Evaluation of STICS model performance for long-term simulation of biomass production and nitrogen nutrition of spring barley and timothy cultivated in two important agricultural regions in Quebec (Canada)

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Evaluation of STICS model performance for long-term simulation of biomass production and nitrogen nutrition of spring barley and timothy cultivated in two important agricultural regions in Québec (Canada)

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Résumé

L'orge de printemps (*Hordeum vulgare* L.) et la fléole des prés (*Phleum pratense* L.) sont des cultures de première importance économique pour la province du Québec et d'autres régions au climat continental froid et humide (Amérique du Nord, les pays nordiques…). Les modèles sol-culture sont des outils puissants capables de calculer de nombreuses variables d'intérêt agronomique et environnemental. Ils sont conçus pour simuler les interactions complexes entre les cultures, l'eau et l'azote (N) du sol dans le continuum sol–plante–atmosphère. Entre autres modèles, STICS (Simulateur mulTIdisciplinaire pour les Cultures Standard) est un modèle sol–culture basé sur les processus, qui a été développé initialement pour des conditions agropédoclimatiques des régions tempérées. Cependant, étant un modèle générique, il est possible de l'adapter aux conditions d'autres agrosystèmes.

Les objectifs de cette thèse étaient d'analyser et d'élargir le domaine d'application de STICS aux deux cultures susmentionnées, cultivées dans des conditions agropédoclimatiques de la province du Québec et d'évaluer ses performances prédictives par des simulations à long terme. Cette thèse est une contribution à l'étude de la généricité de STICS pour des agrosystèmes québécois. Outre le contexte climatique, l'originalité de ce travail porte sur les cultures étudiées, orge de printemps et fléole des prés, et le nombre d'années successives de simulations en continu (sans réinitialisation annuelle). Les performances prédictives de STICS ont été analysées pour la production de biomasse aérienne annuelle, sa teneur en N et la quantité de N exporté pour i) une monoculture d'orge de printemps de 31 ans cultivée avec deux modes de travail du sol et fertilisée avec deux sources de N différentes (engrais azoté minéral et fumier liquide de vaches laitières) ; et ii) une prairie de fléole des prés de 8 ans, fertilisée chaque année avec quatre doses d'engrais azoté minéral (0, 60, 120, 180 kg N ha^{-1}). Nous avons utilisé les bases de données de deux dispositifs expérimentaux au champ d'Agriculture et Agroalimentaire Canada.

Pour la monoculture d'orge, la procédure de calibration de STICS a nécessité l'ajustement des paramètres de cultivar en particulier, confirmant ainsi la généricité de la plupart des paramètres des plantes définis dans STICS. Les valeurs simulées sur une période de 31 ans se sont révélées être correctement en accord avec les valeurs observées des variables d'intérêt pour les différents traitements, mais avec une plus grande dispersion pour la nutrition azotée. Les résultats de la simulation des attributs de la production végétale au moment de la récolte étaient plus précis pour les années où les précipitations étaient proches de la normale. Pour la prairie de fléole des prés suivie pendant 8 ans, la correspondance entre les valeurs observées et simulées était satisfaisante pour la première coupe effectuée au printemps. STICS a correctement simulé l'effet positif de la dose

de fertilisation azotée sur la production de biomasse et la nutrition azotée des plantes. Néanmoins, les valeurs des variables étaient surestimées par le modèle en l'absence de fertilisation azotée, impliquant une carence excessive en N au fil du temps. Si l'on excepte cette situation très particulière, non représentative des pratiques agronomiques, les performances de STICS sont donc satisfaisantes dans le contexte des deux essais au champ étudiés. De plus, STICS a bien reproduit la tendance à la baisse de la productivité de la fléole des prés observée en fonction de l'âge de la prairie. Les résultats ont montré que cette baisse de rendement au fil du temps est fortement corrélée à la réduction de la réserve métabolique dans les organes de réserve.

En conclusion, ce travail de thèse a montré l'applicabilité et la fiabilité du modèle STICS pour la simulation sur le long terme de la production de biomasse et de la nutrition azotée d'orge de printemps et de la fléole des prés dans des conditions agropédoclimatiques de la province de Québec.

Mots clés : Modèle sol-culture STICS, expérimentations de longue durée, climat continental froid et humide, production de biomasse, nutrition azotée.

Abstract

Spring barley (*Hordeum vulgare* L.) and timothy (*Phleum pratense* L.) are crops of prime economic importance for the province of Quebec and other regions with cold and humid continental climate (e.g. north America, Nordic countries). Soil-crop models are powerful tools for calculating, a wide range of agronomic and environmental variables They are designed to simulate the complex interactions between crops, water, and soil nitrogen (N) in the soil–plant–atmosphere continuum. Among the existing models, STICS (*Simulateur mulTIdisciplinaire pour les Cultures Standard*) is a process-based soil-crop model initially developed for temperate agropedoclimatic conditions. However, it can be adapted to other agrosystem conditions.

The objectives of this thesis were to analyze and extend the scope of application of STICS to the two aforementioned crops grown under agropedoclimatic conditions in the province of Quebec. Furthermore, this study aims to evaluate the model's predictive performance on long–term simulations. This thesis is a contribution to the study of the genericity of STICS for the Quebec agrosystems. In addition to the climatic context, the originality of this work lies in the crops studied – spring barley and timothy – and the number of successive years of continuous simulations (without annual reinitialization). The predictive performances of STICS were analyzed for aboveground biomass production, N content and N export for i) 31-year spring barley monoculture grown under two tillage systems and fertilized with two N sources (mineral N and liquid dairy manure); and ii) 8-year timothy grassland, fertilized each year with four application N rates (0, 60, 120, 180 kg N ha^{-1}). To achieve our goals, we used databases from two experimental field trials conducted by Agriculture and Agri-Food Canada.

For the barley monoculture, the STICS calibration procedure particularly required the adjustment of cultivar parameters, thus confirming the genericity of most plant parameters defined in STICS. The results show that there is a good agreement between observed and predicted variables of interest with the various tillage systems and N sources during the 31 successive barley cropping years, but with greater dispersion for the N nutrition. Predictions of crop attributes were more accurate in years with rainfall close to the long-term average. For timothy grassland grown over 8 years, the agreement between observed and predicted values was satisfactory for the first harvest. STICS correctly simulated the positive effect of the N application rates on biomass production and plant N nutrition. Nevertheless, the predicted values were overestimated by the model in the absence of N fertilization, implying an excessive N deficiency over time. Except for this very specific situation, which is not representative of agronomic practices, STICS performed satisfactorily in the context of the two field experiments studied. In addition, STICS reproduced well the decreasing trend in timothy productivity

observed with the age of the sward. The results showed that this decrease in yield over time is strongly correlated with the reduction in metabolic reserve in the perennial organs.

In conclusion, this thesis has demonstrated the applicability and reliability of the STICS model for the long-term simulation of biomass production and N nutrition of spring barley and timothy under agropedoclimatic conditions in the province of Quebec.

Keywords: STICS soil-crop model, long-term field experiments, cold and humid continental climate, biomass production, nitrogen nutrition.

Résumé substantiel

L'orge de printemps (*Hordeum vulgare L.*) et la fléole des prés (*Phleum pratense* L.) sont deux cultures très prisées au Québec et plus généralement pour des régions ayant des caractéristiques climatiques similaires (ex. est du Canada ; les pays nordiques) de climat continental froid et humide. Dans ces conditions climatiques, le facteur agronomique le plus à même de limiter la production agricole est le manque d'azote (N). La gestion de N dans les sols agricoles est au centre d'enjeux majeurs, qu'ils soient agronomiques (production agricole, raisonnement de la fertilisation) ou environnementaux (eutrophisation des eaux de surface, lixiviation, volatilisation, dénitrification…). Pour aider les agriculteurs à mettre au point des modes de production qui répondent à ces multiples enjeux, souvent contradictoires, les agronomes/chercheurs ont développé des modèles décrivant le fonctionnement des systèmes sol-culture afin de prévoir et pouvoir raisonner des pratiques agricoles pour la production de biomasse des agrosystèmes et la préservation de l'environnement. La modélisation du fonctionnement de l'agrosystème est une approche performante qui suppose l'analyse, la compréhension et la quantification de mécanismes clés associés à la croissance et le développement de la culture en même temps qu'à la dynamique des processus importants qui se déroule dans le sol dans les conditions du champ. Les modèles sol-culture ont le potentiel à terme d'améliorer notre compréhension de la façon dont les cultures interagissent avec la gestion agronomique dans l'espace et dans le temps. Ils sont des outils puissants pour calculer en particulier la production de biomasse annuelle et la nutrition azotée des systèmes agricoles, car ils sont capables de simuler les interactions complexes entre les cultures, l'eau et l'azote du sol. Dans le contexte des agrosystèmes du Québec et généralement de l'Est du Canada, ils ont été utilisés essentiellement à l'échelle de l'année culturale. Il y a un manque de connaissances sur leur capacité à prévoir en continu pendant de longues périodes de culture, sans réinitialisation annuelle, les différentes variables d'intérêts de la production.

Dans cette thèse, nous avons étudié les performances d'un modèle sol-culture, appelé STICS, essentiellement paramétré aux caractéristiques agropédoclimatiques des régions tempérées d'Europe. Depuis une décennie, il est utilisé par Agriculture et Agroalimentaire Canada pour quelques cultures d'intérêt économique majeur de la province du Québec. Cette thèse est une nouvelle contribution à l'étude de la généricité de STICS pour des conditions agropédoclimatiques rencontrées dans des agrosystèmes québécois. Deux cultures ont été étudiées dans ce travail : l'orge de printemps et la fléole des prés.

- Pour l'orge de printemps, l'objectif était de calibrer STICS pour un cultivar non encore référencé dans STICS, le cultivar Chapais, variété largement cultivée au Québec, et de tester

la capacité de STICS à prédire, en continu, sans réinitialisation annuelle, et sur de longues périodes de culture, les variables d'intérêt suivantes : production de biomasse aérienne, rendement en grain, teneur en N des récoltes et quantité de N exporté.

- Pour la fléole des prés, STICS a déjà été calibré et validé pour simuler la croissance et la valeur nutritive de la fléole des prés sur quelques années culturales avec une réinitialisation annuelle du modèle (Jégo et al., 2013). L'objectif de cette étude était de valider STICS (sans réinitialisation annuelle) pour ces mêmes variables d'intérêt pour une prairie de fléole maintenue pendant plusieurs années dans une autre situation agropédoclimatique du Québec.

Pour ces deux cultures, nous avons testé l'hypothèse que STICS est à même de simuler correctement, dans des conditions de culture de climat continental froid et humide avec des cultivars adaptés à ces conditions, la production de biomasse et la nutrition azotée pour différentes pratiques de fertilisation azotée.

Pour atteindre ces objectifs, deux dispositifs expérimentaux (traitements répétés 4 fois) de longue durée ont été utilisés. Tous les deux appartiennent au réseau d'expérimentation de longue durée d'Agriculture et Agroalimentaire Canada (AAC) sur la fertilisation azotée dans le contexte des agrosystèmes de la province de Québec.

- L'un, toujours en cours, est localisé dans la ferme expérimentale de Normandin dans la région de Saguenay–Lac-Saint-Jean, QC, Canada. Il est situé en zone nordique à la frontière de la forêt mixte et de la forêt boréale. Il a été mis en place en 1990 sur un sol argilo-limoneux de la série Labarre (Gleysol humique) pour étudier les effets de deux facteurs agronomiques (deux types de fertilisation azotée (engrais minéral ou fumier liquide de vache laitière) et deux modes de travail du sol (labour conventionnel à 20 cm ou passage d'un chisel à 15 cm de profondeur) sur la production annuelle d'une monoculture d'orge de printemps. Nous avons utilisé une base de données regroupant la production de biomasse aérienne à la récolte et le rendement en grain, leur teneur en N et quantité de N accumulé/exporté pendant 31 années successives.

- L'autre dispositif expérimental de longue durée était situé sur le site de la ferme expérimentale d'Harlaka, Lévis, QC, Canada. Le sol était de type Limon sablo-graveleux de la série Saint-André (Podzol). Il portait sur l'effet de doses croissantes (0, 60, 120 et 180 kg N ha^{-1} an^{-1}) d'engrais azoté minéral (ammonitrate de calcium) apportées chaque année au début de la saison de croissance pendant huit ans (1999-2006) sur la fléole des prés.

Ces deux dispositifs expérimentaux de longue durée ont été sélectionnés parce que chacun disposait d'une base de données complète avec en particulier des séries chronologiques de la mesure annuelle de la production de biomasse aérienne, de leur teneur en azote et de la quantité d'azote exporté. Elles ont été utilisées pour analyser et évaluer la capacité de STICS à prédire en continu pendant de longues périodes de cultures ces variables d'intérêts. Les performances de STICS ont été évaluées par des critères statistiques habituels utilisés en modélisation pour analyser la qualité de la prévision des valeurs observées par les valeurs simulées : erreur moyenne normalisée (NME) ; erreur quadratique moyenne normalisée (NMRSE) ; efficience du modèle (EF) ; coefficient de détermination de la régression entre les paires de valeurs observées et simulées (R^2).

Le chapitre 1 présente les résultats pour l'orge de printemps. La base de données a été répartie entre des jeux de données de calibration et d'évaluation du modèle. L'ensemble de données de calibration comprenait 28 paires de données simulées/observées (7 années × 4 traitements) de 1997 à 2003. L'évaluation statistique a été effectuée en utilisant les données des années culturales restantes (de 1990 à 1996 et de 2004 à 2020 pour la biomasse et le rendement en grain (24 années × 4 traitements) et de 2004 à 2020 pour la nutrition azotée (17 années × 4 traitements)). STICS a été calibré pour les caractéristiques écophysiologiques du cultivar Chapais d'orge de printemps, non encore référencé dans STICS, et paramétré pour les caractéristiques pédoclimatiques du site expérimental. La calibration a permis d'obtenir une bonne concordance entre les variables observées et prédites de la production de biomasse aérienne, du rendement en grain, de leur teneur en N et des quantités de N exporté au cours des 31 années de monoculture d'orge de printemps. Nous notons cependant une plus grande dispersion pour les variables de la nutrition azotée. Par exemple, STICS a correctement prédit la production de biomasse aérienne, le rendement en grain et la teneur en azote des plantes avec un biais relatif faible (NME compris entre 0 et 13%) et aussi une faible erreur de prédiction (NMRSE compris entre 6 et 25%). Également, STICS a correctement simulé les tendances observées pour les différents traitements, i.e. les deux modes de travail du sol et les deux sources d'azote. Les erreurs du modèle étaient généralement dues à des erreurs de dispersion plutôt qu'à des erreurs systématiques, ce qui indique que le modèle a été correctement paramétré. Les prédictions des variables d'intérêt étaient plus précises les années où les précipitations annuelles étaient proches de la normale.

Le chapitre 2 présente les résultats pour la fléole des prés, récoltée deux fois, une première récolte à la fin du printemps, suivi d'une seconde récolte faite à la fin de l'été (sans avoir ajouté de N après la première récolte). Pour la première récolte, STICS a simulé de manière satisfaisante le rendement et la nutrition azotée pour les trois traitements 60N, 120N et 180N. STICS n'a pas été très efficace pour simuler les attributs de production de la deuxième récolte. De plus, STICS était beaucoup moins performant à prévoir ces variables d'intérêt en l'absence de tout apport de N, impliquant une

déficience en N trop marquée au fil du temps. Le modèle a correctement simulé l'effet positif des taux d'application de l'azote sur la biomasse fourragère récoltée pour les trois traitements avec fertilisation. Les écarts entre les valeurs simulées et les valeurs observées des variables d'intérêt de la première récolte n'étaient pas expliqués par une variable climatique puisqu'il n'y a pas de corrélation significative avec la somme de température, la température annuelle moyenne, ou la pluviosité annuelle pendant le cycle de croissance. Pendant les huit années de suivi, STICS a également simulé correctement l'évolution à la baisse de la production annuelle de biomasse aérienne lors de la première récolte. Nous avons observé une corrélation positive entre la diminution lente et constante de la production de biomasse aérienne et la baisse des réserves dans les organes pérennes.

En conclusion, ce travail d'analyse des performances de STICS au contexte agropédoclimatique de la province du Québec (climat continental froid et humide) confirme une fois de plus la généricité du modèle. Le paramétrage et la calibration de STICS avec les caractéristiques agropédoclimatiques des sites expérimentaux a permis de simuler correctement les variables d'intérêt. L'originalité du travail était aussi d'analyser les performances de STICS sans le réinitialiser chaque année, mais en l'utilisant en continu sur de longues périodes de cultures dans de telles conditions climatiques. Ainsi, le modèle STICS a montré sa fiabilité pour la simulation à long terme, sans réinitialisation annuelle, de la production de biomasse et de rendement en grain pour l'orge et du rendement en fourrage pour la fléole des prés ainsi que de leur nutrition azotée. L'exploitation de deux bases de données associées aux deux dispositifs expérimentaux de longue durée d'AAC, n'a pas permis de mettre en évidence de difficultés théoriques et méthodologiques. Bien que les résultats de cette étude soient déjà satisfaisants, il est encore possible d'améliorer considérablement le modèle pour obtenir des erreurs de prédictions plus faibles.

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List of Abbreviations

AAC	*Agriculture et Agroalimentaire Canada*
AAFC	Agriculture and Agri-Food Canada
AGB	Aboveground biomass
CP	Chisel plow
CPTAQ	*Commission de protection du territoire agricole du Québec*
DM	Dry matter
EF	Model efficiency
GDD	Growing degree-day
GHG	Greenhouse gas emissions
GR	Global radiation
GY	Grain yield
HI	Harvest index
INRAE	*Institut National de Recherche pour l'Agriculture l'Alimentation et l'Environnement*
LAI	Leaf area index
LDM	Liquid dairy manure applications
MAPAQ	*Ministère de l'Agriculture, des Pêcheries et de l'Alimentation du Québec*
MIN	Ammonitrate applications
MP	Mouldboard plow
NAG	Nitrogen amount in grain
NCG	Nitrogen concentration in grain
NMAE	Normalized mean absolute error
NME	Normalized mean error
NNI	Nitrogen nutrition index
NRMSE	Normalized root mean square error
NU	Nitrogen uptake by shoot
OM	Organic matter
PAR	Photosynthetically active radiation
PLA	Percentage lack of accuracy
PLP	Percentage lack of precision
R^2	Coefficient of determination
RUE	Radiation use efficiency.
SOC	Soil organic carbon
STICS	Simulateur multidisciplinaire pour les Cultures Standard
STN	soil total nitrogen
USM	Simulation unit

To my wife, Manda, and my son, Aiko,

Your unwavering love, patience, and support have been my constant motivation. Every word, every discovery, and every late-night study session are dedicated to both of you. This achievement belongs to our family.

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I sincerely thank my research supervisor from Laval University, Antoine Karam, for his guidance and for sharing his extensive expertise and scientific rigor with me. Each of our meetings reassured me and fueled my motivation to continue.

I also extend my gratitude to my research supervisor from the University of Bordeaux, Christian Morel, for his availability, encouragement, and unwavering commitment. I genuinely appreciate the time and effort he dedicated to reviewing and enhancing this manuscript, undoubtedly elevating its quality and significance.

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Preface

This thesis was conducted within the framework of a cotutelle partnership between Laval University and the University of Bordeaux, with financial support from the Quebec Research and Development Centre, Agriculture and Agri-Food Canada. Additionally, this thesis received financial support from the Excellence Eiffel scholarship program of the French government, as well as the success and completion scholarships from the Faculty of Graduate and Postdoctoral Studies (Laval University).

This thesis consists of four main parts, including a general introduction, two results chapters written in English in the form of scientific articles, and a general discussion and conclusion.

Chapter 1 is a published article included in this thesis, to which I am the first author. It is titled “STICS soil–crop model performance for predicting biomass and nitrogen status of spring barley cropped for 31 years in a gleysolic soil from northeastern Quebec (Canada)” and was published in September 2023 in the journal ‘Agronomy’. The co-authors are Guillaume Jégo, Noura Ziadi, Alain Mollier, Jean Lafond, Antoine Karam, and Christian Morel. For this Chapter 1, the numbering of sections, tables, and figures, as well as the formatting of bibliographic references, have been modified compared to the published version to harmonize with the presentation of this thesis.

Chapter 2, on the other hand, focuses on the “Continuous simulation of biomass production and nitrogen nutrition of an ageing (8 years) timothy sward under various nitrogen application rates in eastern Quebec (Canada)”. This chapter will be published as an article in a peer-reviewed scientific journal.

The databases used in this study were provided by Agriculture and Agri-Food Canada.

My work was supervised by my research advisors, Antoine Karam and Christian Morel, and co-supervised by Noura Ziadi. I also benefited from the guidance of Alain Mollier and Guillaume Jégo.

GENERAL INTRODUCTION

A. General context of Quebec agrosystems

A.1. Agropedoclimatic context of Quebec

A.1.1. Quebec agricultural zone

The agricultural zones of Quebec cover about 4% of the provincial territory, with a surface area of approximately 63,000 km^2 (CPTAQ, 2014). The farmlands are located in southern region of Quebec (between the 45th and 49th parallels north, and the 66th and 80th meridians west) where the biophysical conditions are more conducive to agricultural activities. The agricultural zones extend along the St. Lawrence River from the eastern lowlands through central Quebec to the U.S. border, including Montérégie and the Cantons-de-l'Est, but also alongside major lakes and rivers such as Lake Saint-Jean, the Saguenay River, and the Gatineau River (Figure A.1). Overall, Quebec has a relatively smooth relief, with less than 10% of the province's elevations reaching more than 600 meters. Agricultural areas are mainly located in low-altitude areas or valleys.

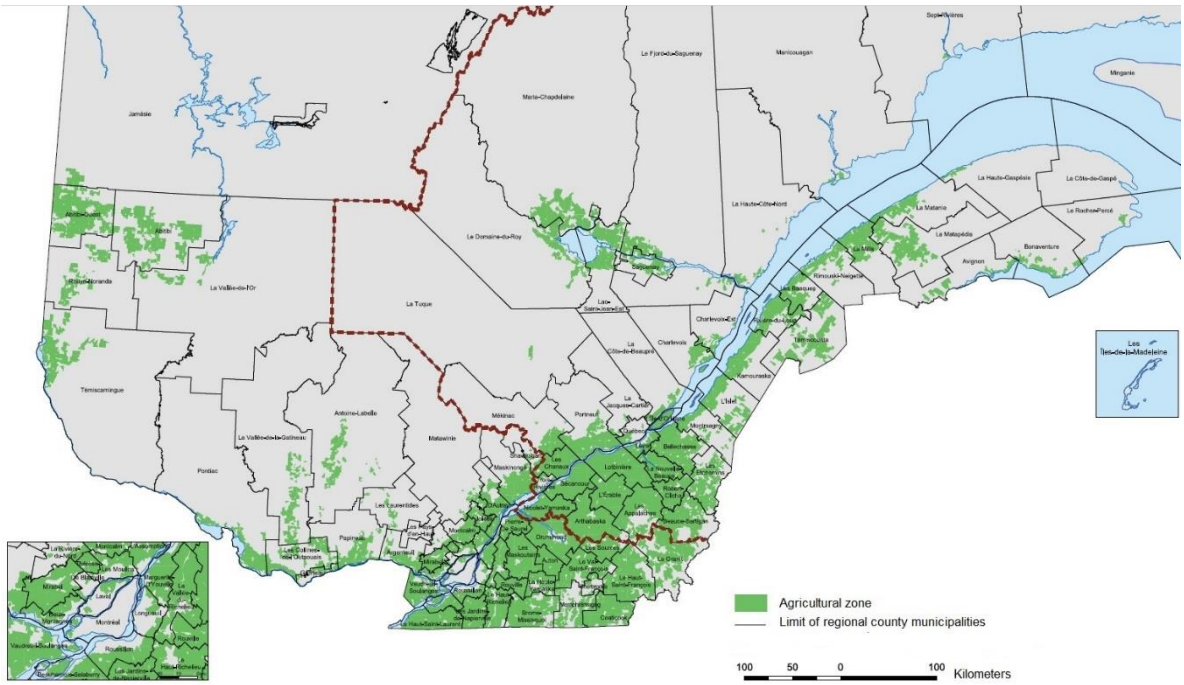

Figure A.1 A general plan of the administrative regions with the agricultural zone of Quebec (CPTAQ, 2014).

The agricultural territories of Quebec can be categorized into 3 zones according to their biogeography:

The first includes the agricultural regions of Saguenay-Lac-Saint-Jean, Côte-Nord and Abitibi-Témiscamingue. They are located in the northernmost agricultural regions of Quebec and are characterized by a forage-based agriculture, dairy production, and beef cattle exploitation. Agricultural activities in these regions are qualified as "Nordic" (Pierre, 2015). It is worth noting that the Saguenay-Lac-Saint-Jean region stands out from the other northern agricultural regions of Quebec for its highly diversified range of agricultural products (Pierre, 2015). From an edaphological point of view, the agricultural zones extend over Humo-Ferric Podzols soils developed from glacial and fluvio-glacial materials are associated with Dystric Brunisols.

The second agricultural region covers the southern Laurentides, the Central St. Lawrence Lowlands and part of the Appalachians in southwestern Quebec. In this region, Dystric Brunisols in association with Humo-Ferric Podzols take on increasing importance.

The third region covers the western St. Lawrence Lowlands, which has the best agricultural potential in Quebec. The climate is much more favorable, despite the presence of a rising seasonal water deficit. Moreover, the frost-free period in the region is up to 180 days per year. The region's soil structure consists of melanic Brunisols, humic Gleysols, on marine limestone and partly well-decomposed organic soils.

A.1.2. Climatic characteristics of Quebec's agricultural regions

Quebec is located in the cold temperate maritime boreal zone. According to the Köppen classification, the region has a cold and humid continental climate (Beck et al., 2018). This climate is characterized by long and cold winters, due to the influence of the cold Labrador Current from the Arctic, which is deflected to the west by the Coriolis force. However, a climatic gradient can be observed between the northern and southern regions of Quebec. The northern regions of Abitibi (e.g. Mont Brun station/48° 25' 6"; 78° 44' 15"/303 m) and Saguenay-Lac-Saint-Jean (e.g. Saint-Ambroise station/48° 34' 7"; 71° 20' 21"/127 m) have an average temperature below zero from the beginning of October until the beginning of April. The annual sum of growing degree-days is between 1100 and 1377 °C d (basis 5.6°C) and the frost-free period varies between 80 and 125 days per year, which limits the range of crops (Figure A.2). Moreover, the average minimum temperature in these regions goes below -15 °C in January and February (Figure A.3).

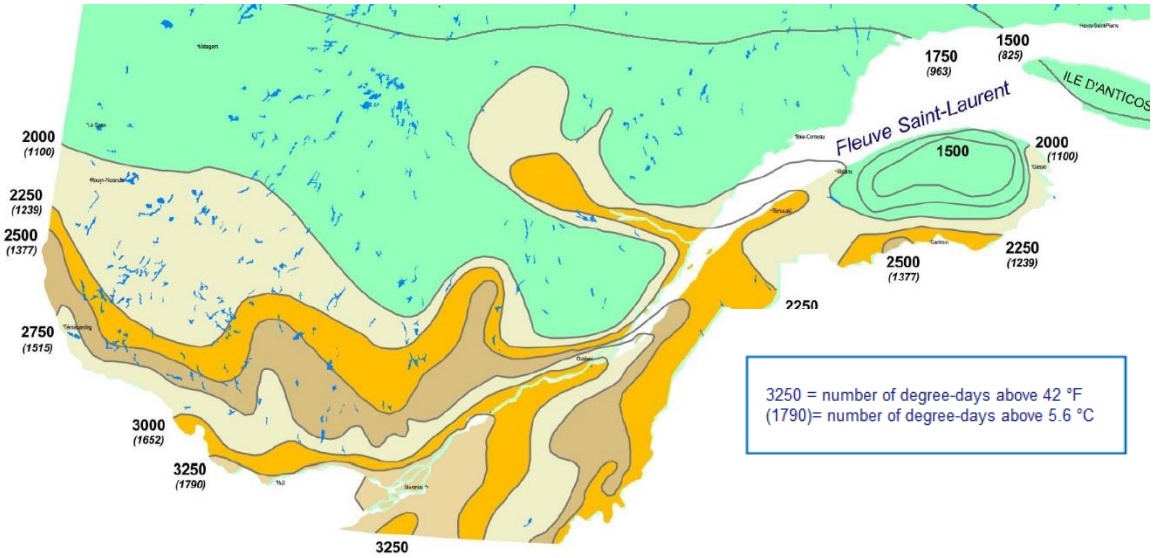

Figure A.2 Climate map of Quebec: growing degree-days (Yves Lemay, IRDA, 2008).

By moving southwards, the length of the winter period with negative temperatures decreases. In the central lowlands of the St. Lawrence (e.g. Louiseville station/46° 16' 25''; 73° 0' 34''/46m), mean negative temperatures are observed between early November to mid-March. They practically correspond to climatic zones with 1377 to 1790 °C d (Figure A.2). In the extreme south of Quebec, mean negative temperatures are observed from mid-November to early March (e.g. Hemmingford-Four-Winds station/45° 4' 21''; 73° 39' 29''/70m). The annual sum of growing degree-days is 1790 °C d or more (Figure A.2).

In Quebec, summer is hot, and the intermediate seasons are short. The hottest month is July, with an average temperature ranging from 17 to 21°C between the northern and southern regions (Figure A.3). In some years, temperatures can reach 35°C in the region near the southern border with Ontario, giving a considerable annual temperature amplitude.

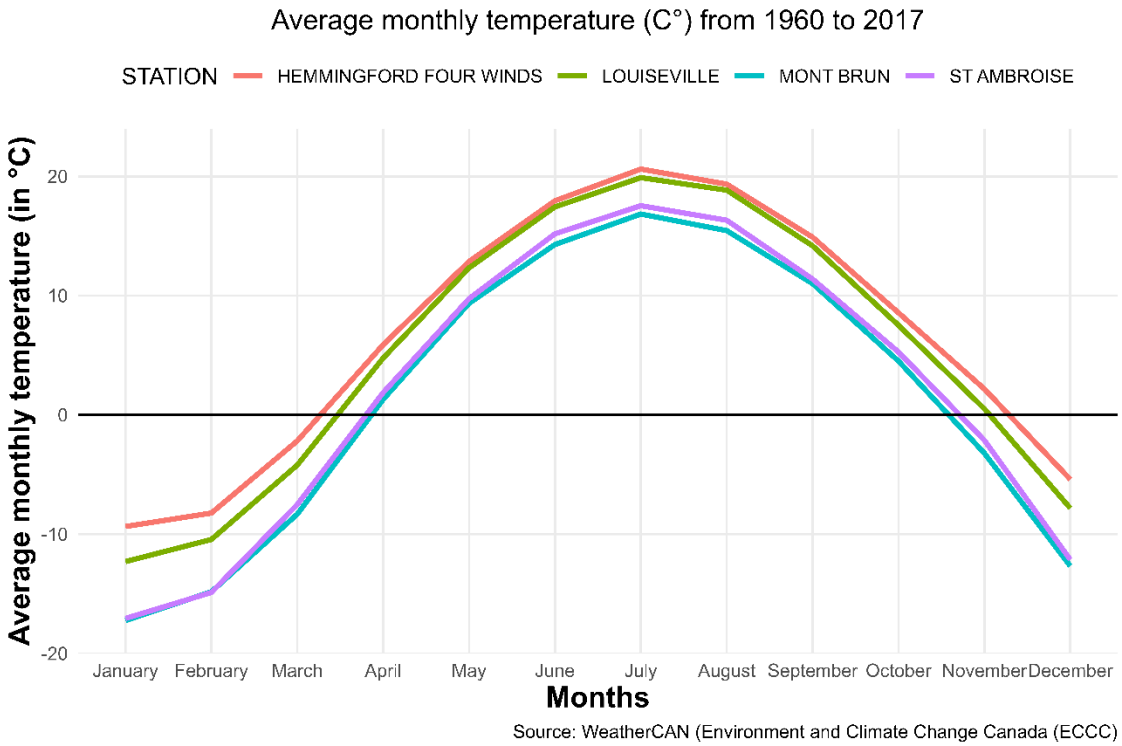

Figure A.3 Average monthly temperature (°C) from 1960 to 2017 at 4 weather stations in Quebec.

Due to its humid climate, precipitations (rain and snow) are relatively abundant in Quebec. Between 1960 (1980 for the Mont Brun station) and 2017, the average annual precipitation was 860 mm at the Louiseville station; 855 mm at the Hemmingford-Four-Winds station; 1005 mm at the Sainte-Ambroise station and 989 mm at the Mont Brun station (Figure A.4). The average amount of rainfall is highest in July, August, and September (Figure A.4). In winter, most precipitations are in the form of snow (Figure A.4, A.5). The abundance of snow in winter is the distinctive trait of this climate. Snow usually covers the ground for 4 to 6 months, depending on the region. The growing season in the province of Quebec is short, ranging from 150 to 180 days between April and October. In the main agricultural regions, the average number of frost-free days, i.e. the period between the last spring frost and the first autumn frost, is about 150 days per year. In terms of photoperiod and photosynthetic radiation received by agricultural regions, there are no major differences with those of western and central Europe, given that southern Quebec is located at the same latitude. The climatic gradient that exists between the north and south of Quebec's agricultural zone explains why the southern regions, which are less cold yet sometimes suffer from water deficits, are the most cultivated and diversified region,

whereas in the northern agricultural regions, where the climate is the harshest, only crops with resistance to extreme conditions are present.

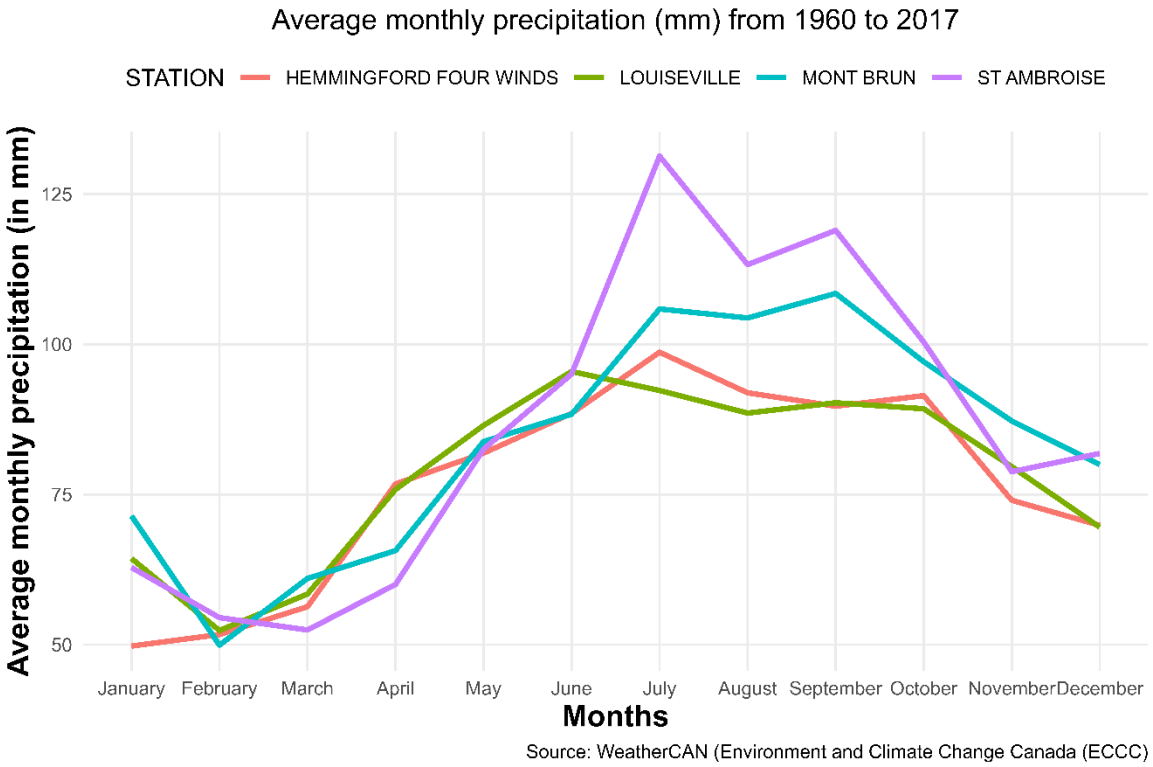

Figure A.4 Average monthly precipitation (rain/snow fall) (mm) from 1960 to 2017 at 4 weather stations in Quebec.

