulateur mulTIdisciplinaire pour les Cultures Standard, STICS) is a model for simulation of agricultural crops and cropping systems 186 187 (Brisson et al., 1998, 2008). It has an add-on module for timothy, including N and nutritive 188 value-related functions (Jégo et al., 2013). The potential radiation use efficiency, setting the growth under non-limiting conditions, varies between juvenile, vegetative and reproductive 189 190 phenological phases. The model simulates soil water dynamics and C and N processes in a multi-layer profile. Plant N demand is driven by the N dilution curve concept for calculating 191 the N requirements of the plants (Bélanger and Gastal, 2000). In the STICS model, the optimal 192 193 crop N uptake is described using the relationship between the critical N concentration and 194 total biomass. The critical N concentration (Nc, % N per DM unit) is defined as the lowest plant N concentration required for maximum growth. As most crops can take up more N than is 195 196 needed for optimum growth, a maximum N concentration curve is also required in STICS, but no additional biomass growth occurs for N uptake between the critical and maximum N 197 concentrations. The effective total N uptake rate is limited either by the crop N demand or by 198 199 the soil N availability. Plant metabolism is affected when the total N concentration is below the critical concentration for a given biomass defined by the critical N concentration curve. 200

Functions to calculate NDF concentration and digestibility are from CATIMO (described brieflyabove).

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204 2.2. Crop data

205 Data on timothy from experimental sites at Fredericton (45°55'N; 66°32'W; 35 m asl),

206 Lacombe (52°28'N; 113°44'W; 860 m asl) and Québec (46°47'N; 71°07'W; 75 m asl) in Canada; 207 Maaninka (63°09'N; 27°17'E; 90 m asl), Rovaniemi (66°35'N; 26°01'E; 106 m asl) and Ruukki (64°40'N; 25°06' E; 48 m asl) in Finland; Særheim (58°46'N; 5°39'E; 90 m asl) in Norway; and 208 209 Umeå (63°45'N; 20°17'E; 12 m asl) in Sweden were used for model calibration and validation 210 (Fig. 1). Data were from the spring growth before and during the first cut and the summer 211 regrowth after the first cut until the second cut. They covered forage dry matter (DM) yield, 212 DM yield of stems and leaves, leaf area index, tiller density, water-soluble carbohydrate concentration and nutritive attributes (CP concentration, NDF concentration, dNDF, ash 213 concentration, digestible DM and digestible organic matter). Data were not available for all 214 215 experimental sites and years (see Table 1). The dataset was divided into combinations of sites, 216 years, cultivars and management regimes, with each unique combination called a "treatment" according to Korhonen et al. (2018). In total, there were 101 treatments. Thirty-three of the 217 218 treatments were previously used in Korhonen et al. (2018) whereas the remaining 68 219 treatments have not been used in any other previous modelling study.

The methods used to measure nutritive value varied slightly between the locations. Nitrogen concentration was analysed using a standard Kjeldahl method at Rovaniemi (Nissinen et al., 2010) and Umeå (Gustavsson and Martinsson, 2004), near-infrared reflectance spectroscopy (NIRS) at Maaninka, Ruukki and Særhiem (Marum, 1990). The NDF concentration at

Fredericton, Lacombe, and Québec was determined using a combination of chemical and NIRS methods. At Fredericton, the NDF analyses were based on methods by Van Soest et al. (1991) without using sodium sulphite, while at Lacombe and Québec the analyses were carried out using an Ankom Fiber Analyzer. At Maaninka, Ruukki and Særheim, the NDF concentration was analysed using NIRS and at Umeå using an ANKOM filter bag technique. The NDF digestibility at Fredericton and Québec was analysed from rumen contents using a method described by Van Soest et al. (1966).

231 Table 1.

232 Figure 1.

233 2.3 Weather and soil data

Daily weather data on minimum and maximum temperature, precipitation, global solar radiation, wind speed and relative air humidity were obtained from weather stations near the experimental sites. The data for Fredericton, Québec and Lacombe were obtained from Environment Canada

(http://climat.meteo.gc.ca/historical_data/search_historic_data_e.html), 238 those for Maaninka, Rovaniemi and Ruukki from the Finnish Meteorological Institute, those for 239 240 Særheim from the Agrometeorology Norway network (http://lmt.nibio.no/) and those for 241 Umeå from the Swedish Meteorological and Hydrological Institute (SMHI) (www.smhi.se). The 242 soil input data comprised texture fractions, bulk density, soil organic material and pH. Soil 243 hydraulic characteristics, including water content at permanent wilting point, field capacity and saturation, which are input to all three models, were either measured or estimated based 244 on available data on soil properties at each site. 245

246

247 2.4. Model calibration and validation

The dataset was divided into calibration and validation data by randomly selecting one treatment for model evaluation from each treatment type from sites with more than two treatments or years except for Rovaniemi, for which no nutritive value data were used in this study (Table 2). Differences in nutritive attribute data availability between sites, geographical location and differences in climate and soil conditions and management practices among sites were taken into account in this division.

254 Table 2.

Two types of calibrations were conducted for each model. In one, parameters were calibrated 255 256 using data for each cultivar separately (cultivar-specific calibration). In the other, a common 257 set of parameter values representing all cultivars was obtained by using the data for all 258 cultivars together (generic calibration). The division between calibration and validation datasets was the same for the two calibration types. In the two calibrations, each model was 259 calibrated using model-specific methods. BASGRA and CATIMO were calibrated using Bayesian 260 261 techniques (Van Oijen et al., 2005). For BASGRA, a prior probability distribution was first 262 defined for each parameter to be calibrated, which was then updated using the observed data, which included nutritive value data as well as observations of biomass, and biomass-related 263 264 data such as leaf area index, specific leaf area and tiller density. For the BASGRA calibration, 265 beta prior distributions were used for all calibration parameters (Table S1). The prior parameter distribution for most parameters was set using information from a previous 266 267 calibration for the cultivar Grindstad in the LINGRA model (the predecessor of BASGRA), in which timothy data from the Nordic region of Europe were used (Persson et al., 2014). For 268 those parameters relating to nutritive value that were introduced into BASGRA later, the prior 269

270 probability distribution was set within a wide, yet plausible, range with the help of literature 271 information and preliminary calibrations. The BASGRA calibration was carried out by sampling 272 from the posterior distribution using the Metropolis algorithm and a chain length of 350 000. A likelihood function by Sivia (2006), which is more robust to outliers than the Gaussian 273 274 distribution, was used in the calibration. For CATIMO, the prior probability distribution of parameters was obtained from a previous calibration (Korhonen et al., 2018) for the same 275 cultivars as used in this study except for cv. Nuutti, for which the prior probability distribution 276 was set based on cv. Tammisto II. The posterior sampling chain length for the Metropolis 277 algorithm was 150 000 iterations for Grindstad, Champ, Climax, Jonatan and generic, 200 000 278 279 iterations for Nuutti and 250 000 iterations for Tammisto II and Iki. For both BASGRA and 280 CATIMO, the maximum *a posteriori* (MAP) vectors from the calibration were used to evaluate the models, not the whole posterior distribution, since uncertainty quantification was not 281 within the scope of this study. In the STICS and CATIMO calibrations, only the parameters 282 283 involved in calculation of NDF concentration and dNDF were calibrated. For STICS, parameters 284 calibrated in Korhonen et al. (2018) were used to simulate plant growth and N uptake except 285 for cv. Nuutti, for which a new calibration was required since this cultivar was not included in the previous study. The parameters of the maximum and critical N dilution curves used in this 286 287 study were those defined by Jégo et al. (2013). These parameters were not calibrated, because in STICS they are supposed to be common to all cultivars of the same species and because it 288 is not recommended to calibrate them directly in the model. If it is considered necessary to 289 290 define new parameters, then this should be done in a separate study following the 291 methodology proposed by Justes et al. (1994). All parameters used to calculate NDF 292 concentration were calibrated simultaneously by minimising the sum of squared differences 293 between measured and simulated NDF values. Two optimisation algorithms available in the

