

# Adding a diversity of legumes to a crop decision-support system: Maintaining satisfactory accuracy while keeping the model simple

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Marine Bedu, L. Lefèvre, Aurelien Dupont, Pascal Dubrulle, Raymond Reau, et al.. Adding a diversity of legumes to a crop decision-support system: Maintaining satisfactory accuracy while keeping the model simple. European Journal of Agronomy, 2023, 151, pp.art. 126999. 10.1016/j.eja.2023.126999 . hal-04288580

# HAL Id: hal-04288580 https://institut-agro-dijon.hal.science/hal-04288580

Submitted on 26 Jan 2024

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1	Adding a diversity of legumes to a crop decision-support system: maintaining satisfactory accuracy
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23	Abstract
24	In a context of economic and environmental concerns in agriculture, legumes appear to be suitable
25	alternative crops to diversify current cropping systems and reduce their dependence on synthetic
26	nitrogen (N) fertiliser and protein from imported soya bean. However, legume-based cropping systems 1

27 may increase N losses through nitrate leaching if the N available from legumes does not coincide with 28 subsequent crop requirements. To help agricultural advisers manage N in these systems, we adapted 29 the decision-support system Syst'N<sup>®</sup>, designed to assess N losses in cropping systems, to simulate 30 three annual and one perennial legume crops: pea, faba bean, soya bean and lucerne. To this end, we 31 adapted and simplified existing submodels of legume functioning to include them in Syst'N, to keep 32 the latter simple. We adapted the submodels "BNF" (i.e. biological N fixation) from the STICS model and "dormancy" from the CropSyst model. We also added the ability to enter the flowering date to 33 34 improve predictions (improvement in N fixation's rRMSE from 57% to 41% and EF from 0.57 to 0.77). 35 The equations and associated parameter set developed for the four legume crops yielded satisfying 36 predictions of crop biomass (rMBE = 9%, EF = 0.82, rRMSE = 39%) and N content (rMBE = 5%, EF = 0.76, 37 rRMSE = 37%). These performances support the philosophy of Syst'N<sup>®</sup> that requires minimising the 38 number of additional parameters for users when representing new crops or processes.

39

40 **Keywords:** nitrogen, legume crops, decision-support system, biological N fixation, model

41

#### 42 **1. Introduction**

43 The agricultural revolution after 1945 led to a major intensification of French agriculture due to the 44 increasingly intensive use of mechanisation and chemically synthesised inputs, which was enabled by 45 technical progress. This intensification and the organisation of agriculture into sectors have fostered 46 specialisation of production systems with a geographical separation between crop and livestock 47 production and increasingly shorter cropping sequences (Ferrant, 2009). These changes, based on 48 choosing crop species that maximise profit in the short term, led to the abandonment of species that 49 provided recognised agronomic and ecosystem services such as legumes (Schott et al., 2010). 50 Moreover, historical choices of public policies (e.g. subsidies for cereal production), research and 51 engineering triggered the marginalisation of legumes (Magrini et al., 2016). Since the 1990s, however, 52 growing awareness of negative externalities associated with cereal-based intensive systems (e.g.

53 environmental pollution, greenhouse gas emissions, loss of biodiversity) has prompted some 54 stakeholders in the agricultural sector to seek more economical and environmentally friendly practices 55 (Voisin et al., 2013). In this context, legumes appear to be good alternative crops to diversify current 56 cropping systems and reduce their dependence on synthetic N fertiliser and protein from imported 57 soya bean (Carof et al., 2019). Comparing N fixed by legumes vs. industrial sources, Crews and Peoples 58 (2004) showed that developing legume-based cropping systems could lead to more sustainable 59 agriculture. Indeed, legumes have the unique ability to fix N from the air  $(N_2)$ , thus reducing their need 60 for N fertilisation; in Europe, legume crops are usually not fertilised (Cernay et al., 2016). Biological N 61 fixation (BNF) by grain/forage legumes also benefits subsequent crops by leaving more N in the soil 62 than cereals do (Herridge et al., 1995) and through mineralisation of N-rich plant residues incorporated 63 into the soil after crop harvest, thus increasing soil N fertility (Justes et al., 2001). However, legume-64 based cropping systems may increase N losses through nitrate leaching if the N available from legumes 65 does not coincide with subsequent crop N requirements (Muller et al., 1993; Cellier et al., 2015; Plaza-66 Bonilla et al., 2015; Voisin et al., 2015). Legumes differ in their N-fixation efficiency, which depends on 67 the response of their BNF to abiotic factors (e.g. soil mineral N content, temperature, soil water content) and their physiological functioning (Guinet et al., 2018). Therefore, legume BNF and N pre-68 69 crop effects must be quantified over time to improve the design of sustainable cropping systems that 70 include legumes. Doing so requires improving quantification of benefits for subsequent crops from 71 legume BNF and its influence on N losses, and thus environmental pollution.

In this context, agricultural stakeholders need to design new cropping systems using decision-making tools that consider legumes and that can estimate their environmental impacts. Since the 1960s, many crop models have been developed to address a variety of objectives, but only a few are directly used by practitioners to simulate N dynamics in legume-based cropping systems. This arises from a lack of user-friendly interfaces, low availability of input parameters and failure to consider users' constraints and knowledge (Prost et al., 2012). Meanwhile, users in the environmental field and agricultural

advisers use indicators or simple tools that fail to simulate N-loss dynamics and to understand
weaknesses of cropping systems.

80 As an operational tool for quantifying N losses at the multi-year scale of a cropping system, Syst'N® 81 predicts N dynamics under the most common crops in France. Syst'N is used mainly by agricultural 82 advisers for regions with strong environmental issues (especially nitrate emissions); thus, it must 83 estimate N losses and help discuss and design more sustainable cropping systems. Stakeholders 84 involved in water and agricultural management who use Syst'N need it to be applicable to a variety of 85 cropping systems that include less common crops, especially legumes (as grain or forage). In the first 86 version of Syst'N (2013), pea (Pisum sativum L.) was the only legume crop parameterised. 87 Consequently, there was a real need to extend the scope of Syst'N for users and adapt it to new 88 cropping systems with a wider variety of legume crops.

Accordingly, this study developed, evaluated and validated Syst'N predictions for several common legume species: faba bean (*Vicia faba* L.), soya bean (*Glycine max* L.) and lucerne (*Medicago sativa* L.). Pea was parametrised again for the new equations added to predict the other legume species considered, and predictions for pea were also evaluated. This adaptation of the model is crucial because satisfactory simulation of growth and N uptake is essential to meet Syst'N's ultimate goal, which is to estimate N emissions to the environment.