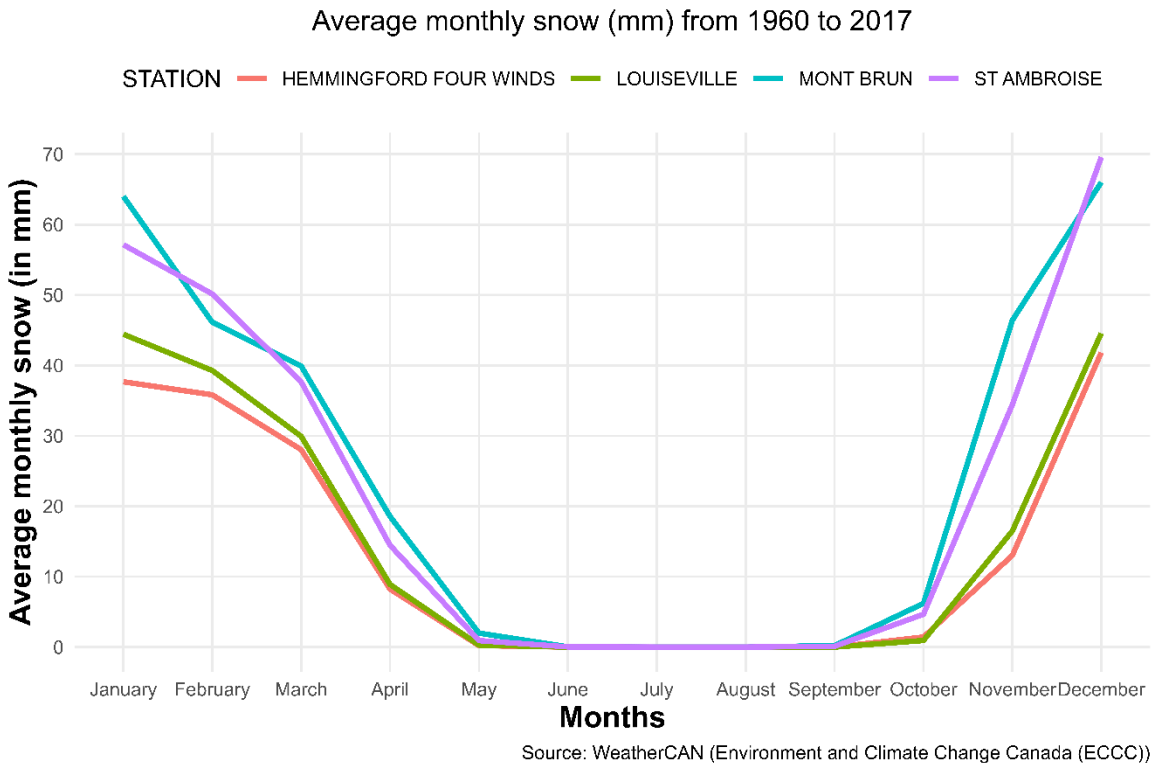

Figure A.5 Average monthly snow fall (mm) from 1960 to 2017 at 4 weather stations in Quebec.

A.1.3. The main agricultural production in Quebec

Dairy and pork production are the most important agricultural activities in Quebec. Crops for animal feed occupy most of the cultivated land. In 2016, field crops and hay/fodder accounted for around 60% and 35% of the cultivated land, respectively, with the remainder land allocated to vegetable and fruit production (Statistics Canada, 2017). Grain corn, soybeans, wheat, oats and barley were the main field crops in terms of acreage (Ministère de l'Agriculture, des Pêcheries et de l'Alimentation, 2020). Timothy is the most widely cultivated grass in Quebec for its adaptability to Quebec's climatic and soil conditions, as well as for its high forage quality, hardiness and appetence (Grant & Burgess, 1979; MAPAQ, 2022). The choice of agricultural species and cultivars, and their spatial distribution are largely influenced by the climatic conditions of the region. The accumulation of growing degree-days in certain agricultural regions is limited, as in the case of more northerly agricultural regions (Saguenay-Lac-Saint-Jean, de la Côte-Nord et de l'Abitibi-Témiscamingue), making it impossible to consider corn and soybean production in the current climatic context (Bélanger & Bootsma, 2002).

Plant hardiness zones are often used as a reference to classify the plants that can overwinter (for perennials) or to describe the ability of plants to tolerate a cool climate (for annuals). Hardiness zones are a division of the territory into different plant growth zones, using various criteria such as minimum winter temperature, maximum summer temperature, frost period, precipitation, wind, altitude.

A.1.4. Quebec soils and the effects of climate on their functioning

Climatic characteristics also influence the conditions and functioning of Quebec soils. In addition to the effects of urban and industrial activities resulting in more acid precipitation, which contribute to the acidification of agricultural soils, under cold and humid climates, soils tend to naturally acidify. Natural acidification results from the process of podzolization and the leaching of soil elements by percolating water, which depends on climatic conditions and the nature of the parent rock. However, it is compounded by the effect of acid precipitation containing sulfuric acid and nitric acid from the volatilization of synthetic ammonia fertilizer. Most soils in Quebec, apart from a few regions, tend to be acidic. The pH level of mineral soil in Quebec varies between 5.6 and 6.4 (based on 110664 observations) (Beaudet et al., 2004). This soil acidification is probably having an impact on crops and soil processes. It affects the potential production, availability of nutrients, biological and enzymatic activities, and decomposition of soil organic matter (Yadav et al., 2020). In addition, most acid soils in Quebec have a high phosphorus (P) fixation capacity due to their high concentration of iron and aluminium oxides and hydroxides (Verma et al., 2005).

The contrasting seasonal temperatures also affect the physical, chemical, and biological processes in the soil. Soil status and processes are affected by fluctuating conditions at the start, during and at the end of the winter period. The risk of soil erosion is increased by the freeze-thaw cycle, which reduces aggregate stability and degrades soil structure (Dagesse, 2013). More specifically, freeze-thaw cycles modify water flow by affecting soil infiltration capacity. Depending on texture and initial water content, freeze-thaw can maintain or reduce infiltration rates, due to the increased viscosity of water around the freezing point, or the formation of ice in soil pores (Fouli et al., 2013). In early autumn and during the snowmelt at the end of winter, the frozen ground slows down the infiltration of soil water and can lead to significant runoff. Greenhouse gas emissions are also influenced by the freeze-thaw cycle, since it stimulate soil N mineralization, which increases NO_3^- availability and induces N_2O emissions, especially in soils without crop residues, where there is no net N immobilization (Pelster et al., 2013). This increase in denitrification is accentuated by the diffusion of organic substrates newly available to denitrifying microorganisms from the disturbance of soil aggregates (Bochove et al., 2000). According to Virkajärvi et al. (2010), N_2O emissions during the winter period in northern regions can be very significant, representing 25% to 78% of the total annual.

In addition, soil organic carbon (C) losses can be significant in cold regions, where decomposition is much more sensitive to small temperature variations (Kirschbaum, 1995). This demonstrates the extent of biological and chemical processes that can take place in the soil during winter under snow cover. The microbial community in northern agricultural soils has probably adapted and acclimatized to the harsh and long-lasting winter conditions through changes in metabolic pathways that enable them to function more efficiently at cold temperatures (Gamache, 2014; Nedwell, 1999). Thus, nitrification and mineralization can occur at potentially significant rates in frozen agricultural soils down to a temperature of -2 °C in loamy soils and -6 °C in clayey soils (Clark et al., 2009). The depth of snow cover during the winter plays an important role, as it acts as a thermal insulator for the soil and the crops underneath, protecting them from frost. If the snow depth is sufficient, the ground surface temperature can be maintained at around 0°C, and the depth of frozen ground can be reduced. In addition to the loss through denitrification, N in humid temperate soils is also subject to high leaching losses due to high soil moisture levels caused by high annual precipitation and snowmelt (Janzen et al., 2003).

A.1.5. Agro-environmental issues in Quebec

Agricultural activities in Quebec have a significant impact on the environment due to the use of organic and inorganic fertilizers, and pesticides, as well as the effects of farming practices and greenhouse gas (GHG) emissions.

In 2008, Quebec's agricultural sector released 7.7% of GHG emissions of Quebec into the atmosphere (MDDEP, 2010). The GHG emissions of the agricultural sector rose by 9.1% in 2008 compared to 1990, mainly due to higher emissions from manure management, as well as agricultural soil management (MDDEP, 2010). Although agriculture contributes only to a relatively small proportion of Quebec's GHG emissions, there are other relevant reasons for taking actions, such as resource conservation, soil fertility maintenance and crop yield stability reason.

Moreover, the evolution of agricultural soil management in Quebec has led to a decline in soil organic C stocks. In contrast to the Canadian Great Plains, soil C levels in eastern Canada, and particularly in Quebec, are now generally declining, compared with much higher levels in the past (Figure A.6). On average, there is a downward trend of over 90 kg ha^{-1} yr^{-1} (AAFC, 2016). This can lead to an increase in CO_2 emissions and a reduction in the fertility of agricultural soils and their resilience to drought. Among other factors, changes in land use in certain parts of eastern Canadian provinces have significantly contributed to this decrease in soil organic C content. In fact, the province of Quebec has experienced major shifts in cropping patterns, with perennial forages and pastures being

converted to annual crops. The area under field crops almost doubled between 1971 and 2016 in the province of Quebec (Debailleul & Mundler, 2018).

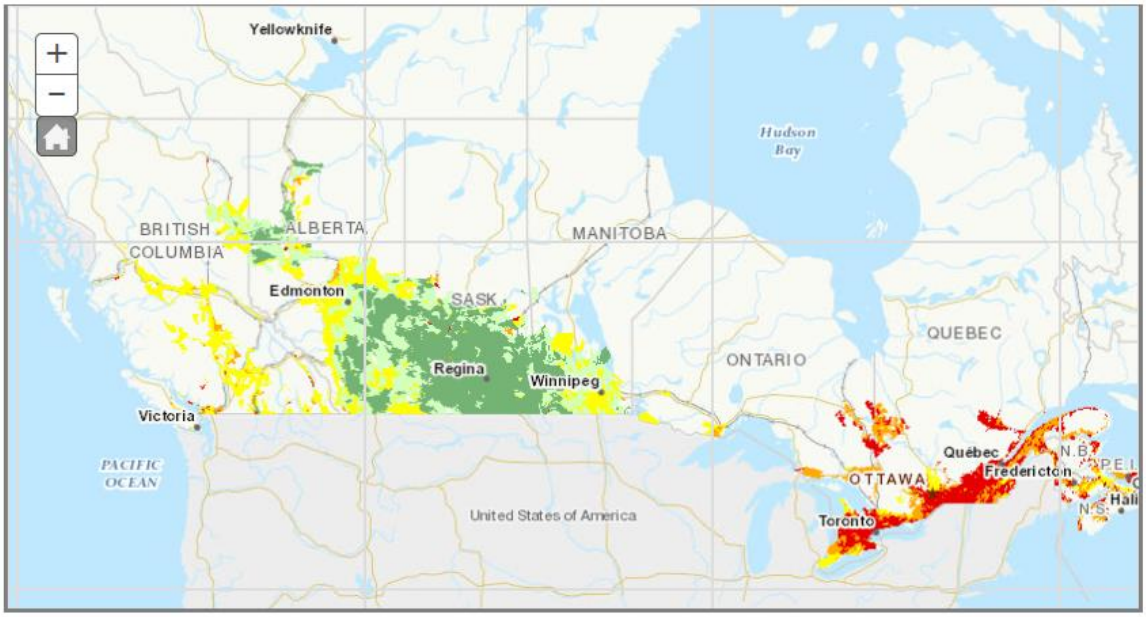

Figure A.6 Change in soil organic carbon (in kilograms per hectare, per year) in Canada in 2011 (AAFC, 2016).

An increasing trend in residual N in Canadian soils has also been observed, particularly in the eastern provinces (e.g. Ontario, Quebec, New Brunswick), as a result of increased inputs of N fertilizers and manure on farmland, combined with greater N fixation by leguminous crops, which have gained in importance (AAFC, 2016). This accumulation of N in soils increases the risk of contamination of surface and ground water.

A.2. Context and challenges of agrosystem modelling

A.2.1. Modeling and model typology

Modeling is characterized as the design and use of models referring to the representation of a complex real-world phenomenon or system. In this way, modeling helps to understand and explain how reality operates, through the observations and analysis of real data (Barreteau et al., 2003); and therefore allows us to control the course of events and predict their occurrence. The practice of modeling existed long before the 20th century in science and technology, but it was around 1920-1940 that modeling took off on a massive scale in several fields, with the switch to essentially mathematical models (Varenne, 2016). Through mathematical modelling, it is also possible to put into the equation the operating processes of our environment.

Historically, modeling of element transfer through the soil-crop system was first developed by soil physicists for P and potassium (K) (Pellerin et al., 2014). As for crop models, which integrate the effects of climate and the biogeochemical cycle of elements on system evolution, they have considerably advanced since the first experiment by De Wit (1965) with the modeling of the effect of environmental factors on photosynthesis intensity. Since then, numerous models have been developed to describe crop ecophysiology, agronomic issues and agro-environmental diagnostics (Pellerin et al., 2014).

For soil-crop models in particular, they can be grouped into two categories: those most often used in science to improve our understanding of plant physiology and environmental interactions in the soil-plant-atmosphere system, and those used in decision-making to provide recommendations or forecasts to farmers and decision-makers (Passioura, 1996). According to other typologies, such as the nature of the mathematical relationships, there are:

- Empirical models, which describe the system through simple statistical relationships between variables without ecophysiological or physical significance;
- Mechanistic models, which describe the system with as much detail as possible, with consideration of the system's mechanisms and processes based on hypotheses about the ecophysiological or physical functioning of the system; and
- Semi-mechanistic models, which combine the two approaches.

Existing soil-crop models can also be classified as “specific models” integrating processes specific to a given crop species or as “generic models” integrating processes that are common to several crops (Guillaume, 2011). From an operational point of view, the main differences between these models

concern the object to be simulated, the spatial scale covered (plot, inter-plot, farm, watershed), the temporal scale covered, the calculation time step (daily, monthly, annual) and the actual use of the model, i.e. the model's main purpose (Jeuffroy et al., 2008). In addition, models differ in terms of the number of input data required to run them, the detail of the mathematical representation of processes, and the accuracy of the results (Addiscott & Wagenet, 1985).

A.2.2. The importance of soil-crop system modelling

Many methods are available for understanding and managing soil fertility and the sustainability of agroecosystems, including the modeling approach, which seems to be an essential and relevant tool for researchers, decision-makers, and agricultural experts. Models are a powerful tool for assessing agricultural production and the environmental impact of farming, by taking into account cultivation practices, soils and climate (Therond et al., 2011). Indeed, the interactions in agroecosystems are very complex to capture over an entire crop cycle, and especially over a longer time scale such as crop rotation, which makes the use of models particularly interesting. Approaches based on experimentation may have their limits, since they do not allow us to provide prompt, appropriate responses to the diversity of agricultural situations (Meynard, 1998). Combined, simulation approaches and long-term field or laboratory experiments are complementary tools for defining sustainable agricultural practices. The data obtained from field trials are valuable and are used upstream of the modeling process for the initialization of models, but also for model calibration, evaluation, and validation. The balance calculation method commonly used by farmers has its limitations regarding the estimation of certain parameters in the calculation. The estimation of the various items in the balance equation (mineralization, organization and the various N transfers in the soil compartment) is very tedious and would require detailed measurements and recommendations based on solid agronomic expertise (Comifer, 2013; Tremblay et al., 2001). As for modeling, this approach offers a panoply of possible agro-environmental uses to answer questions raised by research, crop management and policy. Models are essential for: making evaluation and projection of practices and performance, building strategic management or planning and tactical management or monitoring, and supporting the transfer of knowledge in educational or training courses for farmers or agricultural advisers (Jeuffroy et al., 2008).

In operational terms, depending on the model, they can simulate several variables at the same time, such as agronomic variables (e.g. yield, crop nutrient content) and environmental variables (N and C flux, water balance) (Jeuffroy et al., 2008). Particularly, soil-crop models can help to make management decisions on a wide range of topics, such as soil evapotranspiration and water content (Saadi et al., 2022), fertilization (Basso et al., 2012), irrigation (Constantin et al., 2015), pesticide

application (Lammoglia et al., 2017), soil erosion (Stolpe, 2005), the effects of climate change (Delandmeter et al., 2023; Thivierge et al., 2023) and agricultural productivity at different scales (Kheir et al., 2023; Palosuo et al., 2011; Rötter et al., 2012). Furthermore, modeling represents a cost-effective and time saving alternative which overcomes the difficulty of obtaining data in the field. Some process parameters in the soil-crop system are expensive or laborious to quantify in the field or laboratory (Addiscott & Wagenet, 1985). Hence, modeling provides the opportunity to carry out a multi-criterion evaluation, giving access to the quantification of unmeasured variables. Finally, modeling enables virtual experiments to be performed on various scenarios to propose agronomic solutions or design innovative agricultural practices (Jeuffroy et al., 2008).

Despite its many advantages, modeling also comes with several limitations. Since it involves a simplification based on assumptions about the functioning of the reality, and at some point, an oversimplification risks making the model ineffective. The reliability of the result depends on both the validity of the model (robustness of the equations) and the accuracy with which it is possible to evaluate the variables of interest. According to Passioura (1996), the sources of error in a model are related to the parameters and the complexity of the model. The cumulative errors increase with the number of parameters and the complexity of the model, while the biases decrease with the complexity of the model structures. In some ways, parameter calibration can also be a limitation of modeling, as this step can be very time-consuming.

A.2.3. Existing models of agroecosystem functioning

Different models exist for simulating soil-crop functioning in agroecosystems (Table A.1). The choice of model application often depends on the complexity of its structure and the specific purpose of the model. Models based on an ecophysiological approach, such as SUCROS (Laar et al., 1997) and SWHEAT (Keulen & Seligman, 1987) models have been developed for crop growth and development. Other models was predominantly designed for environmental applications like the DNDC model (Li et al., 1992), which is a model of N and C biogeochemistry primarily developed to predict GHG emissions and to quantify the C sequestration potential of ecosystems, including agrosystems. Moreover, there are the CENTURY (Parton et al., 1989), ROTHC (Jenkinson & Coleman, 2008), and AMG (Saffih-Hdadi & Mary, 2008) models, which are used to predict variations in soil C stocks over several years or even centuries. These models have more complex formalisms (multi-compartmental soil organic C), except AMG, which is a simple model well suited to developing decision support systems (Bouthier et al., 2014; Senapati et al., 2014). These models use monthly or annual data as inputs and have been adapted and validated for different types of ecosystems. A version of CENTURY called DayCent (Parton et al., 1998) has been designed for daily time step predictions.

They are applicable to a wide range of spatial scales, from plot to global. Although these models are primarily designed to model SOC dynamics, they do simulate N dynamics, and even P and sulfuric (S) dynamics for the CENTURY model. These models also consider crop growth and phenology, water balance and soil element movement.

Other models are based on the coupling of a crop model and a decision model, providing a framework for evaluating and proposing irrigation and fertilization practices. For example, MODERATO (Bergez et al., 2001) is a management model initially designed to develop irrigation strategies for irrigated corn crops. The AZOFERT model (Dubrulle et al., 2004) is designed for calculating fertilization on a plot scale and over a crop cycle. This is a dynamic version of the AZOBIL model (Machet et al., 1990), a classic model based on the static mineral N balance aimed at adjusting the provisional dose of N to be applied to the crop to optimize the use of inputs and reduce pollution from agricultural sources. It is based on the complete mineral N balance, including the temporal dynamics of N supplies from the soil and various organic sources. AZODYN models (Jeuffroy & Recous, 1999) are crop models that are available for specific crops (AZODYN-wheat, AZODYN-rapeseed, AZODYN-pea, AZODYN-intercrop) and are used as a reasoning tool for cropping techniques or production forecasting. Currently, generic and agro-environmental models such as DAISY (Hansen et al., 2012), DSSAT-CSM (Hoogenboom et al., 2003), APSIM (Holzworth et al., 2014), CERES-EGC (Drouet et al., 2011), EPIC (Wang et al., 2012), MONICA (Nendel et al., 2011), HERMES (Kersebaum & Nendel, 2014), WOFOST (de Wit et al., 2019), SWIM (Krysanova et al., 2000) , FASSET (Olesen et al., 2002) and STICS (Beaudoin et al., 2022; Brisson et al., 1998) are widely used. They can simulate the combined effects of a wide range of climatic conditions, soil properties, plant characteristics and farming practices on the functioning of the agroecosystem (water-soil-plant-atmosphere system).

Table A.1 Example of existing sol-crop models for simulating agroecosystems.

Models	Main use of the model	Key references
SUCROS (https://www.quantitative-plant.org/model/SUCROS), Netherlands.	Potential growth and water-limited growth of a crop	(Laar et al., 1997; Laar et al., 1992)
SWHEAT	Tool for identifying factors limiting wheat production	(Keulen & Seligman, 1987)
MODERATO (https://www.ndt.net/article/wcndt00/papers/idn322/idn322.htm), France.	Decision tool for corn irrigation	(Bergez et al., 2001)
AZODYN (https://www6.inrae.fr/basc/Recherche/Modeles/AZODYN), France.	Fertilization management tool	(Jeuffroy & Recous, 1999)
AZOFERT (https://www6.hautsdefrance.inrae.fr/agroimpact/Nos-dispositifs-outils/Modeles-et-outils-d-aide-a-la-decision/Azofert) , France.	Decision support tool for mineral N fertilizer recommendations	(Dubrulle et al., 2004)
DNDC (https://www.dndc.sr.unh.edu/), U.S.A.	Quantifying C sequestration and predicting N and CO_2 emissions	(Li et al., 1992)
DayCent (https://www.nrel.colostate.edu/projects/century/index.php), U.S.A.	Simulation of soil gas fluxes (N, CH_4 and CO_2) for terrestrial ecosystems	(Parton et al., 1998)
STICS (https://www6.paca.inrae.fr/stics/Qui-sommes-nous/Presentation-du-modele-Stics), France.	Simulation of soil-crop functioning with agro-environmental output variables	(Brisson et al., 1998)
DAISY (https://daisy.ku.dk/about-daisy/), Denmark.	Soil-plant-atmosphere system model based on agroecosystems	(Hansen et al., 2012)
CENTURY (https://www.nrel.colostate.edu/projects/century-model-information), U.S.A.	Analysis of the effects of changes in management and climate on ecosystems	(Parton et al., 1989)
ROTHC (https://www.rothamsted.ac.uk/rothamsted-carbon-model-rothc), U.K.	Simulation of SOC changes in long-term experiments	(Jenkinson & Coleman, 2008)

AMG (https://www6.hautsdefrance.inrae.fr/agroimpact/Nos-dispositifs-outils/Modeles-et-outils-d-aide-a-la-decision/AMG-et-SIMEOS-AMG/), France.	Simulation of soil C dynamics	(Saffih-Hdadi & Mary, 2008)
DSSAT-CSM (https://dssat.net/about/), U.S.A.	Crop growth and development simulation based on soil and climate conditions	(Hoogenboom et al., 2003)
APSIM (https://www.apsim.info/), Australia.	Simulation of soil-crop functioning with agro-environmental output variables	(Holzworth et al., 2014)
CERES-EGC (https://www6.versailles-grignon.inrae.fr/ecosys/Productions/Logiciels-Modeles/CERES-EGC), France.	Simulation of environmental outputs such as nitrate leaching or N oxide emissions	(Drouet et al., 2011)
EPIC (https://epicapex.tamu.edu/epic/), USA.	Estimation of soil productivity under the effect of erosion, evaluation and management of fertilization and irrigation.	(Wang et al., 2012)
MONICA (http://monica.agrosystem-models.com/), Germany.	Simulation of biochemical transformation of C and N in soil and their transport in soil, air and plants	(Nendel et al., 2011)
HERMES (http://www.zalf.de/en/forschung_lehre/software_downloads/Pages/default.aspx), Germany.	Nitrogen fertilization recommendations and N pollution calculations at plot or regional level	(Kersebaum & Nendel, 2014)
WOFOST (http://www.wofost.wur.nl), Netherlands.	Forecasting crop yields, estimating production potential	(de Wit et al., 2019)
FASSET (https://www.fasset.dk/), Denmark.	Simulation of N transformation and crop production as a function of water and N availability	(Olesen et al., 2002)

A.3. STICS soil-crop model

A.3.1. General presentation of STICS

STICS is a generic soil-crop model developed at INRAE, the French National Research Institute for Agriculture, Food and the Environment, since 1996 (Brisson et al., 1998, 2003). STICS is designed to simulate the soil-crop system at the plot scale, and can simulate agronomic (e.g. yield, plant N, grain/fruit N, soil organic C and N, soil mineral N) and environmental (e.g. drainage, CO2 emissions, N leaching, denitrification, volatilization) outputs over one or several successive crop cycles. It is composed of several modules built by assembling and synthesizing parts or formalisms of existing models (Brisson et al., 1998).

Over the years, STICS has gradually evolved and been enriched by the participation and investment of numerous researchers in its development (Figure A.7). Indeed, the evolution and maintenance of the STICS model are ensured by the model's user group, which constantly capitalizes on the knowledge and experience gained from its use, evaluates the standard model, and provides feedback and proposals on the model's development needs. The STICS project team (https://www6.paca.inrae.fr/stics/Qui-sommes-nous/Equipe-Projet-Stics) is responsible for the governance of the model: from scientific validation of the choice of formalisms and parameterization of the standard version of the model, to the organization of seminars and training courses on its application.

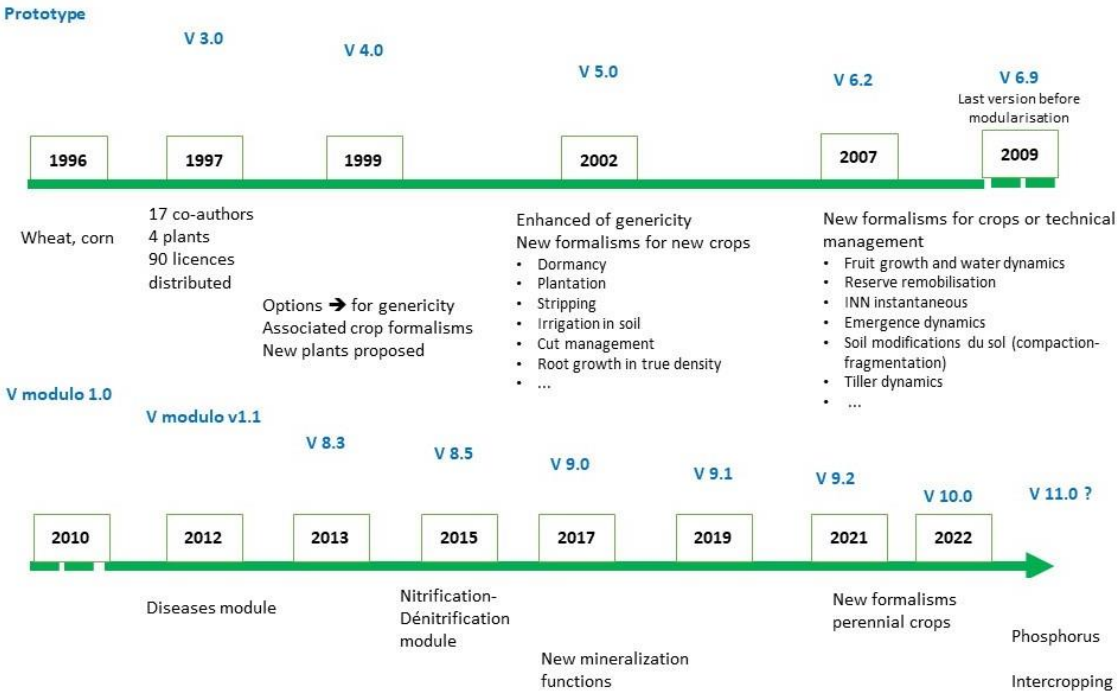

Figure A.7 Timelines of the different versions that have been developed and changes in the formalisms and processes simulated in STICS (Beaudoin et al., 2022).

STICS simulates the functioning of soil-crop systems on a daily calculation time step, as a function of climatic conditions, soil characteristics and crop management (Figure A.8). STICS is currently able to simulate processes linked to crop development and growth, water balance, N and C balance in the soil-crop system. For now, the scope of application of the model remains limited to cropping systems with no limitation in terms of soil P nutrients. The model has hundreds of parameters, which are divided into two categories: i) the global parameters contained in the equations of the model formalism, and considered stable for all simulations, and ii) the local parameters constituting the model input data (soil, climate, and techniques of the case study), which are the responsibility of the model user.

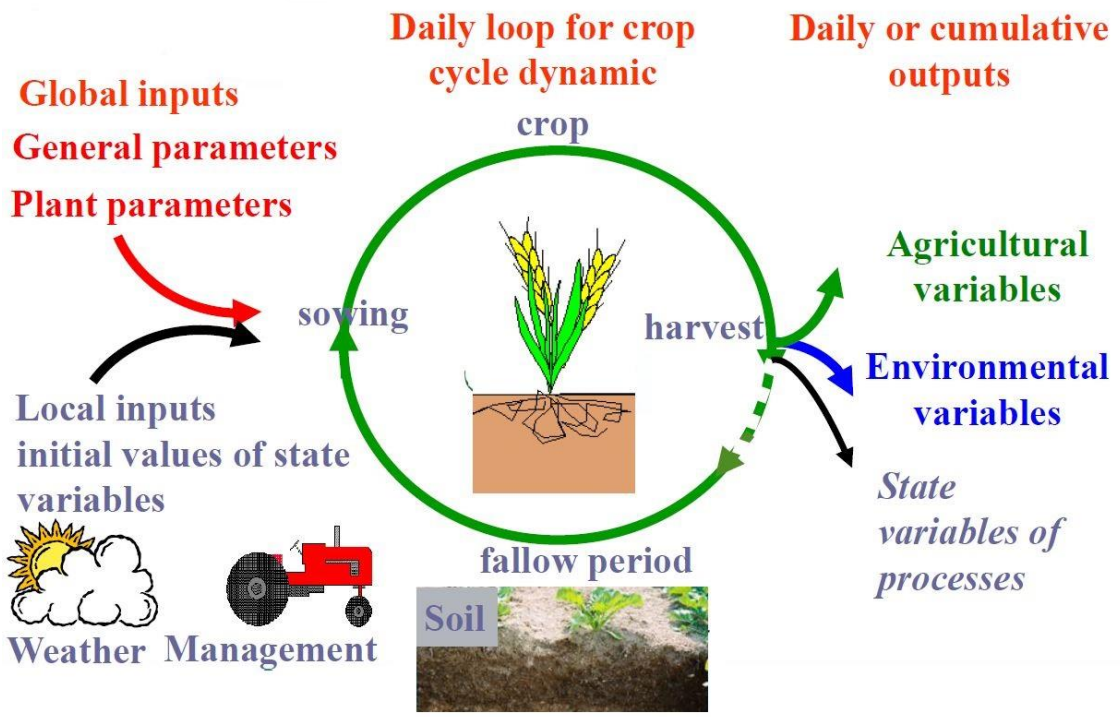

Figure A.8 Simulation design with the STICS model (Beaudoin et al., 2022).

A.3.2. Predictive performance and application of STICS in Europe and worldwide

Since its creation, a large number of studies have been carried out with STICS model on different topics and under various agro-environmental conditions (Figure A.9). These studies were mainly performed in temperate zones where its performance has been demonstrated for genericity and robustness (Coucheney et al., 2015). According to an evaluation of the overall performance of the STICS model conducted by Coucheney et al. (2015) on 15 types of crops and under various soil and climate conditions in France, model errors are mainly related to the model's difficulty in considering dispersion rather than to a bias in predictions. Moreover, the dependence of errors on agro-environmental conditions or crops is low. The simulated variables corresponding to soil water content are well predicted and are rated as very good. As for the mineral N of the soil profile and the upper soil layer, they have been simulated with less precision, especially for the upper layer, respectively falling within the satisfactory and unsatisfactory range. Considering plant simulations, the variables during the growing cycle are very well simulated. On the other hand, the predictive performance for the plant variables at harvest is contrasted. More specifically, aboveground biomass and grain/fruit

biomass were well predicted; plant N prediction was satisfactory, and prediction of grain/fruit N content was unsatisfactory. Model efficiency (EF) for all variables was still satisfactory, with all values above 0.48 and minimum values for soil nitrate and grain/fruit N content.

STICS can be applied to long-term studies to assess N-related environmental processes (Beaudoin et al., 2005, 2008; Constantin et al., 2012). The model satisfactorily predicted crop and soil variables in continuous simulations, although soil water content was better predicted than N leaching and soil NO_3^- content. STICS also performed well in the long-term simulation of COS and soil organic N (SON) dynamics in rotational and organic cropping systems (Autret et al., 2020; Bonilla & Justes, 2015). To obtain an accurate result for SOC and SON, it is sometimes required to modify the proportion of the active/stable fraction of humified OM, with reference to the historical use of the experiments (Autret et al., 2020).

Furthermore, STICS has already been used on several occasions outside the domain in which the model was designed, such as in tropical conditions (Lufuluabo et al., 2011; Sierra et al., 2003, 2010). However, a parameterization of the temperature response of N mineralization and nitrification was necessary to provide reliable estimates of the amount of N available to crops in tropical acid soils (Sierra et al., 2003). In semi-arid regions (Hadria, 2006; Rodriguez et al., 2004), the model was adopted to study the possibilities for improving irrigation water management. These studies have shown that the model is also applicable in semi-arid conditions (low and irregular rainfall, high-temperature dynamics, and high radiation) and can simulate water balance, crop growth, and yield adequately. In high-altitude intertropical areas (Lebonvallet, 2008), where the climatic risks for agriculture are high (frequent frost, low rainfall), the model has been adapted to quinoa crops. For that, the addition and modification of certain model processes were necessary. Among the modification, the consideration of altitude in relation to the calculation of radiation and evapotranspiration by using atmospheric pressure, the representation of limiting conditions for crop establishment (germination and emergence), and the integration of a formalism for sowing in stacks.