Flexible Modelling Environment (FME) package in R were used. The two-step method was used, to avoid the problem of local minima. For both steps, calibrated values were constrained in a calibration range. In the first step, the pseudo algorithm, a pseudo-random search algorithm, was used with the maximum number of iterations (1000). A second algorithm (L-BFGS-B; constrained quasi-Newton method) was then used to refine the calibration. The dNDF parameters were calibrated using the same method.

300

301 2.5. Statistical analysis

The prediction accuracy of the observed CP concentration, NDF concentration and dNDF was evaluated with the root mean square error (RMSE):

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$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (P - O_i)^2}{n}}$$
(1)

where *n* is the number of observations and P_i and O_i are the predicted and observed values for each data pair. The closer the RMSE is to 0, the better the agreement. The RMSE was divided by the mean of the observed values (normalised RMSE) to allow comparison of the prediction accuracy among different nutritive attributes. In addition, predictions were evaluated with the relative mean bias error (rMBE):

310

311
$$rrrrrrr = \frac{\sum_{ii=1}^{nn} PP_{ii} - OO_{ii}}{\sum_{ii=1}^{nn} VOU_{ii}}$$
 (2)

The rMBE provides a measure of the relative magnitude of over- or under-estimation of the nutritive attributes. Willmott's index of agreement (d-index) was also used to evaluate the model predictions:

316
$$dd = 1 - \sum_{\substack{j=1 \\ i \neq j \\ i \neq j}}^{m} \frac{(p - O_{ij})^2}{p} + O_{ij} + O_{ij}$$

where *P_i* and *O_i* are the means of the predicted and observed values and the closer *d* is to 1, the better the agreement between observed and simulated values. According to Willmott (1981), d-index should be used to show the agreement between observations and predictions in a dimensionless way, as a complement to the RMSE. Observed and simulated pairs of nutritive attributes were also plotted against the amount of N applied per cut, mean annual temperature and accumulated annual precipitation, to identify any trends in prediction accuracy across the environmental variability within the calibration and validation datasets.

324

325 **3.** Results

326 3.1. Cultivar-specific calibration and validation

Predictions of CP concentration with BASGRA had a lower normalised RMSE (19%) than those 327 predicted by CATIMO and STICS (50 % and 40 %, respectively) in the cultivar-specific 328 329 calibration (Fig. 2; Table 3). Both STICS and BASGRA had a lower normalised RMSE (24 % and 330 26 %, respectively) than CATIMO (45 %) in the cultivar-specific validation (Table 4). BASGRA 331 under-estimated observed CP concentrations (rMBE = -6 %) in the cultivar-specific calibration (Table 3; Fig. 2), due to under-estimation of high CP concentrations, whereas CATIMO and 332 STICS over-estimated the observed CP concentrations (rMBE = +19 % and +29 % respectively) 333 (Table 3), mostly because of over-estimation of high CP concentrations. In the cultivar-specific 334

335 calibration with data from several locations and cultivars, BASGRA and STICS predicted the NDF concentration with lower normalised RMSE (13 % and 8 %, respectively) and greater d-336 337 index (0.59 and 0.75, respectively) than CATIMO (21 % and 0.43, respectively) (Fig. 3; Table 3). For the cultivar-specific validation, however, there were no clear differences between the 338 339 three models in their ability to predict NDF concentration (Fig. 3; Table 4). The NDF concentration was slightly under-estimated by all three models in the cultivar-specific 340 calibration (Table 3) and validation (Table 4). This under-estimation tended to be greater for 341 BASGRA (rMBE = -9.0 %) than for CATIMO and STICS (rMBE = -0.2 % and -0.4 %, respectively) 342 343 in the cultivar-specific calibration. CATIMO and STICS predicted dNDF with lower normalised 344 RMSE than BASGRA in the cultivar-specific calibration (10%, 6% and 22%, respectively) (Table 345 3) and the cultivar-specific validation (7 %, 5 % and 10 %, respectively) (Table 4). STICS underestimated and CATIMO over-estimated dNDF in both the cultivar-specific calibration and 346 validation, while BASGRA slightly over-estimated dNDF in the cultivar-specific calibration and 347 348 under-estimated it in the cultivar-specific validation. However, the over-estimation in the 349 cultivar-specific calibration with BASGRA was greatly influenced by a large error in one single 350 measurement (Fig. 4), so it can be assumed that BASGRA under-estimated dNDF in both 351 calibration and validation.

352 Figure 2.

353 Figure 3.

354 Figure 4.

355 Table 3.

356 Table 4.

357 When plotted against the amount of N applied per cut, there was a slight increase in both 358 observed and simulated CP concentrations with increasing N level. However, CATIMO and 359 STICS tended to over-estimate CP concentration. For CATIMO, this trend was more noticeable at high than at low N fertiliser levels (Fig. 5; Fig. 6). There were no clear trends in the 360 361 predictability of NDF concentration and dNDF across N fertiliser levels for any of the three models (not shown). Moreover, it was not possible to discern any trends in predictability 362 among climate conditions when the three observed and simulated nutritive attributes were 363 364 plotted against mean annual air temperature and mean annual accumulated precipitation (data not shown). 365

366 Figure 5.

367 Figure 6.

368

369 There was no clear trend between N fertilizer level and DM yield, possibly because many of the measurements of dry matter and nutritive value were taken in between normal cutting 370 times. To further analyse the underlying mechanisms for the differences in the prediction 371 accuracy of CP concentration, simulated CP concentrations with the three models were 372 373 plotted against simulated dry matter yield and, while observed CP concentrations were 374 plotted against observed dry matter yield for the cultivar specific and generic calibration (Fig. 375 7). The plotted relationships indicate that CATIMO, and in some cases the other two models, 376 simulated higher CP concentration than what was observed at a similar dry matter yield, especially at low dry matter yields. 377

