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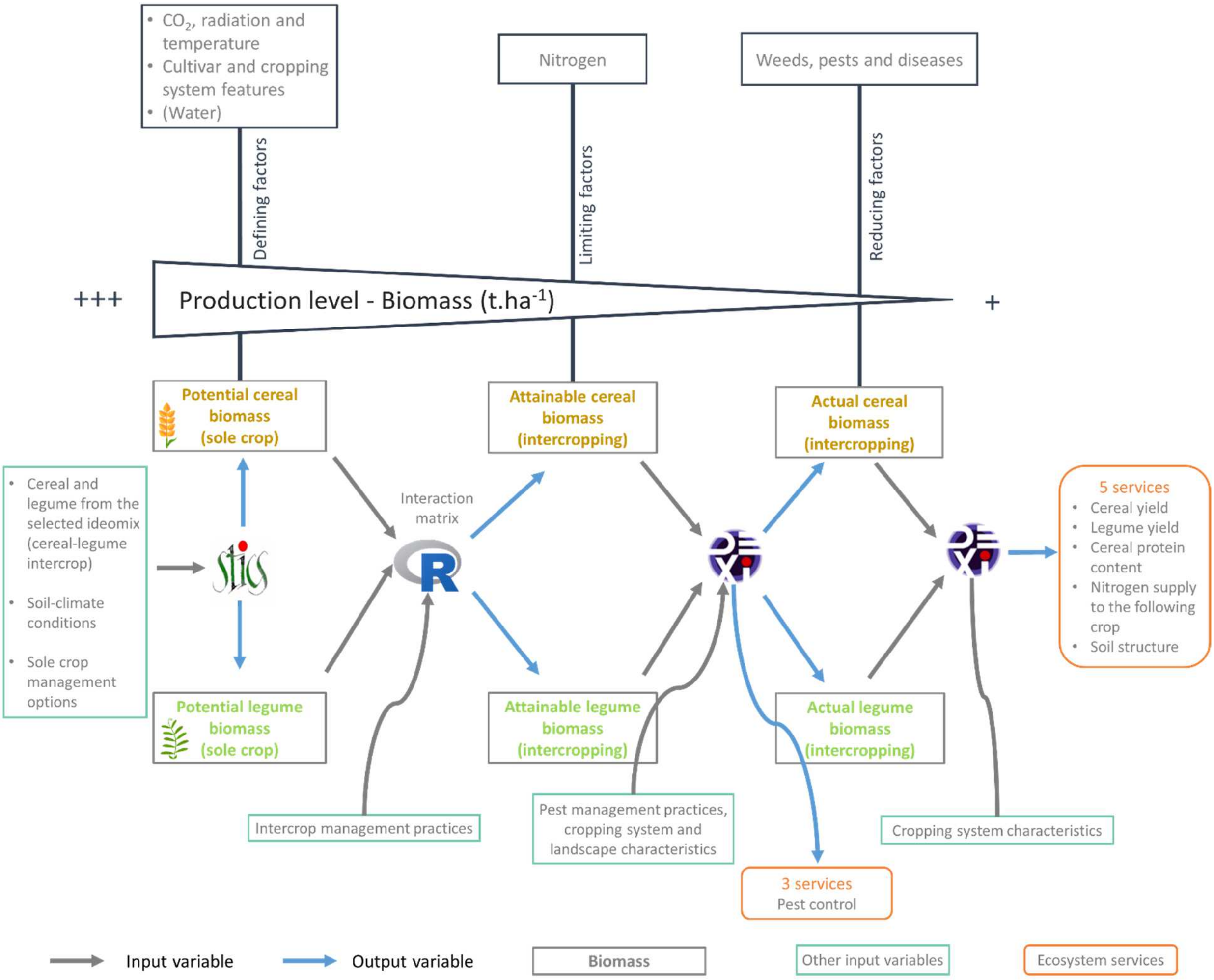
Abstract

Cereal-legume intercropping is known to improve the sustainability of crop production. However, it remains uncommon on commercial farms in Europe due to a number of socio-technical lock-ins and the many practical issues raised when integrating intercrops in cropping systems (e.g. which species, cultivars, sowing densities). Crop modelling is an option to explore integration scenarios and support farmers' decisions. However, available crop models are not able to simulate bundles of ecosystem services provided by a large diversity of binary cereal-legume intercropping scenarios. To address this challenge, we developed a hybrid modelling chain that combines process-based, statistical and knowledge-based models to benefit from the strengths of these three different modelling approaches. The chain (i) simulates potential biomass of the sole cereal and legume crops independently using the crop model STICS; (ii) uses statistical interaction models built in R to convert potential biomass in sole cropping into attainable biomass in intercropping by considering competition effects among species, using a field trial database; (iii) converts attainable biomass into actual biomass by considering pest damage using a knowledge-based multi-attribute DEXi model, and also assesses control of pests (i.e. weeds, insects and diseases); and (iv) uses another set of multi-attribute models to assess five additional ecosystem services (i.e. cereal and legume grain yields, cereal protein content, nitrogen supply to the following crop and impact on soil structure) from the actual biomass of the intercrop at harvest and/or cropping system features. The chain was calibrated for grain cereal-legume intercrops sown simultaneously in a random pattern under low-input French conditions. We used an expert-based approach to assess the performances of each model and evaluate the accuracy of the entire modelling chain. In 18 simulated scenarios, 79% of the predicted levels of ecosystem services were consistent with experts' opinion. Predictions were more accurate for intercropping scenarios that included species from the trial database used to build linear interaction models (relative RMSE of 27-31%) but remained satisfactory for other intercropped species (relative RMSE of 32-37%). This is the first modelling chain able to assess bundles of ecosystem services provided by multiple cereal-legume intercrops in function of their cropping

system contexts. This chain is intended to be included in an educational tool that is used face to face with farmers or students to design cropping systems that include intercrops.

Graphical abstract



Steps of the modelling chain developed to predict ecosystem services provided by a diversity of intercrops according to the production-level model of van Ittersum et al. (2013)

Keywords: intercropping, mixed crop, crop model, mixed model, ecosystem services

1. Introduction

Cultivating annual arable crop species mixtures, also called intercropping, has long been known to improve the sustainability of crop production (Jensen, 1996; Jensen et al., 2020; Maitra et al., 2021; Willey, 1985). In particular, cereal-legume intercropping improves resource-use efficiency (Bedoussac et al., 2015; Duchene et al., 2017; Hauggaard-Nielsen et al., 2003; Jensen et al., 2020), increases productivity per unit area and production stability against weather variability (Pelzer et al., 2012; Raseduzzaman and Jensen, 2017) and supports a wide range of ecosystem services (Maitra et al., 2021), including weed control (Hauggaard-Nielsen et al., 2001) and soil stability and fertility (Stomph et al., 2020).

Despite these known benefits, intercropping remains uncommon on commercial farms in Europe (Machado, 2009) and is associated mainly with low-input systems. This is due, among other factors, to sociotechnical lock-ins that hinder crop diversification on farms (Meynard et al., 2018; Verret et al., 2017): lack of suitable cultivars and machinery for harvesting, sorting and processing, and overall lack of knowledge about best intercrop management practices at all levels of the value chain (e.g. farmers, advisors, processors, researchers) (Casagrande et al., 2017)).

Besides choosing the most suitable species combination (which species and how many), farmers must make multiple decisions when including cereal-legume intercrops in cropping systems, such as the right timing in the crop rotation (considering previous crop effects and consequences on the following crop); the best cultivars for these species; the most appropriate spatial pattern for sowing; when to sow and at what density; how to manage nitrogen fertilization and other inputs; and how to control weeds, pests and diseases. These decisions are also necessary when cultivating sole crops and become even more challenging when combining species. Because field trials alone cannot explore all solutions, crop modelling is one way to explore many scenarios.

Crop modelling has been used extensively to study sole crop functioning, but only a few process-based crop models are available to simulate intercrops: STICS (Brisson et al., 2003), APSIM (Holzworth et al., 2014), CROPSYST (Singh et al., 2013) and FASSET (Berntsen et al., 2004). These models consider a narrower range of annual crop mixtures than those available to farmers (Gaudio et al., 2019). Moreover, they can assess only a few ecosystem services (mainly yield and nitrogen supply), while farmers often expect intercropping to provide a larger bundle of services (Verret et al., 2020). At present, little is known about which input variables are most important to model intercrops reliably, especially when varying crop management practices such as sowing density and weed control. These models still require much research to foster exchanges between modelling and field trials to identify best management practices for a wide range of intercropping practices (Gaudio et al., 2019). In the meantime, complementary approaches (e.g. participatory workshops, expert elicitation, monitoring new knowledge) are needed to support farmers' thoughts about designing and implementing intercropping to further integrate it into cropping systems (Verret et al., 2020).