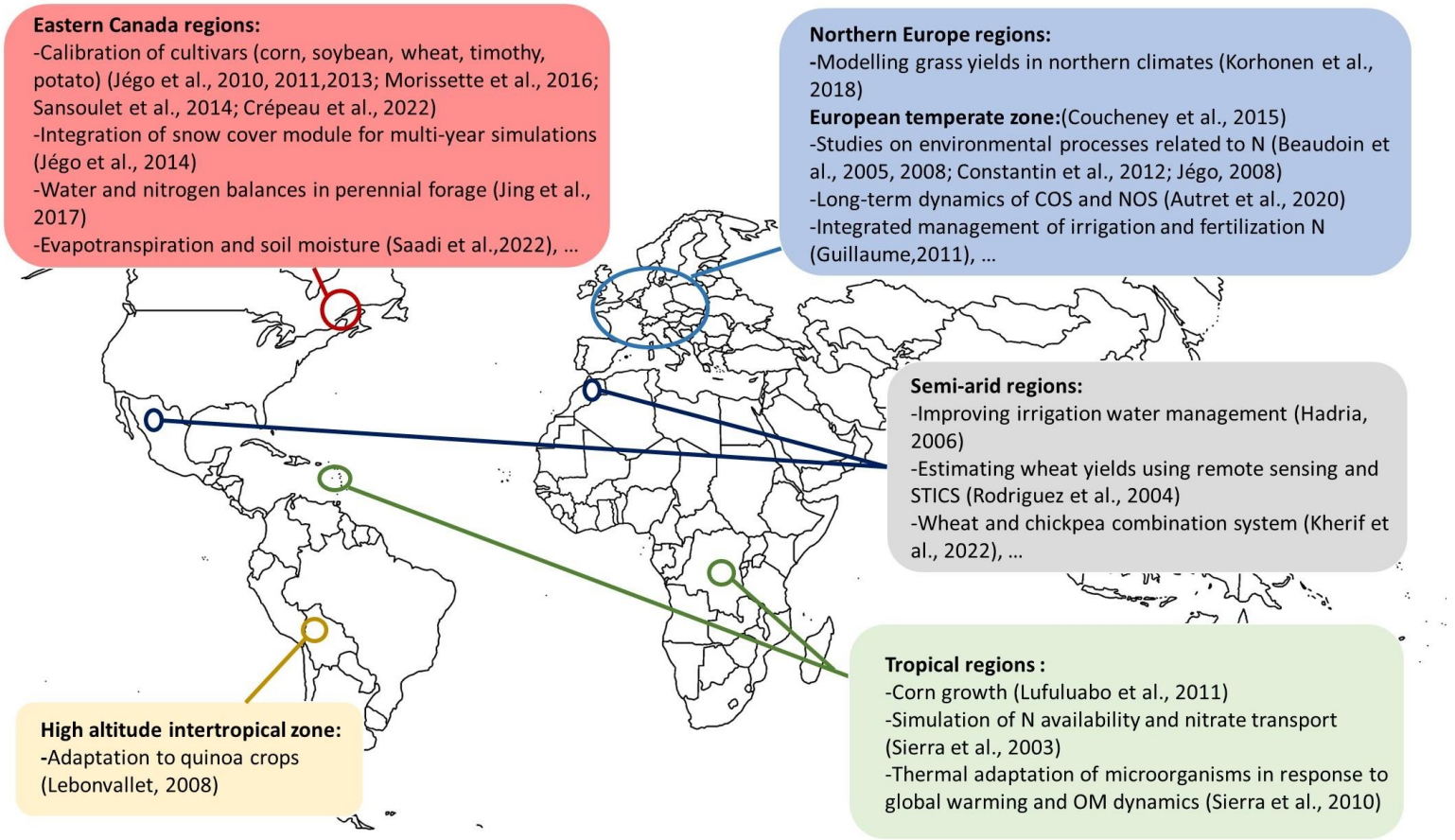

Figure A.9 Example of studies using and applying the STICS model around the world.

A.3.3. Application of the STICS model to agrosystems in eastern Canada

The application of STICS to the context of regions with cold and humid continental climate such as eastern Canada, including Quebec, has been extended more recently (Tableau A.2). The model was calibrated and validated on annual crop cultivars (corn, soybean, spring wheat and potato) adapted to regional conditions. Model evaluation results provided satisfactory accuracy for predicting crop growth and production components such as LAI, biomass, grain yield and plant N content (Crépeau et al., 2021; Jégo et al., 2010, 2011; Morissette et al., 2016). For perennial crops, STICS has been calibrated and validated to simulate the growth and nutritional value of two timothy cultivars (Jégo et al., 2013). All these evaluation studies were carried out over a few years, with the model being reinitialized every growing cycle. It has been shown that new cultivars can easily be calibrated for STICS, even under agro-environmental conditions different from those in which the model was developed.

Since the integration of the snow cover module in the model, multi-year simulation of crop rotation, perennial plants and soil processes (water and N dynamics) under cold conditions including a long period of snow cover has been made possible (Jégo et al., 2014). STICS could be run in a consecutive mode without annual reinitialization for timothy simulation. Nevertheless, the model has never been used for more than three consecutive years under such conditions (Jing et al., 2017). The snow cover module has improved the accuracy of the soil temperature simulation during the winter period by considering the insulating effect of snow cover. In addition, water dynamics have been improved, even though the model's results are better for simulating the deeper soil layer (15-30 cm) than for the first upper soil layer (0-15 cm) (Jégo et al., 2014). A comparison of two methods for calculating evapotranspiration available in STICS showed that the resistive approach (Shuttleworth & Wallace, 1985) provided better results for predicting evapotranspiration under rainfed corn than the crop coefficient method (Penman, 1948). However, the use of either method had practically no impact on the soil moisture simulation (Saadi et al., 2022). The authors nevertheless observed an improvement in soil water content predictions in the surface soil layer (0-10 cm) with a new method that considers the impact of shrinkage cracks on the simulation of water movement at the soil surface in clay soils during dry seasons. In comparison with other models, the results of soil moisture prediction with STICS do not statistically differ from those of North American models such as DNDC or DayCent (Guest et al., 2017).

Concerning the simulation of soil N dynamics, the study on the simulation of soil processes during 3 successive years under a timothy crop showed that soil NO_3^- contents were overestimated by STICS (Jing et al., 2017). The authors suggest that either the overestimation of mineralization/nitrification or

the underestimation of N uptake by the plant or N emitted in gaseous form could be the cause of this overestimation of NO_3^-. Nevertheless, it was shown that the STICS model, coupled with the snow cover model, was able to simulate timothy biomass and soil moisture dynamics. Guest et al. (2017) also observed an overestimation of N concentrations in the soil surface layer during the second half of the growing season, probably due to N mineralization.

The use of remote sensing data to spatialize the STICS model and to estimate crop yield at the plot scale was evaluated under eastern Canadian conditions. When data on soil properties and crop management are not available, using the leaf area index (LAI) extracted from remote sensing data to reinitialize the STICS model improves model performance for biomass and yield predictions (Jégo et al., 2012). Furthermore, it has been reported that in the context of eastern Canada, where soil diversity is high and agricultural units are long and narrow, the use of fine-resolution soil data is recommended as an effective method for improving yield predictions despite the associated uncertainty (Jégo et al., 2012, 2015).

Table A.2 Summary of the main research carried out at AAFC by Guillaume Jégo and collaborators using STICS model to the agropedoclimatic conditions of eastern Canada.

References	Study topics
Jégo et al. (2010, 2011, 2013)	Calibration and performance evaluation of soybean, spring wheat, corn and timothy cultivars using STICS in eastern Canada
Jégo et al. (2014)	Calibration and evaluation of snow cover models under winter conditions in eastern Canada for the implementation of a module considering the effect of snow cover on soil processes and crop growth in the STICS model
Jégo et al. (2012, 2015)	Regional crop yield forecasts (corn, soybeans, spring wheat) in eastern Canada using the STICS model and remote sensing data to reset input parameters; and assessment of the impact of spatial resolution of input data on yield.
Jing et al. (2017)	Evaluation of STICS model for simulation of inorganic N and water fluxes in a timothy forage system in eastern Canada and use of the model for estimation of water and N balances
Sansoulet et al. (2014) ; Guest et al. (2017)	Performance comparison of three soil crop models (STICS, DNDC and DayCent) to simulate the response of yield, N uptake and biomass to fertilizer rates, as well as the simulation of soil moisture and N content for spring wheat experiments in eastern Canada
Morissette et al. (2016)	Calibration and validation of the STICS soil-crop model for potato cultivars under growing conditions encountered in eastern Canada
(Mesbah et al., 2017, 2018)	Identification of optimal ecophysiological N rates and use of new model-based insights for strategic N recommendations for corn using STICS
Crépeau et al. (2021)	Predictions of soybean harvest index and evapotranspiration using the STICS crop model
Saadi et al. (2022)	Evaluation and improvement of simulations of evapotranspiration and soil water content under rain-fed corn with the STICS model

A.3.4. The strengths and limitations of the STICS model

In addition to its genericity and robustness, STICS can also work with limited input data that can be easily obtained at a plot level. In addition, several generic input data are provided with the model. There is also the aspect of future evolution/development of the model without complication, due to its

modularity (Brisson et al., 1998; Coucheney et al., 2015). The model has been designed in a generic way; hence it can be easily adapted to new environmental conditions and new uses. In particular, the parameters of the model equations are easily accessible and modifiable, which facilitates the process of parameterizing the model according to needs and available information (Launay et al., 2005). In addition, STICS includes many original features compared to other well-known soil-crop models, such as crop temperature simulation, the snow module, the simulation of various management techniques and options, and the simulation of bi-specific intercropping. It is among the soil-crop models that use more complex modeling approaches to simulate soil N dynamics by taking into account different processes on soil OM decomposition and mineralization, gaseous N emissions, leaching losses, crop N demand, crop growth and phenological responses to N-related stress (Yin et al., 2017). The snow cover module offers many opportunities for using the model and exploring new issues under a variety of agro-environmental conditions, including in cold regions. In addition to STICS application to both continuous simulation over several years and simulation over a single crop cycle, STICS enables more complex simulations to be carried out with a wide variety of cropping systems: intercropping, alternative cropping systems, perennial crops (Autret et al., 2020; Strullu et al., 2014).

Still, the STICS model also has limitations. Despite its good performance for soil water content prediction, variation in the groundwater table in the soil cannot be accurately considered. In a location with a high water table that may rise towards the simulated soil layers, modelling the NO_3^- concentration in the soil is problematic (Jégo, 2008). The model does not at this stage describe the effects of soil acidity and aluminium toxicity (Al_3^+) on plant growth and development (Sierra et al., 2003). STICS does not include in its formalism the impact of diseases, pests, or weeds on the performance of crop stands. Nevertheless, STICS can be coupled with other models to understand and predict the potential impacts of climate change on the development of crop diseases (Caubel et al., 2014), and to assess pesticide leaching in cropping systems (Lammoglia et al., 2017).

Generally, soil characteristics (e.g. texture, bulk density) are considered permanent in STICS. However, a simple option has recently been added to take into account the effects of tillage on soil compaction and fragmentation (Richard et al., 2007). A value of bulk density was defined after the passage of each type of cultivator, which leads to changes in layer thickness and soil infiltrability, as well as the redistribution of water and N. The effectiveness of this option has not yet been assessed, although the question is of great interest to adequately represent agricultural reality. It represents a first step towards the consideration of structural dynamics in sol-crop models, and its implications for the stabilization or decomposition of soil organic C and soil water processes.

A.4. Summary of the literature review

Soil-crop models are particularly useful and relevant for analyzing the functioning of agrosystems and diagnosing observed constraints on crop growth. To analyze the performance of these models, the first step is to gather information on the agropedoclimatic conditions of the agrosystem under study, using measurements and bibliographical references. In the second stage, the model has to be calibrated to minimize discrepancies between simulation results and observations from field experiments. Finally, model performance must be validated using data independent of those used for calibration.

Like other models with similar features, STICS simulates the dynamics of a soil-crop system over one or more successive crop cycles, in interaction with agricultural practices (including fertilization). STICS has already been used in a wide range of agropedoclimatic conditions, notably in temperate regions of Europe, but also in other parts of the world. For the conditions prevailing in the province of Quebec and, more generally, in eastern Canada and other regions of the world with similar climates, several studies have already been carried out to parameterize, calibrate and, in some cases, validate STICS. Analysis of STICS performance showed satisfactory accuracy in predicting crop growth and production components. However, studies on the simulation of plant N uptake and soil N dynamics remain limited. Most of existing studies consisted of simulations for a limited number of cropping years and with reinitialization of the model at each growing season. No studies have yet been carried out for consecutive simulations (without annual reinitialization) over a long-term cropping period. Moreover, STICS has not yet been calibrated for one of the major economic crops in eastern Canada, such as spring barley. For timothy, STICS needs to be validated for simulating biomass production and N nutrition at different levels of N fertilization and over a long period.

B. Research objectives and hypotheses

The main objective of this thesis is to study and extend the scope of application of STICS to crops of economic importance (spring barley, timothy), grown under the agropedoclimatic conditions of agrosystems in the province of Quebec (cold and humid continental climate). Furthermore, this thesis aims to evaluate the model's predictive performance on long-term simulations. The associated challenge is to analyze the genericity of STICS for situations not yet studied, and/or to show its limits and weaknesses to identify possible points for improvement.

The specific objectives are as follows:

i) To calibrate STICS for simulating annual aboveground biomass production, grain yield and N nutrition of the spring barley cultivar (Chapais) adapted to growing conditions in the province of Quebec.
ii) To analyze the predictive performance of STICS for simulating spring barley crops over several decades without annual reinitialization.
iii) To evaluate the ability of STICS to simulate timothy aboveground biomass production and N nutrition for several consecutive years without annual reinitialization under Quebec agrosystem conditions.
iv) To analyze the ability of STICS to diagnose observed constraints on crop growth in long-term field experiments.

Given the lack of knowledge on the long-term simulation of the impacts of agricultural practices, in particular N fertilization, on agricultural production attributes, this thesis will attempt to answer several research questions:

i) Are the parameters defined in STICS model for spring barley cultivars grown under temperate conditions adapted to the context of agrosystems in the province of Quebec? If not adapted, which one should be changed?
ii) Can STICS correctly simulate the production of aboveground biomass of spring barley and timothy, the grain yield of spring barley, the N concentration in barley and timothy, and the quantity of N exported annually by the crop over long cropping sequences, without annual reinitialization of the model?
iii) Can STICS capture biomass production and N nutrition responses as a function of N fertilization practices or tillage system under the growing conditions of Quebec?
iv) Are there any STICS model formalisms that are not well adapted to the growing conditions of Quebec agrosystems?

The following hypotheses were formulated:

i) The ecophysiological parameters defined in STICS for spring barley grown under temperate conditions require calibration to make the model suitable for the context of agrosystems in the province of Quebec.
ii) The generic plant parameters in STICS are adequately parameterized, so that calibrating a new cultivar of spring barley only requires adjustment of a few parameters.
iii) With the activation of the snow module, the performance of STICS for simulating biomass production and N nutrition for spring barley and timothy is the same for both annual with reinitialization and long-term continuous simulation under cold and humid continental climates.
iv) STICS can correctly simulate the biomass production and N nutrition in response to various crop management, especially for N fertilization, for both crops.

To answer or verify these research questions and hypotheses, the approach adopted in this thesis combined long-term field experiments with modeling of soil-crop system functioning using STICS. The study scale is the experimental field plot. This thesis exploited time series of experimental data collected over long cropping periods to analyze the evolution of variables of interest, to compare the outputs of STICS simulations with values observed in the field, and to test the predictive performance of STICS and its genericity.

Databases from two long-term field experiments were used in this work. Specifically, in the first chapter, the long-term effects of two types of N fertilization (70 kg N ha^{-1} yr^{-1} as mineral fertilizer and 107 kg N ha^{-1} yr^{-1} as liquid dairy manure) on biomass production and N uptake of a spring barley monocrop grown for 31 years were studied.

In the second chapter, the effects of four levels of mineral N fertilization (0, 60, 120, 180 kg N ha^{-1} yr^{-1}) on biomass production and N uptake of a timothy grassland cultivated for 8 years were studied.

C. Materials and methods

C.1. STICS soil-crop model

C.1.1. Model selection criteria

In this thesis, the chosen soil-crop model is STICS. Like other models of this type (Table A.1), STICS offers multiple possibilities for agro-environmental use to answer questions raised by research and crop management. It is particularly useful and relevant for analyzing and diagnosing observed constraints on crop growth, as well as for testing and simulating new practices likely to improve nutrient use efficiency. The predictive performance of STICS has been evaluated for a wide range of applications (e.g. biomass production, soil water and nitrate content) and a wide range of crops and agro-environmental conditions (Coucheney et al., 2015; Kherif et al., 2022; Lebonvallet, 2008; Morissette et al., 2016; Sierra et al., 2003). STICS was able to reproduce the different trends induced by contrasting environmental conditions and management practices (Constantin et al., 2010, 2012).

The choice of STICS was not exclusively motivated by scientific criteria since the different existing soil-crop models (Table A.1) were built on a similar scientific basis. The choice of STICS in this thesis is justified by the fact that many studies have been developed by Agriculture and Agri-Food Canada (AAFC) to adapt STICS and validate it for the growing conditions encountered in eastern Canada. The works done by Guillaume Jégo and collaborators (AAFC, Quebec City research centre; member of the STICS project team) attest to this (Tableau A.2). Another reason is the existence of a team dedicated (STICS project team: https://www6.paca.inrae.fr/stics/Qui-sommes-nous/Equipe-Projet-Stics) to the use and evolution of STICS. This team is composed of more than twenty experts. Since 1996, STICS users have benefited from the latest scientific and technical developments. The team is at the service of STICS users and modelers, and is responsible for the scientific and institutional issues associated with STICS, in line with several objectives (https://www6.paca.inrae.fr/stics/Qui-sommes-nous/Equipe-Projet-Stics/Schema-strategique), which are to structure the governance and working methods of the team, to consolidate the robustness and performance of STICS (parameterization rules, version test database, traceability of modifications), to extend the field of validity of STICS, and to promote its use and international visibility.

C.1.2. STICS input parameters

To run STICS, a certain amount of input information on the agricultural conditions studied is required. STICS operates on a simulation unit basis (USM), corresponding to a simulation period with associated input parameters: an initial state or initialization, climatic conditions, a soil type, one or two

crops in association and a crop management system. An USM can be extended over a maximum of two years. Depending on the needs of the user and the objective of the simulation, the simulation can be run with a single USM (independent USM), or with a set of USMs in succession (successive USM).

C.1.2.1. Initialization

The initialization defines the initial state of the USM. It corresponds to the initial parameters defining the start of the simulation (instant t0 of the simulation). If the USMs are run in successive mode, only the initialization of the first USM in succession is considered by STICS. The initial states of subsequent USMs correspond to the final states of the previous USM. The initialization parameters concern soil state variables, and plant state variables if the simulation starts with a crop already in place. These parameters are soil cover status at the start of the simulation (bare soil, cover corresponding to one of the model's phenological stages, or LAI value), NO_3^- and NH_4^+ content and water content for each soil horizon, and possibly root density for perennial plants.

C.1.2.2. Climatic data

Climatic data correspond to daily weather data retrieved from a station as close as possible to the study plot. At least the following climatic data is required: minimum temperature (C°), maximum temperature (C°), global radiation (MJ m^{-2}) and precipitation (mm). The mean wind speed (m s^{-1}) and air humidity (%) can also be used to have a more precise evapotranspiration calculation (Penman (1948) or Shuttleworth and Wallace (1985)). The activation of the snow module in STICS allows us to incorporate the presence of snow during the winter period in the agricultural regions of Quebec and more widely in eastern Canada, as well as in other regions of the world with similar climatic conditions (e.g. Finland, Norway, Sweden). This module is based on the pre-processing of daily air temperature and precipitation data (Jégo et al., 2014). The method proposed by Trnka et al. (2010) is used in the model with modifications to the equations for calculating snow accumulation, based on the work of Bélanger et al. (2002), and for snowmelt and snow depth calculations, based on the work of de Thorsen et al. (2010).

C.1.2.3. Soil data

The soil is described in the model as a succession of horizontal layers (up to 5 layers), each one characterized by its hydrodynamic parameters: thickness, field capacity, permanent wilting point, bulk density, volumetric content of pebbles, and infiltrability. There are also parameters concerning the properties of the topsoil horizon (of which the depth is an input parameter: 'profhum'): organic N content, C/N ratio, pH, clay and $CaCO_3$ content, albedo. Several other parameters can be specified in the soil characteristics according to the study case, such as the presence of obstacles to rooting

(obstarac), the fraction of runoff in relation to total precipitation (ruisolnu), and the threshold beyond which potential evaporation decreases (Q_0). These parameters can be obtained directly from soil physicochemical analysis or the literature. For some parameters, suggested or recommended values according to soil type are provided with the model.

C.1.2.4. Plant-related parameters

The plant file contains the operating characteristics of a given plant, already parameterized, and supplied with the model. Each plant is defined essentially by its phenology and ecophysiological characteristics. Plant parameters include general plant parameters and one or more subsets of cultivar-specific parameters. These parameters can be directly used without modification, but they can also be adapted or calibrated to the needs of the user to take account of specific conditions.

C.1.2.5. Crop management

Crop management describe the sequence over time of the various cropping operations applied to a plot during a crop cycle or rotation. Different crop management options are considered in the model, such as: sowing/planting (date, depth, density, variety, inter-rows, row orientation), mineral and organic fertilization, irrigation, tillage with residue incorporation, use of specific techniques such as mulching, cutting (for forage crop) or harvesting decision criteria (once or several times, depending on physiological maturity or water, N, sugar, or lipid content).

C.1.3. STICS modules and formalisms

In STICS, the atmosphere representing the upper boundary of the system is characterized by climatic variables. The plant is characterized by its LAI, and the quantity and quality of its aboveground biomass and harvested organs. Interactions between soil and plant take place through the roots and are defined by the distribution of root density in the soil profile. Roots operate solely as absorbers of water and mineral N. The STICS model is structured around several interdependent modules/sub-modules: phenological development, aboveground biomass growth, yield elaboration, root growth, residues and OM decomposition, water balance, N balance, and soil heat, water and N transfer (Brisson et al., 2003). Each of these modules/sub-modules simulates one or more specific ecophysiological or physical processes, and they exchange variables and parameters with each other. The formalisms of each module/sub-module are detailed in Brisson (2009) et Beaudoin et al. (2022).

C.1.3.1 Development module

Several phenological stages divided between two independent vegetative and reproductive scales are considered in the model (Tableau C.1). The periods between successive stages, generally considered to be specific to each cultivar, are expressed in development units and are mainly governed by the sum of degree-days (based on air or crop temperature), and eventually by a photoperiodic or vernalization limiting factor (depending on the species), or by water or N stress. The various stresses are calculated in multiplicative form using indices ranging from 0 (= maximum stress effect) to 1 (= no effect).

Table C.1 List of phenological stages in STICS.

Vegetative stages	Reproductive stages
IPLT: sowing or planting	ILAT: beginning of the critical phase for grain number onset
IGER: germination (sown crop)	IFLO: flowering
IDEBDORM: beginning of dormancy (perennial crops)	IDRP: onset of filling of harvest organs
IFINDORM: end of dormancy (perennial crops)	IDEBDES: onset of water dynamics in fruits
ILEV: emergence or budding	IMAT: physiological maturity
IAMF: maximum acceleration of leaf growth, end of juvenile phase	IREC: harvest
ILAX: maximum leaf area index, end of leaf growth	
ISEN: beginning of net senescence	

C.1.3.2. Shoot growth

Dry aboveground biomass accumulation is simulated in relation to daily leaf C assimilation. It is calculated as a function of LAI evolution and solar radiation interception. LAI evolves according to different phases: growth phase (between ILEV, IAMF and ILAX), stability phase (between ILAX and ISEN) and senescence phase (between ISEN and IMAT). The daily LAI increase is calculated as the product of factors depending on phenological development stages (a logistic function of development units), crop temperature, plant density, and eventual water and N stress (Brisson et al., 2009).

Simulation of leaf senescence follows the concept of natural leaf lifespan applied directly to LAI, which means that part of the leaves and biomass produced at a given time will be lost through senescence once the lifespan has elapsed. The lifespan of the leaf is also conditioned by the same temperature and stress factors as for development.

Aboveground biomass accumulation is the result of a parabolic function of the radiation intercepted by the crop, involving the conversion efficiency of the intercepted radiation. Beer's law is used for homogeneous crops, while another method taking into account the canopy geometry is proposed for radiation transfer in the case of associated crops (Brisson et al., 1999). Daily biomass production is influenced by factors affecting photosynthesis and respiration, such as water and N stress, temperature, anoxia, and CO_2 concentration.

C.1.3.3. Yield formation

The number of harvested organs is calculated from the average growth rate of the crop during a critical grain number determination phase (ILAT-IDRP) that precedes the start of grain filling. The relation is linear (slope of the curve = 'cgrain' parameter) and depends on genetic parameters, i.e. the minimum ('nbgrainmin') and maximum ('nbgrainmax') number of grains. The effects of different stresses during this period are also considered in the calculation to define variations in grain quantity. The quantity of dry matter accumulated in the harvested grains is calculated by applying the evolutive harvest index to the dry biomass. The harvest index is expressed as the ratio between the biomass of harvested organs and the total dry weight of the aerial parts of the plant. Similarly, grain N accumulation is calculated as a function of N harvest index (harvested organ N/total plant N). The progression of these indices follows a linear function from the IDRP stage to the IMAT stage, with the parameters 'vitircarb' and 'vitirazo' as slopes respectively. Grain biomass accumulation dynamics and grain N filling are affected by optimal temperature thresholds ('tminremp', 'tmaxremp'). Other biochemical compounds (oil, sugar) are simulated in a simplified way and assumed to be proportional to the dry matter in the organs.

C.1.3.4. Root growth

Roots are described as a function of front depth and root density profile. Root growth through the soil profile is thus given by 2 series of calculations. The first expresses the speed of progression of the rooting front defined by a linear function of a coefficient that is plant-specific ('croirac') and proportional to soil temperature. Water stress, anoxia or high bulk density reduce root front progression, which stops when soil depth is reached, or a physical obstacle ('obstarac') is encountered in the soil, or when net leaf growth ceases (ILAX).

The second series of calculations gives the root density according to two possible options. The first option calculates the effective root profile for water and N uptake. This sigmoidal profile is defined by the maximum depth reached and an optimum root density profile. The second option, true density, calculates a root density profile comparable to measurements. Root length growth is calculated using a logistic function analogous to that of leaves and is then distributed in each layer of the soil profile in proportion to the roots present and according to soil constraints (drought, anoxia, penetrability). The lifespan of roots in the soil is defined by a species-dependent thermal duration at the end of which roots placed in the layer at a given depth are removed.

Root expansion can be calculated with 2 different methods. The first method is based on the independence of root length expansion from aboveground biomass accumulation. In this way, root length growth is simulated directly, without the need to process root biomass. Conversely, with the second method, root length expansion is driven by aboveground biomass growth and depends on a dynamic sharing coefficient between root biomass and total biomass.

C.1.3.5. Water balance

The water balance module integrates evapotranspiration potential and water availability in the soil, as well as the capacity of the plant to pump water. It can be used to determine the level of water stress, which expresses a gap between supply and demand, which leads to a limitation in aboveground growth. Soil evaporation is calculated in two stages: potential evaporation linked to the energy available at the soil level, followed by actual evaporation linked to water availability and its distribution within the soil profile. Potential evaporation can be calculated in two different ways, either by the LAI or soil cover fraction method (equivalent of Beer's law), or by the energy balance approach. For the actual evaporation, two phases are starting from a rainfall event. During the first stage, the soil is sufficiently moist so that evaporation is potential, and this occurs until cumulative daily evaporation reaches a threshold ('Q0'). During the second phase, the evaporation is reduced depending on the climatic parameter and soil type. The calculation of evaporation distribution is similar to the LIXIM model (Mary et al., 1999), which is based on the decreasing exponential contribution of each elementary soil layer from the surface to a maximum depth.

Two options are available for calculating water requirements for plants. The first option is based on Beer's law and constitutes a crop coefficient approach in which the potential evaporation of the crop is given by a logistic function of the LAI, involving the maximum crop coefficient ('kmax'), assuming that all soil and plant surfaces are not water-limited. Maximum transpiration depends on the energy available within the plant and is estimated by the difference between the potential evaporation of the crop and the potential evaporation of the soil, as well as the state of the atmosphere within the plant

canopy. The resistive approach, on the other hand, is based on the energy balance, which is used when Beer's law cannot be applied, as in the case of associated or row crops.

At the daily time step, root uptake can be considered equal to actual crop transpiration. The root uptake calculated globally is then distributed by the soil layer. Relative transpiration, i.e. the ratio between actual and potential transpiration, is a bilinear function of the water content available in the root zone. Water stress indices affect leaf growth, biomass growth and transpiration. The ratio between actual and potential transpiration represents the stomatal stress index, which operates prior to the leaf growth stress index.

The water balance is calculated from all the variables contributing to water flows in the soil-plant-atmosphere continuum. Inputs flows include rainfall, capillary rise, and irrigation. Outflows are evaporation, transpiration, runoff, deep infiltration and interception of rain and irrigation water by leaves and mulch.

C.1.3.6. Nitrogen transformation

The STICS N balance module considers the main processes affecting organic and/or inorganic N compartments in the soil. These processes are mineralization, immobilization, nitrification, losses through leaching and gaseous emissions (volatilization, denitrification), fertilizer inputs (organic and mineral), symbiotic fixation for leguminous plants, and N uptake by roots. It is worth noting that the N cycle is coupled with the C cycle.

a. Decomposition of organic residues

The module for decomposition and mineralization of organic C and N from residues and organic matter (OM) is derived from the model proposed by Nicolardot et al. (2001), which considers three compartments: crop residues, microbial biomass and humified organic matter (Figure C.1). The model is defined by seven parameters: two decomposition rate constants (k et λ (j^{-1})), two partition parameters (assimilation rate 'Y' (gC g^{-1}C) and humification rate 'h' (gC g^{-1}C), and three C/N ratios (organic residues, microbial biomass and humified OM). Except for the C/N ratio of humified soil organic matter, the other five model parameters were obtained by non-linear adjustment and by minimizing the differences between observed and simulated CO_2 and mineral N values. The module can be applied to 8 residue categories: main crop residues (mature residues), intermediate crop residues (young residues), manure or slurry, compost, sludge, vinasse, horns, and others. Parameters are specific to each category. Part of the residue can be incorporated directly into the stable humified OM compartment.

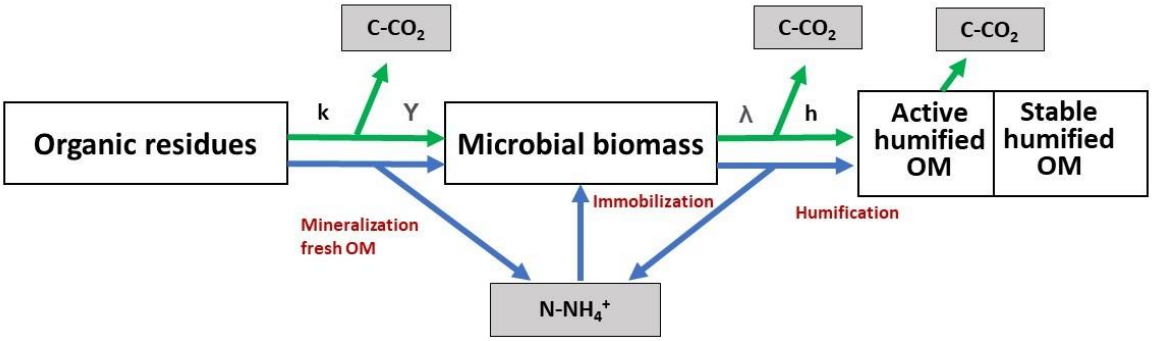

Figure C.1 Flow diagram of the decomposition of organic residues in soil (Nicolardot et al., 2001), the green lines indicate C flows and the blue lines N flows.

The decomposition rate of residues depends on the nature of the organic residues, the depth at which they are incorporated into the soil, and the temperature and humidity of the soil. The nature of organic residues is defined by their origin and C/N ratio. Soil moisture reduces potential mineralization according to a linear relationship with water content. Temperature modifies the rate of residue decomposition, via a logistic-type factor ('ftr').

$$\mathrm{fh} = \frac{\mathrm{hur} - \mathrm{hminm.\ hucc}}{(\mathrm{hoptm} - \mathrm{hminm}).\ \mathrm{hucc}} \qquad \text{(Equation C.1)}$$

Where, 'hur' is the soil water content, 'hminm' is the threshold below which mineralization is stopped, 'hoptm' the threshold where the maximum value is reached, and 'hucc' the moisture at field capacity. The values of these parameters may differ between soils from temperate and tropical regions. (Sierra et al., 2003).

$$\mathrm{ftr} = \frac{\mathrm{ftemra}}{1 + (\mathrm{ftemra} - 1).\exp(-\mathrm{ftemr}.(t - t_{\mathrm{ref}}))} \qquad \text{(Equation C.2)}$$

Where, 'ftemra' (12) is an asymptotic parameter and 'ftemr' (0.103) the action constant (°K-1).