378

379 3.2. Generic calibration and validation

The prediction accuracy across the three models in the generic calibration and validation 380 followed the same pattern as the cultivar-specific calibration and validation. The prediction 381 382 accuracy of CP concentration in the generic calibration was higher for BASGRA (normalised 383 RMSE = 16 %, d-index = 0.89) and STICS (normalised RMSE = 38 %, d-index = 0.92) than for 384 CATIMO (normalised RMSE = 101 %, d-index = 0.36) (Table 5). Similar differences in prediction accuracy between the three models were obtained with the validation dataset (Table 6). In 385 the calibration (Table 5) and validation datasets (Table 6), the observed CP concentration was 386 387 slightly under-estimated by BASGRA, over-estimated by STICS, and greatly over-estimated by CATIMO, based on rMBE. The prediction accuracy for NDF concentration and dNDF was also 388 389 higher for BASGRA and STICS than for CATIMO in the calibration (Tables 5) and validation 390 (Table 6), as indicated by lower normalised RMSE. However, prediction of NDF concentration 391 had a lower d-index with STICS than with BASGRA (Tables 5 and 6). The NDF concentration was slightly under-estimated by CATIMO in the calibration and validation datasets, whereas it 392 was slightly under-estimated in the calibration dataset and over-estimated in the validation 393 394 dataset by BASGRA. CATIMO and to a lesser degree BASGRA under-estimated dNDF in the 395 calibration and validation datasets. STICS slightly over-estimated NDF concentration and dNDF 396 in both datasets (Tables 5 and 6). The generic calibration of BASGRA resulted in slightly better predictions of the three nutritive attributes than the cultivar-specific calibration across 397 locations and cultivars, as indicated by lower normalised RMSE (Table 5). CATIMO predicted 398 399 CP concentration and dNDF less accurately in the generic calibration than in the cultivar-400 specific calibration, whereas it predicted NDF concentration better in the generic calibration (Table 5). STICS predicted NDF concentration better in the cultivar-specific calibration than in 401

the generic calibration, whereas the predictions of dNDF and CP concentration differed only
slightly between the cultivar-specific and generic calibrations (Table 5).

The trends in prediction of CP concentration across N fertiliser levels for the three models were similar to those in the cultivar-specific calibration and validation, but with a tendency for larger over-estimations by CATIMO under conditions with high N-fertiliser levels (Fig. 6). Similarly to the cultivar-specific calibration, simulated NDF concentration and dNDF did not show any trends across N-fertiliser levels for any of the three models. Moreover, there were no discernible trends in predictability of the three nutritive attributes across differences in mean annual air temperature and accumulated precipitation (not shown).

411 Table 5.

412 Table 6.

413 Figure 7.

414 4. Discussion

415 4. 1. Differences in prediction accuracy among nutritive attributes

416 This study examined how models with different structures and calibration procedures affect the prediction of dNDF and concentrations of CP and NDF in timothy under a broad range of 417 environmental conditions in the northern hemisphere. The predictions of NDF concentration 418 419 and dNDF were generally better than those of CP concentration, as indicated by lower 420 normalised RMSE and relative MBE and higher d-index in the calibrations of the three models. 421 This indicates that fibre concentration and digestibility can be predicted with higher accuracy 422 than N or CP concentration. These patterns in prediction accuracy of nutritive attributes that were previously reported from evaluations of CATIMO (Bonesmo et al., 2005; Jing et al., 2013) 423 and STICS (Jégo et al., 2013) against data from field experiments in Canada are confirmed and 424

extended to BASGRA. Even though the timothy CP concentration was less accurately simulated than the NDF concentration and dNDF in the studies cited above, it was generally predicted with better accuracy than in our study. In both CATIMO and STICS, crop N demand is based on critical and maximum N dilution curves. The parameters of those curves established for Canadian cultivars, which were not calibrated in our study, might not be adequate for European cultivars. Our results indicate that existing forage grass models are more efficient at predicting NDF concentration and dNDF than CP concentration.

432

433 4. 2. Differences in predictability between cultivar-specific and generic and calibration

434 The variability in prediction accuracy between cultivar-specific and generic calibrations provides information on the required calibration of forage grass models used to predict 435 436 nutritive value. The fact that CATIMO and STICS tended to have better prediction accuracy with the cultivar-specific calibration than with the generic calibration suggests that separate 437 calibrations for different cultivars could improve their predictive capacity. The overall slightly 438 439 better prediction accuracy of BASGRA in the generic calibration than in the cultivar-specific 440 calibration is, however, surprising. One reason could be that the larger dataset in the generic calibration than in the cultivar-specific calibration limited the influence of outliers and resulted 441 442 in more accurate predictions. Van Oijen et al. (2013) found that a generic calibration of models for Scots pine trees did not result in less accurate growth predictions than calibrations using 443 country-specific data. It should be noted, however, that the cultivar-specific datasets in our 444 445 study were obtained from experiments under different environmental conditions. Hence, differences in prediction accuracy between the cultivar-specific and generic calibrations could 446 be at least partly the result of non-cultivar differences between experimental sites, including 447

differences in climate, soils and crop management. However, this was not confirmed by the 448 449 analyses of observed and simulated nutritive attributes against N fertiliser levels, mean annual 450 air temperature and accumulated annual precipitation, which revealed little information about the impact of environmental variability on model prediction ability. Nevertheless, a 451 452 previous study in which LINGRA, the predecessor of BASGRA, simulated only one timothy cultivar (cv. Grindstad) in a number of field experiments in northern Europe showed better 453 prediction of aboveground DM biomass when the model was calibrated specifically for one 454 experimental site than when it was calibrated using data from several sites (Persson et al., 455 2014). To single out the effects of cultivars on calibration accuracy without any possible 456 457 confounding effects from weather, soil or other environmental factors, comparisons of 458 cultivar-specific and generic calibrations could be performed against data from one single site should there be any such datasets available. Moreover, further knowledge on cultivar-specific 459 traits that are important to the prediction accuracy for nutritive attributes could possibly be 460 obtained by grouping cultivars with similar traits together in the same calibration. 461

462

463 4. 3. Comparisons with dry matter yield predictability

The prediction accuracy of nutritive attributes was generally within the same range or better than the prediction accuracy of the forage DM yield for the same three models and partly the same experimental data (Korhonen et al., 2018). The normalised RMSE for the forage DM yield predictions reported from the study by Korhonen et al. (2018), which varied between 24 and 93 % across calibrations and validations, was generally greater than that for the nutritive attributes in both generic calibrations and validations. Sixty-eight out of the 101 treatments that were used in our study were not included in the study of Korhonen et al. (2018). The

calibration techniques applied for CATIMO and STICS meant that dry matter related 471 472 parameters calibrated in the study of Korhonen et al. (2018) for the other cultivars and the 473 generic calibration did not change. The new Grindstad treatments added here can hence be regarded as an additional validation of the Grindstad and generic calibrations. The normalized 474 475 RMSE for the calibration treatments of the Nuutti (CATIMO 62 %, STICS 27 %) and the newly added Grindstad treatments (CATIMO 66 %, STICS 25 %) from Maaninka and Ruukki 2015 and 476 2016, and the normalised RMSE of the generic calibration as evaluated against the same 477 treatments (CATIMO 129 %, STICS 26 %) were mostly within the same range as the normalised 478 479 RMSE of the DM yield predictions in Korhonen et al. (2018). For comparing models, we 480 calculated the RMSE of the DM predictions for the same treatment also for the BASGRA 481 calibrations in which, unlike the CATIMO and STICS calibrations, the values of all parameters changed during the cultivar-specific calibration of this model. The normalised RMSE for the 482 calibration treatments of the Nuutti and Grindstad cultivars from Maaninka 2015 and 2016 483 was 15 and 20 % respectively. For the generic calibration of BASGRA, the normalised RMSE for 484 485 the same treatments was 32 %. In total, these results illustrate that regardless of the 486 calibration technique the inclusion of nutritive value here was not at the expense of the predictability of the DM yield. 487

In previous evaluations of STICS (Jégo et al., 2013) and CATIMO (Bonesmo et al., 2005; Jing et
al., 2013) for Canadian locations and timothy cultivars, the normalised RMSE for forage DM
yield predictions was between 70 and 120 % greater than for NDF concentration, and between
220 and 440 % greater than for dNDF. Our results confirm that nutritive value predictions can
be as accurate as DM yield predictions in forage grasses.