95 We adapted Syst'N by choosing and adapting generic equations that could simulate N dynamics for 96 several legumes without decreasing its user-friendly aspect. The design criteria for adapting Syst'N to 97 four legumes included: (i) the ability to simulate growth and N uptake of annual and perennial legumes, 98 (ii) the ability to simulate soil N dynamics and content during and after a crop cycle sufficiently well 99 (e.g. residual N effects of legumes), (iii) avoiding the need for users to provide additional input data, 100 (iv) limiting the number of additional parameters needed for new crops and (v) adapting equations 101 from updated knowledge and models. We assumed that adapting Syst'N to a wide range of legumes 102 would meet these criteria.

#### 104 **2.** Materials and methods

#### 105 2.1. The crop model Syst'N

106 Syst'N is a model-based decision-support system (DSS) developed to estimate N losses in cropping 107 systems and promote better N management in rural areas. The French National Research Institute for 108 Agriculture, Food and Environment (INRAE) and eight French agricultural institutes developed Syst'N 109 together. The objective was to meet the needs of stakeholders involved in water and agricultural 110 management for an operational tool that could predict N losses at the multi-year scale of cropping 111 systems. Since 2005, Syst'N has been co-designed with end-users to adapt it further to their needs 112 (Cerf et al., 2012), in an iterative process with agricultural advisers, research and development 113 institutes, applied research institutes and environmental agencies.

114 The Syst'N version described by Dupas et al. (2015) added a soil-crop model to simulate soil N 115 transformations, crop growth, N uptake, water balance and N losses towards water (e.g. nitrate) and 116 air (e.g. ammonia, N<sub>2</sub> and nitrous oxide) on a daily time step. The input data required include the crop 117 sequence, agricultural management practices, soil and climate. The equations in the biophysical model 118 combine existing validated and published submodels from STICS (Brisson et al., 2003) for water and 119 nitrate balances in soils, AZOFERT (Machet et al., 2004; 2017) for N mineralisation of soils and crop 120 residues, AZODYN (Jeuffroy and Recous, 1999) for crop N uptake, NOE (Hénault et al., 2005) for N₂ and 121 nitrous oxide emissions and VOLT'AIR (Génermont and Cellier, 1997) for ammonia emissions.

Syst'N attempts to chart a middle course between complex simulation models such as STICS (Brisson et al., 1998), which simulate many processes but require many input data, and more simple indicators commonly used by agricultural practitioners (e.g. N balance, N-use efficiency) but which have relatively little ability to explain phenomena. Therefore, the equations added to Syst'N were selected to conform to the input data that are generally available to targeted end-users, hence keeping Syst'N user-friendly.

127 **2.2. Experimental data** 

Most of the parameters initially used to calibrate the new legumes (lucerne, faba bean and soya bean)
were derived from previously published studies. The data used to calibrate and evaluate Syst'N were

130 collected in French field experiments, in contrasting pedoclimatic contexts and with different 131 experimental treatments, such as various amounts of N fertilisation or irrigation applied (Table 1; see 132 Table S1 for more details). The objective was to find data with the highest diversity in experimental 133 treatments, including sowing date, amounts of N fertiliser and irrigation applied, as well as cutting 134 dates for lucerne as a perennial crop. Ultimately, fertiliser applications could be tested only for pea, 135 faba bean and lucerne. Site-year-management (SYM) units that covered a wide range of crop-136 management practices with high measurement frequency were chosen for the calibration dataset (6, 137 6, 9 and 17 for pea, faba bean, lucerne and soya bean, respectively), and the remaining SYM units 138 formed the evaluation dataset (12, 3, 32 and 9 SYM, respectively).

139

#### 2.3. Adaptation and calibration method

To begin adapting Syst'N, equations and corresponding parameters that represented plant processes (e.g. phenology, biomass accumulation, BNF) were chosen (Fig. 1). First, specific characteristics of each legume crop were identified. If the existing Syst'N equations could not simulate these characteristics or the resulting N dynamics satisfactorily, the equations were supplemented or modified based on those in existing models. Initial parameters for the crops were set based on a literature review of existing models and plant physiology articles, or directly on measurement datasets if parameter values were not found in the literature.

We then graphically and statistically tested these initial equations and parameters using calibration datasets (Table 1). If predictions were unsatisfactory, some parameters were selected according to a set of criteria (e.g. sensitivity of variables of interest to the parameter, uncertainty) and tested for a range of values to improve prediction accuracy by optimising statistical indicators of accuracy.

151 **2.4. Model assessment** 

As we were adding several legumes to Syst'N, we assessed it by considering important plant variables, such as aboveground biomass and N uptake, as well as BNF and soil mineral N content when datasets included them. Predicted target variables of Syst'N (i.e. N losses) were not evaluated because they were not measured in experiments and because only plant-related equations and parameters were modified in this study.

Model performance (with the optimised parameter set) was evaluated graphically as dynamics over the crop cycle and plots of predictions vs. observations. It was quantified by calculating mean bias error (MBE) and its relative value (rMBE); root mean square error (RMSE) and its relative value (rRMSE); and model efficiency (EF) using data collected at harvest and throughout crop growth. These indicators are commonly used to calibrate and evaluate agronomic models (Dumont et al., 2012).

162 
$$MBE = \frac{1}{N} \sum_{i=1}^{N} (P_i - O_i) \quad (1)$$

163 
$$rMBE = \frac{MBE}{\overline{O}} \times 100 \quad (2)$$

164 
$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(O_i - P_i)^2} \quad (3)$$

165 
$$rRMSE = \frac{RMSE}{\overline{O}} \times 100 \quad (4)$$

166 
$$EF = 1 - \frac{\sum_{i=1}^{N} (O_i - P_i)^2}{\sum_{i=1}^{N} (O_i - \overline{O})^2}$$
(5)

167 where  $O_i$  and  $P_i$  are observed and simulated values for the i<sup>th</sup> measurement, N is the number of these 168 paired values and  $\overline{O}$  is the mean of observed values.

169 MBE and rMBE indicate whether a model underestimates (negative values) or overestimates (positive 170 value) a given variable. Nevertheless, bias is not a sufficient measurement of the quality of a model: 171 low bias can result from small prediction errors in all situations or instead from large prediction errors 172 that compensate each other. Hence, the RMSE was also calculated (expressed in the same unit as the 173 given variable) to identify this latter problem by squaring the difference between simulations and 174 observations. Doing so, however, gives more weight to larger errors, which requires caution when interpreting RMSE, because a large RMSE can result from only one or two major differences. The rRMSE 175 is more relevant for comparing variables with different units. Finally, EF assesses the overall 176 177 performance of a model by comparing it to the mean of observations. EF ranges from  $-\infty$  to 1, which 178 facilitates interpretation: negative EF indicates that the model predicts no better than the mean of 179 observations, whereas EF = 1 indicates a model with perfect accuracy. EF is relevant for comparing 180 models or for comparing the same model's simulations of the same dataset using different sets of 181 parameters/equations. Analysing these five statistical indicators from different groups of correlated 182 indicators give a robust assessment of model prediction accuracy, as recommended by Yang et 183 al. (2014). Like for Beaudoin et al. (2008) and Constantin et al. (2015a, 2015b), Syst'N predictions were considered satisfactory when EF exceeded 0.50 and rMBE was lower than 10% (Table 2). A 20% 184 185 threshold was used for rRMSE, like for Thiebeau (2019a; 2019b), although a higher threshold (40%) 186 was used to evaluate STICS predictions for lucerne (Strullu et al., 2020).