We designed an educational tool to support farmers' assessment of ecosystem services provided by a large diversity of cereal-legume intercropping scenarios. Each scenario is defined as a unique combination of cropping system characteristics (i.e. soil-climate conditions, crop rotations, landscape effects, cereal and legume species and cultivars, and their management practices). This tool is intended for use in low-input farming contexts (whether conventional or organic) under diverse soil-climate conditions for a wide range of binary cereal-legume intercrops sown in a random pattern.

Given our ultimate aim to develop a tool for farmers, it is intended to be relatively simple, reliable, easily scalable and parsimonious in its data requirements.

We developed a modelling chain that combines hard models (process-based) and soft models (statistical and knowledge-based) to evaluate scenarios using the educational tool under development. The chain was used to assess eight ecosystem services which were identified by experts as often expected from cereal-legume intercrops: (i) input services (pest control (i.e. weeds, insects and diseases), impact on soil structure and nitrogen supply to the following crop) and (ii) output services (cereal and legume grain yields and cereal protein content) (Swinton et al., 2007).

2. Materials and Methods

2.1. Overall strategy

2.1.1. Modelling assumptions

We relied on recommendations from a panel of experts to address the diversity (i.e. many intercropping options available) and complexity (i.e. many processes to simulate) of the modelled system. Some of the volunteer experts were French scientists who had performed research on intercropping (Bedoussac et al., 2015; Bedoussac and Justes, 2010a; Gaudio et al., 2019), cereal or legume crop management (Guinet, 2019; Jeuffroy et al., 2015; Voisin et al., 2014), cropping systems (Alletto, 2015), at least one of the ecosystem services considered (Aubertot and Robin, 2013; Casadebaig, 2008; Constantin et al., 2011; Médiène et al., 2019; Nicolardot et al., 2001; Souchère et al., 2005) and/or crop modelling (Aubertot and Robin, 2013; Bergez et al., 2010; Casadebaig, 2008; Constantin et al., 2015b; Gaudio et al., 2019). The other experts were French research and development agents and farm advisers who support farmers with intercrops.

We established the following modelling assumptions:

(i) The diversity of more than 200 binary cereal-legume combinations of the main sole cereals and legumes grown on European farms can be simplified into 23 ideomixes (i.e. groups of cereal-legume intercrops with similar behaviour). Experts objectivized this concept using criteria that were similar for all intercrops in an ideomix: potential biomass, seasonality, architecture (height of the legume), type of legume crop (fodder or grain legume, harvested or not) and some management practices, including sowing date and nitrogen fertilization (Supplementary Material 1). We calibrated the modelling chain only for grain crops sown simultaneously, which represented 7 of the 23 ideomixes.

(ii) Cereal-legume intercrop biomass can be estimated from cereal and legume sole crop biomass if variables that reflect their interactions (i.e. facilitation and competition for resources) are also considered (e.g. sowing density, plants height).

(iii) Five of the eight ecosystem services considered (i.e. soil structure, cereal and legume yields, cereal protein content and nitrogen supply to the following crop) can be estimated from cereal and legume intercrop biomass at harvest.

(iv) Pest control (considering weeds, insects and diseases separately) can be estimated using the approach in the IPSIM model (Aubertot and Robin, 2013; Robin, 2014), which categorizes pests according to their level of endocyclism (i.e. dependence on the cropping system). For example, perennial weeds (e.g. *Rumex crispus*), European cockchafers (e.g. *Melolontha melolontha)* and *Aphanomyces euteiches* are highly endocyclic (i.e. restricted mainly to fields and depending greatly on the field endo-inoculum and history), whereas grassy weeds (e.g.

Bromus sterilis), aphids *(*Aphidoiedea*)* and wheat common bunt (*Tilletia* spp.*)* are slightly endocyclic.

2.1.2. Modelling strategy

We developed a hybrid modelling chain by combining three different modelling approaches to take advantage of their strengths and mitigate their weaknesses. Designing a tool that relies completely on expert knowledge raises the issue of current knowledge gaps for a wide range of intercrops, management practices and levels of ecosystem services provided. Crop models are reliable tools for predicting sole crop biomass and yield for many cereal and legume species (Coucheney et al., 2015), but they can simulate only a narrow range of intercrops and can assess only two ecosystem services: yield and nitrogen supply (Gaudio et al., 2019). Field trials provide a large amount of data to infer effects of cereal and legume interactions on intercrop biomass and yield (Gaudio et al., 2021). These data can be used to build statistical models to predict intercrop biomass and yield from sole crop biomass, but such data is available only for a few types of intercrops and ecosystem services.

We used expert recommendations to construct the modelling chain, as follows (Fig. 1):

(i) The crop model STICS (Brisson et al., 2003) was used to simulate the potential and water-limited biomass of cereal and legume sole crops under diverse soil-climate conditions and management practices.

(ii) A statistical model, built with R software (R Core Team, 2018) using a field-trial database of pairwise cereal-legume intercrops and cereal and legume sole crops (Gaudio et al., 2021), was used to convert the potential and water-limited biomasses into attainable (i.e. water and nutrient-limited) biomasses (Van Ittersum et al., 2013). This model represents competition for resources among intercropped species and how management practices (e.g. sowing density, nitrogen fertilization) influence it.

(iii) A knowledge-based multi-attribute model built in DEXi (Bohanec, 2008) was used to convert attainable biomass into actual biomass considering pest damage and to assess pest-control services. Another set of multi-attribute models was used to assess five additional ecosystem services based on the actual biomass of the cereal-legume intercrop at harvest and/or cropping system features (e.g. late nitrogen input).