493

495 4. 4. Possible explanations for the differences in prediction accuracy

Crude protein concentration in plants results from rather complex soil and plant N processes, 496 which are all affected by soil conditions, weather and crop management. Besides possible 497 498 errors in the input data, errors in the descriptions of processes could have affected the CP 499 concentration predictions. That those parameters, which were related to CP concentration were calibrated in BASGRA, but not in CATIMO and STICS, may have been a reason for the 500 501 difference in prediction accuracy of this attribute among the three models. The higher simulated CP concentration at low simulated dry matter yield than the observed CP 502 concentration at similar observed dry matter yield in CATIMO and to a lesser extent in STICS 503 (Figure 7) indicates that the assumption of N dilution with biomass that was taken from 504 505 previous model development against field trial data in Canada was not applicable to the cultivars and environmental conditions in northern Europe that were investigated here, at 506 507 least not at low dry matter yield. Further experimental studies are needed to demonstrate whether there are differences in N demand and uptake between timothy cultivars. However, 508 the greater difference in CP prediction accuracy between CATIMO and STICS than between 509 510 the latter and BASGRA indicates that there are other underlying reasons than the representation of plant N dilution with biomass or light extinction for the differences in CP 511 prediction accuracy. One reason could be differences in leaf/stem ratio prediction accuracy, 512 which would affect growth and hence N uptake and concentration. Unfortunately, there were 513 insufficient data available to thoroughly analyse correlations between leaf/stem ratio and 514 predictions of CP concentration. Forage NDF concentration increases and dNDF decreases 515 516 with phenological development, and these variables also directly affected by temperature in

CATIMO and STICS. Although severe N stress affects NDF concentration and dNDF in CATIMO 517 and STICS, there is no effect of soil and plant N on NDF concentration and dNDF under normal 518 519 N conditions in any of the three models which, given the complexity of soil-plant N processes, could explain why they are better predicted than CP concentration. Differences between 520 521 models in calculation of leaf/stem ratios could also explain some of the variation in predicted NDF concentration and dNDF among the three models. However, the effect of the leaf/stem 522 ratio on CP concentration is probably larger, due to the complex interaction between N 523 524 distribution in the plant and growth.

525

526 4. 5. Uncertainty in input data

Because the methods used for analysis of the three nutritive attributes were not always the 527 528 same at all sites, there is some uncertainty in the values (Huhtanen et al., 2006). Of the three nutritive attributes included in our study, dNDF most likely has the largest uncertainty 529 associated with the analysis methods and CP concentration the smallest. Different dNDF 530 531 values for the same forage sample analysed *in vitro* in different laboratories may stem from differences in the pore size of the nylon bags in which the samples are incubated and from 532 differences in the incubation time and the rumen liquid used. Similarly, differences in 533 534 methodology between laboratories, such as the use of different extraction chemicals, may result in laboratory differences in NDF concentration estimates (Tavares da Silva et al., 2018). 535 It should also be noted that NIRS often has poorer prediction accuracy for NDF concentration 536 537 and dNDF than for CP concentration, although high accuracy can also be achieved for the former attributes if the method is carefully calibrated with an adequate number of 538 representative reference samples and suitable reference analysis methods (Huhtanen et al., 539

2006). Nevertheless, the better prediction accuracy of NDF concentration and dNDF than of 540 541 CP concentration indicates that other reasons than the uncertainty in nutritive value 542 measurements were more important to the prediction accuracy. Errors related to the weather input data, mainly due to the distance between weather stations and observations in the field, 543 544 could also have affected our results. For most sites, there were no direct measurements of soil hydraulic properties available as input to the soil modules of the grass models and instead 545 these variables were estimated from data on soil texture fractions. For BASGRA and STICS, the 546 547 soil water contents at wilting point and at field capacity were therefore treated as parameters. However, that was not the case for CATIMO. Possible within-field variation in soil texture may 548 also have caused differences between the actual soil properties and those that were input to 549 the simulations. 550

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552

553 4. 6. Suggested further studies

The low prediction accuracy of CP concentration, the importance of CP concentration for 554 nutritive value and the general importance of N for crop performance and for its 555 556 environmental impact emphasise the need for improved descriptions of soil and plant N in the 557 three models. Moreover, studies with synchronised calibration procedures could help assess 558 whether the differences in prediction accuracy between the models were due to differences 559 in calibration methods or the model structure. Such information could increase the performance of models and thus their prospects of being applied in analysis of forage grass 560 performance under various existing or hypothetical environmental conditions. Further 561 562 calibrations with experimental data from other areas, such as Russia, northern Japan and 563 mountainous regions at lower latitudes in Europe, could provide more information about the 564 general applicability of the models. To place the performance of the three models in a broader 565 context, validation of the performance of other grassland models in predicting forage nutritive 566 value could also be valuable.

567

568 5. Conclusions

Three models with different structures (BASGRA, CATIMO and STICS) predicted NDF concentration and digestibility in timothy with similar accuracy to previous predictions of forage DM yield of timothy across a wide range of climate and soil conditions in Canada and northern Europe. However, prediction of CP concentration was rather poor compared with the other nutritive attributes. Cultivar-specific calibrations improved the performance of CATIMO and STICS, but not of BASGRA, compared with calibrations where data on all cultivars were used together.

576

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585 References

- Bélanger, G., and Gastal, F. 2000, Nitrogen utilization by forage grasses. Can. J. Plant Sci.
 80:11-20.
- 588 Bélanger, G., McQueen, R.E., 1999. Leaf and stem nutritive value of timothy grown with
- varying N nutrition in spring and summer. Can. J. Plant Sci. 79, 223-229.
- 590 Bélanger, G., Michaud, R., Jefferson, P.G., Tremblay, G.F., Brégard, A., 2001. Improving the
- nutritive value of timothy through management and breeding. Can. J. Plant Sci. 81, 577-585.
- 592 Bonesmo, H., Bélanger, G., 2002a. Timothy yield and nutritive value by the CATIMO model: I.
- 593 Growth and nitrogen. Agron. J. 94, 337-345.
- 594 Bonesmo, H., Bélanger, G., 2002b. Timothy yield and nutritive value by the CATIMO model:
- 595 II. Digestibility and fiber. Agron. J. 94, 345-350.
- 596 Bonesmo, H., Bélanger, G., Charmley, E., Drapeau, R., McKenzie, D.B., Michaud, R., Tremblay,
- 597 G.F., 2005. Timothy yield and nutritive value by the CATIMO model: III. Validation for eastern
- 598 Canada. Agron. J. 97, 32-40.
- 599 Brisson, N., Launay, M., Mary, B., Beaudoin, N., 2008, Conceptual basis, formalisations and
- 600 parameterization of the STICS crop model. Editions QUAE (Versailles).
- Brisson, N., Mary, B., Ripoche, D., Jeuffroy, M.H., Ruget, F., Nicoullaud, B., Gate, P.,
- 602 Devienne-Barret, F., Antonioletti, R., Durr, C., Richard, G., Beaudoin, N., Recous, S., Tayot, X.,
- Plenet, D., Cellier, P., Machet, J.M., Meynard, J.M., and Delécolle, R. 1998. STICS: A generic
- model for the simulation of crops and their water and nitrogen balances. I. Theory and
- parameterization applied to wheat and corn. Agronomie 18, 311-346.
- Bruinenberg, M.H., Valk, H., Korevaar, H., Struik, P.C., 2002. Factors affecting digestibility of
- temperate forages from seminatural grasslands: a review. Grass Forage Sci. 57, 292-301.