187

188 3. Results

189 190

#### 3.1.1. Mineralisation of crop residues

3.1. Model description and parameterisation for legume crops

Syst'N already used a double exponential equation from the AZOFERT tool to simulate net Nmineralisation from crop residues (Machet et al., 2017):

193

 $N = N_{RO} \times (a_N - b_N e^{-kt} - c_N e^{-lt})$ (6)

194 where N is amount of N mineralised;  $N_{RO}$  is the initial amount of N in crop residues and  $a_N$ ,  $b_N$ ,  $c_N$ , I and 195 k are coefficients that describe the mineralisation kinetics of N.

Before this study, the equation was parameterised for a variety of legume residues. The same parameterisation was used in this study. Inspired by the model TNT2 (Casal et al., 2019) for grazed or cut perennial crops (including lucerne in Syst'N), an additional N sequestration pool was added during crop development depending on grazing or cutting practices. After crop harvest or cover crop destruction, this pool of organic N mineralises.

201 *3.1.2.* Biological nitrogen fixation

As shown by the systematic literature review and quantitative statistical analysis of Anglade et al. (2015), legume species differ significantly in their median percentages of N derived from the 204 atmosphere (%Ndfa), due mainly to the species' sensitivity to abiotic factors (e.g. soil mineral N 205 content, soil water content, temperature) and to their phenological characteristics (e.g. phenological 206 stages, nodule establishment rate) (Guinet et al., 2018; Pampana et al., 2018). In the first version of 207 Syst'N, the equation used to predict BNF was based on the AFISOL-Pea model, but it was adapted only 208 for pea. In the present study, it was necessary to consider the diversity of BNF processes among legume 209 species. The most common method for estimating %Ndfa of legume species in mechanistic crop 210 models is to calculate a potential or maximum BNF rate which is then decreased by the influence of 211 environmental factors: in their review, Liu et al., (2011) identified nine simulation models (Sinclair 212 Model, EPIC, Hurley Pasture Model, Schwinning Model, CROPGRO, SOILN, APSIM, Soussana Model and 213 STICS) that simulated legume BNF. Each model considered one or more of the following factors: soil 214 temperature, soil-plant water, soil-plant N, plant carbon and phenological stage. Some BNF models are 215 calibrated and parameterised for only one legume species, whereas others can simulate a wide range 216 of legume species with different characteristics and geographic ranges.

217 To adapt Syst'N to a variety of legume species (grain and forage), we chose to add the BNF submodel 218 of STICS (Brisson et al., 2009; Corre-Hellou et al., 2007), because it (i) is adapted to the French 219 pedoclimatic context, (ii) is adapted for a wide range of legumes (e.g. field pea, soya bean, faba bean, 220 lucerne) and (iii) considers all the environmental factors mentioned except carbon dynamics (ignored 221 by Syst'N). The BNF equations of STICS were modified slightly to conform to the input data available in 222 Syst'N (i.e. using air temperature instead of soil temperature for the temperature-weighting factor) 223 and to the variables already calculated by Syst'N (beginning of nodulation associated with the 224 beginning of BNF, nodule death associated with the final stage of seed abortion) (Fig. 2). The 225 parameters specific to these equations, which also resulted from parameterisation of STICS, varied 226 among species (Table 3).

## 227 *3.1.3.* Phenology

As for most crops, legume phenology is controlled mainly by air temperature and photoperiod. As a simple crop model, Syst'N calculates phenological stages using only sums of growing degree-days. 230 According to their photo-thermal sensitivity, legumes can be classified into three main categories: 231 photoperiod-insensitive, day-neutral and photoperiod-sensitive (short-day or long-day) (Roberts and 232 Summerfield, 1987). As many studies observed, sensitivity to photoperiod is even more important for 233 legume species, because it drives their transition to the reproductive stage (i.e. flowering) (Baranger 234 et al., 2010; Confalone, 2008; Iannucci et al., 2008; Schneider and Huyghe, 2015). Because flowering 235 stops (e.g. root growth), modifies (e.g. remobilising N, BNF) or triggers (e.g. plant senescence) some 236 plant processes, and thus influences N dynamics, it seemed important for Syst'N to predict flowering 237 time accurately. However, simulating photoperiod and its effects on crop phenology would (i) be too 238 complex for such a DSS, (ii) require new input data (e.g. latitude) and (iii) require new parameters for 239 the photoperiod sensitivity for each crop, which seems difficult to define. Thus, we chose to add the 240 actual flowering date as optional input data. Indeed, a survey of Syst'N users indicated that they often 241 observe it and thus could provide it as input data. When flowering date is provided, Syst'N calculates 242 all phenological stages from it; if not, it calculates stages from the crop parameter that represents the 243 number of degree days from sowing to flowering. When parametrising annual legumes, we decided to 244 distinguish soya bean of types 00 and I, as their stages differ greatly.

245

## 3.1.4. Perennial legumes

246 We modified Syst'N greatly to capture specific characteristics of perennial crops, such as several cuts 247 and regrowth sequences. In the first version of Syst'N, an equation from TNT2 (Casal et al., 2019) that 248 estimated the change in plant biomass and N content when cutting grassland (Nitschelm et al., 2018) 249 was used and adapted to represent other perennial crops such as lucerne. The residual aboveground 250 biomass that remains in the field after a cut is calculated from the cutting height. Nevertheless, plant 251 growth differs between seedlings and crop regrowth (after harvest or dormancy), as observed by 252 Thiébeau et al. (2011) and Lemaire et al. (1985) for lucerne, due to crop defoliation and storage of 253 reserves in roots, which supports regrowth after cutting or after winter. To keep Syst'N relatively 254 simple, it contains two parameter sets to simulate seedlings and crop regrowth separately instead of using complex equations to represent reserve management by perennial crops, as in STICS versions for
 perennial crops (Strullu et al., 2014; 2020).