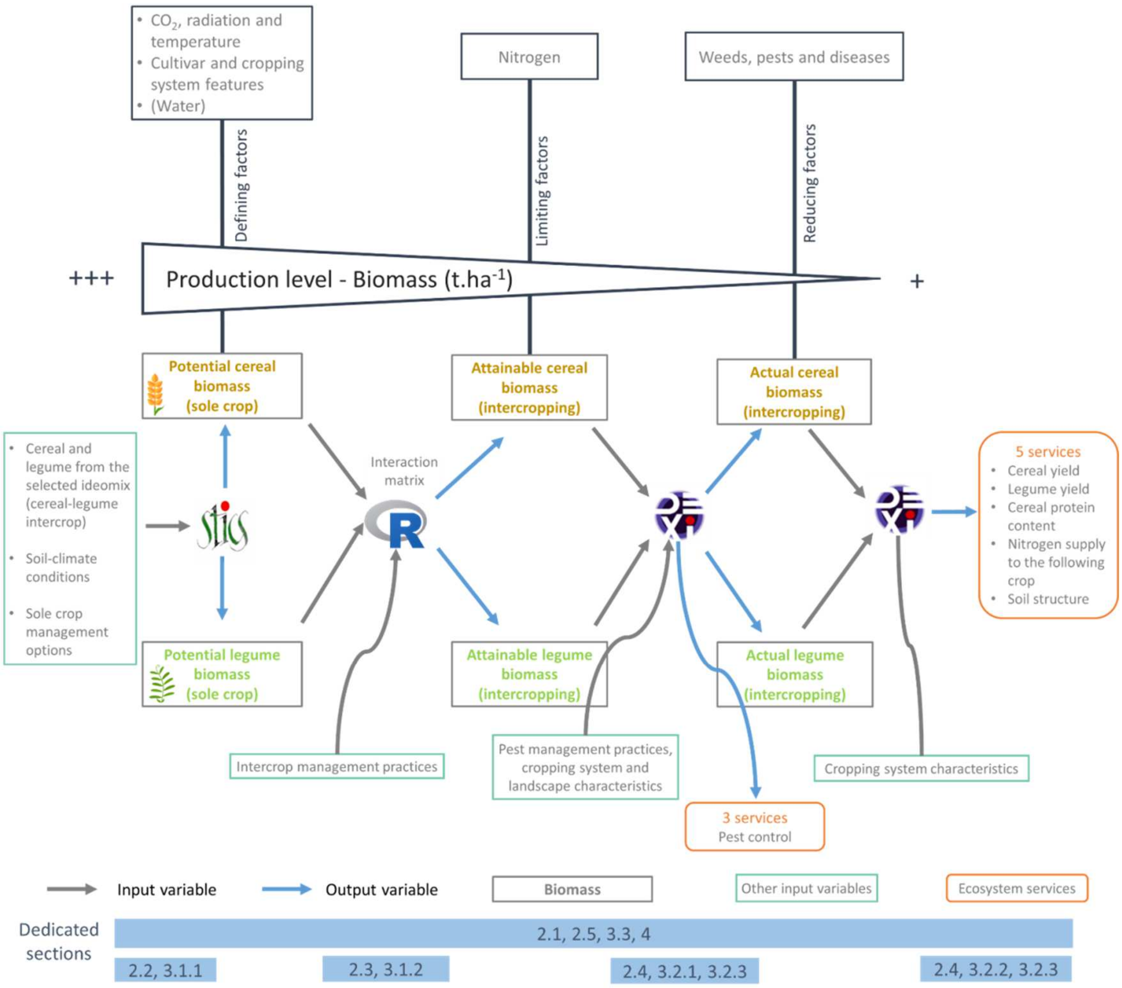


Figure 1. Steps of the modelling chain developed to simulate ecosystem services provided by a diversity of intercrops according to the production-level model of van Ittersum et al. (2013)

2.2. Sole crop simulations

2.2.1. Reasons for choosing the STICS crop model

We used the STICS (v. 9.1) (Brisson et al., 2003) crop model to predict the potential biomass of a wide range of cereal and legume sole crops under diverse soil-climate conditions and management practices (Fig. 1). STICS was chosen as it can predict biomass reliably for many cereal and legume species under a variety of French soil-climate conditions (Coucheney et al., 2015; Kollas et al., 2015). Furthermore, STICS experts were involved in the project (Constantin et al., 2015a) to provide guidance in using the model and interpreting its outputs. We did not use the version of STICS currently under development (Vezy et al., 2020), which is able to simulate intercrops, as the range of intercrops that it can simulate was too narrow to meet our objectives.

2.2.2. Experimental design for simulations

To address the diversity of French soils and climates, we identified 24 climate sites (8×8 km grid cells) across the country from previous projects, which represented 49 soil types (Constantin et al., 2015a). To consider climate variability at each site, we used SAFRAN climate data (Vidal et al., 2010) from

1996-2016. We focused on French soil and climate conditions, although data can be found to run STICS simulations for many other countries.

The STICS plant database does not include all of the cereal and legume species that farmers can combine. Thus, with the support of experts, we created groups of species with similar biomass production potential, in agreement with our list of ideomixes (Table 1, Supplementary Material 1). We then defined ten model species, each of which represented a larger group (Table. 1): winter wheat, spring barley, maize, sorghum, winter and spring pea, winter and spring faba bean (Falconnier et al., 2019), lentil and soya bean. Because lentil and spring faba bean were not available in the STICS database, we estimated their biomasses from simulated spring pea biomass based on empirical biomass ratios defined from legume trial databases (Bourlet et al., 2019; Guinet, 2019) and expert knowledge.

Table 1. Cereal-legume ideomixes of grain crops sown simultaneously and model species used in STICS. Crops in bold and italics are model species available or not available in STICS, respectively. Other crops are species included in the ideomix.

Ideomix	**Cereal species**	**Legume species**
Winter cereal/Annual winter grain legume with height > 40 cm and < 100 cm	**Winter wheat,** winter oat, winter barley, spelt, rye, triticale, durum wheat	**Winter protein pea**
Winter cereal/Annual winter grain legume with height > 100 cm and < 150 cm	**Winter wheat,** winter oat, winter barley, spelt, rye, triticale, durum wheat	**Winter faba bean,** winter lupine, winter fenugreek
Spring cereal/Annual spring grain legume with height < 40 cm	**Spring barley,** spring wheat, spring oat	*Spring lentil*
Spring cereal/Annual spring grain legume with height > 40 cm and < 100 cm	**Spring barley,** spring wheat, spring oat	**Spring protein pea,** chickpea
Spring cereal/Annual spring grain legume with height > 100 cm and < 150 cm	**Spring barley,** spring wheat, spring oat	*Spring faba bean,* spring lupine, spring fenugreek
Maize/Annual summer grain legume	**Maize**	**Soya bean**
Other summer cereal/Annual summer grain legume	**Sorghum,** millet	**Soya bean**

To simulate the widest range of potential biomass for each model species, we considered diverse cultivar choices, sowing dates and irrigation. According to experts, when the cultivar influenced potential biomass strongly (i.e. maize, winter wheat, spring barley and soya bean), we simulated biomass for the cultivars available in STICS that had the most diverse precocity (and, for winter crops, alternativity) and used all values of potential biomass to represent intraspecific diversity. We simulated seven cultivars for maize, four for winter wheat, two for spring barley, three for soya bean and one for all other species. For each cultivar, we simulated three sowing dates and scenarios with or without irrigation. As STICS simulations predicted potential biomass (Fig. 1), experts defined optimal sowing density, and doses and dates of nitrogen fertiliser applications for each model species to avoid nitrogen stress under low-input farming conditions. We did not distinguish organic and conventional low-input situations for fertilization, as the objective was to simulate non-limiting nitrogen conditions. Ultimately, we ran 208 800 simulations (i.e. treatment × site × year combinations).

2.2.3. Evaluation of STICS simulations

We could not compare STICS predictions to observed data, as potential biomass (without pest, nitrogen, and water stress) is a theoretical concept that is difficult to obtain in field trials. However, previous studies that assessed STICS performances showed good accuracy overall and little bias, especially for attainable crop biomass (i.e. relative root-mean-square error (RMSE) of 35%), and an acceptable reproduction of trends induced by contrasting environmental conditions and management practices (Coucheney et al., 2015). We assumed that STICS performances were similar for potential biomass and limited their assessment to verifying the overall consistency of differences in biomass as a function of soil-climate conditions and management practices.

2.3. Integration of interaction effects

2.3.1. Data description

We developed a statistical model using R software v. 3.6.3 (R Core Team, 2018) to predict the attainable biomass of an intercropped cereal and legume based on the potential biomass of their corresponding sole crops (Fig. 1). As few data were available in France, we used a database that included intercrop trials conducted in five European countries from 2001-2017, with several cultivars of four winter species (i.e. durum wheat, soft wheat, pea, faba bean) and seven spring species (i.e. pea, chickpea, soft wheat, barley, lupine, faba bean, lentil) (Gaudio et al., 2021)(Supplementary Material 2). The database included pairwise data on the biomass of cereals and legumes under intercropping and sole-cropping conditions, as well as yields and cereal protein content for certain trials. For 8% of the experimental units, one value (i.e. cereal or legume biomass in sole crop, or intercropped cereal and legume biomass) was missing. We imputed missing data using the R package *MICE* (Van Buuren et al., 2014) (Supplementary Material 3). Ultimately, complete data were available for 183 experimental units at harvest for four ideomixes: winter cereal – pea, winter cereal – faba bean, spring cereal – lentil and spring cereal – pea) (Table 1, Supplementary Material 1).

2.3.2. Statistical modelling

We built two statistical models to predict the attainable biomass of each species of the intercrop (cereal and legume) at harvest. We chose linear models due to the interpretability of their results. The two models included the same input variables, which were selected based on their agronomic effects on the relation between sole crop biomass and intercrop biomass (Table 2). Compared to statistical selection, this agronomic reasoning simplified the explanation of how input variables of the model were selected. In addition, predictor-selection tests showed that these models differed little statistically from those defined from a pre-selected list of variables. To support our decision to include certain variables or not, we compared statistical performances of models with or without these variables using 10-fold cross-validation with the R package *caret* (Kuhn, 2008) and selected the model with the smallest RMSE.