- 608 Buxton, D.R., 1996. Quality-related characteristics of forages as influenced by plant
- environment and agronomic factors. Anim. Feed Sci. Tech. 59, 37-49.
- 610 Casler, M.D., Kallenbach, R.L., 2007. Cool-season grasses for humid areas. Forages. The
- 611 Science of Grassland Agriculture 2, 211-220.
- 612 Chang, J., Viovy, N., Vuichard, N., Ciais, P., Wang, T., Cozic, A., Lardy, R., Graux, A.-I., Klumpp,
- K., Martin, R., 2013. Incorporating grassland management in ORCHIDEE: model description
- and evaluation at 11 eddy-covariance sites in Europe. Geosci. Model Dev. 6, 2165-2181.
- 615 Chapman, D.F., Lee, J.M., Waghorn, G.C., 2014. Interaction between plant physiology and
- 616 pasture feeding value: a review. Crop Pasture Sci. 65, 721-734.
- 617 Ehrhardt, F., Soussana, J.F., Bellocchi, G., Grace, P., McAuliffe, R., Recous, S., Sándor, R.,
- Smith, P., Snow, V., de Antoni Migliorati, M., 2018. Assessing uncertainties in crop and
- pasture ensemble model simulations of productivity and N2O emissions. Global Change Biol.
- 620 24, e603-e616.
- 621 Elgersma, A., Søegaard, K., 2018. Changes in nutritive value and herbage yield during
- extended growth intervals in grass–legume mixtures: effects of species, maturity at harvest,
- and relationships between productivity and components of feed quality. Grass Forage Sci.
- 624 73, 78-93.
- Fulkerson, W.J., Neal, J.S., Clark, C.F., Horadagoda, A., Nandra, K.S., Barchia, I., 2007.
- 626 Nutritive value of forage species grown in the warm temperate climate of Australia for dairy
- 627 cows: Grasses and legumes. Livest. Sci. 107, 253-264.
- 628 Gustavsson, A.-M., Martinsson, K., 2004. Seasonal variation in biochemical composition of
- cell walls, digestibility, morphology, growth and phenology in timothy. Eur. J. Agron. 20, 293-
- 630 312.

- Huhtanen, P., Nousiainen, J., Rinne, M., 2006. Recent developments in forage evaluation
- with special reference to practical applications. Agr. Food Sci. 15, 293-323.

Hurtado-Uria, C., Hennessy, D., Shalloo, L., Schulte, R.P.O., Delaby, L., O'Connor, D., 2013.

- 634 Evaluation of three grass growth models to predict grass growth in Ireland. J. Agr. Sci-
- 635 Cambridge 151, 91-104.
- Höglind, M., Schapendonk, A., Van Oijen, M., 2001. Timothy growth in Scandinavia:
- 637 combining quantitative information and simulation modelling. New Phytol. 151, 355-367.
- Höglind, M., Hanslin, H.M., Van Oijen, M., 2005. Timothy regrowth, tillering and leaf area
- 639 dynamics following spring harvest at two growth stages. Field Crops Res. 93, 51-63.
- Höglind, M., Van Oijen, M., Cameron, D., Persson, T., 2016. Process-based simulation of
- 641 growth and overwintering of grassland using the BASGRA model. Ecol. Model. 335, 1-15.
- 542 Jégo, G., Bélanger, G., Tremblay, G.F., Jing, Q., Baron, V.S., 2013. Calibration and
- 643 performance evaluation of the STICS crop model for simulating timothy growth and nutritive
- 644 value. Field Crops Res. 151, 65-77.
- Jensen, K.B., Robins, J.G., Rigby, C., Waldron, B.L., 2016. Comparative trends in forage
- nutritional quality across the growing season in 13 grasses. Can. J. Plant Sci. 97, 72-82.
- Jing, Q., Bélanger, G., Baron, V., Bonesmo, H., Virkajärvi, P., Young, D., 2012. Regrowth
- simulation of the perennial grass timothy. Ecol. Model. 232, 64-77.
- Jing, Q., Bélanger, G., Baron, V., Bonesmo, H., Virkajärvi, P. 2013. Simulating the nutritive
- value of timothy summer regrowth. Agron. J. 105, 563-572.
- Jokela, V., Trevaskis, B., Seppänen, M.M., 2015. Genetic variation in the flowering and yield
- 652 formation of timothy (Phleum pratense L.) accessions after different photoperiod and
- 653 vernalization treatments. Front. Plant Sci. 6.

- Justes, E., Mary, B., Meynard, J.M., Machet, J.M., and Thelier-Huche, L. 1994. Determination
- of a critical nitrogen dilution curve for winter wheat crops. Ann. Bot-London 74, 397-407.
- 656 Kipling, R.P., Virkajärvi, P., Breitsameter, L., Curnel, Y., De Swaef, T., Gustavsson, A.-M.,
- Hennart, S., Höglind, M., Järvenranta, K., Minet, J., Nendel, C., Persson, T., Picon-Cochard, C.,
- Rolinski, S., Sandars, D.L., Scollan, N.D., Sebek, L., Seddaiu, G., Topp, C.F.E., Twardy, S., Van
- 659 Middelkoop, J., Wu, L., Bellocchi, G., 2016. Key challenges and priorities for modelling
- 660 European grasslands under climate change. Sci. Total Environ. 566–567, 851-864.
- Köchy, M., 2008. Effects of simulated daily precipitation patterns on annual plant
- 662 populations depend on life stage and climatic region. BMC Ecol. 8, 4.
- Köppen, W., 1936: Das Geographische System der Klimate. In: W. Köppen and R. Geiger eds.
- 664 Handbuch der Klimatologie, vol I, Part C. Gebrüder Borntraeger, Berlin. Germany.
- Korhonen, P., Palosuo, T. Persson, T., Höglind, M., Jégo, G., Van Oijen, M., Gustavsson, A-M.,
- 666 Bélanger, G., Perttu Virkajärvi, P., 2018. Modelling grass yields in northern climates a
- 667 comparison of three growth models for timothy. Field Crops Res. 224,37-47.
- 668 Marum, P., 1990. Bestemmelse av kvalitet i forvekster ved hjelp av NIRS og metodens
- 669 muligheter i engvekstforedling. Norsk Landbruksforsking (Norway). Norwegian Agricultural
- 670 Research. no. 9/90 (suppl.).(NLH accession no. NOR).
- Nissinen, O., Kalliainen, P., Jauhiainen, L., 2010. Development of yield and nutritive value of
- timothy in primary growth and regrowth in northern growing conditions. Agr. Food Sci. 19,
- 673 252-268.
- Nordheim-Viken, H., Volden, H., Jorgensen, M., 2009. Effects of maturity stage, temperature
- and photoperiod on growth and nutritive value of timothy (Phleum pratense L.). Anim. Feed
- 676 Sci. Tech. 152, 204-218.