The net N mineralization (positive or negative) resulting from residue decomposition is then calculated as a function of the decomposition rate (C flux) of the N/C ratio of the 3 compartments: organic residues, microbial biomass, and humus.

b. Mineralization of soil organic matter

The mineralization of humified OM ('vminh') is calculated from the potential mineralization rate of the soil ('k2pot'), the organic N stock of the humified active fraction ('nhum') and the soil temperature ('ftm') and humidity ('fthm'). It is assumed to occur up to a maximum depth ('profhum') generally equal to the ploughing depth and negligible below this depth. Soil characteristics affect potential mineralization rates through clay content, CaCO3, soil pH and C/N of soil humus (Clivot et al., 2017). The active organic N stock is calculated from the organic N content 'norg', the bulk density of the soil thickness 'da(1)' corresponding to the depth of humification ('profhum'), and the proportion of the active humus fraction ('1-finert'). Soil moisture affects humus mineralization according to the same law as residue decomposition. Temperature influences the humus mineralization rate according to the same law as residue decomposition, but with different parameter values. The reference temperature (corresponding to potential mineralization) is set at 15 °C in a temperate environment.

$$\mathrm{vminh} = \mathrm{k2pot}.\,\mathrm{nhum}.\,\mathrm{ftm}.\,\mathrm{fh} \qquad \text{(Equation C.3)}$$

With,

$$\mathrm{k2pot} = \mathrm{gmin1}\,.\frac{\mathrm{e}^{-\mathrm{gmin2.\ argi}}}{(1+\mathrm{gmin3.\ calc})}.\,\mathrm{e}^{-\mathrm{gmin4.\ (ph-gmin5)^2}}.\,(0.8\,.\,\mathrm{e}^{-\mathrm{gmin6.(csurn\ sol-gmin7)^2}} + 0.2)$$

(Equation C.4)

Where, '$\mathrm{gmin_x}$' are parameters describing the effect of soil characteristics (N organic, clay, and $CaCO_3$ content, pH, and C/N).

$$\mathrm{nhum} = \mathrm{norg}.\,\mathrm{da}(1).\,\mathrm{profhum}.\,(1 - \mathrm{finert}) \qquad \text{(Equation C.5)}$$

$$\mathrm{fh} = \frac{\mathrm{hur-hminm.\ hucc}}{(\mathrm{hoptm-hminm}).\ \mathrm{hucc}} \qquad \text{(Equation C.6)}$$

Where, 'hur' is the soil water content, 'hminm' is the threshold below which mineralization is stopped, 'hoptm' the threshold where the maximum value is reached, 'hucc' the moisture at field capacity. The values of these parameters may differ for soils in temperate and tropical regions.

$$\mathrm{ftm} = \frac{\mathrm{ftemha}}{1+(\mathrm{ftemha}-1).\exp(-\mathrm{ftemh}.(\mathrm{t}-\mathrm{t_{ref}}))} \qquad \text{(Equation C.7)}$$

, where 'ftemha' is an asymptotic parameter and 'ftemh' is the action constant ($°K^{-1}$).

c. Nitrification

The nitrification defined as the biological process producing nitrates is an option in STICS (Léonard, 2016). It is calculated according to the "profhum" humification depth. The ammonium (formed by mineralization and the addition of mineral and organic fertilizers) is partially transformed into nitrate. Only the nitrate form is affected by leaching. The nitrification rate is calculated as the product of a potential rate and regulatory factors: NH_4^+ substrate availability and environmental conditions: pH, temperature, and soil water content. The effect of pH on nitrification is linear between 2 parameters ('pHminnit' where nitrification is zero and 'pHmaxnit' where nitrification is maximum). The effect of temperature is described either by a piecewise linear model or by a Gaussian function. The effect of water content on nitrification is double: the nitrification increases with water content, but when the soil is completely saturated with water, nitrification ceases. The water content thresholds are: 'hminn' and 'hoptn'. Each of these 3 factors is assigned a coefficient (between 0 and 1) whose effect is multiplicative and non-interacting.

d. Inputs N from mineral fertilizers and organic residues

Exogenous N can be added to the soil through irrigation, rainfall, mineral fertilizers, and organic fertilizers. N supplied by irrigation and rain is calculated from the product of the quantity of rain or water and its average mineral N concentration. With mineral fertilizers, the N is directly integrated and accounted for in the mineral N pool of the soil, and is subject to root uptake, leaching, volatilization, denitrification, or nitrification. The fate of N fertilizers is simulated using fertilizer use efficiency, which corresponds to the proportion of fertilizer N taken up by the crop. In the case of organic fertilizers, N is in mineral form (mainly ammonia) and in organic form. The mineral fraction follows the same process as the N in mineral fertilizers, while the organic fraction is first subjected to decomposition and mineralization.

e. Symbiotic fixation

For legumes, symbiotic fixation of atmospheric N complements the N available in the soil to bring the level of N uptake between the critical and maximum dilution curves. This fixation is calculated in two stages. First, the module calculates potential fixation as a function of the maximum daily fixation specific to the plant and a phenology-dependent coefficient that varies according to the degree-days of growth. Secondly, the constraints on potential fixation (real fixation) are calculated, considering that fixation activity is limited by the N concentration in the root zone. This is inhibited by high levels of mineral N in the nodule zone formed on legume roots by the action of symbiotic atmospheric N-fixing bacteria. It is also limited by water stress, anoxia, and soil temperature.

f. Denitrification and volatilization

The part of the N fertilizer not absorbed by the plant is lost either in gaseous form (denitrification: microbial anaerobic respiration reaction reducing nitrates to gaseous forms of NO, N_2O, and N_2; or volatilization: removal of N from the soil or a fertilizing material, by direct release into the atmosphere of N_2, N oxide or ammonia), or by leaching, or immobilized by microorganisms. Denitrification is calculated as the product of potential rate and regulating factors: NO_3^- substrate availability 'fno3' and environmental conditions: temperature 'ft' and water content 'fh'. By default, denitrification potential is calculated as a function of organic C content in the model. The denitrification depth is defined by a 'profdenit' parameter in STICS (Léonard, 2016). 'vpotdenit' is the potential denitrification rate.

$$\mathrm{dnit} = \frac{\mathrm{vpotdenit}}{\mathrm{profdenit}} . \mathrm{fno3} . \mathrm{ft} . \mathrm{fh} \qquad \text{(Equation C.8)}$$

$$ft = e^{[(t-tdenre1).0.449-0.668]} \quad \text{if t < tdenre1} \qquad \text{(Equation C.9)}$$

$$ft = e^{[(t-tdenre2).0.0742]} \quad \text{if t > tdenre1} \qquad \text{(Equation C.10)}$$

, where T is ground temperature, 'tdenre1' and 'tdenre2' are 11°C and 20°C respectively in temperate conditions.

Volatilization is also pH-dependent, according to a linear function between 2 thresholds 'pHminvol' and 'pHmaxvol'. This module calculates the amount of N that volatilizes as NH_3 after organic fertilizer application. For mineral fertilizers, volatilization is not simulated mechanistically, assuming that potential gaseous losses are proportional to the dose of N fertilizer.

g. Nitrogen uptake by plants

The formalism of N uptake uses the concept of the limiting factor and compares the daily soil N supply with the plant's N demand. Daily uptake is equal to the smaller of these two terms. Crop N requirements are calculated using the concept of maximum (Ncmax) and critical (Nc) N dilution curves on dry aboveground biomass. The Ncmax curve represents the maximum capacity of the plant to accumulate N in the aboveground biomass and is used in STICS to calculate the potential N uptake by the crop. The Nc curve represents the concentration of N in aboveground biomass required to produce maximum aboveground biomass at a given time (Lemaire et al., 2008). It is used to calculate the N nutrition index (NNI), which is the ratio between the actual N concentration and the NNI (Figure C.2). The NNI is used to determine if the plant is under N stress or not. A NNI of less than 1 reduces the growth potential of the crop. For spring barley and timothy, the Nc were calculated using the

following equations: Nc= 6.66×(Shoot Biomass)$^{-0.39}$ (Zhao, 2014) and Nc= 5.7×(Shoot Biomass)$^{-0.33}$, respectively.

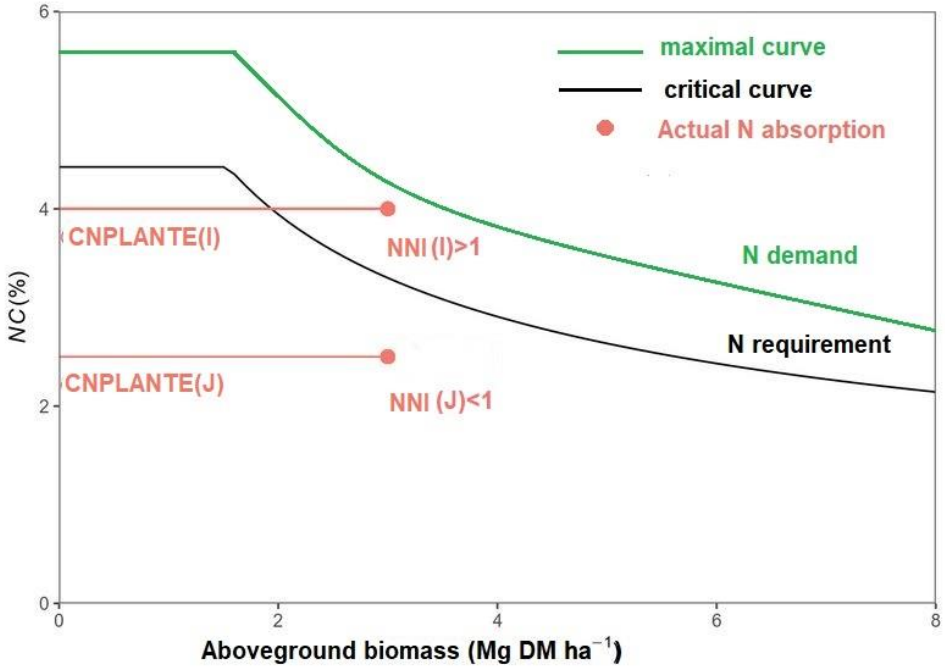

Figure C.2 Maximal and critical dilution curve and NNI calculation as the ratio between N concentration in plante (CNPLANTE) and Nc.

N uptake also depends on the plant's root system in the soil, since soil supply is calculated per elementary layer from 1 cm down to the maximum depth reached by the root system. It is determined by 2 processes: the nitrate transport process in the soil and root uptake. Firstly, the transfer of nitrate from a point in the soil to the nearest root is by convection, which involves the flow of transpiration water and the nitrate concentration of the layer; and by diffusion, which calculates the flow as the product of the apparent nitrate diffusion coefficient and the nitrate concentration gradient. Then there is an active root uptake, which is a flux that depends on intrinsic uptake capacity, root density and nitrate concentration in the root zone. The soil's elementary supply is defined by the smaller of the transfer and absorption fluxes. And the sum of these elementary supplies constitutes the total supply of the soil, which will be confronted with the global demand of the plant. So, if supply is less than demand, absorption equals supply, while if supply is greater than demand, absorption equals demand. No differentiation betweenNH_4^+ et NO_3^- is made for plant N uptake in the model, since the latter is calculated based on the total amount of mineral N in the soil (Brisson et al., 2009).

C.1.3.7. Heat, water, and nitrogen transfer in soil

The evolution of temperature in the soil depends not only on surface conditions, which drive the daily thermal waves, but also on thermal inertia linked to the environment. This inertia is responsible for the damping of average daily temperatures at depth in relation to the surface: this is the annual thermal wave. The temperature at the upper limit for calculating soil temperature is assumed to be the temperature of the crop. At a given depth, the daily thermal amplitude is calculated as a function of the daily thermal amplitude at the soil surface and is used to calculate the soil temperature at the given depth (Brisson et al., 2009).

Soil water storage can be described by 4 compartments, but only the first compartment is mandatory: microporosity, macroporosity, cracking (for clay soils), and pebbles. Microporosity, relating to the textural assembly of particles, forms the basis of water and N transfer calculations in the soil and is managed by 1 cm elementary layers. Macroporosity, relating to structural or biological porosity, is discretized by horizon.

Calculations are made for water transfer in the soil microporosity at each 1 cm elementary layer using a reservoir-type analogy. The permanent characteristics of each elementary layer are deduced from those of the horizon to which it belongs: moisture at wilting point and field capacity, and bulk density. When water content exceeds field capacity, excess water flows down into the lower soil layer. Nitrate transfer through the soil profile is also described by this reservoir analogy, according to the "mixing cell" principle. All the nitrate that arrives by convection with the water in an elementary layer mix with the nitrate already present. The excess water then leaves with the new concentration of the mixture. The macroporosity option is simulated per horizon but not per elementary layer. Downward circulation occurs by overflow from one macroporosity compartment to the next, i.e. from one horizon to another. A parameter is defined for each horizon for daily infiltrability (mm d^{-1}), which determines the maximum amount of water that can pass through each horizon and corresponds to the total excess water in the elementary layers making up each horizon. At the soil surface, the quantity of runoff leaving the system is implicitly calculated from a runoff coefficient (incorporating the effects of slope and soil roughness on runoff) which expresses the proportion of water runoff above the trigger threshold in relation to the incident rainfall for bare soil.

C.1.3.8. Calculation of stress indices

Stresses are represented by indices ranging from 0 to 1, which will reduce the vital functions of the plant. These stresses are abiotic exogenous (N, water, and heat stress, including the effect of frost)

and endogenous (trophic stress: competition between leaves and fruit for available assimilates, and only concerns crops simulated as indeterminate).

Three N stress indices 'NNIs', 'NNIlai' and 'NNIsenes', which are involved in different physiological processes, are calculated from NNI (Brisson et al., 2009). These stress indices reduce RUE and LAI growth, and accelerate senescence, respectively.

For water deficit stress, 4 different stress indices that can affect the plant's physiological functions in different ways. They depend on the water content above the wilting point in the root zone. ‘humirac' delays emergence and slows deep root growth, 'turfac' delays development and slows leaf growth, 'senfac' accelerates leaf senescence, and 'swfac' reduces RUE and transpiration. For water stress due to excess water, 3 indices 'izrac', 'exolai' and 'exobiom' are calculated by STICS from the waterlogging index, called exofac, representing the proportion of root length that is in anoxic conditions during the growing season (exofac = 1 means that all roots are in anoxic conditions). The three indices affect root growth, LAI growth, and RUE, respectively.

For the frost stress, the stress variable is the minimum temperature of the crop. Frost response and damage vary according to the development stage. Different indices of frost stress can affect plant density, foliage (accelerated senescence) and fruit numbers.

C.1.3.9. Microclimate

The microclimate module calculates crop temperature from the energy balance, considering the plant's water status, cover ratio, and climatic conditions. Crop temperature is used to calculate soil temperature.

C.1.3.10. Crop management

This module considers the interactions and effects of the various cultivation techniques applied to the plot (sowing, fertilization, irrigation, tillage, crop residue restitution, mulching, harvesting decision and method) on the evolution of crop growth and development, soil functioning processes and microclimate parameters.

C.2. Experimental conditions

C.2.1. Study sites and experimental data

C.2.1.1. Experimental setup used at Agriculture and Agri-Food Canada's Normandin experimental farm

The long-term experiment initiated in 1989 at Agriculture and Agri-Food Canada's Normandin experimental farm is used in this study. The study site is located in the Saguenay-Lac-Saint-Jean region of eastern Quebec, Canada (48°50'N, 73°33'W, altitude 137 m). The region has a cold and humid continental climate. The Labarre clay-loam soil at Normandin is classified as a humic gleysol (Humic Cryaquept). In the first 15 cm, the soil contains 490 g kg^{-1} soil clay and 430 g kg^{-1} soil silt, pH_{water} is 5.6 and bulk density is 1.36 g cm^{-3}. The initial soil organic C content is 26.1 g C kg^{-1} soil, while the initial soil organic N content is 1.7 g N kg^{-1} soil. Further information on soil and site characteristics can be found in Bissonnette et al. (2001) and Maillard et al. (2016). The site had been cultivated under a spring barley (*Hordeum vulgare* L.) –alfalfa (*Medicago sativa* L.) rotation for about 10 years prior to 1990.

The experimental setup comprises 8 treatments and 4 replications, for a total of 32 plots measuring 10 m x 5 m. The 2 types of cropping sequences include a monoculture succession (M) of spring barley (*Hordeum vulgare* L., cv. 'Chapais' or 'Alyssa') and a 3-year cereal-perennial forage rotation (R) (1st year: under-seeding of barley with a mixture of timothy (*Phleum pratense* L. cv. 'Champ') and red clover (*Trifolium pratense* L. cv. 'Prosper'); 2nd and 3rd years: forage production). Only the plots cropped with continuous barley in monoculture, equivalent to 16 plot units, were considered in this study. The two tillage systems were a moldboard plow down to a 20–cm depth (MP) and a chisel plow down to a 15–cm depth (CP), performed yearly in the fall after harvest. The two N sources were ammonium nitrate (MIN) and N-based liquid dairy manure (LDM), applied according to local recommendation rates. Before seeding, plots under the MIN treatment received 70 kg N ha^{-1} yr^{-1}, 17.5 kg P ha^{-1} yr^{-1} as triple superphosphate, and 58 kg K $ha^{-1}yr^{-1}$ as potassium chloride. For the LDM plots, about 50 m^3 $ha^{-1}yr^{-1}$ of liquid dairy manure obtained from a local farm was applied in early spring, providing an average of 107 ±24 kg total N $ha^{-1}yr^{-1}$, 17 ±4 kg total P $ha^{-1}yr^{-1}$, and 119 ±29 kg total K ha^{-1} yr^{-1}.

For soil analysis, total soil C and N concentration (g kg^{-1}) was measured by dry combustion with a CNS analyzer (LECO, TRUSPEC, Leco Corp., St-Joseph, MI, USA) on air-dried soil, ground to pass 0.5 mm sieve. To limit the bias that could be introduced on the gain or loss in C and N by soil compaction or fragmentation, the total C and N concentration results will be adjusted by taking into

account the bulk density of the soils using the equivalent soil mass approach (Ellert & Bettany, 1995). Carbonates in the soil samples were negligible, so total C was equal to organic C. Bulk density measurements were carried out only in 1989, 1993, 2002, 2010. Stainless steel cylinders were used to determine the bulk density of each layer: 5.5 cm in diameter and 3 cm in height for the top layer (0-15 cm), and 5 cm in diameter and 5 cm high for the deeper layers. The bulk density for the years for which we have no measured data was calculated as an average of the measured bulk density of two years, preceding and following, for which we have measurements. Soil organic C and total N were then calculated at a depth of 0-20 cm. For plant analysis, grain, straw, and forage samples were mineralized with a solution of H_2SO_4 and H_2O_2 (Isaac & Johnson, 1976). The N concentration in digested solutions was measured by automated colorimetry using Lachat QuikChem 8000 autoanalyzer (QuikChem Method 13-107-06-2-E; Lachat Instruments, Milwaukee, WI, USA). The amount of N absorbed by the plant is then calculated from the product of plant N concentration and dry matter yield. Details of the measurement protocols are described in (Bissonnette et al., 2001; Lafond et al., 2016; Maillard et al., 2016).

C.2.1.2. Experimental setup used at Agriculture and Agri-Food Canada's Harlaka experimental farm

The second experimental setup was located at the site of Agriculture and Agri-Food Canada's Harlaka research farm, Lévis, QC, Canada (46°47′N, 71°07′W, altitude 65 m). Timothy (*Phleum pratense* L. cultivar "Champ") had been sown alone on a gravelly loam soil in May 1998 (Bélanger & Ziadi, 2008). A split-plot experimental design with four replicates was used with 16 combinations of 4 annual doses of P (0, 15, 30 and 45 kg P ha^{-1}) and 4 annual doses of N (0, 60, 120 and 180 kg N ha^{-1}). Calcium ammonium nitrate and triple superphosphate were applied each year before the start of forage growth in the first week of May from 1999 to 2006. A dose of 67 kg K ha^{-1} yr^{-1} was also applied to the plots at the same time as the N and P inputs, to ensure that K did not limit plant growth. Only the 32 experimental plots receiving 30 and 45 kg P ha^{-1} yr^{-1} were considered in this study to ensure that P was not limiting for plant growth throughout the experiment.

Timothy aboveground biomass was harvested once a year in the sowing year (1998) and biannually during the eight subsequent years (1999–2006). The harvests of aboveground biomass for both harvests were carried out at 5-cm height on 0.91 m × 2.1 m areas with a self-propelled flail forage harvester (Carter MGF Co., Inc., Brookston, IN). The first harvest was made at late heading during spring growth (mid-June) and the second harvest was made during summer regrowth (early August).

Forage yield dry matter (DM) content was determined on a 500 g fresh sample after weighing and drying at 55 °C in a forced-draft oven for 3 days. Dried samples were then ground using a Wiley mill

(Standard model 3, Arthur H. Thomas Co., Philadelphia, PA) fitted with a 1-mm screen for plant analysis. The N concentration in forage yield was determined by automated colorimetry using Lachat QuikChem 8000 autoanalyzer (QuikChem Method 13-107-06-2-D; Lachat Instruments, Milwaukee, WI) on subsamples previously mineralized by the method of Isaac & Johnson (1976). Briefly, this method consists of mineralizing dry, and ground (<1 mm) plant tissues subsamples with a mixture of sulfuric and selenious acids. The amount of N exported by forage yield was calculated by multiplying N concentrations by its yield DM content.

C.2.2. Climatic conditions

For both sites, according to the Köppen-Geiger classification, the climate is classified as cold and humid continental with no dry season ("Dfb" - strong seasonal variations in temperature and abundant, evenly distributed precipitation throughout the year). Nevertheless, variations and differences are observed between these two sites in terms of mean annual air temperature, precipitation, the sum of degree-days, and solar radiation.

C.2.2.1. Site de Normandin

For the Normandin site, the mean annual temperature between 1990 and 2020 was 2.0 °C (with a mean minimum of -3.7 °C and maximum of 7.6 °C). Over the 31 years of experimentation, annual precipitation averaged 850 mm, of which 511 mm (60%) occurred during the growing season. The average annual sum of degree-days (0°C basis) was 2441 °C d at Normandin. In terms of solar radiation, the Normandin site received an average of 2941 MJ m^{-2} per year between May and October (Tableau C.2).

C.2.2.2. Site d'Harlaka

For the Harlaka site, the mean annual temperature between 1998 and 2006 was 4.7°C (with extreme values ranging from -0.7°C to 10.2°C). The mean annual sum of degree-days (0°C basis) was 2797°C d. Over the years of experimentation, although somewhat irregular, average precipitation was 1142 mm, of which 683 mm (60%) fell between the beginning of May and the end of October. In terms of solar radiation, the Harlaka site received an average of 3027 MJ m^{-2} per year between May and October (Tableau C.2).

Table C.2 Data on annual growing degree-day (GDD) sums, air temperature (mean, minimum and maximum), precipitation (annual and during the May to October growing season), and global radiation (GR) (May to October) recorded at the environment Canada stations closest to the 2 experimental sites.

Site	**Normandin**						**Harlaka**					
Year	**GDD** [0°C basis]	**Temperature** [°C]			**Precipitation** [mm]	**GR** [MJ m^{-2}]	**GDD** [0°C basis]	**Air Temperature** [°C]			**Precipitation** [mm]	**GR** [MJ m^{-2}]
		Moy.	**Min.**	**Max.**				**Moy.**	**Min.**	**Max.**		
1990	2518	3.0	-2.0	8.0	858(495)	2822	-	-	-	-	-	-
1991	2531	2.6	-2.5	7.7	717(407)	3000	-	-	-	-	-	-
1992	2308	1.5	-3.4	6.4	839(503)	2858	-	-	-	-	-	-
1993	2483	1.9	-3.1	6.8	867(616)	2753	-	-	-	-	-	-
1994	2496	2.1	-2.8	7.0	814(489)	2945	-	-	-	-	-	-
1995	2629	2.9	-2.0	7.8	790(388)	3202	-	-	-	-	-	-
1996	2517	2.9	-2.0	7.7	1134(663)	2956	-	-	-	-	-	-
1997	2402	1.9	-2.9	6.7	733(443)	2719	-	-	-	-	-	-
1998	2533	3.4	-2.7	9.4	732(405)	2899	2943	5.9	1.4	10.3	1125(726)	3071
1999	2542	2.7	-3.5	8.8	875(552)	2992	2986	5.7	0.2	11.1	988(635)	3157
2000	2224	1.5	-4.6	7.5	702(379)	2878	2677	4.2	-0.6	9.0	1206(609)	2979
2001	2547	2.6	-3.4	8.7	832(555)	2861	2893	5.3	-0.5	11.0	994(644)	3130
2002	2221	0.9	-5.3	7.2	779(392)	3057	2658	4.4	-1.3	10.1	945(595)	3087

2003	2417	1.3	-4.7	7.3	805(441)	2907	2713	3.8	-1.6	9.1	1329(662)	2958
2004	2104	0.1	-6.1	6.3	785(461)	2782	2578	3.3	-2.7	9.3	1109(707)	2955
2005	2497	2.0	-4.1	8.1	702(398)	2973	2767	4.2	-2.0	10.4	1318(762)	2994
2006	2432	2.8	-2.8	8.5	1033(625)	2825	2955	5.8	0.4	11.3	1261(810)	2908
2007	2373	1.4	-4.9	7.7	697(464)	3089	-	-	-	-	-	-
2008	2423	1.2	-4.8	7.3	800(475)	2716	-	-	-	-	-	-
2009	2263	1.2	-4.7	7.1	683(440)	2807	-	-	-	-	-	-
2010	2510	3.8	-2.0	9.5	758(428)	2944	-	-	-	-	-	-
2011	2508	2.4	-3.4	8.3	890(614)	3076	-	-	-	-	-	-
2012	2641	3.1	-2.8	9.0	804(567)	2945	-	-	-	-	-	-
2013	2507	1.9	-3.9	7.7	965(557)	2990	-	-	-	-	-	-
2014	2519	1.4	-4.5	7.4	982(596)	2986	-	-	-	-	-	-
2015	2555	1.7	-4.5	7.8	958(529)	3002	-	-	-	-	-	-
2016	2486	2.0	-3.9	7.9	1291(757)	3034	-	-	-	-	-	-
2017	2413	1.6	-4.2	7.4	1117(688)	3129	-	-	-	-	-	-
2018	2388	1.6	-4.4	7.5	843(562)	3050	-	-	-	-	-	-
2019	2257	0.7	-5.1	6.6	742(372)	2953	-	-	-	-	-	-
2020	2440	2.8	2.2	3.4	838(588)	3026	-	-	-	-	-	-
Moy.	2441	2.0	-3.5	7.6	850(511)	2941	2797	4.7	-0.7	10.2	1142(683)	3027

C.3. Model evaluation

To calibrate and evaluate the STICS ability to predict the variables of interest, we calculated various complementary statistical criteria based on the comparison of predicted and observed data (Coucheney et al., 2015). A revisited linear regression procedure was used to test the model performance (Correndo et al., 2021b).

The normalized mean error (NME) (Equation C.11) estimates the model relative bias. A |NME| < 10% is considered a low bias (Falconnier et al., 2019; Morissette et al., 2016). The normalized root mean square error (NRMSE) (Equation C.12) allows for determination of the error of prediction of the model by giving more weight to high errors, which represents the relative mean deviation of the predicted values to the observed values. NRMSE is particularly useful when comparing results from different studies. According to Jamieson et al. (1991), the model is considered excellent when NRMSE ≤ 10%, good when 10% < NRMSE ≤ 20%, fair when 20% < NRMSE ≤ 30%, and poor when NRMSE > 30%. For the STICS calibration, the best sets of parameters were identified by minimizing NRMSE.

The efficiency of the model (EF) (Equation C.13) measures agreement between predicted and observed values. If the model is perfect, predicted values are equal to observed values, and EF= 1. Negative EF values mean that the model is not a better predictor than the average of the observations. Positive EF values greater than 0.40 are considered satisfactory (Beaudoin et al., 2008).

The coefficient of determination (R^2) (Equation C.14) was calculated for the linear regression between predicted and observed values to evaluate the strength ($R^2 < 0.25$: very weak; $0.25 \leq R^2 < 0.50$: weak; $0.50 \leq R^2 < 0.75$: moderate: $R^2 \geq 0.75$: substantial) of the linear model using the standardized major axis (SMA) regression. This approach proposed by Correndo et al. (2021b) overcomes the axis orientation problem of the traditional ordinary least squares method (y vs. x or x or y) (Piñeiro et al., 2008) and provides a single line regression (symmetric) defining the relationship regardless of which variable is x or y. Thus, the bivariate regression SMA model is likely to provide a more reliable regression line and error decomposition. The mean square error was also decomposed into percentage lack of precision (PLP) (Equation C.15) and percentage lack of accuracy (PLA) (Equation C.16), which refer to the percentage of dispersion and the systematic error, respectively. These criteria estimate the dominant type of the model error (either dispersion or systematic error). Statistical criteria were computed using the "STICSevalR" library and R-Code provided by Correndo et al.(2021a). Plots were made with the "ggplot2" library R.

$$\mathrm{NME}\ (\%) = 100\frac{\frac{1}{n}\sum_{i=1}^{n}(Obs_i - Pred_i)}{\overline{Obs}} \qquad \text{(Equation C.11)}$$

$$\mathrm{NRMSE}\ (\%) = 100\frac{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(Pred_i - Obs_i)^2}}{\overline{Obs}} \qquad \text{(Equation C.12)}$$

$$\mathrm{EF} = 1 - \frac{\sum_{i=1}^{n}(Pred_i - Obs_i)^2}{\sum_{i=1}^{n}(Obs_i - \overline{Obs})^2} \qquad \text{(Equation C.13)}$$

$$\mathrm{R}^2 = \left[\frac{\frac{1}{n}\sum_{i=1}^{n}(Pred_i - \overline{Pred})(Obs_i - \overline{Obs})}{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(Pred_i - \overline{Pred})^2}\sqrt{\frac{1}{n}\sum_{i=1}^{n}(Obs_i - \overline{Obs})^2}}\right]^2 \qquad \text{(Equation C.14)}$$

$$\mathrm{PLP}\ (\%) = 100\frac{\frac{1}{n}\sum_{i=1}^{n}\left(|Pred_i - \widehat{Pred_i}|\right)\left(|Obs_i - \widehat{Obs_i}|\right)}{\frac{1}{n}\sum_{i=1}^{n}(Pred_i - Obs_i)^2} \qquad \text{(Equation C.15)}$$

$$\mathrm{PLA}\ (\%) = 100\frac{\frac{1}{n}\sum_{i=1}^{n}\left(Obs_i - \widehat{Pred_i}\right)^2}{\frac{1}{n}\sum_{i=1}^{n}(Pred_i - Obs_i)^2} \qquad \text{(Equation C.16)}$$

$Pred_i$: predicted values; $\overline{Pred}$: mean of predicted values; Obs_i: observed values; $\overline{Obs}$: mean of observed values; $\widehat{Pred_i}$: value given by the linear regression of predicted *vs.* observed values; $\widehat{Obs_i}$: value given by the linear regression of observed *vs*. predicted values. *n*: number of predicted/observed pairs.

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CHAPTER 1: STICS soil–crop model performance for predicting biomass and nitrogen status of spring barley cropped for 31 years in a gleysolic soil from northeastern Quebec (Canada)

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Article

STICS Soil–Crop Model Performance for Predicting Biomass and Nitrogen Status of Spring Barley Cropped for 31 Years in a Gleysolic Soil from Northeastern Quebec (Canada)

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Abstract

Spring barley (*Hordeum vulgare* L.) is an increasingly important cash crop in the province of Quebec (Canada). Soil–crop models are powerful tools for analyzing and supporting sustainable crop production. STICS model has not yet been tested for spring barley grown over several decades. This study was conducted to calibrate and evaluate the STICS model, without annual reinitialization, for predicting aboveground biomass and N nutrition attributes at harvest during 31 years of successive cropping of spring barley grown in a soil (silty clay, Humic Gleysol) from the Saguenay–Lac-Saint-Jean region (northeastern Quebec, Canada). There is a good agreement between observed and predicted variables during the 31 successive barley cropping years. STICS predicted well biomass accumulation and plant N content with a low relative bias (|normalized mean error| = 0–13%) and small prediction error (normalized root mean square error = 6–25%). Overall, the STICS outputs reproduced the same trends as the field-observed data with various tillage systems and N sources. Predictions of crop attributes were more accurate in years with rainfall close to the long-term average. These 'newly calibrated' parameters in STICS for spring barley cropped under continental cold and humid climate require validation using independent observation datasets from other sites.

Keywords: STICS, soil–crop model, gleysol, spring barley, long-term experiment, cold and humid continental climate

Résumé

L’objectif de ce chapitre était de calibrer et d’évaluer le modèle STICS, sans réinitialisation annuelle, pour prédire la biomasse aérienne et les attributs de nutrition azotée à la récolte pendant 31 années de cultures successives d'orge de printemps cultivée dans un sol de la région du Saguenay-Lac-Saint-Jean (nord-est du Québec, Canada). Une bonne concordance entre les variables observées et prédites pendant les 31 années de culture est obtenue. STICS a bien prédit l'accumulation de biomasse et la teneur en azote des plantes avec un biais relatif faible (|erreur moyenne normalisée| = 0-13%) et une faible erreur de prédiction (erreur quadratique moyenne normalisée = 6-25%). Dans l'ensemble, les sorties STICS ont reproduit les mêmes tendances que les données observées sur le terrain avec différents systèmes de travail du sol et sources d'azote. Les prédictions des attributs des cultures étaient plus précises les années où les précipitations étaient proches de la normale.

Mots clés: STICS, modèle sol–culture, gleysol, orge de printemps, essai de longue durée, climat continental froid et humide.

1.1 Introduction

Spring barley (*Hordeum vulgare* L.) is used as cattle feed and for malting but grain barley production remains insufficient to meet the demand in the province of Quebec (Canada) (Ministère de l'Agriculture, des Pêcheries et de l'Alimentation du Québec, 2020). Even with the use of high-performance cultivars and improved crop management over the last decades, grain barley yields remain lower than in western Europe (Bulman et al., 1993; Holland et al., 2021). Average annual barley grain yields in Canada were 2.0 Mg DM ha^{-1} between 1960 and 1989, and 2.7 Mg DM ha^{-1} between 1990 and 2021 (Statistics Canada, 2021) compared to about 4.4 Mg DM ha^{-1} for western Europe (Friedt et al., 2011).

The cold and humid continental climate of eastern regions of Canada, including the province of Quebec, poses significant constraints for crop production (Bélanger & Bootsma, 2002). About 52% of the barley acreage in the province of Quebec is located in areas with limiting soil and climate conditions such as the Bas-Saint-Laurent, Gaspésie, Îles-de-la-Madeleine and Saguenay-Lac-Saint-Jean (Ministère de l'Agriculture, des Pêcheries et de l'Alimentation du Québec, 2020). In these areas, the mean annual temperature ranges from 1 to 3°C, and the last spring frost occurs late, up to the end of May. The sum of growing degree-days (GDD, basis 0 °C) between April and October ranges from 1800 to 2200 °C d, which corresponds to severe to moderate limitations for spring sown small grains according to climatic suitability ratings (Agriculture and Agri-Food Canada, 2010). Moreover, soils with excess water and poor fertility also limit crop production in these areas (Moore, 2021). For barley, waterlogging can reduce yields by 20 to 85% depending on the duration and intensity of the waterlogging at different stages of the plant's development and the cultivar tolerance (Setter et al., 1999).

The short growing season in several regions of northeastern Quebec dictates the choice of cultivars that can be grown successfully. Cultivars are known to differ in their phyllochron, which is positively corelated with temperature and daylength (Cao & Moss, 1989). Phenological traits were also shown to vary with locations (Juskiw et al., 2001). For instance, the time needed to reach anthesis from sowing is about 55 days (860-940 °C d) for two spring barley cultivars, Cadette (a semidwarf lodging-resistant type) and Leger (a standard lodging-susceptible type) grown under climatic conditions of Montreal region (province of Quebec) (Ma & Smith, 1992), but 10-20 days longer (up to 1200 °C d) in western Europe (Ma & Smith, 1992; Russell, 1990). Differences in cultivars and length of the growing season between western Europe and northeastern Quebec should therefore be taken into account in process-based models of barley growth and development. Understanding the growth and development of barley cultivars adapted to the cold and humid conditions of northeastern Quebec, which has short growing season is crucial for improving cultivars and crop management practices.