Table. 2. Relevant variables used in linear interaction models to predict cereal-legume intercrop biomass from sole crop biomass. (P = precipitation, ETP = evapotranspiration, GR = global radiation, T = temperature)

Variable type	Input variable	Definition	Unit	Impact on cereal/legume intercrop biomass
Biomass	Cereal and legume biomass for sole crops at harvest	Biomass of cereal and legume sole crops at harvest	$t.ha^{-1}$	Ability to produce biomass in the sole crop directly determines biomass production in the intercrop
Species and cultivar	Crop season	Sowing period of the cereal and legume (winter or spring/summer)		Sowing period of each species determines the degree of competition over time
	Cereal and legume height	Potential height of the cereal and legume sole crop	cm	Height is a known determinant of a plant species' ability to compete for light
Management practices	Relative nitrogen fertilization of the cereal and legume	Absolute difference in fertilization between the intercrop and the sole crops (cereal and legume)	kg $N.ha^{-1}$	Relative decrease in nitrogen fertilization determines nutrient competition among species
	Relative sowing density of the cereal and legume	Ratio of the sowing density of the intercropped cereal or legume to that of the corresponding sole crop (cereal or legume)		Sowing density is a known determinant of competition for abiotic resources among species
Climate	∑(P-ETP) at harvest	Sum of daily climatic water balance from sowing to harvest	mm	Water availability determines biomass production of each species when intercropped
	∑GR at harvest	Sum of daily global incident radiation from sowing to harvest	$J.cm^{-2}$	Incident radiation determines biomass production of each species when intercropped
	∑Tmean at harvest	Sum of daily mean air temperature from sowing to harvest	°C	Degree days determine biomass production of each species when intercropped

The two linear interaction models (one for cereal biomass, one for legume biomass) were defined to infer interaction effects (see Supplementary Material 4 for model coefficients). They included cereal and legume characteristics, management practices and climate variables (P = precipitation, ETP = evapotranspiration, GR = global radiation, T = temperature) :

$$\textbf{Associated cereal biomass} = \mathrm{f}\,(\text{Sole cereal biomass} + \text{Sole legume biomass} + \text{crop season} + \text{cereal potential height} + \text{legume potential height} + \text{relative nitrogen fertilization of the cereal} + \text{relative sowing density of the cereal} + \text{relative sowing density of the legume} + \sum(\mathrm{P}-\mathrm{ETP}) + \sum\mathrm{GR} + \sum\mathrm{Tmean})$$

$$\textbf{Associated legume biomass} = \text{f (Sole cereal biomass} + \text{Sole legume biomass} + \text{crop season} + \text{cereal potential height} + \text{legume potential height} + \text{relative nitrogen fertilization of the legume} + \text{relative sowing density of the cereal} + \text{relative sowing density of the legume} + \sum(\text{P} - \text{ETP}) + \sum\text{GR} + \sum\text{Tmean})$$

2.3.3. Statistical model evaluation

We assessed the statistical performances of the two models using adjusted coefficients of determination (Adj. R^2) and its range (min and max R^2) in k-fold cross-validation and RMSE. We calculated R^2 and its range using the full dataset. RMSE was calculated for three datasets: (i) the full dataset, (ii) a random split of the dataset (75% of individuals to train the model and 25% to test it) and (iii) a predetermined split of the dataset (3 of the 4 ideomixes to train the model and the 4th to test it).

2.4. Expert-based assessment of ecosystem services

2.4.1. Expert knowledge elicitation and modelling

The multi-attribute model was built in DEXi (Bohanec, 2008) to assess eight expert-chosen ecosystem services provided by intercrops in diverse scenarios and to compare their levels among scenarios. Each scenario corresponded to a combination of STICS input variables (ideomix × cereal cultivar × legume cultivar × irrigation × sowing date × site × year) × R input variables (cereal-legume density ratio × intercrop nitrogen fertilization × crop season × climate variables) × DEXi input variables for pest damage (crop sequence × tillage × sowing date × curative actions × cultivar susceptibility × landscape effect) × other input variables specific to each DEXi tree. The multi-attribute model was intended to be simple (i.e. to include a few readily available input variables and to be applicable to all ideomixes). The services were assessed qualitatively (i.e. pest control and soil structure) or quantitatively (i.e. cereal and legume yields, cereal protein content and nitrogen supply to the following crop) and, when relevant, using actual intercropped cereal and legume biomass as the main input variable, along with other cropping system features (Fig. 1), as suggested by experts.

To design this model, we organized four meetings with experts to define input variables (i.e. basic attributes) relevant for estimating each ecosystem service and for building multi-attribute DEXi models based on “if-then” decision rules through an iterative process of discussion and revision. Experts also defined, in mutual agreement, aggregation rules for each tree and aggregated attributes, i.e. internal knots. Pest damage was included to convert attainable intercrop biomass predicted by STICS and interaction models into the actual biomass needed to estimate five of the eight ecosystem services considered. We organized two additional meetings with intercrop and pest experts to build the multi-attribute model following the same method as that for ecosystem services. Experts also defined potential losses in attainable biomass due to low, medium and high pest damage (i.e. < 5%, 5-20% and > 20% biomass loss, respectively).

2.4.2. Defining the classes

We defined classes for all input and output variables of the multi-attribute model in DEXi. We selected five classes for attainable and actual biomass, as recommended by experts and frequently done in DEXi tools (Craheix et al., 2015). To define actual biomass classes, we used potential sole crop biomass predicted by STICS (Fig. 1) for multiple soil-climate conditions and management practices. Potential biomass was then converted into attainable biomass using statistical models and considering multiple intercrop management practices for nitrogen fertilization levels and sowing densities (Fig. 1). To estimate actual biomass, we decreased attainable biomass by the median of percentage classes defined by experts for low, medium and high pest damage.

We also tested the application of three commonly used distributions (i.e. uniform, normal and lognormal) to the actual biomass for each ideomix. We chose rounded to one decimal quantiles of a normal distribution, which was the closest to that of the observed data, to define five actual biomass classes for each ideomix. We used the same approach on the dataset of attainable biomass to define five attainable biomass classes for each ideomix.

We also defined classes for other input variables and for ecosystem services. For other input variables (e.g. tillage after harvesting the previous and pre-previous crop (i.e. the crop preceding the previous crop), landscape effects on pest damage, late nitrogen input), we relied on the literature and expert knowledge to define two classes for each input variable. For output variables (i.e. ecosystem services), we defined three classes based on expert recommendations (Craheix et al., 2015). For yield, we defined a harvest index for each cereal and legume species, which was applied to actual intercropped cereal and legume biomass. We then adjusted the normal distribution to define three yield classes for each ideomix. For cereal protein content, we used a threshold of 12% as the class boundary. For nitrogen supply to the following crop (here, potential nitrogen restored to the soil by the intercrop at harvest), experts defined the class boundaries based on STICS' prediction of residual soil nitrogen available after each type of sole crop. For soil structure and pest control, we defined three levels of services (i.e. low, medium and high) (see Supplementary Materials 5, 6 and 7 for the classes defined for all input and output variables).

2.4.3. Model evaluation

We analysed the sensitivity of the nine multi-attribute DEXi models (i.e. the tree that assessed actual biomass from attainable biomass considering pest damage (for the cereal and legume) and the eight ecosystem service trees). We first studied the mean contribution of each input variable to the overall variance of the output variable (Carpani et al., 2012). To do so, we used normalized local weights provided by the DEXi software (i.e. the weights of input variables and subtrees on the value of the output variable) (Aubertot and Robin, 2013). We also compared these results to an analysis of variance (ANOVA) of the ecosystem service multi-attribute models, which were simple enough that ANOVA could be performed quickly (Carpani et al., 2012).

We then assessed the probability of occurrence of each value of the output variable (i.e. actual biomass or ecosystem service) using Monte-Carlo analysis, which randomly selects input scenarios based on their probability of occurrence. To perform this analysis, we assumed that input variables were independent, in agreement with Carpani et al. (2012): "by default, the scenarios are all sampled with equal probability, thus giving equal weight to all possible input combinations". We first analysed each of the nine multi-attribute models based on this assumption of a uniform distribution of input variables, using 1000 samples. We then challenged this assumption, because the DEXi models were part of a modelling chain. We thus used the observed distribution of attainable cereal and legume biomasses as the probability of occurrence for attainable cereal and legume biomass in the DEXi model considering pest damage. We then performed a second Monte-Carlo analysis of this multi-attribute DEXi model (still using 1000 samples) and used the probabilities of occurrence of actual cereal and legume biomass obtained as the distribution of cereal and legume biomass input variables in the ecosystem service models. Finally, we performed a third Monte-Carlo analysis of each ecosystem service multi-attribute model that considered these new probabilities of occurrence of biomass. For all other variables, scenarios were sampled with equal probability.