- 677 Persson, T., Höglind, M., Gustavsson, A.-M., Halling, M., Jauhiainen, L., Niemeläinen, O.,
- 678 Thorvaldsson, G., Virkajärvi, P., 2014. Evaluation of the LINGRA timothy model under Nordic
- 679 conditions. Field Crops Res. 161, 87-97.
- 680 Pontes, L.S., Carrère, P., Andueza, D., Louault, F., Soussana, J.F., 2007. Seasonal productivity
- and nutritive value of temperate grasses found in semi-natural pastures in Europe:
- responses to cutting frequency and N supply. Grass Forage Sci. 62, 485-496.
- 683 Sándor, R., Barcza, Z., Acutis, M., Doro, L., Hidy, D., Köchy, M., Minet, J., Lellei-Kovács, E., Ma,
- 684 S., Perego, A., 2017. Multi-model simulation of soil temperature, soil water content and
- biomass in Euro-Mediterranean grasslands: Uncertainties and ensemble performance. Eur. J.
- 686 Agron. 88, 22-40.
- 687 Sándor, R., Barcza, Z., Hidy, D., Lellei-Kovács, E., Ma, S., Bellocchi, G., 2016. Modelling of
- grassland fluxes in Europe: evaluation of two biogeochemical models. Agr. Ecosyst. Environ.215, 1-19.
- 690 Schapendonk, A., Stol, W., van Kraalingen, D.W.G., Bouman, B.A.M., 1998. LINGRA, a
- 691 sink/source model to simulate grassland productivity in Europe. Eur. J. Agron. 9, 87-100.
- 692 Sivia, D.S., 2006. Data Analysis: A Bayesian Tutorial. Oxford University Press, Oxford, UK.
- Tavares da Silva, R.S., Fernandes A.M., dos Santos Gomez, R., Ramos Bendia, L.C., da Costa e
- 694 Silva, L., Mendonca Viera, R.A. 2018. On the specificity of different methods for neutral fiber
- and related problems. Anim. Feed Sci. Tech. 240, 128-144.
- Thornton, P.K., 2010. Livestock production: recent trends, future prospects. Philos. T. Roy.
- 697 Soc. B. 365, 2853-2867.
- Van Oijen, M., Reyer, C., Bohn, F., Cameron, D., Deckmyn, G., Flechsig, M., Härkönen, S.,
- Hartig, F., Huth, A., Kiviste, A., 2013. Bayesian calibration, comparison and averaging of six

- forest models, using data from Scots pine stands across Europe. Forest Ecol. Manag. 289,255-268.
- Van Oijen, M., Rougier, J., Smith, R., 2005. Bayesian calibration of process-based forest
- models: bridging the gap between models and data. Tree Physiol. 25, 915-927.
- Van Soest, P.J., Robertson, J.B., Lewis, B.A., 1991. Methods for dietary fiber,
- neutraldetergent fiber, and non starch polysaccharides in relation to animal nutrition. J.
- 706 Dairy Sci. 74, 3583–3597.
- Van Soest, P.J., Wine, R.H., Moore, L.A., 1966. Estimation of the true digestibility of forages
- by the in vitro digestion of cell walls. Proc. Int. Grassland Congress, 10th, Helsinki, Finland, 7–
- 709 16 July 1966. Finnish Grassl. Assoc., Helsinki (1966), pp. 438-441.
- Vital, J.-A., Gaurut, M., Lardy, R., Viovy, N., Soussana, J.-F., Bellocchi, G., Martin, R., 2013.
- 711 High-performance computing for climate change impact studies with the Pasture Simulation
- 712 model. Comput.Electron. Agr. 98, 131-135.
- 713 Wilkinson, J.M., Rinne, M., 2018. Highlights of progress in silage conservation and future
- 714 perspectives. Grass Forage Sci. 73, 40-52.
- 715 Willmott, C.J., 1981. On the validation of models. Phys. Geogr. 2, 184-194.
- 716 Wu, L., McGechan, M., McRoberts, N., Baddeley, J., Watson, C., 2007. SPACSYS: integration
- of a 3D root architecture component to carbon, nitrogen and water cycling—model
- 718 description. Ecol. Model. 200, 343-359.

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Table 1. Cultivars, nutritive value (crude protein (CP) concentration, neutral detergent fibre
(NDF) concentration, digestibility of NDF (dNDF)) and N fertilizer treatments at the
experimental sites

Location	Mean	Köppen	Soil	Datase	Cultivar	Nutritiv	N fert.
	annual	climate	type	t year		e values	regim
	temp (°C)	classification					e (kg
	/annual acc.	1					ha⁻¹ yr⁻
	precipitatio						¹)
	n (mm)						
Fredericto	5.7/1108	Dfb (Warm-	Loam	1991-	Champ	NDF,	0, 70,
n (45°55'N;		summer		1993		dNDF	140,
66°32′W;		humid					168,
35 m asl)		continental					200,
		climate)					210
Lacombe	3.5/429	Dfb (Warm-	Silty	2004-	Climax	NDF	100
(52°28′N;		summer	clay	2005			
113°44′W;		continental	loam				
860 m asl)		climate)					
Québec	5.3/1009	Dfb (Warm-	Loam	1999-	Champ	NDF,	0, 60,
(46°47′N;		summer		2001		dNDF	120
71°07′W;		humid					
75 m asl)		continental					
		climate)					

Maaninka	4.2/560	Dfc	Silt	2006-	Tammist	NDF, CP	0, 150
(63°09′N;		(Continental	loam	2007,	o II,		180,
27°17′E;		Subarctic	/	2015-	Nuutti,		190,
90 m asl)		Climate).	loam	2016	Grindsta		200,
			2		d		250,
							300,
							350,
							400,
							450
Rovaniemi	1.0/610	Dfc	Silt	1999-	Iki	-	160,
(66°35′N;		(Continental	loam	2001			200
26°01′E;		Subarctic					
106 m asl)		Climate).					
Ruukki	2.6/513	Dfc	Silt	2015-	Nuutti,	NDF, CP	0, 150
(64°40′N;		(Continental	loam	2016	Grindsta		200,
25°06' E;		Subarctic			d		250,
48 m asl)		Climate).					300,
							350,
							400,
							450
Særheim	8.0/1392	Cfc (Cool	Sand	2000-	Grindsta	NDF, CP	220
		oceanic	у	2002	d		
		climate)	loam				

(58°46′N;							
5°39'E; 90							
m asl)							
Umeå	3.3/595	Dfc	Silt	1995-	Jonatan	NDF, CP	18
(63°45′N;		(Continental	loam	1996			
20°17′E;		subarctic					
12 m asl)		climate).					