257 Some vigorous perennial legumes, such as lucerne, become dormant during winter (Undersander et 258 al., 1997). Dormancy is triggered mainly in autumn by two factors: photoperiod and temperature 259 (Mauriès, 2003). As mentioned, simulating photoperiod would require new input data from users and 260 make Syst'N more complex. An equation from CropSyst (Confalonieri and Bechini, 2013) was a good 261 compromise to add dormancy to Syst'N in a relatively simple way (Fig. 3). This equation was adapted 262 slightly in Syst'N to fit with its existing equations of biomass growth and N uptake. The parameters 263 used in these equations were calculated from the optimisation measurement dataset. For simulated 264 plant N content, this adaptation delays crop regrowth after winter and resets crop-stage variables, 265 thus avoiding the unexpected early physiological maturity predicted without the dormancy equation 266 (Fig. 4).

267 3.2. Results of model evaluation

268 The final parameters for legumes in Syst'N were set by the calibration method described (Table S2).

269

#### 3.2.1. Calculating phenological stages from the actual flowering date

270 To evaluate effects of calculating phenological stages from the observed flowering date on the 271 accuracy of Syst'N predictions, the statistical indicators were calculated for predictions based on a 272 dataset with or without the actual flowering date. The latter dataset was smaller than the 273 measurement dataset, as it contained only the site-year-management (SYM) units in which flowering 274 had been observed. The accuracy of predicted total aboveground plant N (Fig. 5C and 5D) content and BNF (Fig. 5E and 5F) increased, and that of predicted aboveground biomass remained good (Fig. 5A 275 276 and 5B), which indicated the relevance of calculating phenological stages from the actual flowering 277 date (as input data), as flowering is an important stage for BNF and N uptake. The rMBE were low (-6% 278 to 19%) and showed Syst'N's tendency to overestimate total aboveground plant N (rMBE = 19%, Fig. 279 5C) but underestimate BNF (rMBE = -6%, Fig. 5E). However, the relatively good EF (0.73-0.85) of predictions of all plant variables confirmed that Syst'N predicted growth and N assimilation (uptake plus BNF) throughout the crop cycle (from juvenile to mature stages) better when stages were calculated from the actual flowering date. All rRMSE were satisfactory (< 41%).

283

## 3.2.2. Accuracy of predictions over the crop cycle

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## 3.2.2.1. Aboveground biomass

285 Predicted biomass agreed with observations throughout each legume crop's growing season for both 286 calibration and evaluation datasets (EF > 0.75, 9% < rMBE < 13%), considering a dataset with or without 287 flowering date (Fig. 6A and 6B). Positive rMBE showed Syst'N's tendency to overestimate aboveground 288 biomass, especially for lucerne with the calibration dataset (data not shown). Prediction error was high 289 (rRMSE of 40% for both datasets) due to senescence defoliation and the loss of biomass related to 290 respiration during dormancy (Justes et al., 2002), which Syst'N ignores for all crops. Hence, Syst'N 291 assumes that aboveground biomass does not change during dormancy. Nevertheless, it can be 292 considered a time-lag in growth dynamics that does not influence Syst'N prediction, as they became 293 more accurate after dormancy (Fig. 7).

For each legume crop, all statistical indicators were good: rMBE was low (i.e. -13% < rMBE < 20%), EF</li>
was satisfactory (> 0.59) and rRMSE was rather satisfactory (< 48%) (Table 4).</li>

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#### 3.2.2.2. Plant nitrogen content

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#### 3.2.2.2.1. Total aboveground nitrogen content

298 Total aboveground N content was predicted accurately using both the calibration and evaluation 299 datasets considering a dataset with or without flowering date for evaluation (Fig. 6C and 6D): rMBE 300 was low (19% and 5%, respectively), EF was high (> 0.70) and rRMSE was satisfactory (< 40%). 301 Prediction of aboveground N content was satisfactory for faba bean and pea, with good rMBE (< 16%), 302 high EF (0.87) and low rRMSE (< 25%) (Table 4). Despite lower EF (0.61) and higher rRMSE (44%), 303 predictions for lucerne using the evaluation dataset remained satisfactory, with a slight overestimation 304 of the dynamics. In contrast, rMBE (23%), EF (0.48) and rRMSE (44%) for soya bean showed a tendency 305 for Syst'N to overestimate aboveground N content (Table 4).

#### 3.2.2.2.2. Aboveground nitrogen fixation

307 The parameters related to BNF defined for each crop (Table 3) yielded good predictions (Fig. 6E and 308 Fig. 6F), with a high EF (> 0.78) and low rMBE (-13% < rMBE < 6%) for pea, faba bean and soya bean 309 (Table 4). Because observed data were not available for lucerne, we compared predictions to data from 310 the literature (Kelner et al., 1997; Schneider and Huyghe, 2015; Wivstad et al., 1987; Xie et al., 2015). 311 They showed highly variable %Ndfa of 20-90%, which seemed to be explained in part by variable 312 amounts of mineral N in the soil. These percentages were found in the predictions, with a mean %Ndfa 313 of 70% for unfertilised plots and 50% for plots that had received mineral N fertiliser. For the other 314 legume crops, this good accuracy was verified throughout growing season (EF=0.80, low rMBE). EF 315 remained high and bias remained low with the evaluation dataset, indicating that Syst'N was able to 316 reproduce the wide range of cumulative BNF at harvest (33-265 kg N.ha<sup>-1</sup>).

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#### **3.2.2.3.** Soil water content and soil mineral nitrogen content

Syst'N predicted soil water content better during evaluation (EF = 0.44) than calibration (EF = -2.38), despite lower rMBE (-7% and 20%, respectively) and higher rRMSE (33% and 24%, respectively) (Fig. 8). Despite satisfactory indicators, we observed threshold effects. Syst'N had difficulty predicting the wide range of soil water content observed (2.5-33.2%), as it was constrained by threshold values of the pedotransfer classes used to define field capacity ( $\theta_{FC}$ ) and wilting point ( $\theta_{WP}$ ) as a function of soil texture (9.1-26.4%).

324 Soil N content was predicted less well using the calibration and evaluation datasets, with negative EF 325 (-0.19 and -0.24, respectively) and high rRMSE (45% and 67%, respectively) (Fig. 8). The low EF (-0.76) 326 and high rRMSE (69%) for lucerne (Table 4) could be explained mainly by temporal shifts (data not 327 shown). First, nodule activation, which enables BNF, and moderate N uptake from the soil can occur 328 sooner than predicted. This delay in prediction by a few days may cause Syst'N to underestimate soil 329 N content at a given date significantly. Secondly, the simple equation used to simulate dormancy may 330 delay N uptake during biomass regrowth and cause Syst'N to overestimate soil N content for a few 331 weeks, which has little influence on predicted N losses.

332

#### 3.2.3. Nitrogen effect of legumes on subsequent crops

Dynamics of N mineralisation after a legume crop were evaluated only for lucerne because of the specific calculations in Syst'N for grazed or cut perennial crops. For the other crops, the N effect of legumes is calculated directly with the AZOFERT equation, which has already been evaluated (Machet et al., 2017).