2.5 Analysis of the modelling chain

We could not formally analyse the entire modelling chain for all ecosystem services due to (i) the combination of three very different types of models (process-based, statistical and knowledge-based) with diverse inputs, (ii) the lack of observed data on some ecosystem services (for soil and pests) and ideomixes and (iii) the inability to compare predictions to observed data on production services (i.e. cereal and legume yields, cereal protein content). As data from field trials to estimate pest damage were lacking, we could not select an appropriate simulated scenario to which to compare observed data. Thus, we assessed the performances of each model independently to estimate the performances of the entire modelling chain indirectly.

In addition, we organized three meetings with experts to verify the consistency of ecosystem service levels estimated by our modelling chain for diverse intercrop scenarios. We defined 18 scenarios for three well-known ideomixes (i.e. winter cereal-pea, spring cereal-pea and spring cereal-faba bean) to maximize the expert knowledge. We tested each of the three ideomixes with two soil-climate conditions, two levels of nitrogen input, two cereal cultivars, two sowing densities for the cereal and legume in the intercrop and two levels of pest damage. For each scenario and ecosystem service, each expert assessed the level of ecosystem service provided by allocating ten poker chips to represent the probability of attaining each level under the specific scenario. We then summed experts' chips for each level of ecosystem service and compared the level chosen most to the modelling chain output to identify one of four levels of prediction performance: (i) correct (i.e. experts chose the predicted level), (ii) nearly correct (i.e. the experts' level was one class away from the predicted level (e.g. "low" vs. "medium" yield)), (iii) incorrect (i.e. the experts' level was more than one class away from the predicted level (e.g. "low" vs. "high" yield)) and (iv) uncertain (i.e. the experts' disagreed on the level or lacked knowledge, which made it impossible to evaluate the predictions). When the experts' level and predicted level differed, we discussed the consistency of the prediction and why it differed. When the error was due to an inaccurate estimate by one of the DEXi models and occurred for several scenarios, we modified aggregation rules to correct the modelling chain predictions according to expert knowledge. When the error was due to an inaccurate prediction of attainable biomass, however, we could not modify STICS or the linear interaction models to correct it.

3. Results

3.1. Attainable biomass estimate

3.1.1. Potential biomass estimate

We used STICS to predict potential biomass for a wide range of cereals and legumes in sole crops under diverse French soil-climate conditions and management practices (see Supplementary Material 8 for main results). For the potential biomass of spring faba bean and lentil, which STICS could not predict, the mean (± standard deviation) empirically defined ratios of biomass to spring pea biomass were 1.06 (± 0.29) and 0.86 (± 0.20), respectively.

3.1.2. From potential to attainable biomass

Adj. R^2 was 0.6 and 0.7 for the linear interaction models for the legume and cereal, respectively (Table 3). Large differences in R^2 between folds during k-fold cross-validation were due in part to data heterogeneity, especially for intercropped legumes (Fig. 2). Relative RMSE ranged from 27-37% for the two models, regardless of which dataset they had been trained with, which corresponded to a mean RSME of 1.0 $t.ha^{-1}$ (from 1.2-1.8 $t.ha^{-1}$ for cereals and 0.9-1.2 $t.ha^{-1}$ for legumes). The relative and absolute RMSE were slightly higher when models were trained with a predetermined split of the dataset (Table 3). Similarly, only the model that predicted intercropped cereal biomass based on a predetermined split of the dataset underpredicted biomass for almost all individuals (Fig. 2). Model predictions for intercropped cereal and legume biomass were thus reliable for all ideomixes, although they were more accurate when using the full dataset or a random split of the dataset (i.e. for one of the four ideomixes available in the database of trials).

Table 3. Statistical performances of the linear interaction models used to predict intercropped cereal and legume biomass from sole cereal and legume biomass according to the type of dataset used to evaluate the model.

	Full dataset				**Random split of the dataset**		**Predetermined split of the dataset**	
Model	**Adj R^2**	**Adj R^2 min – max**	**RMSE** ($t.ha^{-1}$)	**Relative RMSE**	**RMSE** ($t.ha^{-1}$)	**Relative RMSE**	**RMSE** ($t.ha^{-1}$)	**Relative RMSE**
Cereal	0.7	0.4 – 0.9	1.2	30%	1.2	27%	1.8	37%
Legume	0.6	0.2 – 0.9	0.9	30%	0.9	31%	1.2	32%

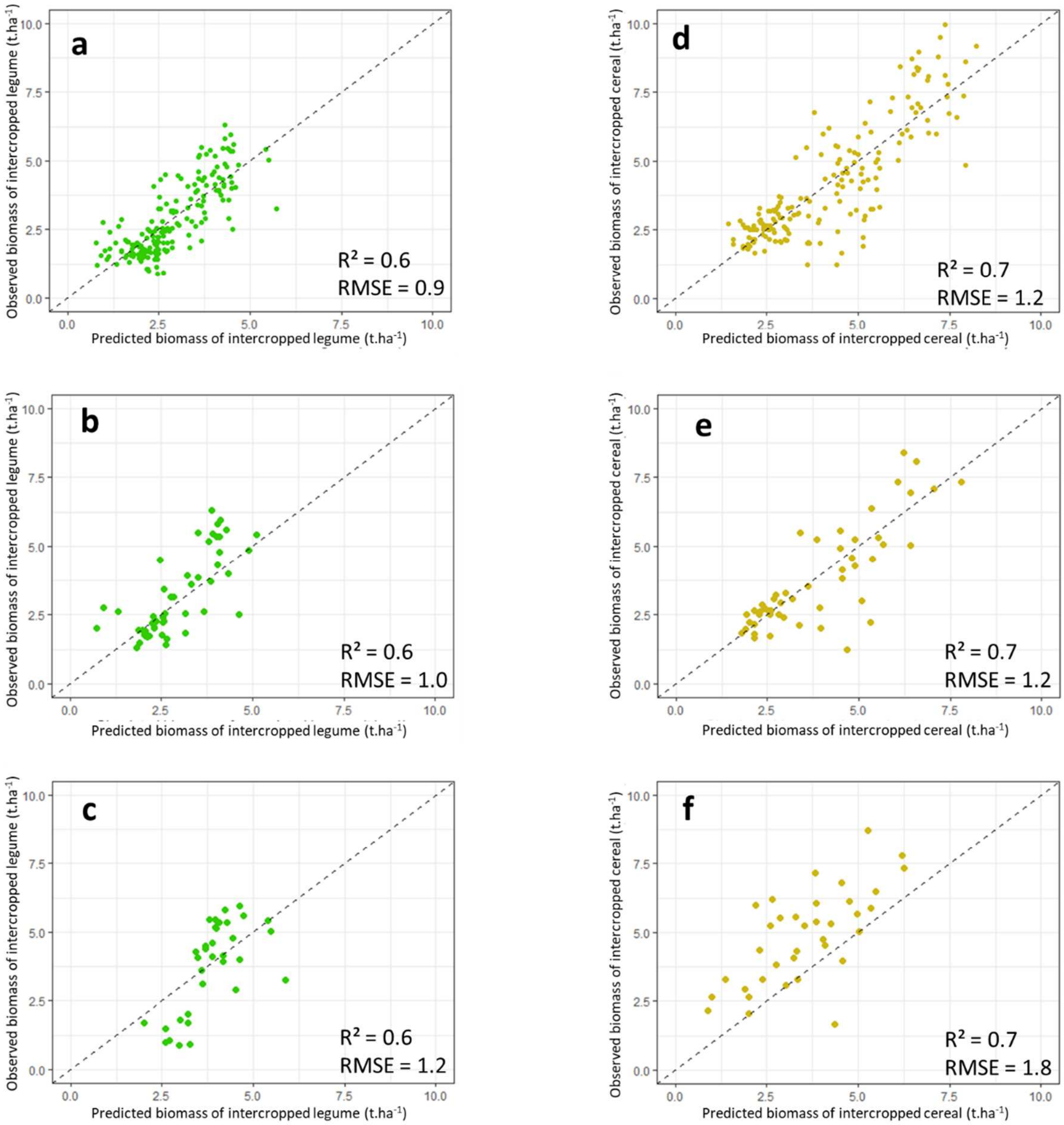


Figure 2. Observed vs. predicted intercropped biomass. (a) Legume observed vs. predicted intercropped biomass for the full dataset. (b) Legume observed vs. predicted intercropped biomass for a random split of the dataset. (c) Legume observed vs. predicted intercropped biomass for a predetermined split of the dataset. (d) Cereal observed vs. predicted intercropped biomass for the full dataset. (e) Cereal observed vs. predicted intercropped biomass for a random split of the dataset. (f) Cereal observed vs. predicted intercropped biomass for a predetermined split of the dataset.