Soil–crop models are valuable and powerful tools for understanding many complex processes in agroecosystems (Oteng-Darko et al., 2013). They can be used to predict and analyze crop growth attributes (Quintero & Díaz, 2020) and the use of nitrogen (N) (Basso et al., 2010; Salo et al., 2016) and water (Cheng et al., 2022; Saadi et al., 2022), to assess the environmental impacts of agriculture by taking into account crop management, soils and climate (Lammoglia et al., 2017; Yin, Beaudoin, et al., 2020; Yin, Kersebaum, et al., 2020); and to test longer-term scenarios in the context of global warming (Constantin et al., 2012; Gardi et al., 2022). Several soil–crop models have been developed that differ in their structure, simulated process and approach (Yin et al., 2017), scales (plant, field, watershed, or regional) (Pasquel et al., 2022), and objectives (Di Paola et al., 2016). A number of process-based soil–crop models (e.g. DAISY, DSSAT-CERES, HERMES, MONICA, and WOFOST) are available for spring barley crops grown in Europe (Rötter et al., 2012; Salo et al., 2016). In western Canada, Jame et al. (1997) developed crop model using DSSAT for wheat and barley grown on the Great Plains of the Canadian province of Alberta. STICS (*Simulateur mulTIdisciplinaire pour les Cultures Standard*) is a generic soil–crop model initially developed in France for wheat (*Triticum turgidum* L. subsp. *durum*) and maize (*Zea mays* L.) and then for other annual and perennial crops in Europe (Brisson et al., 1998, 2003). STICS simulates crop growth and development along with soil water, C, and N processes (Beaudoin et al., 2008; Constantin et al., 2012). It has been tested in a large number of soil-plant agroecosystems and was designed to adapt easily to various crops and diverse climatic conditions (Coucheney et al., 2015; Lebonvallet, 2008; Sierra et al., 2003). STICS was tested and validated for spring barley cultivars cropped in the temperate climate of western Europe (Beaudoin et al., 2008; Corre-Hellou et al., 2009)

In Canada, STICS was calibrated and validated for soybean (*Glycine max* L. Merr) and spring wheat (*Triticum aestivum* L.) cultivars cropped in several sites distributed between southwestern Quebec province and southern Ontario province, which highlighted the opportunities for using STICS in areas with a short growing season (Jégo et al., 2010). The integration of a snow-cover module has extended the possibility of using STICS for cold and humid continental regions (Jégo et al., 2014). STICS has also been calibrated and evaluated for non-consecutive simulations with annual resetting under these conditions for maize (Jégo et al., 2011), potato (*Solanum tuberosum* L.) (Morissette et al., 2016), and timothy (*Phleum pratense* L.) (Jégo et al., 2013).

No crop growth model has been yet calibrated and evaluated over long-term cropping periods without annual resetting for spring barley in the soil and climate conditions of the Saguenay–Lac-Saint-Jean region (northeastern Quebec, Canada). This region occupies an immense territory (106.5 million km^2) relatively far from the rest of the province of Quebec (Ministère de l'agriculture, des pêcheries et de l'alimentation du Québec, 2014) and constitutes the northern limit of the practice of agriculture in Quebec. Its 149,204 hectares of soils with agricultural potential (Lapointe, 2006) and the combination of the cool climate and isolated geographic location provide the region with a unique place in the

agricultural industry due to its geographical position within the boreal zone. The objectives of this study were (i) to statistically analyze a dataset of dry matter aboveground biomass, grain yield, grain and shoot N concentration and N uptake at harvest over 31 successive cropping years of spring barley cultivars selected for the pedoclimatic conditions of the Saguenay–Lac-Saint-Jean region, (ii) to calibrate and evaluate the ability of STICS to predict the above-mentioned variables over several decades without annual reinitialization; and (iii) to compare the two approaches: Are STICS predictions for the experimental site and the associated database better or not than a statistical model?

1.2 Materials and methods

1.2.1 Experimental site and field database

The study was conducted using a long-term experiment that was initiated in the fall of 1989, at the Agriculture and Agri-Food Canada's Normandin Experimental Farm, at Normandin city, located in the regional county municipality of Maria-Chapdelaine, in the Saguenay–Lac-Saint-Jean region of the Canadian province of Quebec (lat. 48° 50' N; long. 72° 33' W; alt. 137 m). Since 1936, research conducted there has significantly helped to improve farming practices in Quebec's Saguenay—Lac-Saint-Jean region (Agriculture and Agri-Food Canada, 2024). The region has a cold and humid continental climate. For the 31 years considered in this study, cumulative rainfall from 10 days before seeding date to grain harvest ranged from 176 to 498 mm with an average of 317 mm. The average temperature was 16.0 °C (14.3–18.4 °C), the sum of GDD above 0 °C ranged from 1,431 to 1,775 °C d, and the cumulative global radiation ranged from 1,543 to 2,259 MJ m^{-2}. Values for each of the 31 years are presented in Table 1.S1 for the growing season and the entire year. The soil is a Labarre series silty clay (Humic Gleysol). Soil characteristics are presented in Table 1.1. The site had been cultivated under a spring barley–alfalfa (*Medicago sativa* L.) rotation for about 10 years prior to 1990.

Table 1.1 Properties of the soil layers at the initiation of Normandin experimental setup.

Soil characteristics	**Values**
Soil texture	Silty clay
Soil classification (Food and Agriculture Organization, 2014)	Humic gleysol
Clay <2 µm (g kg^{-1}) at 0-20 cm	490
Silt (2-50 µm) (g kg^{-1})	430
Sand (50-2000 µm) (g kg^{-1})	80
Organic N (g kg^{-1})	1.7
$CaCO_3$ (%)	<1
pH_{water} at 0-20 cm	5.6
Field capacity (% dry-mass soil): 0-20 cm 20-40 cm 40-100 cm	 29.0 26.7 25.6
Wilting point (% dry-mass soil): 0-20 cm 20-40 cm 40-100 cm	 20.0 19.2 18.6
Bulk density (g_{soil} cm^{-3}_{soil}): 0-20 cm 20-40 cm 40-100 cm	 1.36 1.50 1.60

The experimental design was a factorial split-split-plot replicated four times with two types of crop rotation randomized into main plots (a continuous barley in monoculture and a 3-year cereal-perennial forage rotation), two tillage systems randomly assigned to subplots and two N sources randomly assigned to sub-subplots (Lafond et al., 2016). Only the plots cropped with continuous barley in monoculture (16 plot units 10 m × 5 m in size) were considered in this study. Six-row spring barley cultivars Chapais (1990−2014) and Alyssa (2015−2020) (Kong et al., 1994), both having similar ecophysiological parameters, were sown between 9 and 31 May at a rate of 360 grains m^{-2} using a conventional cereal seeder. Details of N application along with dates of seeding, harvest and tillage for each year are provided in Table 1.S2. The two tillage systems consisted of a moldboard plow operated to a 20-cm depth (MP) and a chisel plow to a 15-cm depth (CP), with tillage performed yearly in the fall after harvest. The two N sources were ammonium nitrate (MIN) and N-based liquid dairy manure (LDM), applied according to local recommendations. The LDM were analyzed annually, and N concentrations were determined using a LECO CNS-1000 analyzer (LECO Corp., St. Joseph, MI, USA). Before seeding, plots under the MIN treatment received 70 kg N ha^{-1} yr^{-1} as ammonium nitrate, 17.5 kg P ha^{-1} yr^{-1} as triple superphosphate, and 58 kg K ha^{-1} yr^{-1} as potassium chloride. For the LDM plots, about 50 m^3 $ha^{-1}yr^{-1}$ of liquid dairy manure obtained from a local farm was applied in

early spring, providing an average of 107 ±24 kg total N ha^{-1} yr^{-1}, 17 ±4 kg total P ha^{-1} yr^{-1}, and 119 ±29 kg total K ha^{-1} yr^{-1}. Annual amounts of N applied as LDM from 1990 to 2020 are reported in Table 1.S2.

1.2.2 Plant analysis

Grain yield (GY) and straw yield were determined every year from 1990 to 2020 in the 16 experimental plots. Grain and straw yields were measured in a 8.2 m × 1.62 m area at grain maturity between mid-August and mid-September depending on the year (Table 1.S2), using a Wintersteiger plot harvester (Salt Lake City, UT, USA). Dry matter content of grain and straw was determined on a fresh 500 g subsample after drying in a forced draft oven at 55 °C to constant weight. Straw residues were returned to the soil after harvest. Nitrogen-concentrations in grain (NCG) and straw were measured only from 1997 to 2020. Dried and ground (to pass through a 1 mm screen) subsamples of grain and straw were digested using a mixture of sulfuric and selenious acids, as described by Isaac and Johnson (1976). The N concentration in digested solutions was measured by automated colorimetry using a Lachat QuikChem 8000 autoanalyzer (QuikChem Method 13-107-06-2-E; Lachat Instruments, Milwaukee, WI). Dry matter aboveground biomass (grain+straw) (AGB), N concentration in AGB (NCAGB), and N accumulation in AGB (NU) and grain (NAG) were then calculated.

1.2.3 STICS soil–crop model overview

STICS is a generic soil–crop model applicable to a wide variety of agroecosystems which has been in development since 1996 (Beaudoin et al., 2022; Brisson et al., 1998, 2003). Based on general ecophysiological concepts and soil processes that describe the functioning of soil-plant systems, STICS simulates the dynamic of soil–plant systems on a daily time step as a function of climatic conditions, crop and soil characteristics, and management practices (Figure 1.1). It calculates agricultural (e.g., crop yield and grain N content) and environmental (e.g., soil water and mineral N contents, N leaching, and soil organic carbon dynamic) variables simultaneously (Constantin et al., 2012). STICS has several interdependent modules and sub-modules which were built by assembling and synthesizing parts or formalisms of existing models (Beaudoin et al., 2022; Brisson et al., 2009). Each module or sub-module deals with a particular physical or ecophysiological process, and variables are exchanged between modules and sub-modules. The description of these processes mostly relies on a unique set of general parameters. In STICS, two types of plant parameters are defined: cultivar parameters and generic parameters that are assumed to be the same for all cultivars of the same species. An in-depth description of STICS concepts, mathematical equations, general parameterization, and uses can be found in Brisson et al. (2009) and Beaudoin et al. (2022).

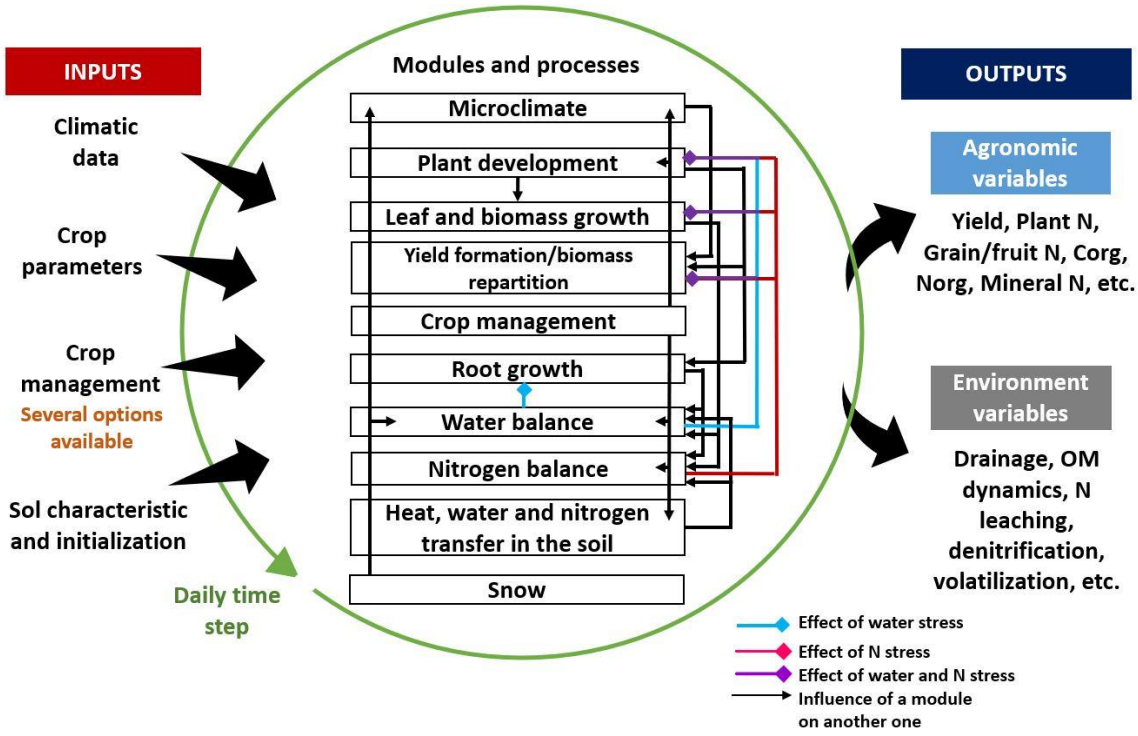

Figure 1.1 STICS soil–crop model: inputs, outputs, the different modules/processes, and their respective influences.

Briefly, the phenological development stages of a given crop cultivar, are expressed in development units that are mainly governed by thermal (degree-day), photothermal, or vernal-photothermal indices (according to the species) but are also affected by limiting factors such as soil water and N content. Shoot biomass accumulation is calculated from the leaf area index (LAI) by converting intercepted radiation into biomass using the radiation use efficiency (RUE) concept. These processes are closely influenced by the phenological development stage, temperature, and plant density along with water stress and N stress. The grain C content is derived from the retranslocation of vegetative C as well as from the continued assimilation of C during grain filling. The GY is calculated by applying a progressive “harvest index” to the AGB dry weight of the plant (Beaudoin et al., 2022), i.e. the ratio of the biomass accumulated in the GY from the beginning of grain filling until maturity is an increasing proportion of the AGB.

Plant N accumulation depends on soil mineral N availability in the soil–root system (and symbiotic fixation for legumes) and on crop N requirements. Crop N requirements were calculated using the concept of maximum (N_{cmax}) and critical N (N_c) dilution curves. The N_{cmax} curve represents the plant’s maximum capacity to accumulate N in its shoot biomass and is used in STICS to calculate potential crop N uptake. The N_c curve represents the N concentration in shoots required to produce the maximum AGB at a given time (Lemaire et al., 2008). It can be used to calculate the N nutrition index

(NNI), which is the ratio of the actual N concentration to N_c. The NNI is used to determine if the plant is under N stress or not. An NNI below 1 will reduce potential crop growth. For spring barley, the N_{cmax} and N_c were calculated using the following equations: N_{cmax}= 6.66×(Shoot Biomass)$^{-0.39}$ and N_c= 4.76×(Shoot Biomass)$^{-0.39}$, respectively (Zhao, 2014). As with C, NAG is calculated as a function of a dynamic N harvest index, i.e., the amount of N accumulated in grains from the beginning of grain filling until maturity is an increasing proportion of the amount of N in the AGB.

In STICS, the soil is described as a succession of up to five horizontal layers with their hydrodynamic and pedological characteristics. Soil dependent modules calculate water, C, and N balances and, consequently, the effects of water stress and N stress on crops. Humus mineralization depends on soil characteristics (clay and $CaCO_3$ content), soil organic N content, temperature, and soil water content. Mineralization of organic residues is calculated as a function of the C/N ratio based on the model of Nicolardot et al. (2001). Interactions between soil and crops occur through the roots, which operate exclusively as mineral N and water absorbers. Root growth is derived from root density, which is calculated separately from AGB growth in the model, unless the “trophic-link root length expansion” option is selected. STICS simulates crop water stress due to excess or lack of water, based on soil water content available to roots and crop requirements, which are directly linked to climatic conditions (rainfall) or crop management (absence/presence of irrigation). In case of water excess, a waterlogging index (exofac), which is the proportion of root length that is under anoxic conditions during the growing season, is calculated and used in the model to calculate three anoxic stress indices that affect root growth, LAI growth, and RUE.

STICS considers commonly used farming practices such as soil tillage, irrigation, and the use of mineral or organic fertilizers. The model includes eight types of mineral N fertilizers which differ in term of ammonium fraction, microbial immobilization, and volatilization. There are 10 categories of organic fertilizers, each with specific decomposition parameters (Beaudoin et al., 2022).

1.2.4 Model inputs and simulation options

The V10 version of STICS was used (Beaudoin et al., 2022). The model was initialized only once, in the spring of 1990, and used without resetting to simulate successive cropping cycles of spring barley over 31 years (1990-2020) continuously.

Soil input parameters (clay and $CaCO_3$ contents, pH, organic N, and bulk density) were obtained from soil analyses carried out at the beginning of the experiment (Table 1.1). Gravimetric soil water content at field capacity and wilting point was calculated or derived from analyses using a pedo-transfer function (Saxton & Rawls, 2006). In STICS, mineralization is assumed to occur up to a maximum depth (profhum) and to be negligible below this depth. This ‘profhum’ was assumed to be 20 cm. Soil depth and maximum rooting depth were set to 1 m. Initial soil water content was set to field capacity,

which is representative of the soil moisture status in early spring when soils are recharged with moisture from snowmelt. We assumed that the mineral N amounts were 30, 35, and 20 kg N ha^{-1} for the 0-20, 20-40, and 40-100 cm soil layers, respectively. These values are consistent with soil mineral N contents measured in spring after an alfalfa stand termination (Malhi et al., 2007). In keeping with the finding of Martel and Lasalle (1977) reported for a gleysolic Ap horizon, sampled on the experimental farm of Agriculture Canada at La Pocatière, Quebec (lat. 47° 20´00˝ N; long. 70° 2'00˝ W), the proportion of inactive soil organic matter (finert) was set to 55% rather than 65% , which is used as default value in STICS.

Climate inputs include minimum and maximum air temperatures, global radiation, precipitations, wind velocity, and relative humidity. Daily weather data from 1990 to 2020 (Table 1.S1) were obtained from Environment Canada's Normandin weather station (lat. 48°50´30˝ N; long. 72°32´49˝ W, alt. 137 m). Missing values (about 2% of the total) were imputted by using data obtained from the Saint-Prime weather station (lat. 48°37´00˝ N; long. 72°25´00˝ W, alt. 121 m), located approximately 20 km from Normandin. Management practices such as dates and rates of sowing and N fertilization as well as harvesting dates were carefully recorded (Table 1.S2).

1.2.5 Calibration of crop parameters for new cultivars and STICS performance evaluation

Although default values of parameters for several crop species and cultivars are provided in STICS, these values can be adapted or modified for new cultivars. Two datasets, designated the "calibration dataset" and the "evaluation dataset", were used to calibrate these parameters and evaluate the performance of STICS. The calibration dataset included data with 28 predicted/observed data pairs (7 years × 4 treatments) from 1997 to 2003. AGB, GY, NCAGB, NCG, NU, and NAG data were available for those seven years and cumulative rainfall during the growing season was near the 31-year average. STICS was statistically evaluated using the calibrated crop parameters and the remaining cropping years (from 1990 to 1996 and 2004 to 2020 for AGB and GY, and from 2004 to 2020 for NCAGB, NCG, NU, and NAG).

Calibration, which consists of adjusting the values of the parameters used in specific equations to fit the output to a set of measured state variables, was performed using a method proposed by the STICS development team (Guillaume et al., 2011; Jégo et al., 2010). Among the cultivars already available in STICS, we selected the European spring barley cultivar Scarlett as a reference, as it gave better evaluation results with our data set. Scarlett is a modern European two-row spring barley cultivar (Hickey et al., 2017). We reviewed the literature to identify key parameters of barley cultivars cropped in the province of Quebec that could be directly integrated into STICS. Then we took values directly from the literature or our experimental dataset for six parameters: maximum number of grains

per surface area (*nbgrmax*), maximum grain weight (*pgrainmaxi*), maximum crop height (*hautmax*), sum of degree-days between emergence and beginning of grain filling (*stlevdrp*), and sum of degree-days between beginning of grain filling and maturity (*stdrpmat*). Finally, parameter optimization was carried out in successive steps following the structure of the model, with each step corresponding to a key process in the simulation of the variables of interest. Priority was given to the cultivar-related parameters in order to preserve the genericity of the model as much as possible. Parameter optimization was performed with the Javastics application using the simplex method, which involves minimizing the mean square error for a given target variable (Buis et al., 2011).

1.2.6 Statistical analysis and model evaluation

Linear mixed model using the "*lme"* function in the R package "nlme"(Pinheiro et al., 2022) was performed with field-observed data considering replicates as a random factor and both years, N source type, tillage system, and their interactions as fixed factors. The year factor was used to fit a first-order autoregressive covariance structure to consider the repeated measurements across 31 years. Residuals were analyzed for normality using the Shapiro-Wilks and Levene's test for homogeneity of variances. Where treatment or interaction effects were significant at the 0.05 probability level, means were compared using LSMEANS. We evaluated the predictive ability of the fitted mixed model using 5-fold cross validation with the "cvFit" function in the R package "cvTools" (Alfons, 2023).

To calibrate and evaluate the ability of STICS to predict AGB, GY, NCAGB, NCG, NU, and NAG of spring barley, we calculated various complementary statistical criteria based on the comparison of predicted and observed data (Coucheney et al., 2015). A revisited linear regression procedure was used to test model performance (Correndo et al., 2021b).

The mean absolute error (MAE) (Equation 1.1) quantifies the average magnitude of the errors between the observed value and the predicted value. The normalized mean error (NME) (Equation 1.2) estimates the model's relative bias. An $|NME| < 10\%$ is considered a low bias (Falconnier et al., 2019; Morissette et al., 2016). The normalized root mean square error (NRMSE) (Equation 1.3) is used to determine the error of prediction of the model by giving more weight to larger errors and it represents the relative mean deviation of the predicted values to the observed values. The NRMSE is particularly useful when comparing results from different studies. According to Jamieson et al. (1991), a model is considered excellent when $NRMSE \leq 10\%$, good when $10\% < NRMSE \leq 20\%$, fair when $20\% < NRMSE \leq 30\%$, and poor when $NRMSE > 30\%$. For the STICS calibration, the best sets of parameters were identified by minimizing the NRMSE.

The efficiency of the model (EF) (Equation 1.4) measures the level of agreement between predicted and observed values. If the model is perfect, predicted values are equal to observed values, and

EF = 1. Negative EF values mean that the model is not a better predictor than the average of all the observations. Positive EF values greater than 0.40 are considered satisfactory (Beaudoin et al., 2008).

The coefficient of determination (R^2) (Equation 1.5) was calculated for the linear regression between predicted and observed values in order to assess the strength ($R^2 < 0.25$: very weak; $0.25 \leq R^2 < 0.50$: weak; $0.50 \leq R^2 < 0.75$: moderate: $R^2 \geq 0.75$: substantial) of the linear model by using the standardized major axis (SMA) regression. This approach proposed by Correndo et al. (2021b) overcomes the axis orientation problem of the traditional ordinary least squares method (y vs. x or x vs. y) (Piñeiro et al., 2008) and provides a single line regression (symmetric) defining the relationship regardless of which variable is x or y. Thus, the bivariate regression SMA model is likely to provide a more reliable regression line and error decomposition. The mean square error was also decomposed into percentage lack of precision (PLP) (Equation 1.6), which refers to the percentage of dispersion, and percentage lack of accuracy (PLA) (Equation 1.7), which refers to the systematic error. These criteria estimate the dominant type of model error (either dispersion or systematic error). Statistical criteria were computed using the "STICSevalR" library and R-Code provided by Correndo et al. (2021a). Plots were created with the R library "ggplot2".

$$\mathrm{MAE} = \frac{1}{n}\sum_{i=1}^{n} |Obs_i - Pred_i| \qquad \text{(Equation 1.1)}$$

$$\mathrm{NME}\ (\%) = 100\frac{\frac{1}{n}\sum_{i=1}^{n}(Obs_i - Pred_i)}{\overline{Obs}} \qquad \text{(Equation 1.2)}$$

$$\mathrm{NRMSE}\ (\%) = 100\frac{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(Pred_i - Obs_i)^2}}{\overline{Obs}} \qquad \text{(Equation 1.3)}$$

$$\mathrm{EF} = 1 - \frac{\sum_{i=1}^{n}(Pred_i - Obs_i)^2}{\sum_{i=1}^{n}(Obs_i - \overline{Obs})^2} \qquad \text{(Equation 1.4)}$$

$$\mathrm{R}^2 = \left[\frac{\frac{1}{n}\sum_{i=1}^{n}(Pred_i - \overline{Pred})(Obs_i - \overline{Obs})}{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(Pred_i - \overline{Pred})^2}\sqrt{\frac{1}{n}\sum_{i=1}^{n}(Obs_i - \overline{Obs})^2}}\right]^2 \qquad \text{(Equation 1.5)}$$

$$\mathrm{PLP}\ (\%) = 100\frac{\frac{1}{n}\sum_{i=1}^{n}(|Pred_i - \widehat{Pred}_i|)(|Obs_i - \widehat{Obs}_i|)}{\frac{1}{n}\sum_{i=1}^{n}(Pred_i - Obs_i)^2} \qquad \text{(Equation 1.6)}$$

$$\mathrm{PLA}\ (\%) = 100\frac{\frac{1}{n}\sum_{i=1}^{n}(Obs_i - \widehat{Pred}_i)^2}{\frac{1}{n}\sum_{i=1}^{n}(Pred_i - Obs_i)^2} \qquad \text{(Equation 1.7)}$$

$Pred_i$: predicted values; $\overline{Pred}$: mean of predicted values; Obs_i: observed values; $\overline{Obs}$: mean of observed values; $\widehat{Pred}_i$: value given by the linear regression of predicted *vs.* observed values; $\widehat{Obs}_i$: value given by the linear regression of observed *vs*. predicted values. *n*: number of predicted/observed pairs.

Prediction performance was also evaluated based on the waterlogging index (exofac) calculated by STICS which is the proportion of root length that is under anoxic conditions during the growing season (exofac = 0; 0 < exofac < 0.06; 0.06 ≤ exofac < 0.14). A value of 1 means that all roots are under anoxic conditions.

1.3 Results

1.3.1 Statistical analysis of field-observed data

The analyses of variance and the means of treatments or interactions are presented in Table 1.2. All crop production attributes (AGB, GY, NCAGB, NCG, NU, and NAG) at harvest differed significantly among years, and N source type in this study. The differences between years are likely to be related to climatic conditions rather than treatment effects since the lowest AGB and GY were generally associated with unfavorable rainfall conditions (1991, 1993, 1994, 1995, 2003, 2014, 2018 and 2020). For these years, the amount of rainfall in June or during the growing season was either too low or too high when compared with the norm of 78 mm and 317 mm, respectively (Table 1.S1). The MIN treatment performed better than the LDM treatment in terms of AGB and GY (4.7 vs. 3.9 Mg DM ha^{-1} yr^{-1} and 3.0 vs. 2.4 Mg DM ha^{-1} yr^{-1}, respectively). The NU and NAG were greater, while NCAGB and NCG were lower for the MIN treatment than for the LDM treatment (Table 1.2). The tillage system had a low but significant impact on GY, NCAGB and NAG. The GY, NCAGB and NAG were slightly greater for the MP treatment than for the CP treatment. In addition, significant interactions between years and N source type, year and tillage system, and N source type and tillage system were observed except for NCG (Table 1.2; Figure 1.S1). However, there was no significant effect of the interactions between year, N source type and tillage system for all the variables. Although we have excluded the data from the first 3 years following initiation (1990, 1991, 1992), probably influenced by the preceding alfalfa crop rotation, a slight drop in yield was observed over time for the 2 N sources and the 2 tillage systems (Figure 1.S2).

Table 1.2 Analysis of variance of the effects of year, N source type and tillage system on the field-observed aboveground biomass (AGB), grain yield (GY), N concentration in aboveground biomass (NCAGB) and in grain (NCG), N uptake by plant (NU), and N amount in grain (NAG); and mean of field-observed values. LDM: liquid dairy manure; MIN: ammonium nitrate; MP: moldboard plow; CP: chisel plow. Different letters (a, b, c, d) indicate significant differences among treatment according to a Lsmeans post hoc test ($P < 0.05$).

Source	AGB (Mg DM ha^{-1})	GY (Mg DM ha^{-1})	NCAGB (g kg^{-1} DM)	NCG (g kg-1 DM)	NU (kg N ha^{-1})	NAG (kg N ha^{-1})
	p-value					
Year (Y)	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
N source type (N)	**<0.0001**	**<0.0001**	**<0.0001**	**0.0008**	**<0.0001**	**<0.0001**
Tillage system (T)	0.9464	**<0.0001**	**<0.0001**	0.1857	0.3647	**0.0007**
Y×N	**<0.0001**	**<0.0001**	**<0.0001**	0.0535	**<0.0001**	**<0.0001**
Y×T	**<0.0001**	**<0.0001**	**0.0002**	0.1805	**0.0003**	**0.0002**
N×T	**0.0002**	**0.0007**	**0.0328**	0.4104	**0.0332**	**0.0199**
Y×N×T	0.6422	0.4050	0.9160	0.9316	0.3748	0.6536
Mean of field-observed values						
N source type						
MIN	4.7 a	3.0 a	16.1 b	19.8 b	73.2 a	57.1 a
LDM	3.9 b	2.4 b	16.6 a	20.2 a	62.0 b	45.7 b
Tillage system						
MP	4.3 a	2.8 a	16.6 a	20.1 a	67.2 a	52.2 a
CP	4.3 a	2.6 b	16.2 b	20.0 a	68.0 a	50.6 b
N source type × Tillage system						
MIN-MP	4.8 a	3.1 a	16.2 b	19.8 b	74.1 a	58.8 a
MIN-CP	4.6 b	2.9 b	16.0 b	19.8 b	72.3 a	55.4 b
LDM-MP	4.0 c	2.4 c	17.0 a	20.3 a	60.3 c	45.6 c
LDM-CP	3.8 d	2.4 c	16.3 b	20.1 ab	63.7 b	45.7 c

The evaluation of the ability of the mixed model considered in this study to predict the AGB, GY, NCAGB, NCG, NU and NAG is presented in Table 1.3. For each variable, the model had low MAE and RMSE from 5-fold cross-validation. For NCAGB and NCG, the model predictions were excellent with NRMSE of 8% and 7%, respectively. For AGB, GY, NU and NAG, the model prediction was good with NRMSE of 17% or 18%.

Table 1.3 Linear mixed model evaluation metrics from 5-fold cross-validation. Independent variables were aboveground biomass (AGB), grain yield (GY), N concentration in aboveground biomass (NCAGB) and in grain (NCG), N uptake by plant (NU), and N amount in grain (NAG).

Independent variable	MAE	RMSE	NRMSE (%)
AGB (Mg DM ha^{-1})	0.6	0.7	17
GY (Mg DM ha^{-1})	0.4	0.5	17
NCAGB (g kg^{-1} DM)	1.0	1.3	8
NCG (g kg^{-1} DM)	0.9	1.3	7
NU (kg N ha^{-1})	8.7	11.3	17
NAG (kg N ha^{-1})	7.1	9.3	18

MAE: mean absolute error; RMSE: root mean square error; NRMSE: normalized root mean square error.

1.3.2 Calibration to add new cultivar adapted to northeastern Quebec conditions in STICS

Default parameter values for the European reference cultivar (Scarlett) defined in STICS and newly calibrated parameter values for the Chapais spring barley cultivar adapted to the short-growing season area are presented in Table 1.4. Based on the literature and data from our experimental site, the sum of GDD from emergence to the beginning of grain filling (*stlevdrp*) was reduced to 800 °C d and the duration of grain filling (*stdrpmat*) was reduced to 565 °C d (Table 1.4). Thus, the sum of GDD between emergence and physiological maturity (*stlevdrp+stdrpmat*) decreased from 1,555 °C d for the Scarlett cultivar to 1,365 °C d for the Chapais cultivar.

Predictions of LAI dynamics were not assessed because measured LAI data were not available. To improve the overestimated AGB predictions obtained with the default parameters, we set out to optimize the parameters controlling LAI dynamics (*dlaimaxbrut, stlevamf, stamflax, durvief*, and *innsen*) (Table 1.4). The maximum rate of leaf growth during LAI development (*dlaimaxbrut*) decreased. The sum of GDD between emergence and the end of the juvenile stage (*stlevamf)* and between the end of the juvenile stage and the maximum LAI (*stamflax)* both increased by 80 °C d relative to the default values after the optimization procedure. Therefore, the maximum LAI occurred at about 900 °C d after emergence. The parameters describing potential RUE (efcroijuv, efcroiveg, and efcroirepro), which is used for the calculation of shoot biomass were also reduced (Table 1.4).

Table 1.4 Default values of parameters of the Scarlett cultivar of spring barley in the standard version of STICS and the newly calibrated values for the Chapais cultivar adapted for short-growing season area (specific cultivar parameters are shown in italics).

Parameter name and definition	Default values in STICS	Newly calibrated values	Source
Phenological stages			
stlevamf: sum of degree-days between the beginning of growth and maximum acceleration of leaf growth (°C d)	400	480	Optimization
stamflax: sum of degree-days between the maximum acceleration of leaf growth and the maximum LAI (°C d)	340	420	Optimization
stlevdrp: sum of degree-days between the beginning of growth and the beginning of the reproductive stage (°C d)	940	800	(Ho et al., 1995, 2000, 2002) /Calculation
stdrpmat: sum of degree-days between the beginning of grain filling and the maturity (°C d)	615	565	Calculation
Leaves			
dlaimaxbrut: maximum rate of daily increase of LAI (m^2 $plant^{-1}$°C d^{-1})	0.00077	0.00028	Optimization
durvief: maximal lifespan of an adult leaf (Q_{10})	200	180	Optimization
hautmax: maximum height of crop (m)	1.00	0.85	(Ho et al., 1995, 2000, 2002)
Innsen: N stress function active on senescence	-0.17	-0.18	Optimization
Innturgmin: N stress function active on leaf expansion	-0.65	-0.73	Optimization
Shoot biomass growth			
*teopt: b*eginning of the thermal optimum plateau for net photosynthesis (°C)	12	16	Optimization
efcroijuv: maximum radiation use efficiency during the juvenile phase (g DM MJ^{-1})	2.25	1.75	Optimization
efcroiveg: maximum radiation use efficiency during the vegetative phase (g DM MJ^{-1})	4.5	2.2	Optimization
efcoirepro: maximum radiation use efficiency during the reproductive phase (g DM MJ^{-1})	4.5	4.1	Optimization
Nitrogen			
INNimin: instantaneous NNI corresponding to INNmin	-0.5	-0.77	Optimization
Yield formation			
*nbgrmax: m*aximum number of grains per surface area (grain m^{-2})	26000	17500	(Spaner et al., 2001)
pgrainmaxi: Maximum weight of one grain (g)	0.044	0.046	(Ho et al., 1995, 2000, 2002)

Table 1.4 – Continued from previous page			
Parameter name and definition	**Default values in STICS**	**Newly calibrated values**	**Source**
nbjgrain: Number of days used to compute viables grains number (d)	20	30	Optimization
cgrain: slope of relationship between grain number and growth rate	0.028	0.132	Optimization
*vitircarb: r*ate of increase of the C harvested index vs. time (g $g^{-1}d^{-1}$)	0.0192	0.031	Optimization
*vitirazo: r*ate of increase of the N harvest index vs. time (g $g^{-1}d^{-1}$)	0.0308	0.038	Optimization

When the default parameters of the Scarlett cultivar were used, AGB was poorly predicted and largely overestimated with NME = -42% (Table 1.S3). Differences in AGB accumulation and crop cycle duration between the Scarlett and the Chapais cultivar (Figure 1.2) reflect the overall effects of differences in the cultivars' phenological parameters. For the same seeding date, the Chapais cultivar reached maturity on average 18 days earlier than the Scarlett cultivar under the conditions of northeastern Quebec. On average for the seven years and the four management units, the predicted AGB was 4.4 ±0.3 Mg DM ha^{-1} for the Chapais cultivar and 6.4 ±1.0 Mg DM ha^{-1} for the Scarlett cultivars, respectively. This reduction in AGB for the norteastern Quebec cultivar resulted from the decrease in the parameters relative to the maximum rate of daily increase in LAI and the potential RUE. In addition, the *vitircarb* and *vitirazo* values were adjusted (Table 1.4) to increase the annual GY and NCG values, respectively, which were underestimated with the Scarlett parameters (NME = 16 and 38%, respectively).