337 Predicted N mineralisation in the soil after lucerne was compared to measurements from Justes et al. (2001). In this experiment, mineralisation from humus and from residues returned to the soil after 338 339 lucerne destruction were differentiated. Dynamics of simulated N mineralisation from lucerne residues 340 and soil organic matter accurately reproduced observations for two years in two situations: lucerne 341 cut just before destruction (3% error between prediction (331 kg N ha<sup>-1</sup>) and observation (340 kg N 342 ha<sup>-1</sup>) after two years) and lucerne cut one week before destruction (8% error between prediction (368 343 kg N ha<sup>-1</sup>) and observation (400 kg N ha<sup>-1</sup>) after two years). Thus, with less than 10% error, predictions 344 of N mineralisation were satisfactory and confirmed Syst'N's ability to represent long-term effects of 345 lucerne residues.

346

#### **4. Discussion**

## 348 **4.1.** A generic and user-friendly crop model able to simulate a diversity of legumes

This study showed that the generic equations of Syst'N can simulate a variety of legumes species: those with cool-season adaptation (pea and faba bean), warm-season adaptation (soya bean) and a perennial cycle (lucerne). The accuracy of predicted aboveground biomass and N assimilation (uptake plus BNF) was satisfactory for all 4 legume species, with rMBE less than 10% (2-9%) and EF greater than 0.50 (0.74-0.81), which are consistent with the guidelines of Beaudoin et al., (2008) and Constantin et al. (2015a, 2015b). Moreover, the accuracy of these predictions are similar to those for other species parameterised in Syst'N (unpublished).

Prediction of BNF was improved by adding the actual flowering date as input data. Users in the field can obtain the actual flowering date easily, which allows Syst'N to remain adapted to its purpose and user-friendly. In addition, the flowering date can also be estimated using a simple phenology algorithm
(Schoving et al., 2020) and then used as an input variable for Syst'N.

#### 360 **4.2. Water balance prediction**

Syst'N's ability to simulate soil water and mineral N contents, both of which are used to calculate N leaching, is less satisfactory than that for biological variables, as all statistical indicators except rMBE lay above satisfactory thresholds. Our predictions of soil N content were similar to those of STICS with faba bean (Falconnier et al., 2019), whose rMBE, EF and rRMSE were -10%, -1.42 and 51%, respectively, using an evaluation dataset.

366 Syst'N predicted both low and high observed soil water contents poorly (Fig. 8) due to the pedotransfer 367 classes it uses to estimate  $\theta_{FC}$  and  $\theta_{WP}$  as a function of percentages of clay, silt and sand. Indeed, large 368 differences in soil texture can yield the same characteristic water contents, as observed for 9 site-year-369 management (SYM) in this study (Fig. 8). For example, because silty-clay loam (30% clay, 62% silt, 8% 370 sand) and sandy-clay loam (14% clay, 32% silt, 54% sand) are considered to be the same in Syst'N's 371 pedotransfer classes, both have  $\theta_{FC}$  of 32.3% and  $\theta_{WP}$  of 14.0%. Many studies have related soil texture 372 to water-retention characteristics of the soil (Gupta & Larson, 1979) using pedotransfer classes or 373 functions. Classes were used in the first version of Syst'N instead of functions based on the results of 374 Al Majou et al., (2007), who showed that "simple" texture-based pedotransfer classes allowed water-375 retention characteristics to be predicted as accurately as with more sophisticated pedotransfer classes 376 or functions. However, using pedotransfer classes inevitably leads to threshold effects, which 377 decreases the accuracy of predictions of water balance and thus nitrate leaching. Toth et al. (2015) developed new hydraulic pedotransfer functions valid for the pedoclimatic context in France. The most 378 379 accurate predictions were obtained using the clay percentage, silt percentage, bulk density, organic 380 carbon and pH as parameters, all of which are available as input data in Syst'N. In future versions, using 381 pedotransfer functions could improve predictions of soil water content, in particular by overcoming 382 the threshold effect caused by pedotransfer classes. Soil water content has a strong influence on BNF 383 and soil N content, but also on water transfer and thus on N leaching, which is one of the main outputs

of the model. In addition, the parameters  $\theta_{FC}$  and  $\theta_{WP}$  could be used as input data if they are available. Nevertheless, we have noted that the end-users of Syst'N do not often know the values of these parameters.

### 387 **4.3.** Specifying a large number of plant parameters

388 Using the actual flowering date to calculate phenological stages and the new BNF equation required 389 adding 2 and 16 new plant parameters, respectively, specific to legume species. Thus, 77 agro-390 physiological parameters for each species must now be defined to simulate a new legume crop in 391 Syst'N. Although some of these parameters require good knowledge of the agro-physiological 392 behaviour of the crop, particularly for N processes (e.g. parameters of N-dilution curves), many of them 393 can be approximated easily using knowledge of other crops already parameterised in Syst'N. 394 Moreover, despite the large number of plant parameters, Syst'N is easier to adapt than most other 395 models, such as STICS, which requires specifying over 200 crop- and cultivar-specific parameters; 396 however, it was developed by researchers to investigate a wider diversity of cropping systems and 397 consider many more processes (Brisson et al., 2009).

398

#### 4.4. Strong simplification of biological processes for perennial legumes

399 Predictions highlight high overestimation of aboveground biomass and N content immediately after 400 dormancy due to the lack of equations to simulate senescence and mobilisation of reserves in Syst'N. 401 However, this trend is relatively brief: along with rapid biomass regrowth in the spring, reserves stored 402 in roots during autumn and winter are remobilised to shoots (Justes et al., 2002). The accuracy of 403 predicted aboveground biomass and N content increased after a few weeks and became satisfactory 404 during the cuts in spring. This simplification in Syst'N delays N uptake from the soil in the spring but 405 has little influence on soil N content during winter, a key variable used to predict nitrate leaching. As 406 shown by Strullu et al. (2014) for Miscanthus × giganteus, total aboveground N content decreases only 407 slightly in winter despite a strong decrease in aboveground biomass. Rapid remobilisation of N 408 temporarily stored in perennial organs has also been observed for other legumes, such as white clover 409 (Trifolium repens L.) (Robin et al., 1999), which supports this hypothesis. In the future, the simple 16

410 equation that maintains aboveground biomass and N content constant during winter could be applied411 to other perennial crops in Syst'N.

412 As mentioned, Syst'N has two parameter sets to simulate seedlings and crop regrowth separately, 413 instead of using a complex model to represent reserve management by perennial crops, as in STICS 414 versions for perennial crops. These STICS versions, initially developed for Miscanthus reserves (Strullu 415 et al., 2014) and then for lucerne (Strullu et al., 2020), consider the N fluxes between perennial organs 416 (e.g. the taproot) and non-perennial organs (i.e. leaves, stems and roots) as a function of abiotic stress, 417 photoperiod and phenological stages using a single set of parameters, but they required defining more 418 compartments in the model and are thus complex. STICS version for lucerne resulted in EF values of 419 0.70 for aboveground biomass and 0.60 for N content, while Syst'N using less complex equations gave 420 similar EF (0.60 for both biomass and N content). However STICS predictions were slightly more 421 accurate (rRMSE of 31% vs 36% for Syst'N). So, despite being less accurate, the predictions of Syst'N 422 were reasonable for perennial crops given it uses simpler equations than STICS.