3.2. Actual biomass estimate and ecosystem services assessment

3.2.1. From attainable to actual biomass

The multi-attribute models that converted attainable biomass into actual biomass considering pest damage included 21 attributes (12 basic, 3 linked (i.e. attributes occurring several times with the same name and classes) and 6 aggregated) (Fig. 3). They estimated (i) actual cereal and legume biomass and (ii) pest damage to cereal and legume biomass (%) for slightly, moderately and highly endocyclic pests, which was used to assess three pest-control ecosystem services. Input variables used to estimate pest damage included effects of genetics, crop management and the cropping system. Experts estimated that 55% of actual cereal (or legume) biomass depended on attainable cereal (or legume) biomass, while 45% depended on total pest damage (Fig. 3, Supplementary Material 5). They assumed that total pest damage was divided equally between slightly, moderately and highly endocyclic pests. They did not weight curative actions differently by the type of pest, and decided it accounted for 33% of the resulting pest damage each time. Cultivar susceptibility, representing both its ability to compete with weeds and susceptibility to pathogens and pests, also had a relatively large influence for all types of pests (i.e. 25-33%, depending on the level of endocyclism). For highly endocyclic pests, the interaction between crop sequence and tillage accounted for 33% of the resulting pest damage, which is consistent with their strong dependence on the field cropping history. For slightly endocyclic pests, the proximity of host plants and agroecological infrastructure, both of which represent the influence of the landscape on their population, accounted for 25% of the resulting pest damage, while sowing date accounted for 17%, as delaying sowing decreases endocyclic pest damage slightly. Moderately endocyclic pests were in an intermediate situation, with a stronger influence of the crop sequence and tillage practices (28%) and a smaller influence of the landscape (6%) (Fig. 3).

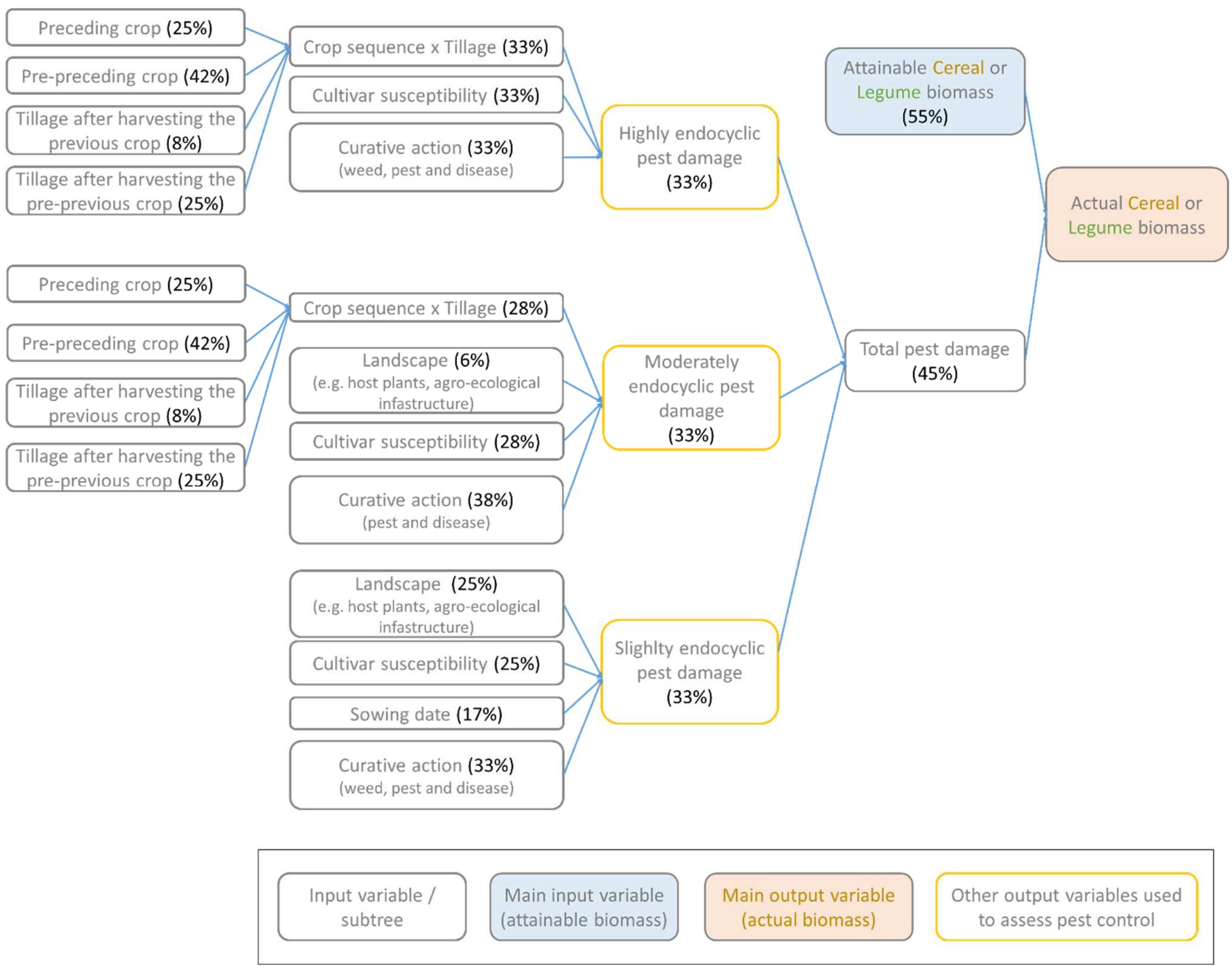


Figure 3. Multi-attribute DEXi model used to convert attainable cereal intercrop biomass to actual biomass considering pest damage. The percentages correspond to normalized local weights of input variables provided by the DEXi software.

3.2.2. From actual biomass to ecosystem services assessment

To assess the eight ecosystem services considered, we built one multi-attribute decision model for each. For the three DEXi models used to assess pest damage, we used the highly, moderately and slightly endocyclic pest damage estimated independently for cereal and legume (Fig. 3) and built a DEXi model to aggregate them to estimate total damage to the intercrop, assuming an equal weight for cereal and legume damage. We then defined the intercrop's ability to control highly, moderately and slightly endocyclic pests as the inverse of pest damage. For the other six ecosystem services, we used actual intercropped cereal and/or legume biomass as the main input variable, as the experts suggested. Based on expert recommendations, we then added variables for genetic and cropping system effects that had not been considered in previous steps of the modelling chain, while maintaining a simple DEXi model structure.

For yields, experts defined cereal yield as a function of actual cereal biomass (77%) and cereal lodging risk (23%) (Table 4, Supplementary Material 5). Cereal lodging risk had a low weight because lodged cereals are usually harvestable, which results only in minor losses in yield. For legume yield, experts also considered actual legume biomass and lodging risk, giving a higher weight to lodging risk than that for cereals due to the difficulty in harvesting lodged legumes (e.g. pea, lentil). They also considered cereal biomass and lodging risk, as the cereal can physically support the legume when it has sufficient biomass to prevent the legume from lodging. Experts determined that cereal protein content is negatively correlated with actual cereal biomass, and depends strongly on late nitrogen uptake. The relatively low weight allocated to cereal biomass (24%) was based on the experts' hypothesis that cereal protein content in the intercrop is never low, even with high biomass production.

Experts considered that nitrogen supply to the following crop depends mainly on actual legume biomass and the legume C:N ratio, with a cumulative weight of more than 75%. The remaining 25% was equally divided between cereal biomass and C:N ratio, and represented a decrease in nitrogen supply to the following crop by the legume due to the cereal. The impact of the intercrop on soil structure was divided equally between the cereal and the legume, each depending on its actual biomass (67% for cereal and legume together) and root system (33% for cereal and legume together, and corresponding to both depth and density).