728 ² Treatments 1-3, 33-37: Silt loam soil. Treatments 38-68: Loam soil

Treatment	Location	Cultivar	N fertiliser	Calibration/validation
number			application	
			(kg ha ⁻¹ yr ⁻¹)	
1-2	Maaninka	Tammisto II	180	Calibration
3-8	-8 Rovaniemi Iki		160, 200	Calibration
9, 11-12, 14	Særheim	Grindstad	220	Calibration
10, 13	Særheim	Grindstad	220	Validation
15-21,23	Québec	Champ	0,60,120	Calibration
22	Québec	Champ	60	Validation
24-25	Lacombe	Climax	100	Calibration
26-27	Umeå	Jonatan	180	Calibration
28, 30-32	Fredericton	Champ	0, 70, 140,	Calibration
			168, 210	
29, 33	Fredericton	Champ	200, 210	Validation
34-35, 37, 46-	Maaninka	Nuutti	0, 150, 190,	Calibration
50, 52-53, 62-			200, 250,	
68			300, 350,	
			400, 450	
36, 51, 69	Maaninka	Nuutti	190, 350,	Validation
			450	
38-40, 42-45,	Maaninka	Grindstad	0, 150, 200,	Calibration
54-59, 61			250, 300,	

730 Table 2. Division between calibration and validation data within the dataset

			350, 400,	
			450	
41,60	Maaninka	Grindstad	250, 400	Validation
71-77, 86-91,	Ruukki	Grindstad	0, 150, 200,	Calibration
93			250, 300,	
			350, 400,	
			450	
70, 92	Ruukki	Grindstad	0, 400	Validation
78-82, 84-85,	Ruukki	Nuutti	0, 150, 200,	Calibration
94-97, 99-101			250, 300,	
			350, 400,	
			450	
83, 98	Ruukki	Nuutti	300, 350	Validation

Table 3. Statistics on the cultivar-specific calibration: Observed and simulated means, root
mean squared error (RMSE), normalised RMSE, relative mean bias error (rMBE) and Willmott's
index of agreement (d-index) for crude protein (CP) concentration, neutral detergent fibre
(NDF) concentration and digestibility of NDF (dNDF)

	Number of	Mean of	Mean of RMSE		Normalised	rMBE	d-		
	observations	observation	simulation		RMSE (%)	(%)	index		
		CP concer	ntration (g g ⁻¹	DM)					
BASGRA			0.13	0.027	19	-6.0	0.82		
CATIMO	173	0.14	0.17	0.070	50	19.0	0.57		
STICS			0.18	0.055	40	29.0	0.88		
NDF concentration (g g ⁻¹ DM)									
BASGRA			0.51	0.072	13	-9.0	0.59		
CATIMO	252	0.56	0.57	0.120	21	-0.2	0.43		
STICS	252		0.56	0.045	8	-0.4	0.75		
		dND	PF (g g ⁻¹ NDF)						
BASGRA			0.71	0.170	22	0.7	0.72		
CATIMO	28	0.78	0.82	0.077	10	5.0	0.64		
STICS			0.78	0.046	6	-3.0	0.82		

Table 4. Statistics of the cultivar-specific validation: Observed and simulated means, root
mean squared error (RMSE), normalised RMSE, relative mean bias error (rMBE) and Willmott's
index of agreement (d-index) for crude protein (CP) concentration, neutral detergent fibre
(NDF) concentration and digestibility of NDF (dNDF)

	Number of	Mean of	Mean of	RMSE	Normalized	rMBE	d-			
	observations	observation	simulation		RMSE (%)	(%)	index			
CP concentration (g g ⁻¹ DM)										
BASGRA			0.13	0.037	26	-5.0	0. 72			
CATIMO	48	0.14	0.17	0.063	45	18.0	0.67			
STICS			0.16	0.034	24	11.0	0.93			
		NDF conce	ntration (g g ⁻	¹ DM)						
BASGRA			0.52	0.063	11	-0.1	0.63			
CATIMO	62	0.55	0.55	0.077	14	-0.7	0.64			
STICS			0.55	0.047	9	-0 5	0.71			
		dND	F (g g ⁻¹ NDF)							
BASGRA			0.70	0.081	10	-0.1	0.70			
CATIMO	14	0.78	0.81	0.053	7	0.5	0.81			
STICS			0.75	0.041	5	-3.0	0.87			

Table 5. Statistics of the generic calibration: Observed and simulated means, root mean
squared error (RMSE), normalised RMSE, relative mean bias error (rMBE) and Willmott's index
of agreement (d-index) for crude protein (CP) concentration, neutral detergent fibre (NDF)
concentration and digestibility of NDF (dNDF)

	Number of	Mean of	Mean of	RMSE	Normalised	rMBE	d-		
	observations	observation	n simulation		RMSE (%)	(%)	index		
CP concentration (g g ⁻¹ DM)									
BASGRA			0.15	0.022	16	-0.8	0.89		
CATIMO	173	0.14	0.26	0.14	101	87	0.36		
STICS			0.17	0.052	38	25	0.92		
		NDF conce	ntration (g g ⁻	¹ DM)					
BASGRA			0.56	0.050	8.8	-0.4	0.72		
CATIMO	252	0.56	0.55	0.095	17	-3	0.49		
STICS			0.56	0.066	12	0.8	0.46		
		dND	F (g g ⁻¹ NDF)						
BASGRA			0.75	0.072	9.3	-4	0.59		
CATIMO	28	0.78	0.51	0.29	38	-34	0.34		
STICS			0.79	0.050	6.4	0.23	0.82		

Table 6. Statistics of the generic validation: Observed and simulated means, root mean
squared error (RMSE), normalised RMSE, relative mean bias error (rMBE) and Willmott's index
of agreement (d-index) for crude protein (CP) concentration, neutral detergent fibre (NDF)
concentration and digestibility of NDF (dNDF)

	Number o	of Mean	of	Mean	of	RMSE	Normalized	rMBE	d-
	observatior	ns observa	tion	simulat	ion		RMSE (%)	(%)	index
		СР сс	ncer	ntration	g g ⁻¹	DM)			
BASGRA				0.15		0.025	18.0	-0.2	0.91
CATIMO	48	0.14		0.26		0.130	92.0	86.0	0.47
STICS				0.16		0.032	23.0	11.0	0.95
		NDF c	once	ntration	(g g ⁻	¹ DM)			
BASGRA				0.56		0.043	7.8	2.0	0.77
CATIMO	62	0.56		0.55		0.095	17.1	-2.0	0.51
STICS				0.56		0.069	12.4	0.9	0.49
			dND)F (g g⁻¹ N	IDF)				
BASGRA				0.75		0.050	6.5	-4.0	0.99
CATIMO	14	0.78		0.51		0.290	37.0	-36.0	0.34
STICS				0.79		0.047	6.0	0.2	0.99

Figure captions

Figure 1. Geographical location of the eight experimental sites in Canada and Northern Europe.

Figure 2. Observed crude protein concentration plotted against the simulated concentrations produced by BASGRA, CATIMO and STICS in the cultivar-specific calibration (upper row) and validation (lower row). Statistics on the cultivar-specific calibration and validation are presented in Tables 3 and 4.

Figure 3. Observed neutral detergent fibre concentration plotted against the simulated concentrations produced by BASGRA, CATIMO and STICS in the cultivar-specific calibration (upper row) and validation (lower row). Statistics on the cultivar-specific calibration and validation are presented in Tables 3 and 4.

Figure 4. Observed digestibility of neutral detergent fibre (dNDF) plotted against the simulated values produced by BASGRA, CATIMO and STICS in the cultivar-specific calibration (upper row) and validation (lower row). Statistics on the cultivar-specific calibration and validation are presented in Tables 3 and 4.

Figure 5. Observed crude protein concentration and concentration simulated by BASGRA, CATIMO, and STICS with cultivar-specific parameters as a function of amount of N applied per cut. Upper row: calibration dataset, lower row: validation dataset.