423 Comparing Syst'N's lucerne predictions to those of CropSyst highlights the difficulty in applying a model 424 to contrasting environments using a single set of crop parameters. Using CropSyst, Confalonieri and 425 Bechini (2013) obtained an rRMSE of 3-6% for predictions of total aboveground biomass after 426 calibrating crop parameters that partly considered local conditions, especially for dormancy and 427 development temperature. We used a submodel of CropSyst for dormancy in Syst'N, but due to the 428 small amount of measurement data over the period, Syst'N's parameters were not calibrated to local 429 conditions of the datasets, which may explain the lower rRMSE for Syst'N. Moreover, lucerne 430 parameters were calibrated based on a variety grown in northern France, and the influence of 431 decreasing photoperiod varies among lucerne varieties. Syst'N represents the effect of photoperiod 432 on crops indirectly using two fixed calendar dates that can stop growth during a period with a short 433 photoperiod. Unfortunately, this study could not test the ability of Syst'N and this parameter set to 434 simulate southern varieties of lucerne, which may start growing earlier in the spring.

435

#### 436 5. Conclusion

437 Legumes can play a key role by providing N to cropping systems and thus enhancing the N self-438 sufficiency of farms (Cellier et al., 2016; Vertès et al., 2010; 2015). Therefore, farmers and their advisers 439 increasingly attempt to insert legume species into their crop sequences; besides the effects on their 440 crop production that they can observe, they need results for and knowledge about N fluxes that they 441 cannot assess themselves, such as N supply to subsequent crops and emissions to the environment. Adapting Syst'N to several legumes with different crop cycles and BNF capacities but keeping it 442 443 relatively simple was both a challenge and an expected development, given its utility to non-researcher 444 users.

445 We chose and combined equations from research crop models such as STICS and CropSyst to maintain 446 the simplicity of Syst'N for end users. Although some BNF equations required many parameters, users 447 need to supply only one additional parameter (flowering date) if they want to predict BNF. Based on 448 the literature, experiments and optimisation, we developed a set of parameters that provided 449 satisfactory predictions of legume aboveground biomass and N content. In contrast, Syst'N predicted 450 soil N content less well, mainly due to temporal shifts. Nevertheless, they remain relevant and are an 451 important prerequisite for simulating N emissions that are of particular interest to users. The next step 452 will be to improve predictions of soil N and water content, to evaluate the accuracy of Syst'N 453 predictions of N emissions (i.e. nitrate leaching, nitrous oxide emissions) and to do so at the scale of a 454 cropping sequence that includes legumes.

455

#### 456 Acknowledgements

We thank the French Ministry of Agriculture and Food and the French Biodiversity Agency, which funded this study. We also thank the "Sojamip" research project, which involved the Occitanie/Pyrénées-Méditerranée region and several stakeholders (Euralis Semences, INRAE, RAGT2n, Terres Inovia, Terres Univia, Toulouse INP), for soya bean experimental data, and UMR FARE and the Alsace Chamber of Agriculture for lucerne experimental data.

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Table 1. Experimental data used to parameterise Syst'N

		Total site-year-management units with available measurements					References	
Species	Dataset	Total	Leaf area index	Aboveground biomass	Aboveground N content	N fixed	Soil N content	
Lucerne	Calibration	9	9	9	9		3	Thiébeau et al., 2011
(Medicago sativa L.)	Evaluation	32	13	30	30		22	Justes et al., 2002, 2001; Lemaire et al., 1985; Thiébeau et al., 2011, 2004
Pea (Pisum	Calibration	6	4	6	6	6	6	Guinet et al., 2018
sativum L.)	Evaluation	12	8	12	9		12	Voisin <i>et al.</i> , 2002; Corre-Hellou <i>et al.</i> , 2009; Launay <i>et al.</i> , 2009; Naudin, 2009; Pelzer <i>et al.</i> , 2016
Faba bean	Calibration	6	4	6	6	6	6	Guinet et al., 2018
(Vicia faba L.)	Evaluation	3		3	3			Schneider et al., 2019; Schneider et al., 2021
Soya bean	Calibration	17	12	16	16	16	4	Guinet et al., 2018
(Glycine max L.)	Evaluation	9	0	9	9	0	0	Schoving et al., 2022

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Table 2. Indicators used to assess model accuracy. MBE=relative mean bias error, rMBE=relative mean bias error, RMSE=root mean square error, rRMSE=relative root mean square error, EF=model efficiency.

Indicator	Range of values	Ideal value	Satisfactory range
EF	[-∞ ; 1]	1	> 0.5
MBE	[-∞ ; +∞]	0	
rMBE	[-∞ ; +∞]	0	rMBE  < 10%
RMSE	[0;+∞]	0	
rRMSE	[0 ; +∞]	0	< 20%