Table 4. Input variables chosen by experts to assess the five ecosystem services considered and their weights. Variables in italics are actual cereal and legume biomass.

Type	**Ecosystem service**	**Input variable**	**Weight**	**References that supported experts' choices**
Output service	Legume yield	*Actual legume biomass*	53%	(Bedoussac et al., 2015; Viguier et al., 2018)
		Actual cereal biomass	2%	
		Legume lodging risk	36%	
		Cereal lodging risk	9%	
	Cereal yield	*Actual cereal biomass*	77%	
		Cereal lodging risk	23%	
	Cereal protein content	*Actual cereal biomass*	24%	(Jeuffroy and Oury, 2012)
		Late nitrogen intake	76%	(Bedoussac et al., 2014)
	Nitrogen supply to the following crop	*Actual legume biomass*	49%	(Anglade et al., 2015)
		Actual cereal biomass	11%	
		Legume C:N ratio	28%	
		Cereal C:N ratio	12%	
Input service	Soil structure	*Actual legume biomass*	40%	(Postic et al., 2012)
		Actual cereal biomass	27%	
		Legume root system	10%	
		Cereal root system	23%	

3.2.3. Sensitivity analysis

The ANOVA confirmed the hierarchy of variables established with the normalized local weights of DEXi. For example, cereal biomass accounted for most of the total variance (87%) in cereal yield (Fig. 4), while lodging risk and its interaction with yield accounted for only 5% and 8%, respectively. Similarly, legume biomass, cereal biomass, the cereal root system and legume root system accounted for 44%, 19%, 11% and 2%, respectively, of the variance in intercrop impact on soil structure, which was consistent with the normalized DEXi weights. The remaining 14% corresponded to interactions among factors.

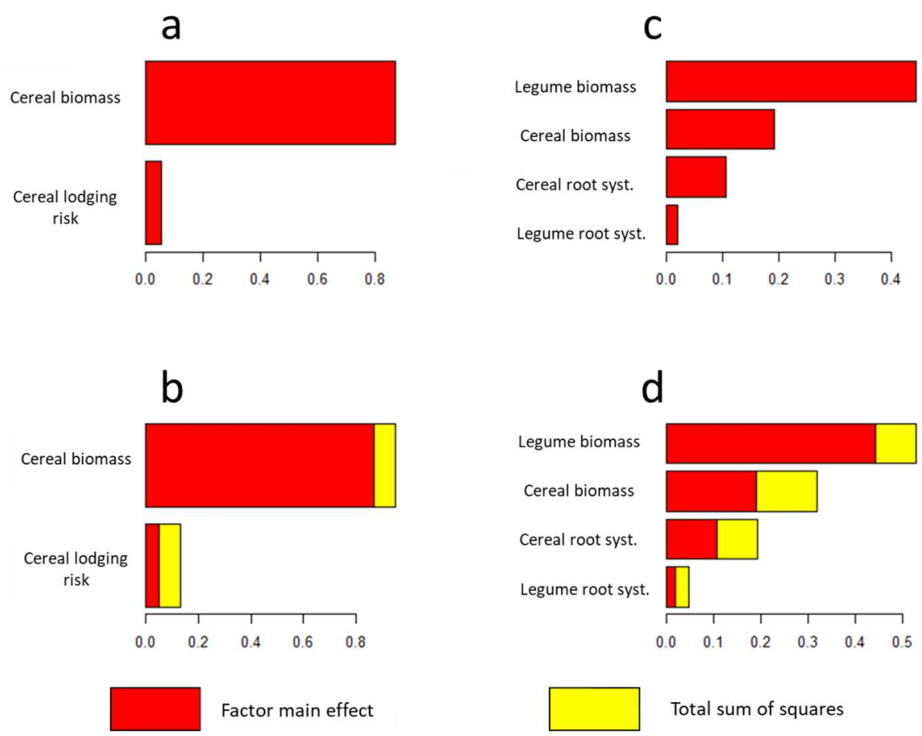


Figure 4. Example of analysis of variance of factors used to determine the ecosystem services of cereal yield (a, b) and intercrop impact on soil structure (c, d). Graphs a and c focus on factor main effects, b and d represent factor main effect and total sum of squares.

For the Monte Carlo analysis, when equal probabilities of occurrence were used for all input variables of all DEXi models, low classes were overrepresented for actual biomass (46% very low actual cereal biomass) and ecosystem services (47% low cereal yields, 69% low potential nitrogen supply) (Fig. 5). When the observed distribution of attainable biomass was used as the probability of occurrence, the distribution of actual biomass differed little, as the observed distribution of attainable biomass was similar to a uniform distribution (Fig. 5). However, when the distribution of actual biomass was used as the probability of occurrence for biomass in the ecosystem service DEXi models, the overrepresentation of low classes increased (72% low cereal yield, 83% low potential nitrogen supply). Low classes were already represented more often with this new distribution than with a uniform distribution (Fig. 5). High classes for some ecosystem service models (e.g. nitrogen supply to the following crop) were underrepresented (occurrence < 10%).

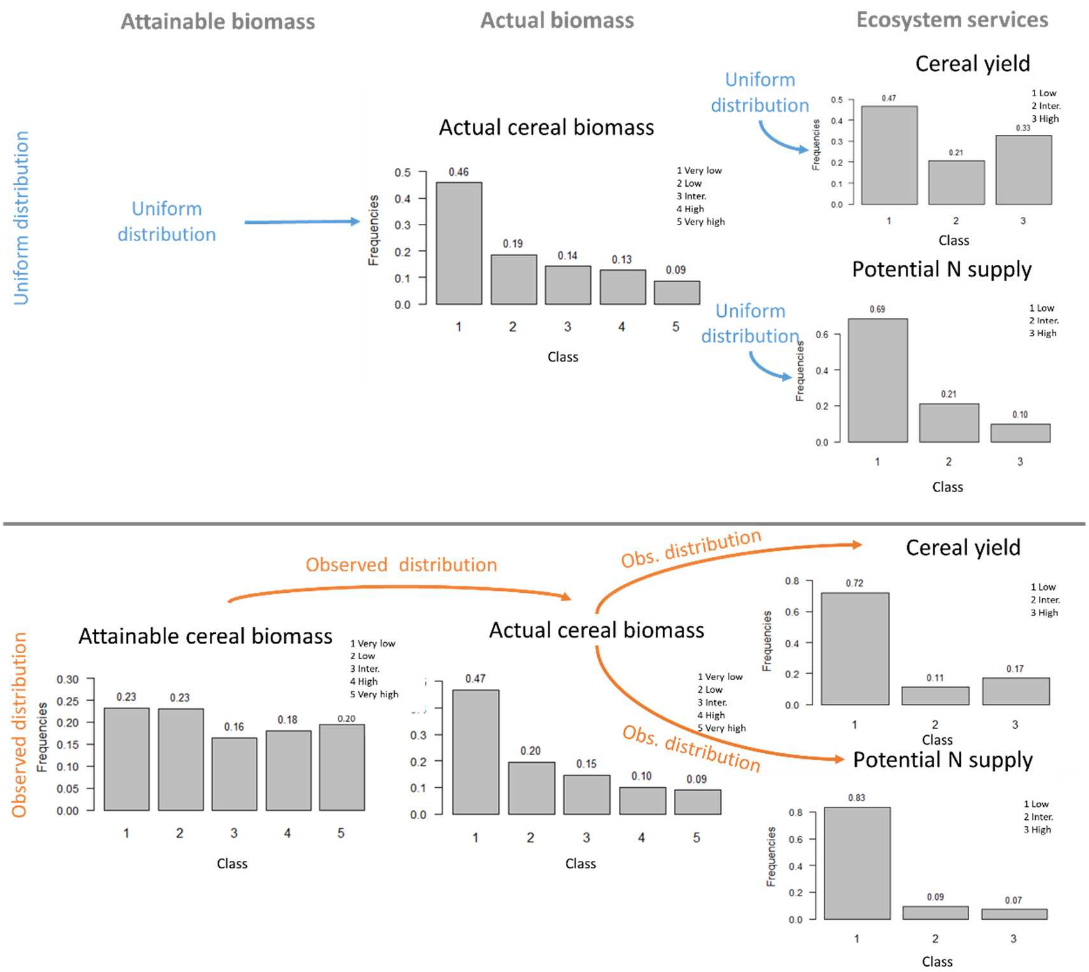


Figure 5. Results of the Monte-Carlo sensitivity analysis of two selected DEXi models of the modelling chain considering (top) a uniform distribution for all variables or (bottom) the observed distribution for biomass and uniform distribution for the other variables.