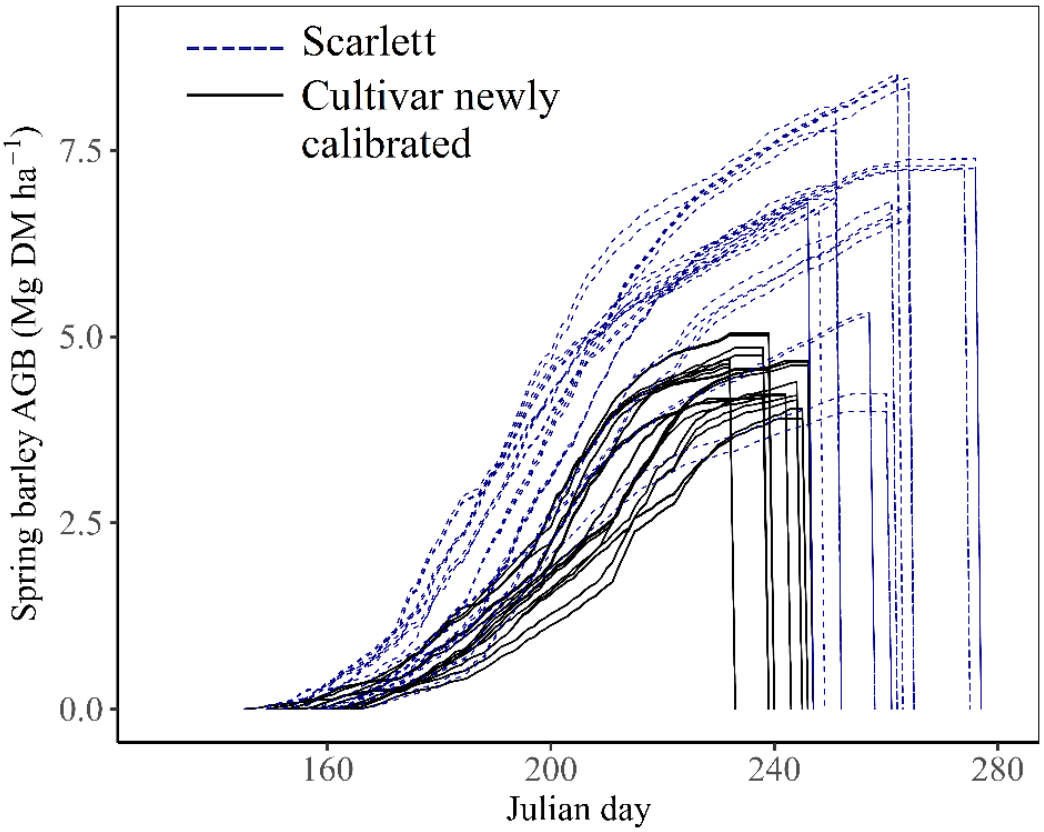

Figure 1.2 Predicted aboveground biomass (AGB) of cultivar Scarlett (blue dashed line) and the newly calibrated cultivar Chapais (black solid line) with calibration dataset (7 years and 4 treatments per year making 28 AGB curves).

1.3.3 Comparison between observed and predicted values

1.3.3.1 Aboveground biomass and grain yield at harvest

The observed AGB values for all treatments over 31 years of the cropping experiment ranged from 2.2 to 7.8 Mg DM ha^{-1} yr^{-1} with a mean of 4.3 ±1.2 Mg DM ha^{-1} yr^{-1} whereas the predicted AGB values ranged from 2.8 to 6.4 Mg DM ha^{-1} yr^{-1} with a mean of 4.3 ±0.6 Mg DM ha^{-1} yr^{-1} (Figure 1.3a). The mean of observed GY values was 2.7 ±0.8 and the mean of predicted GY values was 2.8 ±0.4 Mg DM ha^{-1} yr^{-1} (Figure 1.3b), with a narrower range for predicted values (1.8–4.0) than for the observed values (0.9–5.2).

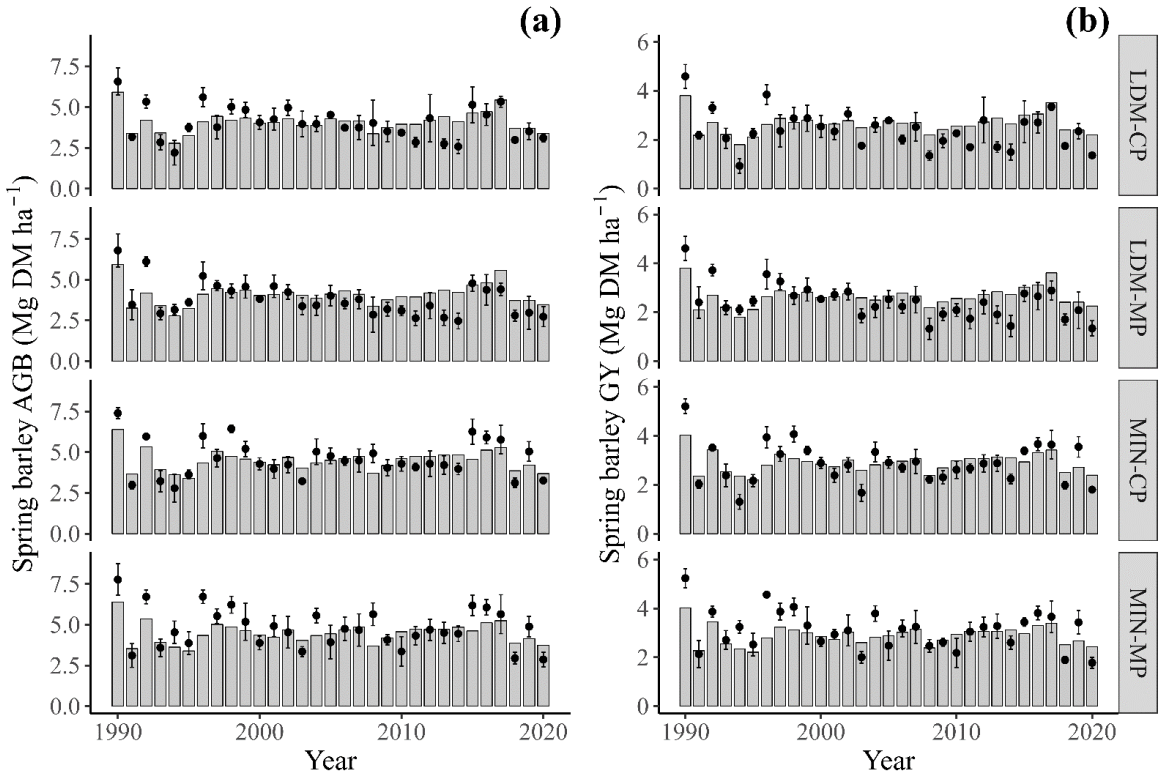

Figure 1.3 Annual mean of observed (dots) and predicted (grey bars) (a) spring barley aboveground biomass (AGB) and (b) grain yield (GY) from 1990 to 2020 for soil tillage and N fertilization source treatments. Bars on dots are standard deviation (n=4). LDM: liquid dairy manure; MIN: ammonium nitrate; MP: moldboard plow; CP: chisel plow.

After the calibration, STICS performed well in predicting AGB and GY with a low bias (NME = 3% and 0%, respectively), good NRMSE (14% and 16%, respectively), and moderate R^2 (0.44 and 0.69, respectively) (Figures 1.4a, 1.4c). The STICS evaluation with the 24 remaining cropping years gave similar performance for AGB and GY with a low bias (NME = 0% and -3%, respectively), a small NRMSE (21% and 23%, respectively), a moderate R^2 and a satisfactory EF (Figures 1.4b, 1.4d).

The error decomposition indicated that, for the evaluation dataset, the model errors for AGB and GY are due to dispersion error rather than systematic error (PLP > PLA); however, the opposite was true for the calibration dataset (Figure 1.4).

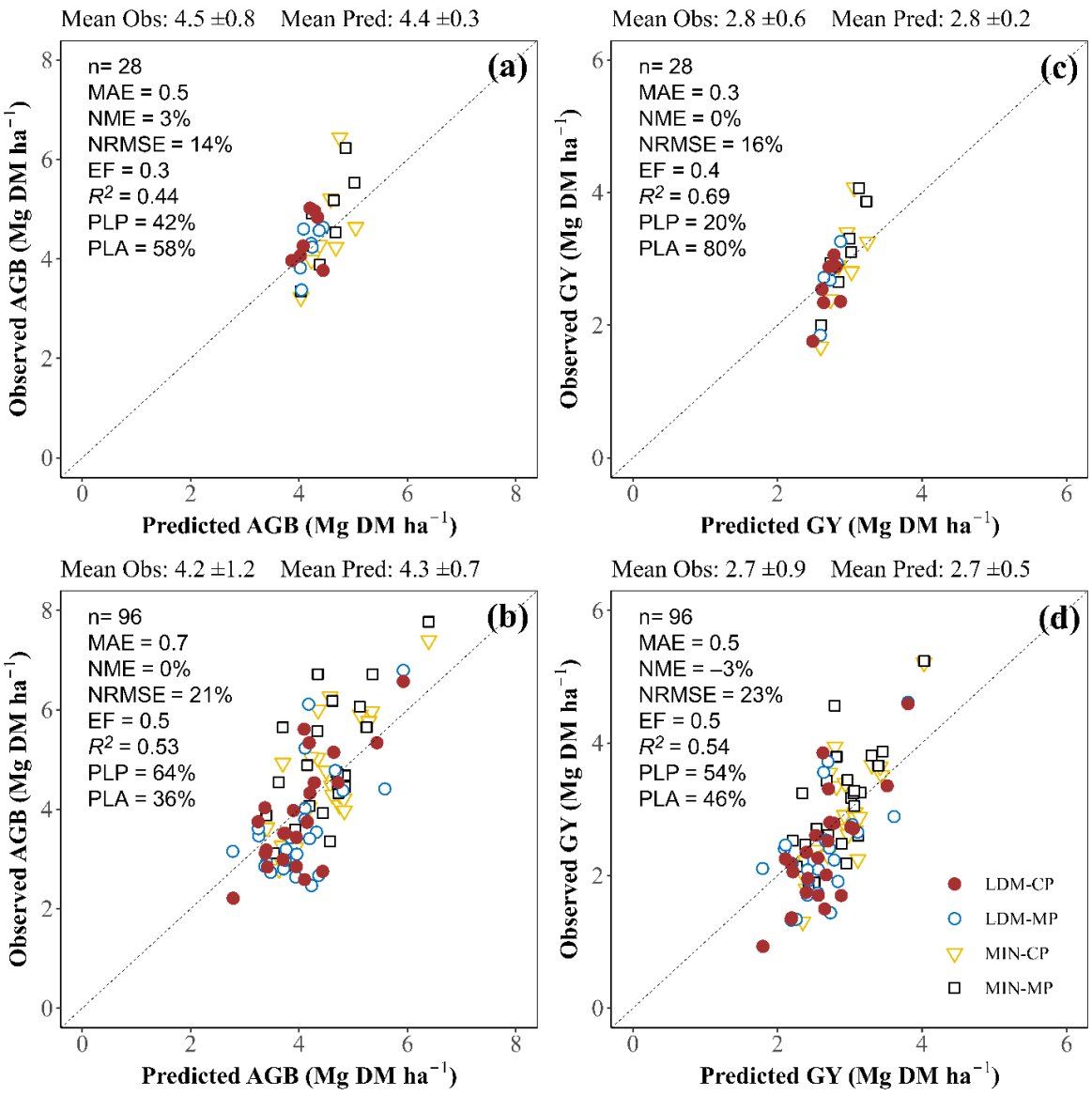

Figure 1.4 Observed versus predicted spring barley aboveground biomass (AGB) and grain yield (GY) for 'calibration' (a, c) and 'evaluation' (b, d) dataset. Each point is the mean of four replicates. Mean Obs: mean of observed values; Mean Pred: mean of predicted values; n: number of simulation units; MAE: mean absolute error; NME: normalized mean error; NRMSE: normalized root mean square error; EF: model efficiency; R^2: coefficient of determination; PLP: percentage lack of precision; PLA: percentage lack of accuracy; LDM: liquid dairy manure; MIN: ammonium nitrate; MP: moldboard plow; CP: chisel plow.

1.3.3.2 Nitrogen concentration in aboveground biomass and in grain at harvest

Annual values of observed NCAGB at harvest over 24 years of measurement for the four treatments ranged from 12 to 20 g kg^{-1} DM with a mean of 16 ±2 g kg^{-1} DM (Figure 1.5a). The mean (17 ±2 g kg^{-1} DM) and the range (13–20 g kg^{-1} DM) of predicted NCAGB values were very close to the observed values. For NCG, the annual observed values ranged from 14 to 24 g kg^{-1} DM with a mean of 20 ±2 g kg^{-1} DM. The range (17–25 g kg^{-1} DM) and the mean (20 ±2 g kg^{-1} DM) of the annual predicted NCG values were also quite similar to the observed values (Figure 1.5b).

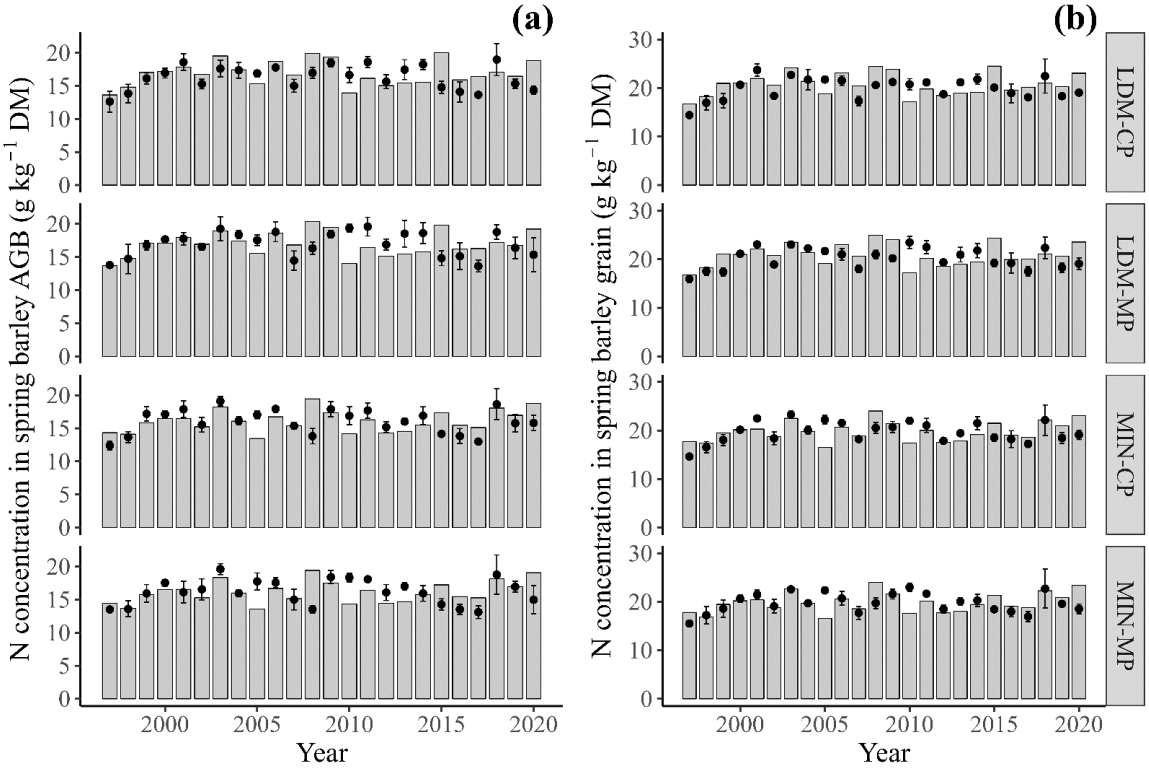

Figure 1.5 Annual mean of observed (dots) and predicted (grey bars) (a) N concentration in spring barley aboveground biomass and (b) grain from 1997 to 2020 for soil tillage and N fertilization source treatments. Bars on dots are standard deviation (n=4). LDM: liquid dairy manure; MIN: ammonium nitrate; MP: moldboard plow; CP: chisel plow.

Calibration led to good prediction of NCAGB and NCG with a low relative bias, excellent NRMSE, and satisfactory EF; however, R^2 was substantial for NCAGB and moderate for NCG, respectively (Figures 1.6a, 1.6c). For the evaluation dataset, the relative bias and the NRMSE were low (NME = -1% and NRMSE ≤ 16%) but the EF was negative and R^2 was very weak for both variables (Figures 1.6b, 1.6d). The error decomposition showed that most of the error for NCAGB and NCG was due to dispersion (PLP > PLA), for both datasets (Figure 1.6).

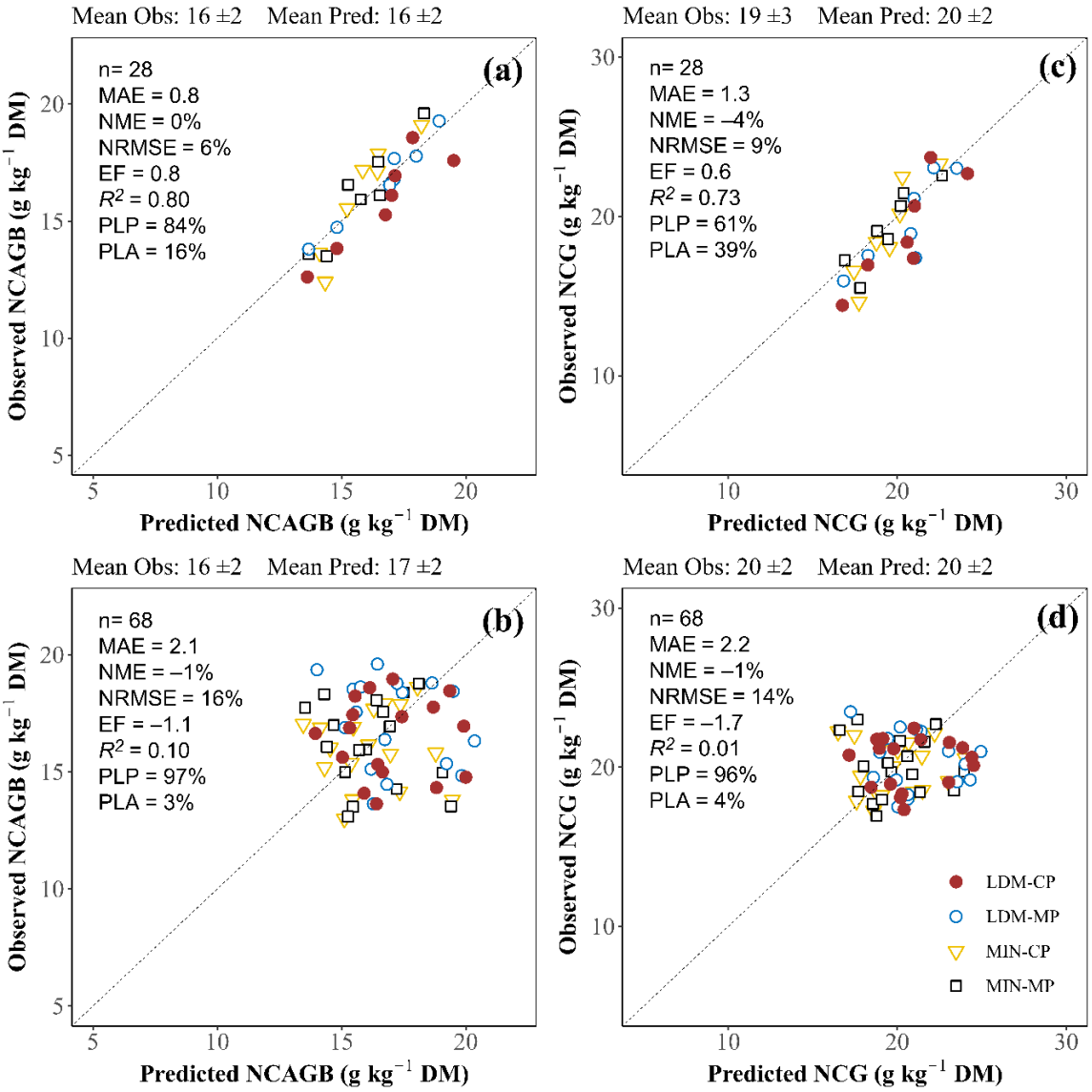

Figure 1.6 Observed versus predicted N concentration in aboveground biomass (NCAGB) and in grain (NCG) for the 'calibration' (a, c) and 'evaluation' (b, d) dataset. Each point is the mean of four replicates. Mean Obs: mean of observed values; Mean Pred: mean of predicted values; n: number of simulation units; MAE: mean absolute error; NME: normalized mean error; NRMSE: normalized root mean square error; EF: model efficiency; R^2: coefficient of determination; PLP: percentage lack of precision; PLA: percentage lack of accuracy; LDM: liquid dairy manure; MIN: ammonium nitrate; MP: moldboard plow; CP: chisel plow.

1.3.3.3 Plant N uptake and amount of N in grain

The mean observed NU value for the 24 years of cropping and four treatments was 67.4 ±11.9 kg N ha^{-1} yr^{-1} with values ranging from 41.2 to 89.3 kg ha^{-1} yr^{-1}. In comparison, the predicted NU ranged from 55.1 to 92.8 kg ha^{-1} yr^{-1} with a mean of 70.9 ±7.0 kg ha^{-1} yr^{-1} (Figure 1.7a). The mean observed NAG value was 51.4 ±11.2 kg N ha^{-1} yr^{-1} with values ranging from 25.3 to 74.7 kg N ha^{-1} yr^{-1} (Figure 1.7b). For the predicted NAG, there was a narrower range of values (43.9–74.4 kg N ha^{-1} yr^{-1}) but the mean (56.5 ±5.6 kg N ha^{-1} yr^{-1}) was similar compared to observed values.

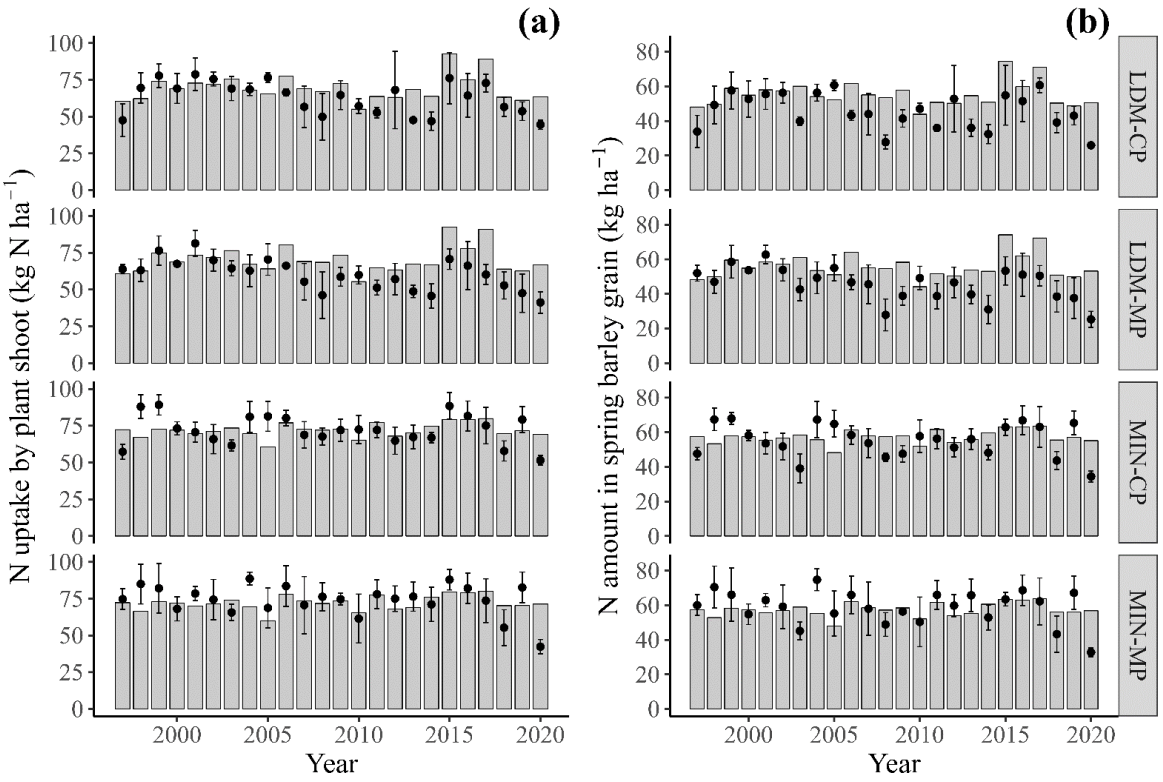

Figure 1.7 Annual mean of observed (dots) and predicted (grey bars) (a) N uptake by spring barley shoot (NU) and (b) N amount in grain (NAG) from 1997 to 2020 for soil tillage and N fertilization source treatments. Bars on dots are standard deviation (n=4). LDM: liquid dairy manure; MIN: ammonium nitrate; MP: moldboard plow; CP: chisel plow.

According to the statistical criteria, NU predictions were satisfactory for the calibration and the evaluation dataset, with a small NRMSE (13% and 19%, respectively) and low bias (NME = 2% and -8%, respectively) but relatively low EF and R^2 (Figures 1.8a, 1.8b). The NAG predictions were satisfactory for the calibration dataset, with a good NRMSE and a low bias, but a negative EF (-0.1) (Figure 1.8c). For the evaluation dataset, the NRMSE was fair (25%), and the EF and R^2 were weak

(Figure 1.8d). The relative contributions to the model error for NU and NAG indicate that most of the error was due to dispersion, for both datasets (PLP ≥ 57%) (Figure 1.8).

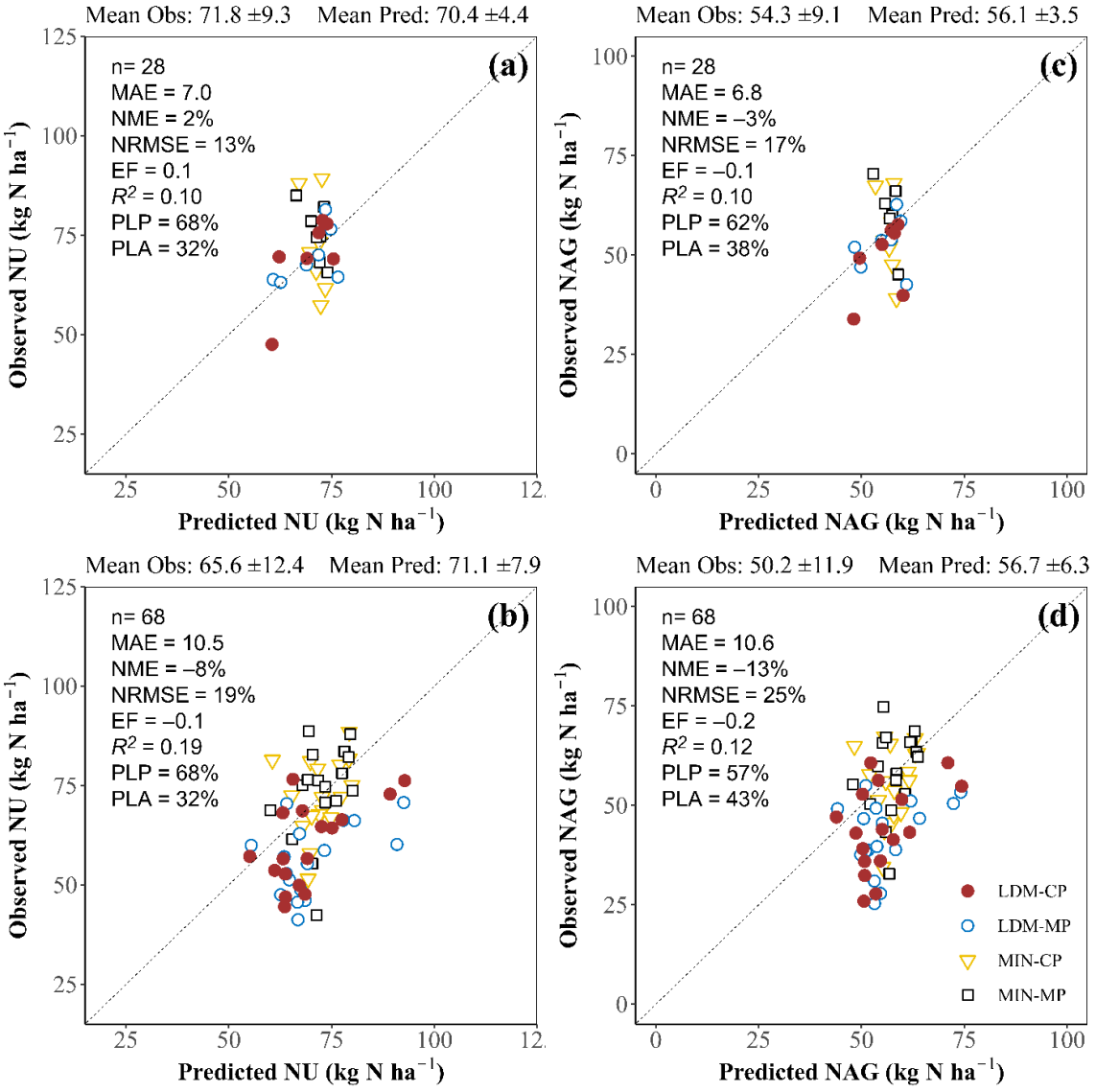

Figure 1.8 Observed versus predicted shoot N uptake (NU) and N amount in grain (NAG) for the 'calibration' (a, c) and 'evaluation' (b, d) dataset. Each point is the mean of four replicates. Mean Obs: mean of observed values; Mean Pred: mean of predicted values; n: number of simulation units; MAE: mean absolute error; NME: normalized mean error; NRMSE: normalized root mean square error; EF: model efficiency; R^2: coefficient of determination; PLP: percentage lack of precision; PLA: percentage lack of accuracy; LDM: liquid dairy manure; MIN: ammonium nitrate; MP: moldboard plow; CP: chisel plow.

1.3.4 STICS performance in relation to climatic conditions

STICS identified a slight degree of anoxia stress in the majority of cropping years in this study. This may be due to the soil texture (silty clay), which has a low infiltration capacity, and the high intensity rainfall events in the region. Five of the 24 years in the evaluation dataset were not subject to anoxic conditions (exofac = 0), but they were subject to water deficit stress. The other years had waterlogged conditions which varied in intensity and duration depending on the amount and distribution of rainfall over the growing season. Situations with $0 < \text{exofac} < 0.06$ were observed for 9 of the 24 years and situations with $0.06 \leq \text{exofac} < 0.14$ for 10 of the 24 years. Conditions with $0 < \text{exofac} < 0.06$ correspond approximately to years with evenly distributed rainfall throughout the growing season and close to the average level of rainfall over 31 years of experimentation (317 mm) (Table 1.S1).

Predictions of the variables of interest were better for years with a low waterlogging index ($0 < \text{exofac} < 0.06$), giving small biases ($|\text{NME}| < 7\%$), NRMSE values ranging from 10% to 22%, and high EF, except for NAG (Table 1.5). Under water deficit conditions, relatively higher NME values ($|\text{NME}| \geq 8\%$) were obtained for biomass accumulation variables and lower values for the amount of N in plant shoots and grain. The opposite was true for conditions with a significant waterlogging index. EF values were negative for all variables simulated under water deficit conditions. The NRMSE values were greater when the waterlogging index was high ($\text{exofac} \geq 0.06$). The other climate variables such as temperature, GDD, and global radiation varied from year to year but appear not to have affected the performance of STICS in predicting AGB, GY, NCAGB, NCG, NU, and NAG (data not shown).

Table 1.5 Performance evaluation of STICS by waterlogging stress level to predict spring barley aboveground biomass (AGB), grain yield (GY), N concentration in AGB (NCAGB) and grain (NCG), plant shoot N uptake (NU) and N amount in grain (NAG). Waterlogging stress was estimated in STICS by the waterlogging index, denoted exofac, i.e. the fraction of root length that is under anoxic conditions during the growing season.

Variables	n	Mean Obs	Mean Pred	NME	NRMSE	EF
0.06 ≤ exofac < 0.14						
AGB (Mg DM ha^{-1})	36	4.4(1.4)*	4.2(0.8)	5	23	0.4
GY (Mg DM ha^{-1})	36	2.7(1.0)	2.7(0.5)	-1	26	0.5
NCAGB (g kg^{-1} DM)	20	15(2)	17(2)	-14	21	-1.7
NCG (g kg^{-1} DM)	20	19(2)	21(2)	-10	15	-2.5
NU (kg N ha^{-1})	20	62.5(13.9)	74.3(7.8)	-19	25	-0.3
NAG (kg N ha^{-1})	20	47.0(14.9)	59.1(6.2)	-26	34	-0.2
0 < exofac < 0.06						
AGB (Mg DM ha^{-1})	40	4.4(1.3)	4.4(0.7)	-1	18	0.6
GY (Mg DM ha^{-1})	40	2.8(0.9)	2.9(0.4)	-3	22	0.6
NCAGB (g kg^{-1} DM)	36	17(2)	17(1)	-1	11	-0.4
NCG (g kg^{-1} DM)	36	20(2)	21(2)	-4	10	-0.6
NU (kg N ha^{-1})	36	67.3(12.0)	71.8(7.3)	-7	16	0.1
NAG (kg N ha^{-1})	36	51.0(10.6)	57.2(5.9)	-12	23	-0.3
exofac = 0						
AGB (Mg DM ha^{-1})	20	3.7(0.6)	4.0(0.6)	-9	20	-0.5
GY (Mg DM ha^{-1})	20	2.4(0.4)	2.6(0.4)	-8	19	-0.5
NCAGB (g kg^{-1} DM)	12	17(1)	15(1)	17	18	-11.5
NCG (g kg^{-1} DM)	12	22(1)	18(1)	17	19	-12.3
NU (kg N ha^{-1})	12	65.7(10.9)	63.9(5.1)	3	18	-0.2
NAG (kg N ha^{-1})	12	53.1(9.2)	50.9(4.0)	4	18	-0.2

*Mean with SD in parentheses
n: number of simulation units; Mean Obs: mean of observed values; Mean Pred: mean of predicted values; NME; normalized mean error; NRMSE: normalized root mean square error; EF: model efficiency.