## Table 3. Parameters of the biological nitrogen fixation submodel added to Syst'N

		Сгор							
		Lucerne		Faba bea	an	Реа		Soya be	an
Parameter name (unit)	Description	Initial	Regrowth	Winter	Spring	Winter	Spring	Type I	Type 00
CONC_N_NOD_SEUIL (kg N.ha <sup>-1</sup> .mm <sup>-1</sup> water)	Maximum soil nitrogen concentration threshold for nodule establishment	1.6	1.6	4.5	4.5	2.0	2.0	2.14	2.5
VIT_NOD (nodules.degree-day <sup>-1</sup> )	Nodule establishment rate	0.0037	0.0015	0.0068	0.0068	1.0	1.0	0.003	0.003
FIX_MAX_VEG (kg N.t DM⁻¹)	Maximum nitrogen fixation capacity per t of dry matter produced before the grain-filling stage (DRG)	-	-	32	40	28	30	-	-
FIX_MAX_GR (kg N.t DM⁻¹)	Maximum nitrogen fixation capacity per t of dry matter produced after the grain-filling stage (DRG)	-	-	17	17	9.5	9.5	-	-
FIX_MAX_CONST (kg N.day <sup>-1</sup> )	Constant capacity for maximum nitrogen fixation by the crop	6.0	6.0	-	-	-	-	6.0	6.0
TEMP_NOD_MIN (°C)	Minimum cardinal temperature for nodule activity	0	0	0	0	0	0	0	0
TEMP_NOD_OPT_B (°C)	Low optimal cardinal temperature for nodule activity	15	15	12	12	10	10	20	20
TEMP_NOD_OPT_H (°C)	High optimal cardinal temperature for nodule activity	25	25	25	25	25	25	36	36
TEMP_NOD_MAX (°C)	Maximum cardinal temperature for nodule activity	35	35	40	40	35	35	50	50
N_RAC_100 (kg N.ha <sup>-1</sup> .cm <sup>-1</sup> soil)	Nitrogen concentration threshold for full activity of nodules	0.12	0.12	1.6604	1.6604	0.3612	0.3612	1.6604	1.6604
N_RAC_0 (kg N.ha <sup>.1</sup> .cm <sup>.1</sup> soil)	Nitrogen concentration threshold that inhibits nodule activity	0.82	0.82	9.4759	9.4759	1.2058	1.2058	4.4804	4.4804
PROF_NOD_MAX (cm)	Maximum nodulation depth	40	40	30	30	30	30	40	40
ECARTTEMP_FIN_NOD (degree days)	Degree-day difference between the phenological reference stage and end of nodulation (FIN NOD)	-100	0	550	550	1200	1316	700	530
ECARTTEMP_FSLA (degree days)	Degree-day difference between the phenological reference stage and final stage of seed abortion (FSLA)	300	300	800	1000	1200	1316	1000	750
ECARTTEMP_DRG (degree days)	Degree-day difference between the phenological reference stage and beginning of grain-filling (DRG)	0	0	250	250	200	150	400	400
SOMTEMP_DEBUT_FIX (degree days)	Sum of degree days from sowing to the beginning of fixation	250	0	340	310	235	235	320	320

Table 4. Statistical indicators of predictions of aboveground biomass, aboveground nitrogen (N) content and biological N fixation (BNF) for each legume crop with the evaluation dataset. EF=model efficiency, MBE=relative mean bias error, rMBE=relative mean bias error, RMSE=root mean square error, rRMSE=relative root mean square error.

Indicator	Prediction	Faba	Реа	Soya bean	Lucerne
		bean			
EF	Biomass	0.82	0.90	0.71	0.59
	N content	0.87	0.87	0.48	0.61
	BNF	0.78	0.78	0.83	NA
	Soil water content	-28.71	0.44	-3.72	No data
	Soil N content	-0.2	0.49	-2.97	-0.76
MBE	Biomass	0.70	0.24	-0.65	0.43
	N content	16.21	0.08	31.52	5.63
	BNF	-9.24	-0.25	4.03	NA
	Soil water content	5.55	-0.75	5.21	No data
	Soil N content	-9.09	-5.93	-0.49	4.1
rMBE	Biomass	20%	5%	-13%	19%
	N content	16%	0%	23%	7%
	BNF	-13%	0%	6%	NA
	Soil water content	22%	-4%	22%	No data
	Soil N content	-14%	-11%	-1%	6%
RMSE	Biomass	0.94	1.28	1.59	1.08
	N content	20.45	32.99	59.83	36.19
	BNF	20.64	32.54	26.55	NA
	Soil water content	7.21	6.35	6.33	No data
	Soil N content	26.35	26.53	16.19	43.79
rRMSE	Biomass	27%	27%	33%	48%
	N content	20%	25%	44%	44%
	BNF	30%	45%	38%	NA
	Soil water content	29%	32%	27%	No data
	Soil N content	42%	50%	41%	69%

Table 4. Statistical indicators of predictions of aboveground biomass, aboveground nitrogen (N) content and

3 biological N fixation (BNF) for each legume crop with the evaluation dataset. EF=model efficiency, MBE=relative

mean bias error, rMBE=relative mean bias error, RMSE=root mean square error, rRMSE=relative root mean square error.

Indicator	Prediction	Faba	Реа	Soya bean	Lucerne
		bean			
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	N content	0.87	0.87	0.48	0.61
	BNF	0.78	0.78	0.83	NA
	Soil water content	-28.71	0.44	-3.72	No data
	Soil N content	-0.2	0.49	-2.97	-0.76
MBE	Biomass	0.70	0.24	-0.65	0.43
	N content	16.21	0.08	31.52	5.63
	BNF	-9.24	-0.25	4.03	NA
	Soil water content	5.55	-0.75	5.21	No data
	Soil N content	-9.09	-5.93	-0.49	4.1
rMBE	Biomass	20%	5%	-13%	19%
	N content	16%	0%	23%	7%
	BNF	-13%	0%	6%	NA
	Soil water content	22%	-4%	22%	No data
	Soil N content	-14%	-11%	-1%	6%
RMSE	Biomass	0.94	1.28	1.59	1.08
	N content	20.45	32.99	59.83	36.19
	BNF	20.64	32.54	26.55	NA
	Soil water content	7.21	6.35	6.33	No data
	Soil N content	26.35	26.53	16.19	43.79
rRMSE	Biomass	27%	27%	33%	48%
	N content	20%	25%	44%	44%
	BNF	30%	45%	38%	NA
	Soil water content	29%	32%	27%	No data
	Soil N content	42%	50%	41%	69%

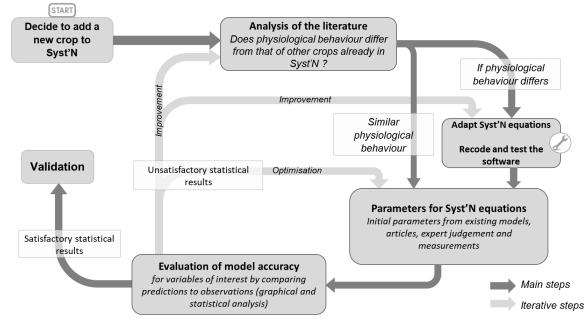
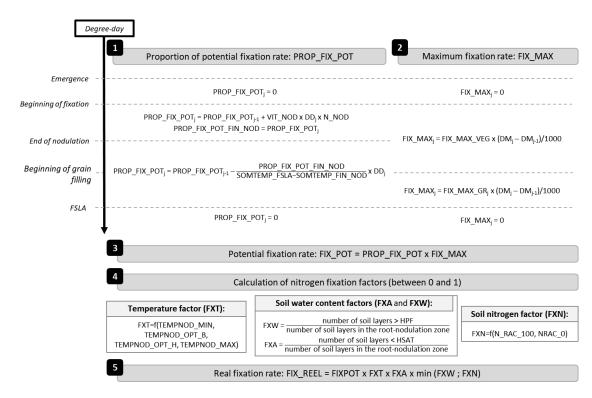


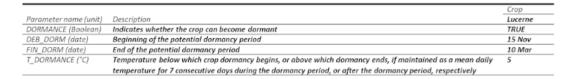
Figure 1. Flowchart for adding a new crop to the Syst'N model

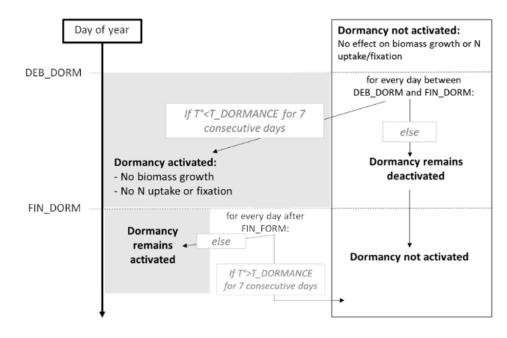
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- 12 Figure 2. Description of the biological nitrogen fixation (BNF) submodel added to Syst'N (adapted from the
- 13 STICS model). See Table 3 for definitions of variables not defined in the figure. Numbers in black boxes indicate
- 14 the order of the calculation steps.