Figure 6. Observed crude protein concentration and concentration simulated by BASGRA, CATIMO, and STICS with generic parameters as a function of the amount of N applied per cut. Upper row: calibration dataset, lower row: validation dataset.

Figure 7. Observed crude protein concentration vs observed dry matter yield, and simulated crude protein vs simulated dry-matter yield for the cultivar-specific (left) and generic (right) calibrations.

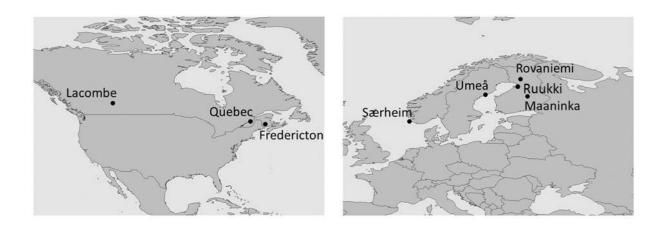


Figure 1. Geographical location of the eight experimental sites in Canada and Northern

Europe.

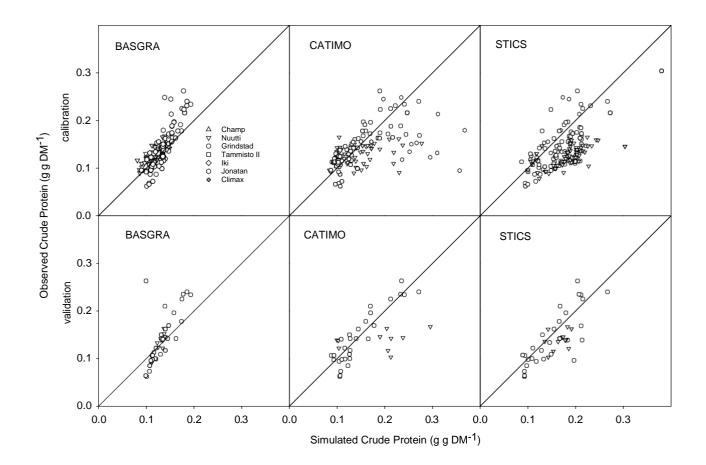


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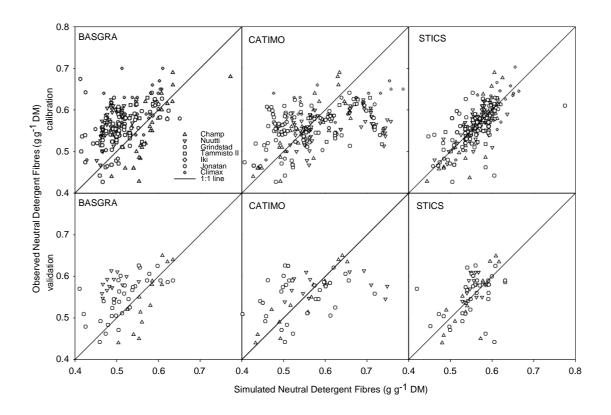


Figure 3. Observed neutral detergent fibre concentration plotted against the simulated concentrations produced by BASGRA, CATIMO and STICS in the cultivar-specific calibration (upper row) and validation (lower row). Statistics on the cultivar-specific calibration and validation are presented in Tables 3 and 4.

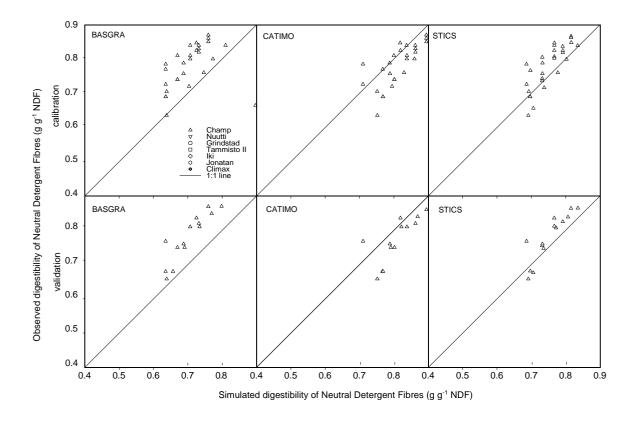


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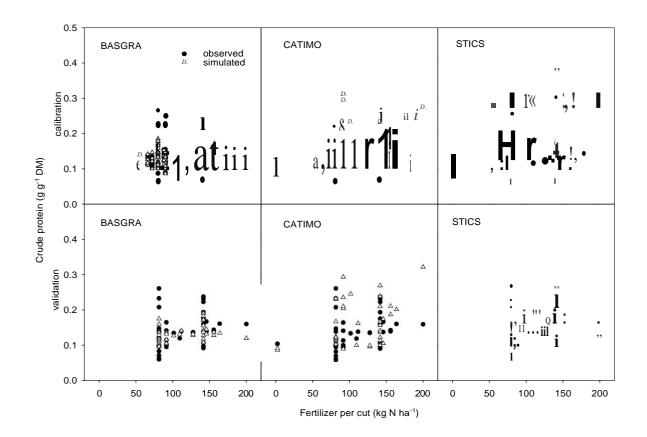
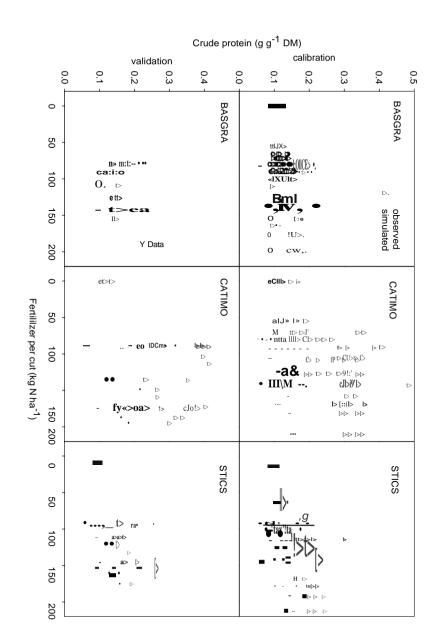


Figure 5. Observed crude protein concentration and concentration simulated by BASGRA, CATIMO, and STICS with cultivar-specific parameters as a function of amount of N applied per cut. Upper row: calibration dataset, lower row: validation dataset.



Upper row: calibration dataset, lower row: validation dataset. Figure 6. Observed crude protein concentration and concentration simulated by BASGRA, CATIMO, and STICS with generic parameters as a function of the amount of N applied per cut.

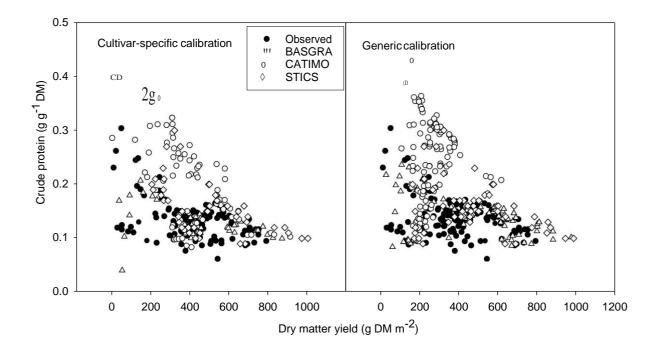


Figure 7. Observed crude protein concentration vs observed dry matter yield, and simulated crude protein vs simulated dry matter yield for the cultivar specific (left) and generic (right) calibrations.