1.4 Discussion

1.4.1 STICS calibration for spring barley cultivars adapted to climatic conditions of northeastern Quebec

The biomass and plant N uptake of a spring barley cultivar adapted to pedoclimatic conditions of the Saguenay–Lac-Saint-Jean region (northeastern Quebec) had never been simulated with STICS. Our results for spring barley confirm that the model can be successfully calibrated for a new cultivar and new pedoclimatic conditions such as those found in northeastern Quebec. This is consistent with the results previously reported with the same model for soybean and spring wheat cultivars (Jégo et al., 2010) as well as for maize cultivars (Jégo et al., 2011).

Although the calibration was based on a limited set of target variables, all of them measured at the end of the growing season, it significantly improved the simulation of biomass accumulation and N nutrition for spring barley cultivars grown in silty clay soil at Normandin. This is consistent with the findings of Guillaume et al. (2011) that STICS can be calibrated without integrating additional observed data from sequential sampling during the growing season to improve the prediction of crop variables at harvest (e.g. AGB and GY). However, this is not always the case for other crop models where restricted calibration can create substantial uncertainty in crop growth predictions (Rötter et al., 2012; Yin et al., 2017).

Although the calibration procedure should give priority to adjusting parameters by using direct measurements and data from the literature, this is not always possible, for many reasons (Falconnier et al., 2019). In this study, crop height and yield component traits were adjusted according to data found in the literature and other parameter values were derived from the sequential optimization performed using observed values. This underscores the importance of ensuring that the values of the parameters calibrated by optimization are plausible. The sum of GDD between emergence and physiological maturity obtained during calibration falls in the range of GDD values (1,268 to 1,702 °C d) reported for spring barley grown at three locations in the northern Great Plains of the Canadian province of Alberta (Botha, Lacombe, and Olds) from 1993 to 1996 (Juskiw et al., 2001) as well as in the range of values (1,250 to 1,850 °C d) reported for barley grown in agricultural area of the western Canadian province of Manitoba (Mapfumo et al., 2023). The reduction of *stlevdrp* and *stdrpmat* is consistent with the shorter growing season characterizing the study location in northeastern Quebec. In addition, the sum of GDD required to reach maximum LAI is in line with results from Alberta, where reported values ranged from 756 to 1,109 °C d, depending on site location, year, and cultivar (Juskiw et al., 2001). Furthermore, it is generally expected that post-anthesis RUE (efcroirepro) will be equal to or lower than pre-anthesis RUE (efcroiveg) since no new

leaves are produced after heading and the photosynthetic activity of existing leaves decreases with age (Calderini et al., 1997; Gallagher & Biscoe, 1978). However, Raj Singh et al. (Raj Singh et al., 2012) found that RUE for spring barley is not constant throughout the growing season. It has also been reported that post-anthesis RUE values can be high for six-row barley under short growing season conditions: 1.6 to 3.0 g DM MJ^{-1} for pre-anthesis RUE vs. 2.1 to 3.8 g DM MJ^{-1} for post-anthesis RUE (Bingham et al., 2007; Muurinen & Peltonen-Sainio, 2006). This higher post-anthesis RUE value can be attributed to the significant contribution of the cereal spike to photosynthetically active radiation interception (PAR) and to grain yield (Ahmadi et al., 2009; Maydup et al., 2012; Zhang et al., 2020). Furthermore, Zhang et al. (2020) suggested that RUE for cereal spike (spike light interception) should be included in crop models in addition to the RUE derived from leaf light interception in order to capture the contribution of spike photosynthesis to grain yield and to improve simulation results, notably in the high yield range. For STICS, the interception of PAR by cereal spikes has not been explicitly documented.

1.4.2 STICS performance

After the calibration using 28 predicted/observed data pairs (7 years × 4 treatments) of the dataset, the ability of STICS to predict AGB, GY, NCAGB, NCG, NU, and NAG (Figures 1.4, 1.6, 1.8) was tested with the remaining 96 predicted/observed data pairs (24 years × 4 treatments) by regressing field-observed vs STICS-predicted values using the standard major axis procedure proposed recently by Correndo et al. (2021b).

The NRMSE values for AGB (Figures 1.4a, 1.4b) were low compared to those reported in previous studies where STICS was used for European spring barley cultivars (NRMSE of about 25–35%) (Constantin et al., 2012; Corre-Hellou et al., 2009). For GY (Figure 1.4c, 1.4d), the NRMSE values were in the same range as those obtained by Rötter et al. (2012) (NRMSE = 24%) in northern and central Europe and by Salo et al. (2016) (NRMSE = 10–26%) in southern Finland. For NCG, the NRMSE values of 9% and 14% for calibration and evaluation, respectively, were low compared to the values obtained by Salo et al. (2016) (NRMSE = 13–27%) and Yin et al. (2017) (NRMSE > 30%) for spring barley. Our results for NU prediction were comparable to those reported for spring wheat grown at three locations in the Mixedwood Plains Ecozone of eastern Canada (Quebec and Ontario) (NRMSE = 14–20%) (Sansoulet et al., 2014). In general, plant N attributes variables are more difficult to model than plant biomass. The simulation of these variables is closely dependent at the same time on the simulation of biomass as well as the dynamic of mineral N in the soil, which is itself the result of multiple simultaneous biotransformation processes that interact with several other parameters.

With respect to error decomposition, it has been reported that complex models with a large number of parameters generally tend to have a low systematic error but a large dispersion error (Hastie et al.,

2009). In their overall performance evaluation, Coucheney et al. (2015) concluded that STICS errors are mostly related to dispersion error rather than systematic error, and this is also what we observed in our study.

The annual variability of biomass and N accumulation in plant parts was generally well captured, with predicted values being close to observed values, even several years after the start of the simulation. This indicates that STICS performed well in predicting spring barley production over 31 years in a continuous simulation mode without simulations being reset each year, which is consistent with the results of previous studies (Beaudoin et al., 2008; Yin et al., 2017). This was tested for the first time with STICS under northern climatic conditions with a heavy snow cover every winter. The model's continuous simulation mode is especially useful for predicting the effects of climate change, which requires long-term simulations. In addition, the STICS evaluation showed that all the output variables were well predicted for the Alyssa cultivar, which has been used since 2015 in the long-term field experiment (Figures 1.3, 1.5, 1.7). After a validation step using independent observations from other sites, the new set of calibrated parameters could be used for other cultivars in northeastern Quebec with characteristics similar to those of the Chapais and Alyssa cultivar. This aspect is important, especially since these cultivar are well adapted to the environmental conditions found in Canada, in both the eastern and western regions (Kong et al., 1994; Spaner et al., 2000).

Overall, the STICS outputs reproduced the same trends as the observed data for the various treatments (Table 1.S4). Concerning N sources, higher yields observed for the MIN than for the LDM treatment in this study contradict some observations that dairy manure can increase long-term soil fertility. Lafond et al. (2016) found that LDM and MIN treatments can affect barley grain yields differently depending on the cropping system (rotation or monoculture). The mean predicted AGB and GY values were lower for the LDM treatment than for the MIN treatment. However, the model overestimated NU and NAG for the LDM treatment (Figure 1.7). Although the model predictions of AGB, GY, NCAGB, and NCG for the LDM treatment in 2011, 2013 and 2014 were poor, the predicted values were close to the observed values for all the other years (Figures 1.3, 1.5). For the tillage systems, the predicted values for the MP and CP treatments were comparable (Table 1.S4). As is the case for most currently available models, the variables and processes simulated by STICS are still limited to the incorporation and redistribution of residues and nutrients in the soil down to the tillage depth. Yet, tillage affects soil functioning and, ultimately, crop yield through multiple processes such as microbial activity and biomass, weed seeds and soil texture redistribution, as well as soil hydraulic properties (Maharjan et al., 2018). In addition, the differences in the observed values of some variables such as GY due to the tillage treatments were low (7%), even if statistically significant (Table 1.2). The two tillage treatments did not differ in the observed AGB values.

1.4.3 STICS process-based model vs statistical model

Given that the performance metrics from the cross-validation method are equal to the average of the performance metrics calculated for each of the 5 iterations (5 folds), we can state that the overall predictive performance of STICS obtained with the 2 datasets was comparable to that of the mixed model approach for all production attributes variables (Table 1.2, Figure 1.4, 1.6, 1.8). The 2 models, which represent the two extremes of a spectrum of modeling approaches gave similar good performances although the process-based model STICS integrates both soil and plant processes as well as agri-environmental conditions. This is not surprising, since we only used the database from one experimental site. As well as the great flexibility in the type of input that can be used, the main advantage of the statistical model is that it relies solely on the data for its parameterization, by minimizing the difference between observed and predicted values of the training datasets. However, their results can not be extrapolated to new contexts. On the other hand, process-based approaches require a significant of input data to run, some processes are better understood than others, and calibration often requires a lot of time before achieving satisfactory performance predictions. Therefore, the sources of error in a process-based model can be multiple (model structure, model parameters, uncertainty in model inputs, uncertainty in evaluation/validation data) (Maestrini et al., 2022). To be applied to broader conditions, although process-based models are theoretically universal in scope, as they are based on ecophysiological and biological laws, validation steps with independent data are needed to see how the model behaves outside the conditions under which it has been calibrated.

1.4.4 Suggestions to improve model performance

The STICS evaluation indicated that predictions of plant variables were less accurate when the waterlogging index level was high (Table 1.5). For example, the large underestimation of AGB and GY that occurred in 1996 (Figures 1.3a, 1.3b) was partly due to the large amount of rainfall in July (200 mm), which induced transitory stress from waterlogging (exofac = 0.09 during the reproductive stage) that the model captured too intensely in the AGB growth and GY predictions. This suggests that some plant parameters related to root, LAI or biomass growth are sensitive to excess water and, should be adjusted to improve the simulations under excessive water conditions. The assessment of the soil water content (at 0-20 cm depth) was carried out with the measured data collected on the adjacent plots belonging to the experimental set-up under spring barley and forage in 2011, a year characterized by above-average rainfall most of the growing season (402 mm), and showed a very satisfactory soil water content prediction with an excellent NRMSE (9.8%), a satisfactory EF, and a moderate R^2 (data not shown). In general, soil water content is one of the variables that is best predicted by the STICS model (Coucheney et al., 2015), and this is also true under eastern Canadian (Ontario and Quebec provinces) climatic conditions (Jing et al., 2017; Saadi et al., 2022).

The predicted values of AGB and GY were much greater than the observed values for the LDM treatment in 2011, 2013 and 2014, but not for the MIN treatment (Figure 1.3). In contrast to the other years, STICS failed to reproduce the low observed values of AGB and GY in the LDM for these three cropping years. The observed AGB and GY values were the lowest, and the yield gap compared to the MIN treatment was particularly large. It has been reported that cereal GY in monoculture systems using organic fertilizers is lower than with a mineral fertilizer due to low N use efficiency (Lafond et al., 2016; Rieux et al., 2013). Significant differences in observed AGB and GY values between the MIN and LDM treatments (Table 1.2, Figure 1.S1) can also be explained by the proportion of mineral N, the mineralization rate of organic N in LDM, or poor synchronization of the availability of organic N in the soil for the critical phases of crop growth (Rakotovololona, 2018). The amount of N applied as organic fertilizer in 2011, 2013 and 2014 was large compared with other years (103, 138 and 123 kg total N ha^{-1}, respectively, with at least 30% in mineral form) and STICS output showed that predicted soil mineral N content down to the 100-cm depth was comparable between LDM and MIN in 2013 and 2014 (Figure 1.S3). It is therefore likely that grain yields were affected and exacerbated by factors related to biotic pressures, which are not accounted for by STICS. The slight NCAGB and NCG underestimations can be explained in part by a dilution effect due to the strong overestimation of AGB and GY (Figures 1.3a, 1.3b), even though NU and NAG were overestimated for these years (Figures 1.7a, 1.7b). It would be interesting in the future to evaluate the model's performance in simulating spring barley yield and N plant status in response to contrasting N application rates of a given fertilizer. In this study, the MIN (70 kg N ha^{-1} yr^{-1}) and LDM (107 kg N ha^{-1} yr^{-1} corresponding to about 40 kg N ha^{-1} yr^{-1} of mineral N) treatments provided an amount of available N to the crop that differed slightly, taking into account immobilization of mineral N from mineral fertilizer (on average 15 kg N ha^{-1} yr^{-1}) and net mineralization for the LDM treatment (on average 9 kg N ha^{-1} yr^{-1}), as predicted by STICS.

To further refine consideration of the effect between MIN and LDM treatment, STICS could be further improved by taking better account of N supply. In this study, all the parameters of the model equations used to simulate soil N transformation processes are model default values adopted for temperate regions. In the absence of measured field data, the accuracy with which STICS simulates N transformation processes in the soil could not be assessed. These processes influence the dynamics of soil mineral N and its availability to plants (Yin, Beaudoin, et al., 2020; Yin, Kersebaum, et al., 2020). Previous studies conducted on a sandy loam field near Quebec City (Quebec, Canada) cultivated with perennial timothy (*Phleum pratense* L.) showed that total soil mineral N was reasonably well simulated, although soil nitrate content was overestimated during a certain period of the crop cycle (Jing et al., 2017). Assessing the ability of STICS to simulate N transformation processes under spring barley cropping system in soils from northeastern Quebec province should be included in future studies. This lack of soil measurement data and the absence of observations from a different (independent) site constitute the main limitation of this study.

In 2005 and 2010, predicted NCAGB and NCG values were lower than the observed values for all treatments (Figure 1.5). Rainfall was significantly below the 31-year average for these two years, with only 176 and 179 mm of cumulative rainfall during the cropping period, respectively (Table 1.S1). The crop was under water stress and STICS predicted low NU values (Figure 1.7a). Drought is known to affect the acquisition of nutrients by roots and their transport to shoots, resulting in reduced N uptake and plant N in barley (Bista et al., 2018; Farooq et al., 2009). STICS thus exaggerates the depressive effect of water stress on N nutrition. A study of spring wheat at three sites in the Mixedwood Plains Ecozone of eastern Canada showed that the model's performance was sensitive to the amount of rainfall during the growing season (Sansoulet et al., 2014). It showed that the model's performance was better when rainfall was close to normal in the early growing season.

Field data during the growing season (e.g., AGB and NCAGB) that could be used in the calibration procedure would help to further improve the prediction of AGB, GY, NCAGB, NGY, NU, and NAG. This would also make it possible to assess and adjust the prediction of NU during the crop vegetative stage and N remobilization/uptake during the grain filling period, as well as the effects of possible N stress. Kherif et al. (2022) stated that the performance of soil–crop models refers not only to the overall accuracy of model predictions, but also to the ability of models to capture the temporal dynamics of plant and soil variables. The verification of LAI dynamics which plays a key role in predicting plant biomass accumulation and the validation of the critical N dilution curve parameters for spring barley may also be required to predict AGB and NU more precisely. Morissette et al. (2016) concluded that using cultivar-specific N dilution curves instead of the default curve improves STICS performance and is essential for adequately predicting the N cycle of potato growing systems. To our knowledge, no critical N dilution curve for spring barley grown in agricultural soils from the six provinces of eastern Canada (New Brunswick, Newfoundland, Nova Scotia, Prince Edward Island, Quebec, and Ontario) has been established or at least validated to date. The default critical N dilution curve parameters used in this study are those proposed by Zhao (2014) for winter barley from data obtained in China. For wheat, a specific critical N dilution curve was developed for spring wheat in Canada, which differed from the reference curve used for winter wheat in Europe (Ziadi et al., 2010). For maize, the critical N dilution curve established in France was found to be valid in several agricultural sites within the province of Quebec (Ziadi et al., 2008), although Jégo et al. (2022) have proposed a specific critical N dilution curve for Canada using the Bayesian approach for data analysis.

1.5 Conclusion

This study enabled us to calibrate STICS for spring barley cultivars grown on gleysolic soil under the climatic conditions (continental cold and humid climate) of Saguenay-Lac-Saint-Jean (northeastern Quebec). The STICS calibration procedure required the adjustment of cultivar parameters in particular, thus confirming the genericity of most plant parameters defined in STICS. Good agreement

was obtained between annual observed and predicted values of AGB, GY, NCAGB, NCG, NU and NAG during 31 years of spring barley monoculture, although there was a greater dispersion for the plant N attributes. STICS also reproduced the trends of observed values effectively with different tillage systems and N sources applied at the locally recommended N rates. Model errors were generally due to dispersion error rather than systematic error, indicating that the model was correctly parameterized. Although the simulation results for the spring barley grown at the studied experimental site were satisfactory, they could be improved with additional data, particularly data obtained during the growing season to capture the temporal dynamics of plant and soil variables. The validation of the STICS predictions for the temporal dynamics of spring barley growth and N uptake in response to various crop management approaches and contrasting soil types is also needed using observations from independent datasets obtained from different sites. Our results will serve as the basis for future studies aimed at understanding and quantifying long-term changes in C and N fluxes in cropping systems with spring barley in the same site and experimental set-up.

1.6 Supplementary information

Table SI.1.1 Weather data during the cropping period of spring barley from 1990 to 2020 recorded at the Normandin and the Saint-Prime weather station of Environment Canada, the closest of the studied field experiment.

Year	**Precipitations** [mm]		**Mean temperature** [°C]		**GDD*** [°C-d]	**Sum Radiation** [MJ m^{-2}]
	From early May to harvest	**Annual**	**From sowing to harvest**	**Annual**	**From sowing to harvest**	
1990	338	858	15.8	3.0	1641	1912
1991	245	717	17.0	2.6	1597	1931
1992	402	839	14.9	1.5	1699	1944
1993	387	867	17.0	1.9	1715	1845
1994	371	814	16.1	2.1	1639	1960
1995	230	790	18.4	2.9	1492	1866
1996	379	1134	16.4	2.9	1607	1921
1997	315	733	15.4	1.9	1744	2067
1998	310	732	15.4	3.4	1775	2166
1999	371	875	15.7	2.7	1510	1840
2000	260	702	14.4	1.5	1456	1840
2001	325	832	16.1	2.6	1605	1828
2002	263	779	15.8	0.9	1553	1928
2003	262	805	16.1	1.3	1597	1819
2004	311	785	14.3	0.1	1497	1804
2005	176	702	16.3	2.0	1431	1821
2006	297	1033	16.0	2.8	1555	1839
2007	292	697	14.3	1.4	1635	2259
2008	324	800	15.5	1.2	1438	1543
2009	311	683	14.8	1.2	1674	2008
2010	179	758	16.4	3.8	1550	1891
2011	402	890	16.4	2.4	1540	1859
2012	298	804	16.4	3.1	1609	1989
2013	296	965	16.1	1.9	1463	1813
2014	340	982	16.9	1.4	1610	1895
2015	349	958	16.0	1.7	1644	1910
2016	417	1291	16.3	2.0	1598	1854
2017	498	1117	14.9	1.6	1687	2157
2018	269	843	17.4	1.6	1722	1962
2019	249	742	15.8	0.7	1591	1980
2020	355	838	18.1	2.8	1663	1823
Average	317	850	16.0	2.0	1598	1912

*Sum of growing degree-days on 0°C basis

Table SI.1.2 Key cropping practices (date of N application, seeding, harvest, and soil tillage) and measurements at harvest of the 'Chapais' (1990-2014) and 'Alyssa' (2015-2020) spring barley cultivars.

Year	Fertilization date	Seeding date	Harvest date	Fall tillage date	N total LDM* [kg N ha^{-1}]
1990	8/05	9/05	20/08	21/09	73
1991	20/05	21/05	22/08	16/10	121
1992	23/05	25/05	15/09	15/10	79
1993	30/05	30/05	7/09	13/10	90
1994	20/05	20/05	29/08	27/09	89
1995	26/05	26/05	14/08	28/09	77
1996	17/05	17/05	22/08	25/09	75
1997	15/05	15/05	4/09	25/09	110
1998	11/05	12/05	3/09	25/09	79
1999	16/05	17/05	20/08	25/09	79
2000	23/05	23/05	31/08	25/09	110
2001	22/05	23/05	30/08	25/09	141
2002	28/05	29/05	3/09	25/09	105
2003	26/05	27/05	2/09	17/09	115
2004	27/05	27/05	8/09	22/10	105
2005	19/05	20/05	15/08	20/09	120
2006	19/05	19/05	23/08	12/09	120
2007	14/05	14/05	4/09	24/09	142
2008	19/05	20/05	20/08	18/09	75
2009	21/05	21/05	10/09	24/09	153
2010	20/05	21/05	23/08	4/10	87
2011	25/05	25/05	26/08	28/09	103
2012	14/05	15/05	20/08	27/09	134
2013	27/05	28/05	26/08	16/10	138
2014	27/05	27/05	29/08	15/10	123
2015	21/05	22/05	1/09	28/09	134
2016	26/05	26/05	31/08	5/10	84
2017	31/05	31/05	20/09	4/10	118
2018	28/05	29/05	4/09	1/10	138
2019	28/05	28/05	5/09	2/10	85
2020	22/05	25/05	24/08	24/09	110

*Liquid dairy manure

Table SI.1.3 Performance of STICS with defaults parameters (Scarlett cultivar) and newly calibrated parameters to predict spring barley aboveground biomass (AGB), grain yield (GY), N concentration in AGB (NCAGB) and in grain (NCG), plant shoot N uptake (NU) and N amount in grain (NAG).

Variables	n	Mean Obs	Mean Pred	NME (%)	NRMSE (%)	EF
With defaults parameters (Scarlett cultivar)						
AGB (Mg DM ha^{-1})	28	4.5(0.8)	6.4(1.0)	-42	50	-7.9
GY (Mg DM ha^{-1})	28	2.8(0.6)	2.4(0.7)	16	29	-0.8
NCAGB (g kg^{-1} DM)	28	16(2)	9(1)	47	48	-14.4
NCG (g kg^{-1} DM)	28	19(3)	12(2)	38	41	-7.2
NU (kg N ha^{-1})	28	71.8(9.3)	55.2(12.3)	23	32	-5.2
NAG (kg N ha^{-1})	28	54.3(9.1)	44.2(16.3)	19	39	-4.7
With newly calibrated parameters (Chapais cultivar)						
AGB (Mg DM ha^{-1})	28	4.5(0.8)	4.4(0.3)	3	14	0.3
GY (Mg DM ha^{-1})	28	2.8(0.6)	2.8(0.2)	0	16	0.4
NCAGB (g kg^{-1} DM)	28	16(2)	16(2)	0	6	0.8
NCG (g kg^{-1} DM)	28	19(3)	20(2)	-4	9	0.6
NU (kg N ha^{-1})	28	71.8(9.3)	70.4(4.4)	2	13	0.0
NAG (kg N ha^{-1})	28	54.3(9.1)	56.1(3.5)	-3	17	-0.1

n: Number of predicted/observed data pairs, Mean Obs: mean of observed values, Mean Pred: mean of predicted values, NME; normalized mean error, NRMSE: normalized root mean square error, EF: model efficiency

Table SI.1.4 Mean of field-observed and STICS-predicted values for aboveground biomass (AGB), grain yield (GY), N concentration in aboveground biomass (NCAGB) and in grain (NCG), N uptake by plant (NU), and N amount in grain (NAG) as affected by N source type and tillage system. LDM: liquid dairy manure; MIN: ammonium nitrate; MP: moldboard plow; CP: chisel plow.

Source	AGB (Mg DM ha^{-1})	GY (Mg DM ha^{-1})	NCAGB (g kg^{-1} DM)	NCG (g kg^{-1} DM)	NU (kg N ha^{-1})	NAG (kg N ha^{-1})
Mean of field-observed values						
N source type						
MIN	4.7	3.0	16.1	19.8	73.2	57.1
LDM	3.9	2.4	16.6	20.2	62.0	45.7
Tillage system						
MP	4.3	2.8	16.6	20.1	67.2	52.2
CP	4.3	2.6	16.2	20.0	68.0	50.6
Mean of STICS-predicted values						
N source type						
MIN	4.5	2.9	16.1	19.8	72.1	57.4
LDM	4.1	2.6	16.9	20.8	69.8	55.6
Tillage system						
MP	4.3	2.8	16.5	20.3	71.2	56.7
CP	4.3	2.8	16.4	20.3	70.7	56.3

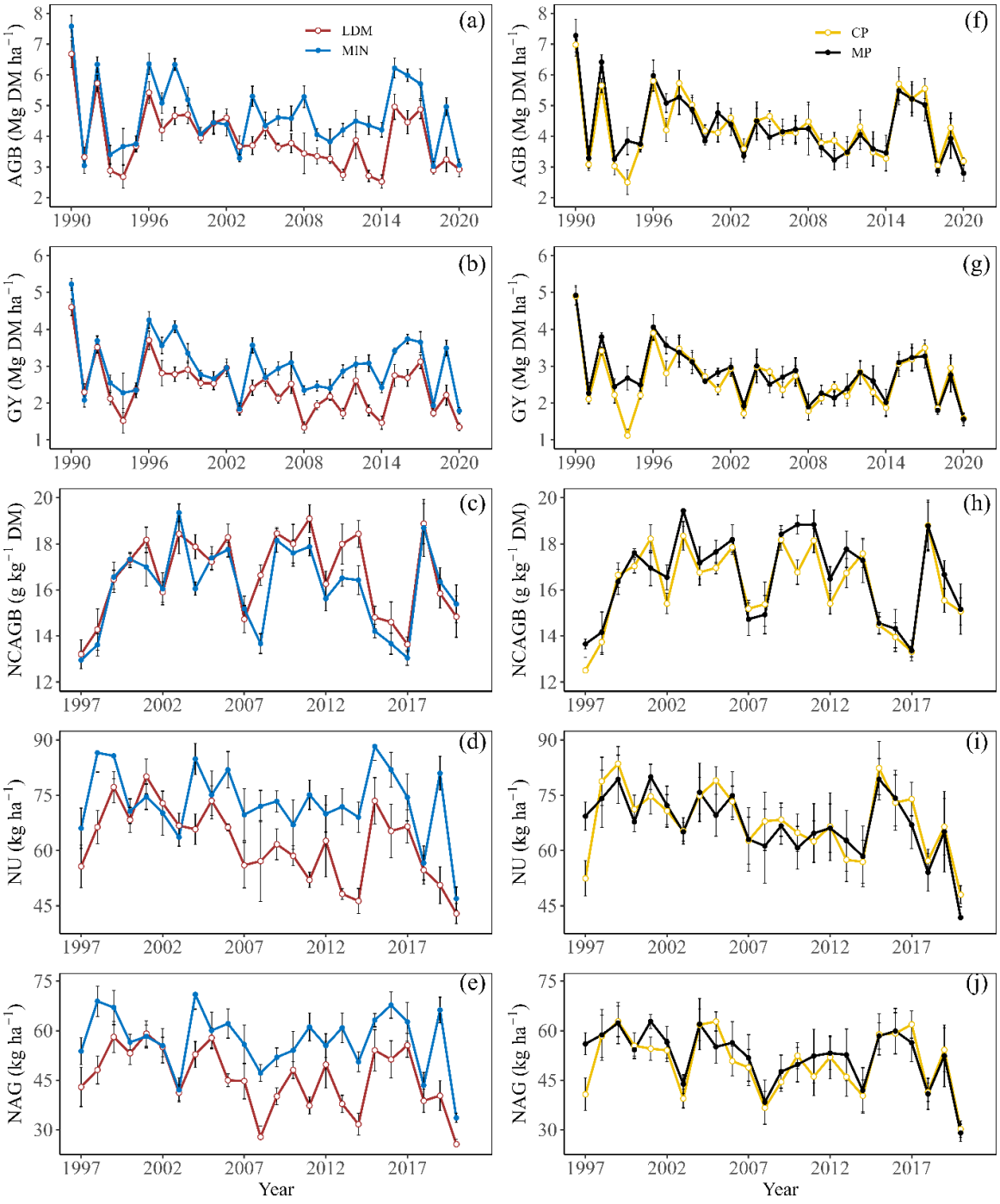

Figure SI.1.1 Aboveground biomass (AGB), grain yield (GY), N concentration in aboveground biomass (NCAGB), N uptake by plant (NU), and N amount in grain (NAG) as affected by N source type (a, b, c, d, e) or tillage system (f, g, h, i, j). Dots represent the means. Bars on dots are standard error of the mean (n=4). LDM: liquid dairy manure; MIN: ammonium nitrate; MP: moldboard plow; CP: chisel plow.

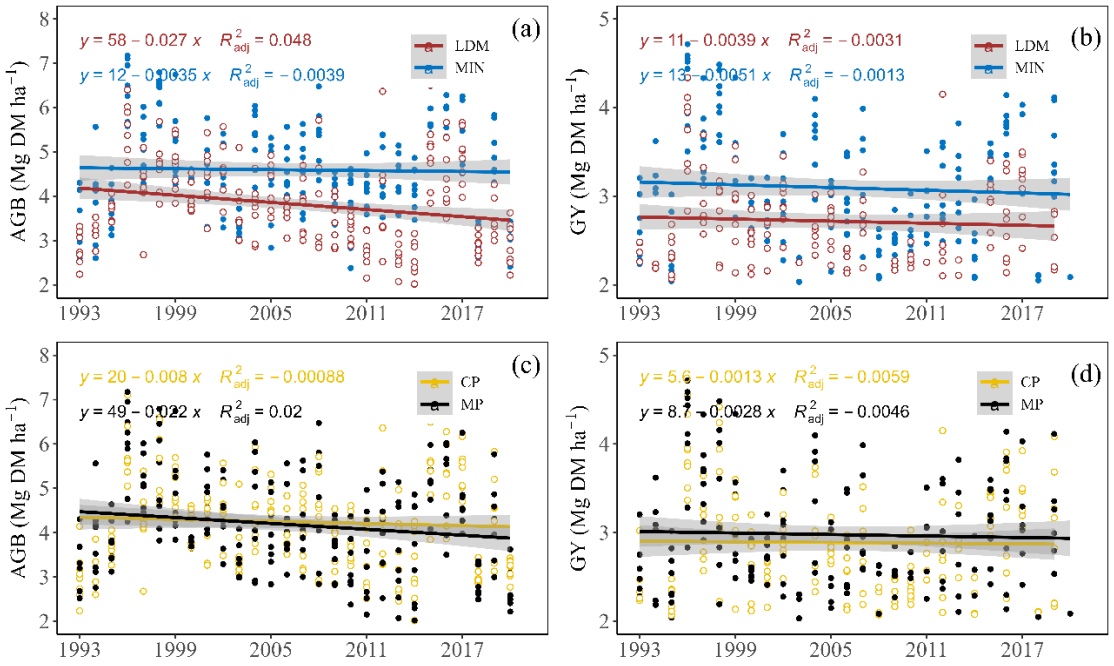

Figure SI.1.2 Scatterplots showing the trend in field-observed spring barley AGB and GY as a function of N source type (a, b), and tillage system (c, d) between 1993 and 2020. LDM: liquid dairy manure; MIN: ammonium nitrate.

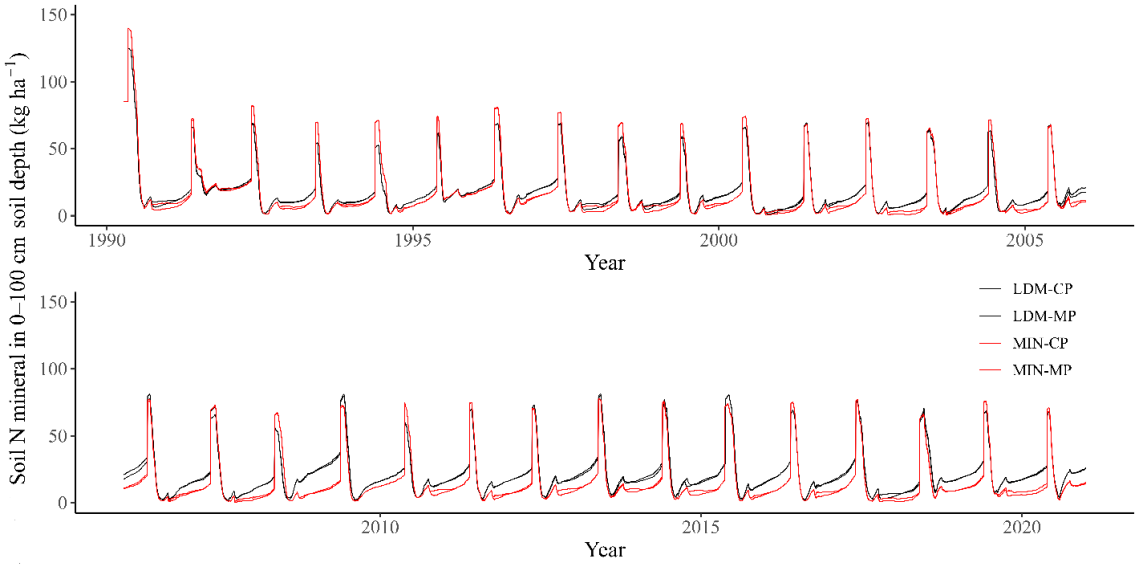

Figure SI.1.3 STICS-predicted soil mineral N content (kg ha^{-1}) down to 100 cm depth over 31 years according to crop management system. LDM: liquid dairy manure; MIN: ammonium nitrate; MP: moldboard plow; CP: chisel plow.

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CHAPTER 2: Continuous simulation of biomass production and nitrogen nutrition of an ageing (8 years) timothy sward under various nitrogen application rates in eastern Quebec (Canada)

Abstract

Timothy (*Phleum pratense* L.) is a perennial crop of prime economic importance in cool and northern regions such as Canada. The STICS soil-crop model has been calibrated and validated to these region conditions for simulating the growth and nutritive value of timothy only for a few successive years. It has not been validated for the continuous simulation of long period of cropping. Our objectives were twofold: (i) to evaluate multi-year (8 years) performance of STICS (version V 9.2) without annual reinitialization to simulate timothy forage yield and nitrogen (N) nutrition for increasing N fertilization rates; and (ii) to explore with STICS the possible causes of yield decreasing trend with time of the timothy forage production. The database of an 8-year timothy field experiment on N rates (0, 60, 120, 180 kg N ha^{-1} yr^{-1}), located in eastern Quebec, was used. STICS performed well over 8 years for simulating the forage yield for the first harvest, but it was not very good for the second harvest at summer regrowth. The normalized mean error (NME = -9%) and root mean square (NRMSE = 22%) were small, with a substantial coefficient of determination (R^2 = 0.77) and high model efficiency (EF = 0.7) for the first harvest. The correspondence between observed and predicted values was also satisfactory with respect to N concentration and amount in harvested biomass for the first growth, with NME of -1 and 2%, respectively, and NRMSE values of 14 and 22%, respectively. STICS satisfactorily simulated the positive effect of N fertilization rate on harvested forage biomass, N concentration and on N amount exported, except for the unfertilized treatment. STICS reproduced well the decrease of annual yield of timothy sward with years of cropping. Results showed that this yield drop could be due to the reduction of metabolic reserve in the perennial organs. The next stage of this research will be to calibrate the new STICS formalism specific to perennial crops for timothy, to enable better simulation of crop reserves and more realistic simulation of regrowth.