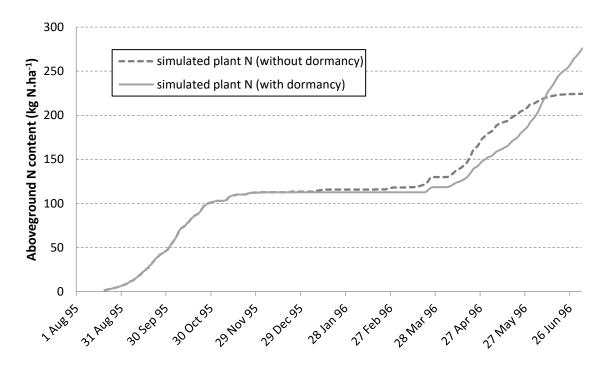




17 Figure 3. Description of the dormancy submodel added to Syst'N (adapted from that in the CropSyst model).



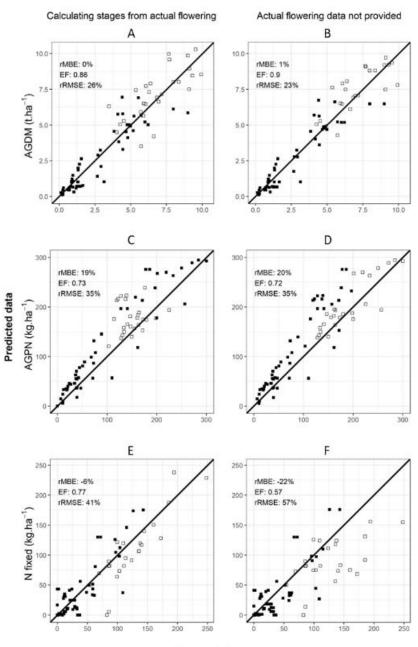
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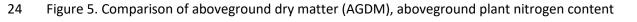
20 Figure 4. Syst'N predictions of lucerne aboveground N content before and after adding equations to simulate

21 dormancy

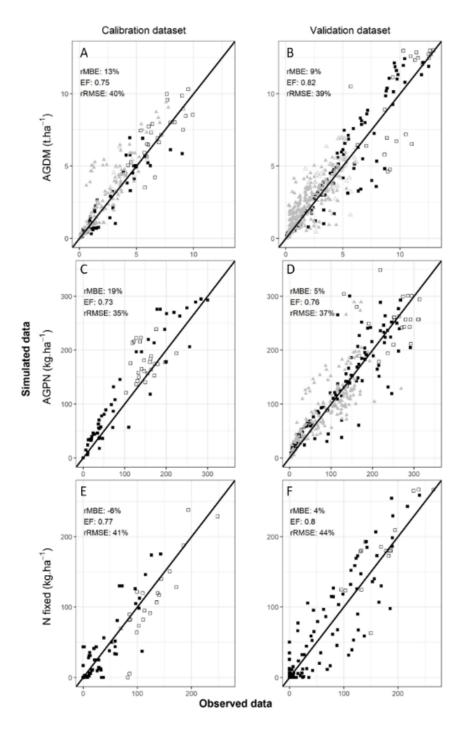




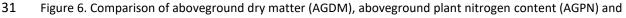
Observed data



- (AGPN) and biological N fixation observed vs. that predicted by Syst'N with the calibration dataset,
   with or without calculating phenological stages from the actual flowering date. rMBE=relative mean
- bias error, EF=model efficiency, rRMSE=relative root mean square error. The black line is the 1:1 line.
- 27 bias error, Li model enciency, rivise-relative root mean square error. The black line is the 1.1 lin
- 28 White symbols correspond to the end of the growing season. Black symbols correspond to earlier
- 29 stages.



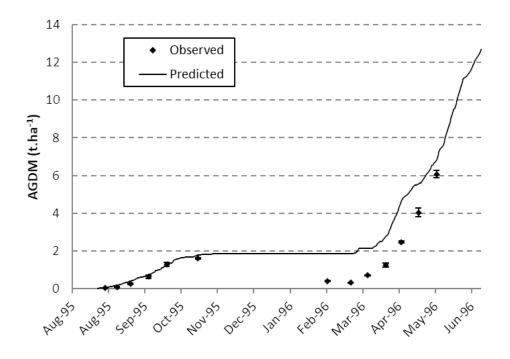




biological N fixation observed vs. that predicted by Syst'N with the calibration and evaluation datasets.

rMBE=relative mean bias error, EF=model efficiency, rRMSE=relative root mean square error. The black line is
 the 1:1 line. White symbols correspond to the end of the growing season. Black symbols correspond to earlier

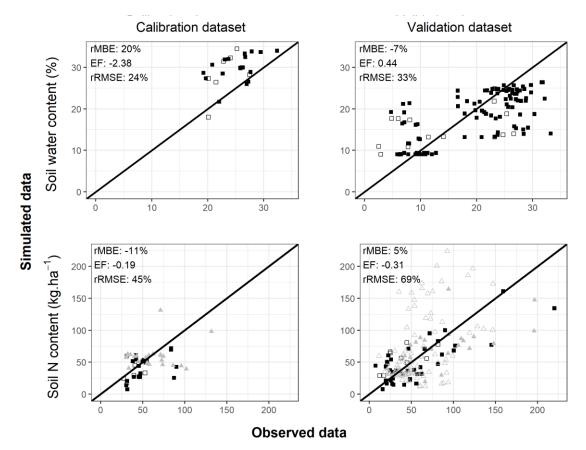
35 stages.



## 37

38 Figure 7. Example of observed and predicted aboveground dry matter before and after dormancy using the

39 evaluation dataset (site: Châlons-en-Champagne). Error bars indicate standard deviations.



40

41 Figure 8. Comparison of soil water content and soil nitrogen content observed and that predicted by Syst'N

42 using calibration and evaluation datasets. rMBE=relative mean bias error, EF=model efficiency, rRMSE=relative

43 root mean square error. The black line is the 1:1 line. White symbols correspond to the end of growing season.

44 Black symbols correspond to earlier stages.

45

46