3.3. Evaluation of the modelling chain

The experts considered modelling chain predictions correct, nearly correct and incorrect for 79%, 19% and 2%, respectively, of the ecosystem services assessed in the 18 scenarios (Table 5). No prediction was considered uncertain, as even when experts' choices differed initially, they ultimately agreed. When comparing their mutual choices to modelling chain predictions, the performances of the latter were similar for all ecosystem services and scenarios tested (Table 5). Predictions had a higher variance and slightly lower percentage of correct values for nitrogen supply to the following crop, which experts expected to be higher than the model predicted. This conclusion was consistent with the overrepresentation of low levels of nitrogen supply, as highlighted by the sensitivity analysis of DEXi models. We thus adjusted two values of the nitrogen supply DEXi model from low to intermediate to conform to expert recommendations. Other incorrect predictions, including cereal yield and protein content, occurred randomly for several scenarios and services, and were due mainly to an inaccurate estimate of one ecosystem service, while actual biomass seemed accurate. As the error did not occur frequently and experts did not suggest an adjustment, we did not modify the DEXi models.

Table 5. Mean (and standard deviation (SD)) percentages of predictions of ecosystem services of the modelling chain that experts considered correct from 18 scenarios.

Prediction	Mean	SD
Cereal yield	67%	17%
Cereal protein content	67%	17%
Legume yield	89%	10%
Nitrogen supply	72%	26%
Impact on soil structure	89%	10%
Pest control	89%	10%
Total	**79%**	**17%**

4. Discussion

4.1 A variety of intercropping scenarios, processes and ecosystem services

To integrate the diversity and complexity of intercropping scenarios, we built an original modelling chain to consider a wide range of possibilities, such as species and management practices about which little is known. The chain can compare intercropping scenarios to scenarios of sole cereal or legume crops. Bundles of ecosystem services are often expected from intercrops, and the chain is able to assess them, including some services at the forefront of research. This assessment is original and considers both abiotic stresses (i.e. water stress with STICS, nitrogen stress with linear interaction models) and biotic stresses (i.e. pest damage with DEXi models). Most crop models (e.g. STICS (Brisson et al., 2003), APSIM (Holzworth et al., 2014), CROPSYST (Singh et al., 2013)) do not consider the latter. Some models can assess damage by a specific category of pests (e.g. IPSIM (Aubertot and Robin, 2013) for several insects and diseases, FLORSYS (Colbach et al., 2021) for weeds) or by weeds, insects and diseases to a single crop (e.g. WHEATPEST (Willocquet et al., 2008)). However, only our modelling chain considers pest damage holistically (i.e. weed, insect and disease damage to a wide range of crops).

Given the heterogeneity of existing knowledge about intercropping practices, we made several modelling assumptions and simplifications to address the large diversity of intercropping scenarios and ecosystem services. For example, we created ideomixes and groups of model species for STICS simulations under the expert-defined assumption that species in each ideomix had the same biomass potential under the same cropping system conditions and behaved similarly when intercropped. We also designed linear interaction models using a training database that did not contain all of the ideomixes simulated with the modelling chain. The relative RMSE of the linear interaction models decreased slightly when the models predicted an ideomix that was not in the training database (from 27-31% to 32-37%) (Table 3). These performances were satisfactory compared to those of other crop models (e.g. relative RMSE of 35% for attainable biomass with STICS; Coucheney et al., 2015). Finally, we assessed several ecosystem services for which few data are available. Accordingly, experts were less confident in defining input variables and decision rules for them than for production trees, resulting in a potential omission of some impacting factors and a more uncertain assessment of these services. The corresponding DEXi trees will need to be updated (e.g. considering new input variables, revising variables weight) as new knowledge is produced.

To date, we have tested this modelling chain only for a cereal and grain legume sown simultaneously in France. Future studies will adapt the chain for a wider variety of intercropping scenarios and soil-climate conditions. Further experimental and modelling studies will be necessary to consider other ideomixes, including fodder legumes and/or relay cropping.

4.2 A hybrid modelling chain that combines diverse sources of knowledge

We built an original modelling chain that combines, for the first time, hard models (process-based) and soft models (statistical and knowledge-based) to design a tool that accurately predicts levels of ecosystem services provided by a wide variety of intercropping scenarios. Few studies have combined process-based and statistical models (e.g. Casadebaig et al., 2020). Hybridizing these approaches allowed us to use their strengths to address their weaknesses. Doing so required processing different types of data (quantitative and qualitative) of varying degrees of precision and ranking hundreds of thousands of STICS simulations with multiple input variables into three-level classes of predicted ecosystem services. The overall structure of the modelling chain designed considers potential biomass and decreases it at each step of the chain (Fig. 1, Van Ittersum et al., 2013). This approach overrepresented low levels of ecosystem services in the final DEXi models. Our modelling chain thus provides a conservative and relatively pessimistic assessment of the ecosystem services provided, especially as low-input systems have lower levels of certain services (e.g. yield and cereal protein content) despite promoting other services (e.g. pest control). This hybrid approach also required identifying where to express each effect of a crop management practice along the modelling chain, as some practices influenced potential biomass, attainable biomass and some ecosystem services independently. It sometimes required re-using variables along the modelling chain when their effects could not be allocated clearly to a single step. For example, sowing date was used to predict potential biomass in STICS simulations and was re-used in the DEXi tree to consider pest damage as a strategy to avoid pests. This first-known combination of three diverse modelling approaches is an original addition to the conceptual modelling of intercropping from a cropping-system perspective (Gaudio et al., 2019).

In overall performance and compared to other more traditional crop models (Coucheney et al., 2015), this modelling chain is a promising first attempt to combine three modelling approaches. The uncertainty in the outputs should decrease as the research community improves crop models. For example, input files for new plant cultivars in STICS will allow it to predict the potential biomass of each species more accurately. Similarly, simulating a wider range of intercrops using crop models would enable the STICS sole crop and linear interaction models to be replaced with a single crop model. Research developments in intercropping, especially field trials on more diverse intercrops, would increase the number of ideomixes in the database used to build linear interaction models. Finally, ongoing studies on intercropping, whether in field trials or with farmers, will increase expert knowledge, which was essential throughout our study.

4.3 A transparent and easily understandable modelling chain

The modelling chain is planned to be included in an educational tool such as Forage Rummy (Martin et al., 2011). This tool will be used face to face with farmers or students to design cropping systems, including intercrops. Our modelling strategy was based on this framework (Prost et al., 2012). Accordingly, our goal extended beyond obtaining the most accurate assessment of the eight ecosystem services for all possible intercropping scenarios. Instead, we designed a modelling chain whose logic and rationale are simple to understand by users, even though its structure may appear complicated to modellers. The main processes and variables considered along the chain are meant to be easily available, understandable and explainable to achieve salience, credibility and legitimacy (Cash et al., 2003). Indeed, we relied on a well-established model of biomass development (Van Ittersum et al., 2013), beginning with potential biomass and progressively applying a variety of stresses to reduce it (i.e. interaction effects with linear models, pest damage with the first DEXi model), and based assessment of most of the ecosystem services on the actual biomass estimated with this model. Having an explicit conceptual model is crucial when modelling with stakeholders (Voinov and Bousquet, 2010), as planned with the educational tool under development.

Besides the underlying conceptual model, we selected variables and processes for each model in the chain to obtain easily explainable and transparent decisions:

- We could not simplify STICS input variables, so instead we selected easily explainable processes involved in biomass development.
- We selected variables for the linear interaction models based on their known agronomic effects on intercropped cereal-legume interactions according to the literature (e.g. Bedoussac et al., 2014).
- We built DEXi models with a simple structure that highlighted the main cropping system and crop management practices that affect each ecosystem service.

Once integrated into the educational tool, the modelling chain will enable farmers to explore and think outside the box. Farmers will be able to assess multiple intercropping scenarios and determine their ability to provide expected ecosystem services in their specific context. These outputs could stimulate discussions and knowledge sharing among farmers, as previously reported for this type of tool (Martin et al., 2011; Michalscheck et al., 2020).

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