Keywords: STICS crop-model, timothy, nitrogen fertilization, continuous simulation, cold and humide climate

Résumé

Les objectifs de ce chapitre étaient d'évaluer la performance pluriannuelle de STICS sans réinitialisation annuelle pour simuler le rendement et la nutrition azotée (N) de la fléole des prés pour des taux de fertilisation N croissants ; et d'explorer avec STICS les causes possibles de la tendance à la baisse du rendement avec le temps. La base de données d'une expérimentation de 8 ans avec quatre taux d'azote (0, 60, 120, 180 kg N ha^{-1} an^{-1}) située au Québec, a été utilisée. STICS a bien fonctionné pour simuler le rendement et la nutrition N de la fléole pour la première récolte. STICS a simulé de manière satisfaisante l'effet positif du taux de fertilisation N sur la production de biomasse et la nutrition azotée, à l'exception du traitement non fertilisé. STICS a bien reproduit la diminution du rendement annuel d'une prairie de fléole des prés avec les années de culture.

Mots clés : Modèle sol-culture STICS, fléole des prés, fertilisation azotée, simulation continue, climat froid et humide

2.1 Introduction

Timothy (*Phleum pratense* L.) grassland is widespread in regions with cold and humid continental climates such as Canada and northern regions of Europe and provides high-quality forage for livestock. In the province of Quebec, it is often grown in mixtures with leguminous (e.g, alfalfa). Timothy is by far the most important cultivated grass species in terms of production and occupies the greatest proportion of the forage acreage in Quebec (McCartney & Horton, 1997). Timothy is winter-hardy and adapted to a wide range of soil and to the growing conditions in these regions, where the climate is characterized by a short growing season, heavy rainfall, relatively high summer temperatures, and harsh winters with long periods of snow cover. Although its yield peaks at around 9 Mg DM ha^{-1} yr^{-1} in the best conditions, timothy productivity remains much higher than any other forage crop under unfavorable and restricted growing conditions (e.g., acidic soil, poorly drained soil, droughty soils) (Grant & Burgess, 1979).

A well-reasoned and balanced fertilization plan is needed to obtain strong stands and maintain long-term timothy productivity without the need for reseeding (Bélanger et al., 1989). However, among other elements, nitrogen (N) is most often the major limiting nutrient in timothy hay production and quality (Bélanger & Ziadi, 2008; McKenzie, 2009). Improved N fertilization practices are necessary to reduce the risks of environmental losses. Inappropriate use of N fertilizers on grassland can lead to contamination of surface and groundwater (Decau et al., 2004; Rechcigl, 1994), as well as air pollution (Rahman & Forrestal, 2021). In addition, excessive N application beyond crop needs, lead to nutrient imbalances, reduce resistance to parasites, and generally result in soil acidification (Altieri & Nicholls, 2003; Zeng et al., 2017).

Although timothy stands can last for many years, as with other forage grasses (Robbins et al., 1987; Smith & Allcock, 1985), a reduction in herbage productivity with ageing swards was also reported (Bélanger et al., 2008; Gilliland & Mann, 2001). Some authors have argued that the accumulation of plant litter in ageing grasslands can lead to N immobilization, resulting in N deficiency (Robbins et al., 1987). Hoogerkamp (1984) suggested that this decreasing trend could be due to changes in some soil factors (e.g., organic matter content, activity of the earthworm population, occurrence of "soil disease") but also the insufficient longevity of the sown species. Jing & Bélanger (2012), in their simulation analysis of the first harvest of timothy, also speculated that this drop in yield could be due to the reduction in the accumulation root N and carbon (C) reserves in the previous fall. The reasons for this decrease in productivity with increasing sward age remain to be explored.

Modelling is a useful approach for diagnosing the agronomic constraints of crop production, providing estimates of indicators that are crucial for assessing crop growth, but tedious or costly to quantify in experimental plots. Therefore, it can assist to explore the interactive relationship between

agropedoclimatic conditions and crop growth and development (Matthews et al., 2013). Different models have been parameterized to simulate timothy biomass production under eastern Canada pedoclimatic conditions. For example, the CATIMO (Canadian Timothy Model) process-based model was specifically developed to simulate the growth (Bonesmo & Bélanger, 2002a) and nutritive value of timothy (Bonesmo & Bélanger, 2002b) (Jing & Bélanger, 2012). Soil−crop model STICS (*Simulateur mulTIdisciplinaire pour les Cultures Standard*), developed by INRAE (France), was initially calibrated for annual crops (e.g. corn, wheat, barley, soybean) (Brisson et al., 1998; Jégo et al., 2010) but was later adapted to perennial crops such as timothy, alfalfa, and Miscanthus (Jégo et al., 2013; Strullu et al., 2014, 2020). STICS has been calibrated and validated for two cultivars of timothy in eastern Canada (Jégo et al., 2013), but it has never been used beyond three consecutive years without annual reinitialization of the model (Jing et al., 2017). Previous studies showed the reliability of STICS predictions for timothy biomass under various N application rates (Jégo et al., 2013; Jing et al., 2017).

The objectives of this study were (i) to evaluate multi-year (8 years) performance of STICS (version V 9.2) without annual reinitialization to simulate timothy spring growth and summer regrowth and N nutrition under increasingly N application rates, including the zero N application; and (ii) to explore with STICS the possible causes of yield decreasing trend with years of cropping of the timothy primary growth in an ageing sward. The analysis was performed by using a dataset from an 8−year field experiment on timothy located in eastern Quebec (Canada) including four fertilizer N rates. The variables evaluated were forage yield, N concentration and N amount exported in forage yield.

2.2 Materials and methods

2.2.1 Site description and experimental design

The study was conducted on a grassland experiment at the Agriculture and Agri-Food Canada's Harlaka Research Farm, Lévis, QC, Canada (lat. 46°47′ N, long. 71°07′ W, alt. 65 m) from 1998 (seeding year) to 2006. The local climate is continental humid. Over this period, the annual average temperature was 4.7 °C (average minimum of −0.7 °C and maximum of 10.2 °C), and the average precipitation, although somewhat irregular, was 1141 mm, with 683 mm (60%) in the period from early May to late October. The soil is a Saint-André series gravely-sandy loam classified as Podzol (FAO, 2014) with slope <2%. The amount of coarse material (>2 mm) was variable among replicates (from 12 to 28%). The bulk densities of the plough layer (0–15 cm) were 1.23, 1.14, 1.08, and 1.14 g cm^{-3} for replicates 1–4, respectively.

Timothy (*Phleum pratense* L. cv. "Champ") grassland was established in May 1998 in individual plots of 2.1 m × 1.5 m arranged in split-plot design replicated four times. The overall experiment included

four P application-rates (0, 15, 30 and 45 kg P ha^{-1} yr^{-1}, applied as triple superphosphate) as main plots, and four N application rates (0 [0N], 60 [60N], 120 [120N] and 180 [180N] kg N ha^{-1} yr^{-1}, applied as calcic ammonium nitrate), as subplots. The P and N fertilizers were applied at early spring each year from 1999 to 2006, with a potassium fertilizer dose of 67 kg K ha^{-1}. Only the 32 experimental plots receiving 30 and 45 kg P ha^{-1} yr^{-1} were considered in this study to ensure that P was not limiting for plant growth over the period of experiment.

2.2.2 Plant analysis

Timothy aboveground biomass was harvested once in the sowing year (1998) and then twice every year during the eight subsequent years (1999–2006). The harvests of aboveground biomass for both harvests were carried out at 5-cm height on 0.91 m × 2.1 m areas with a self-propelled flail forage harvester (Carter MGF Co., Inc., Brookston, IN). The first harvest was made at late heading during spring growth (mid-June) and the second harvest was made during summer regrowth (early August). The aboveground biomass harvested in 1998 was not recorded. Harvest dates are presented in Table 2.1.

Table 2.1 Harvest dates, sum of growing degree-days basis 0°C (GDD), and cumulative rainfall during the first growth and regrowth period for the eight successive years of cropping. Daily temperature and rainfall data were taken at the Lauzon station (lat. 46°49´ N; long. 71°06´ W, alt. 69 m), approximately 5 km from the experimental site.

Year	First growth period (from May 01 to 1st cut)				Regrowth (between dates of the 1st harvest to the 2nd one)			
	1st harvest date	Sum GDD (°C d)	Cumul. rainfall (mm)	Mean Temp. (°C)	2nd harvest date	Sum GDD (°C d)	Cumul. rainfall (mm)	Mean Temp. (°C)
1999	16-06	719	118	15.3	07-08	997	214	19.2
2000	20-06	590	146	11.6	26-07	646	143	17.9
2001	20-06	734	157	14.4	07-08	886	170	18.5
2002	19-06	504	190	10.1	05-08	899	179	19.1
2003	17-06	542	183	11.3	13-08	1093	237	19.2
2004	14-06	494	159	11.0	28-07	752	245	17.1
2005	20-06	580	157	11.4	08-08	960	129	19.6
2006	13-06	521	168	11.8	17-07	676	151	19.9

Forage yield dry matter (DM) content was determined on a 500 g fresh sample after weighing and drying at 55 °C in a forced-draft oven for 3 days. Dried samples were then ground using a Wiley mill (Standard model 3, Arthur H. Thomas Co., Philadelphia, PA) fitted with a 1-mm screen for plant analysis. The N concentration in forage yield was determined by automated colorimetry using Lachat QuikChem 8000 autoanalyzer (QuikChem Method 13-107-06-2-D; Lachat Instruments, Milwaukee, WI) on subsamples previously mineralised by the method of Isaac & Johnson (1976). Briefly, this method consists of mineralising dry, and ground (<1 mm) plant tissues subsamples with mixture of sulfuric and selenious acids. Amount of N exported by forage yield was calculated by multiplying N concentrations by its DM yield.

2.2.3 STICS model overview

STICS is a processed-based model that describes the functioning of soil–crop systems over one crop cycle or several successive cycles with a daily time step (Brisson et al., 2009). It was developed to simulate the effects of climatic conditions, soil characteristics and management practices on crop growth and development, crop N nutrition, and environmental variables (e.g. N leaching, gaseous N emissions, and soil organic C dynamic).

Crop phenological development stages are simulated using a thermal index (sum of degree-days [◦C d]). The crop is described by its leaf area index, root growth and shoot dry biomass, which can be affected by temperature, water, and N stress. Shoot growth is driven by C accumulation in the plant through the conversion of intercepted radiation into biomass using the radiation use efficiency (RUE) concept. Then crop biomass is partitioned between structural aboveground organs (stems, green leaves, and dead leaves) and metabolic aboveground biomass, pooled in a virtual reserves compartment which represent the metabolic reserve in the perennial organs in this version of STICS (restemp). The STICS V9.2 used in this study simulates C and N remobilisation during regrowth for perennial crop (Brisson et al., 2009). However, the C remobilisation is limited and driven by the source/sink ratio and occur independently of the N remobilization. The lack of compartmentation of the reserves in the plant (the C and N reserves that can be remobilized by the plant and the structural part of organs that cannot be remobilized by the plant) and the absence of parallelism between the C and N pools mean that the remobilization of C and N from non-perennial organs (organs with a lifespan of less than one year: leaves and stems) to perennial organs (organs that last for more than a year and are used as storage organs by the plant: rhizomes or taproots) at the end of the growing season and after a hay cut is not simulated by the model.

The water and N balances are calculated using the concept of limiting factor between soil supply and crop demand, allowing water and N stress indices to be defined. For water deficit stress, four different stress indices are calculated, affecting the plant's physiological functions in different ways (delay

emergence and slow deep root growth, delay development and slow leaf growth, accelerate leaf senescence and to reduce RUE and transpiration). They depend on the water content above the wilting point in the root zone, calculated from the balance of all variables contributing to water flux in the soil-plant-atmosphere continuum. For water stress due to excess water, three indices are calculated by STICS from the waterlogging index, called exofac, representing the proportion of root length that is in anoxic conditions during the growing season (exofac = 1 means that all roots are in anoxic conditions). The three indices affect root growth, LAI growth and RUE, respectively.

Crop N requirement is calculated according to the concept of N dilution curves in the aboveground biomass. This approach enables to calculate the potential crop N uptake with the maximum N dilution curve (N_{cmax}), and the critical N concentration in shoots required to produce the maximum aboveground biomass at a given time with the critical N (N_c) dilution curve. For Timothy, N_c was calculated using the following equations: $N_c = 4.8 \times (\text{Shoot Biomass})^{-0.32}$.(Lemaire & Salette, 1984). The ratio of the actual N concentration to N_c, defined as N nutrition index (NNI) is used to determine the presence (NNI < 1) or absence (NNI ≥ 1) of N stress on potential crop growth. Three N stress indices, which are involved in different physiological processes, are calculated from NNI. These stress indices reduce RUE and LAI growth, and accelerate senescence, respectively.

The soil is described as a succession of horizontal layers (up to 5) with their hydrodynamic and pedological characteristics. The crop interacts with the soil via the roots, which are defined in terms of root density distribution in the soil profile. Root expansion can be calculated in 2 different ways. The first option is based on the independence of root length expansion from shoot biomass accumulation. Conversely, with the second option, root length expansion is driven by shoot growth and relies on a dynamic underground/total biomass partitioning coefficient (Trophic-linked root length expansion). The latter option has two other variants: either the specific root length to root mass ratio parameter is taken into account in the root length growth calculation function (continuous link), or act as a threshold (Beaudoin et al., 2022).

Soil N supply is calculated per 1-cm layer along the rooting depth and takes into account mineral fertilizers, mineralization of organic matter (humus and crop residues), denitrification, nitrification, NH_3 volatilization, and NO_{3-} leaching. Soil N transformations are closely influenced by soil characteristics (pH, clay and $CaCO_3$ content), soil organic N content, temperature, and soil water content.

The fate of N fertilizer is simulated empirically, using the fertiliser use efficiency (FUE) which refers to the proportion of N fertilizer recovered in the crop at harvest. The complement of this efficiency (1-FUE) is partitioned into gaseous losses (volatilisation and denitrification), lixiviation and microbial immobilisation in soil organic matter. Details about all algorithms and equations are available in Brisson et al. (2009).

2.2.4 STICS parametrization

STICS version V9.2 has been calibrated and validated to simulate the growth and nutritive value of timothy under Canadian growing conditions (Jégo et al., 2013). Crop parameters for the cultivar Champ given in this previous study were used.

Timothy (cultivar Champ) was sown at rate of 10 kg ha^{-1} equivalent to 2000 plants m^{-2}. The main variables defining the initial state and the permanent characteristics of the soil system are set only once at the beginning of simulation in spring 1998. Multi-year continuous simulations without annual reinitialization were made from seeding to the end of the experiment. Soil water content and soil mineral N were not available neither at the initiation of the experiment neither for years of experiment. Based on topsoil (0-20 cm depth) analysis in 2008, the concentration of organic N and the soil pH_{water} were set, based on soil analysis in 2008, at 2.0 g kg^{-1} and 5.9, respectively. Initial soil water content was fixed at field capacity, which is representative of the soil moisture status in early spring. We assumed mineral N content of 20, 10, and 10 kg N ha^{-1} for the 0-20, 20-40, and 40-120 cm soil layers, respectively. Because the proportion of mineral soil particles was not measured, soil clay content (<2 µm) was then assumed to be 180 g kg^{-1} by referring to the amount of clay for a soil with a sandy loam texture (clay content between 0 and 20 g kg^{-1}) according to Canadian soil type texture triangle. The soil bulk density was defined to 1.16, 1.25 and 1.36 g cm^{-3}, for the 0-20, 20-40, and 40-120 cm soil layers, respectively, with a volumetric content of coarse materials (>2 mm) per soil layer of 20%. The water content for the three soil layers at field capacity (19.2, 18.6 and 16.4% dry-mass soil, respectively) and at permanent wilting point (9.3, 9.0 and 7.9% dry-mass soil, respectively) were estimated using a pedo-transfer function (Saxton & Rawls, 2006). The thickness of the biologically active layer for mineralisation was assumed to be 20 cm. The proportion of inactive soil organic matter (finert) was set to 55% rather than 65% used as default value (Martel & Lasalle, 1977).

Daily weather data (minimum and maximum temperatures, solar radiation, rainfall, wind speed, and relative humidity) were obtained from the Lauzon weather station of Environment Canada (lat. 46°49´ N; long. 71°06´ W, alt. 69 m) located at 5 km from the Harlaka experimental site. Daily minimum and maximum temperatures and precipitation were pre-processed by the snow module to take account of snow cover. In this study, potential evapotranspiration was calculated using the equation proposed by Shuttleworth and Wallace (1985).

Management practices such as N fertilization application dates and rates, and dates of the first and second harvests required in the management file of STICS were used. Harvest dates, the sum of growing degree-days and rainfall in each year during each growing cycle are presented in Table 2.1.

2.2.5 Model evaluation and statistical analysis

STICS performance was evaluated by comparing the mean observed data, collected over the eight production years (1999–2006) for the eight (N*P) treatments with the predicted values. The studied variables included forage yield, N concentration and N amount exported in forage yield for the two harvests.

Various complementary statistical criteria were used to evaluate the model performance and were calculated as follows:

Normalized mean error (NME) with an optimal value of 0%:

$$\mathrm{NME}\ (\%) = 100\,\frac{\frac{1}{n}\sum_{i=1}^{n}(Obs_i - Pred_i)}{\overline{Obs}} \qquad \text{(Equation 1)}$$

Normalized root mean square error (NRMSE). According to Jamieson et al. (1991), the model is considered excellent when NRMSE ≤ 10%, good when 10% < NRMSE ≤ 20%, fair when 20% < NRMSE ≤ 30%, and poor when NRMSE > 30% :

$$\mathrm{NRMSE}\ (\%) = 100\,\frac{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(Pred_i - Obs_i)^2}}{\overline{Obs}} \qquad \text{(Equation 2)}$$

Model efficiency (EF) with an optimal value of 1.0:

$$\mathrm{EF} = 1 - \frac{\sum_{i=1}^{n}(Pred_i - Obs_i)^2}{\sum_{i=1}^{n}(Obs_i - \overline{Obs})^2} \qquad \text{(Equation 3)}$$

And coefficient of determination (R^2) between observed and predicted data pairs using the standardized major axis (SMA) regression (Correndo et al., 2021b):

$$\mathrm{R}^2 = \left[\frac{\frac{1}{n}\sum_{i=1}^{n}(Pred_i - \overline{Pred})(Obs_i - \overline{Obs})}{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(Pred_i - \overline{Pred})^2}\sqrt{\frac{1}{n}\sum_{i=1}^{n}(Obs_i - \overline{Obs})^2}}\right]^2 \qquad \text{(Equation 4)}$$

The mean square error was also decomposed into percentage lack of precision (PLP) and percentage lack of accuracy (PLA), which refer to the percentage of dispersion and the systematic error, respectively. These criteria estimate the dominant type of the model error (either dispersion or systematic error). These two criteria were calculated as follows:

$$PLP\ (\%) = 100\,\frac{\frac{1}{n}\sum_{i=1}^{n}\left(|Pred_i - \widehat{Pred_i}|\right)\left(|Obs_i - \widehat{Obs_i}|\right)}{\frac{1}{n}\sum_{i=1}^{n}(Pred_i - Obs_i)^2} \qquad \text{(Equation 5)}$$

$$PLA\ (\%) = 100\frac{\frac{1}{n}\sum_{i=1}^{n}(Obs_i - \widehat{Pred}_i)^2}{\frac{1}{n}\sum_{i=1}^{n}(Pred_i - Obs_i)^2} \qquad \text{(Equation 6)}$$

Pred$_i$ and *Obs*$_i$: annual predicted and observed values, respectively; $\overline{Pred}$ and $\overline{Obs}$: mean of predicted and observed values for the 1999-2006 period, respectively; *n*: number of predicted and observed data pairs.

All statistics were carried out using R software, version 4.3.1 (R Core Team, 2023). Statistical criteria for STICS evaluation were computed using the "STICSevalR" library. Plots were made with the "ggplot2" library R. Field-observed data at each forage harvest and each year were analyzed by analysis of variance. It was performed to evaluate the effect of N fertilization on forage yield, N concentration, and N amount in forage yield under the two P rate treatments (30 and 45 kg P ha^{-1}). Residuals were analyzed for normality using the Shapiro-Wilks and Levene's test for homogeneity of variances. Where treatment effects were significant at the 0.05 probability level, means were compared using Tukey's Honest Significant Difference (HSD) test. Standard errors of the mean were also calculated. To identify the agronomic optimum N rate, ANOVA and post-hoc test were computed for annual forage yields during the eight production years.

2.3 Results

2.3.1 Field-observed data

Forage yield increased significantly with increasing N fertilization rates in all production years, except in 2006 for the second harvest (Table 2.2). The 8-year average of forage yield for the first harvest was 2.4, 4.9, 5.7, and 5.8 Mg DM ha^{-1} yr^{-1} for 0, 60, 120, and 180 kg N ha^{-1} yr^{-1}, respectively. For the second harvest, the 8-year average of forage yield was much lower with 0.5, 0.7, 0.9, and 1.5 Mg DM ha^{-1} yr^{-1} after applying 0, 60, 120 and 180 kg N ha^{-1} yr^{-1}, respectively. Forage yields obtained with 120 and 180 kg N ha^{-1} were not significantly different in all 8 production years for the first harvest and in 4 out of 8 for the second harvest (Table 2.2). For all treatments, forage yields for the first harvest represent between 78 to 94% of annual production depending on the year (with an average of 84%). A slow but constant drop in forage yield was observed all along years of cropping for all treatments, particularly from the 5th year of cropping (from 2003 to 2006) for the first harvest and to a lesser extent in the second harvest also (Table 2.2).

Table 2.2 Annual mean (n = 8) of measured timothy forage yield (Mg DM ha^{-1}) grown under four N application rates (for the first and second harvests) during eight successive cropping years.

N rate (kg N ha^{-1})	1999	2000	2001	2002	2003	2004	2005	2006
First harvest								
0	5.1 c	3.4 c	2.8 c	2.6 c	1.4 b	0.7 c	1.8 c	1.7 b
60	7.4 b	6.5 b	6.1 b	5.5 b	3.2 a	2.9 b	3.9 b	3.8 a
120	8.2 ab	7.7 ab	7.2 a	6.3 a	3.7 a	4.0 a	4.6 a	4.3 a
180	8.9 a	7.9 a	7.2 a	6.5 a	3.6 a	3.8 a	4.4 ab	4.2 a
SEM [a]	0.4	0.3	0.3	0.2	0.1	0.2	0.1	0.2
p-value [b]	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001
Second harvest								
0	0.6 b	0.7 c	0.4 c	0.7 ab	0.4 c	0.2 b	0.1 b	0.9 a
60	2.5 a	1.0 c	0.4 c	0.4 b	0.4 c	0.2 b	0.1 b	0.9 a
120	1.9 ab	1.7 b	0.8 b	0.6 ab	0.7 b	0.4 b	0.3 a	1.1 a
180	3.3 a	2.8 a	1.6 a	1.0 a	1.0 a	1.1 a	0.5 a	1.2 a
SEM	0.4	0.2	0.1	0.1	0.1	0.1	0.1	0.2
p-value	0.002	<0.001	<0.001	0.0371	<0.001	<0.001	<0.001	0.273

[a] SEM: Standard error of the mean for the comparison of N rates within a year
[b] p-value: probability of a significant effect of N rate

For annual forage yield (sum of 1st and 2nd harvest), although the yield obtained with 180N was slightly higher than with 120N, the difference between the 2 treatments was not significant (Table 2.3).

Nitrogen application rates increased significantly ($P < 0.05$) N concentration in all production years for the first harvest and in five production years for the second harvest (Table 2.4). The 8-year average of N concentration was 16.3, 18.5, 21.9 and 24.4 g N kg^{-1} DM for the first harvest and 20.3, 20.4, 21.1 and 22.5 g N kg^{-1} DM for the second harvest with 0, 60, 120 and 180 kg N ha^{-1} yr^{-1}, respectively.

Table 2.3 Annual mean (n = 8) of measured timothy forage yield (sum of the annual two harvests) (Mg DM ha^{-1}) grown under four N application rates during eight successive cropping years.

N rate (kg N ha^{-1})	1999	2000	2001	2002	2003	2004	2005	2006
0	5.6 c	4.2 c	3.2 c	3.3 c	1.8 c	0.9 c	1.9 c	2.6 b
60	9.6 b	7.5 b	6.6 b	5.9 b	3.6 b	3.1 b	4.0 b	4.7 a
120	10.1 ab	9.4 a	8.0 a	6.8 ab	4.3 a	4.4 a	4.9 a	5.3 a
180	12.1 a	10.7 a	8.8 a	7.5 a	4.7 a	4.9 a	4.9 a	5.5 a
SEM [a]	0.6	0.4	0.3	0.2	0.2	0.2	0.1	0.3
p-value [b]	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001

[a] SEM: Standard error of the mean for the comparison of N rates within a year
[b] p-value: probability of a significant effect of N rate

Table 2.4 Annual mean (n = 8) of measured N concentration in forage yield (g N kg^{-1} DM) grown under four N application rates (for the first and second harvests) during eight successive cropping years.

N rate (kg N ha^{-1})	1999	2000	2001	2002	2003	2004	2005	2006
First harvest								
0	14.6 c	15.6 c	13.0 b	21.5 b	16.9 d	17.4 c	15.3 d	15.9 c
60	18.7 b	18.7 b	13.8 b	19.6 b	19.9 c	19.7 c	18.7 c	19.1 b
120	22.1 a	19.0 b	18.5 a	22.4 ab	24.3 b	24.2 b	21.8 b	23.0 a
180	23.1 a	21.9 a	19.3 a	25.1 a	27.0 a	28.4 a	25.6 a	24.7 a
SEM [a]	0.5	0.6	0.5	0.8	0.6	0.7	0.4	0.5
p-value [b]	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001
Second harvest								
0	19.6 a	17.7 a	22.4 a	26.0 a	22.2 c	17.0 a	19.9 b	17.3 b
60	18.0 a	18.4 a	20.9 ab	24.9 ab	23.3 bc	20.4 a	20.3 ab	17.3 b
120	20.7 a	19.0 a	19.1 b	23.3 ab	24.2 b	22.4 a	21.4 ab	18.8 ab
180	22.4 a	19.1 a	20.2 ab	21.9 b	27.6 a	22.9 a	23.2 a	22.5 a
SEM	2.1	0.5	0.6	0.9	0.4	2.0	0.8	1.2
p-value	0.517	0.177	0.003	0.016	<0.001	0.157	0.025	0.014

[a] SEM: Standard error of the mean for the comparison of N rates within a year
[b] p-value: probability of a significant effect of N rate

Increasing N fertilization rates had also significant (P > 0.05) effect on N amount exported in forage yield in all the 8 years of the study, except in 2002 for the second harvest (Table 2.5). The 8-year average of N amount exported in forage yield was 39, 90, 123 and 138 kg N ha^{-1} for the first harvest, and 11, 15, 19 and 34 kg N ha^{-1} for the second harvest with 0, 60, 120 and 180 kg N ha^{-1} yr^{-1}, respectively.

Table 2.5 Annual mean (n = 8) of observed N amount exported in forage yield (kg N ha^{-1}) grown under four N application rates (for first and second harvests) during eight successive cropping years.

N rate (kg N ha^{-1})	1999	2000	2001	2002	2003	2004	2005	2006
First harvest								
0	74 c	55 c	36 c	56 d	24 c	12 c	27 d	27 c
60	139 b	122 b	85 b	109 c	64 b	58 b	73 c	73 b
120	180 a	147 ab	132 a	140 b	88 a	95 a	100 b	98 a
180	206 a	174 a	139 a	163 a	98 a	108 a	113 a	103 a
SEM [a]	8.5	8.0	4.8	5.1	3.5	3.4	2.8	4.7
p-value [b]	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001
Second harvest								
0	15 c	13 c	9 b	19 a	9 c	4 b	2 b	14 b
60	50 ab	19 c	10 b	10 a	9 c	4 b	2 b	14 b
120	40 bc	33 b	16 b	13 a	17 b	9 b	7 a	19 ab
180	73 a	53 a	32 a	21 a	28 a	25 a	11 a	28 a
SEM	8.0	2.9	1.8	3.6	1.6	1.4	1.2	2.6
p-value	<0.001	<0.001	<0.001	0.155	<0.001	<0.001	<0.001	0.002

[a] SEM: Standard error of the mean for the comparison of N rates within a year
[b] p-value: probability of a significant effect of N rate

2.3.2 Agreement between field-observed and STICS predicted values

2.3.2.1 Timothy forage yield

Observed values for the forage yield varied between 0.7 and 8.9 Mg DM ha^{-1} and predicted ones between 3.2 and 8.7 Mg DM ha^{-1} for the first harvest. Mean of predicted yield values (5.2 ±1.5 Mg DM ha^{-1}) was higher than the mean of observed yield values (4.7 ±2.2 Mg DM ha^{-1}). The model bias and NRMSE were small (NME = -9 %; NRMSE = 22%), with a substantial coefficient of determination (R^2 = 0.77) and high model efficiency (EF=0.7) (Figure 2.1). For the second harvest, observed forage yield values varied between 0.1 and 3.3 Mg DM ha^{-1} and predicted ones between 0.0 and 5.0 Mg DM ha^{-1}. The mean observed and predicted values were 0.9 ±0.8 and 1.2 ±1.0 Mg DM ha^{-1}, respectively. The NME was relatively high (-19%) and the NRMSE was very large (99%) with a very weak R^2 and a negative EF, showing the poor agreement between predicted and observed forage yield (Figure 2.1). The model errors, especially for the second harvest, were mainly due to dispersion error (PLP > PLA) for forage yield.

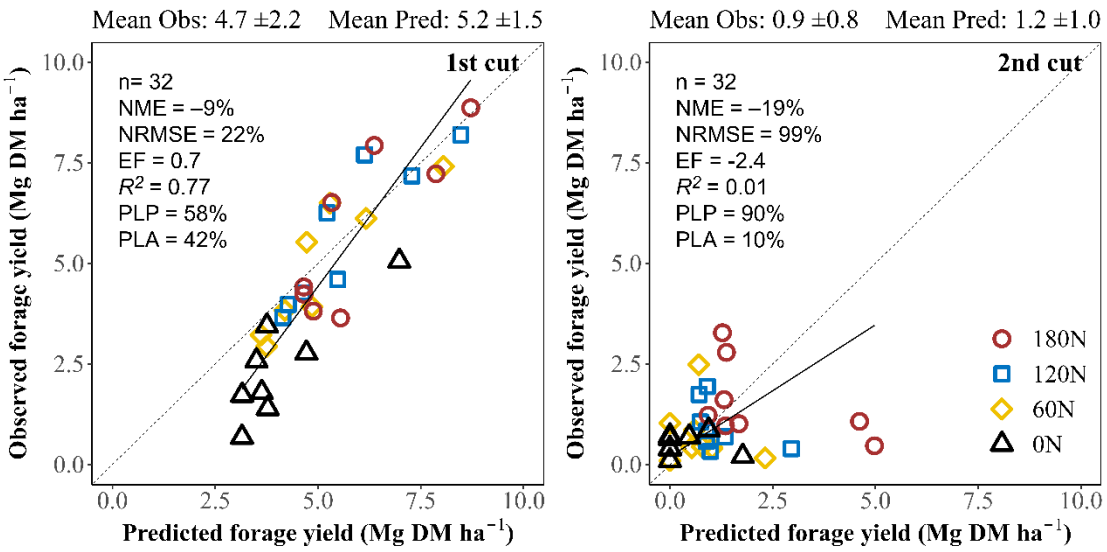

Figure 2.1 Observed versus predicted forage yield for the 1st and 2nd harvest as a function of N application rates. Each point is an average of 8 measurements (=4 replicates × 2 P application-rates) for the observed values. Mean of observed value (Mean Obs), mean of predicted value (Mean Pred), number of predicted and observed data pairs (n), normalized mean error (NME), normalized root mean square error (NRMSE), model efficiency (EF), coefficient of determination (R2), percentage lack of precision (PLP), and percentage lack of accuracy (PLA).

2.3.2.2 N concentration in forage yield

For the first harvest, the mean of predicted (20.4 ±5.2 g N kg^{-1} DM) and observed values (20.3 ±3.8 g N kg-1 DM) of N concentration in forage yield were similar. The model bias (NME = -1%) and the NRMSE (14%) were low, with a moderate R^2 and a satisfactory EF (0.6 and 0.5, respectively) (Figure 2.2). Considering N concentration in forage yield for the second harvest, the bias was relatively high (mean of observed and predicted values of 21.4 ±2.5 and 13.0 ±3.9 g N kg^{-1} DM, respectively, with NME of 38%). The NRMSE was poor (43%) and there is a great dispersion (R^2 = 0.01 and EF = -13.5) (Figure 2.2). For N concentration in forage yield, the errors of the model were mainly due to unsystematic error (PLP = 99%) for the first harvest, and conversely for the second harvest.

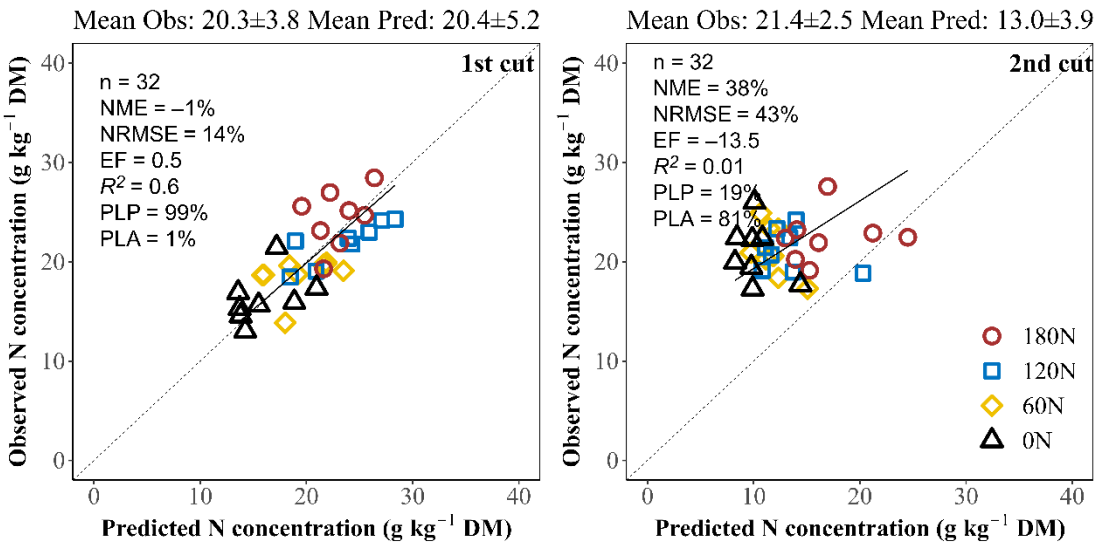

Figure 2.2 Observed versus predicted N concentration in forage yield for the 1st and 2nd harvest as a function of N application rates. Each point is an average of 8 measurements (=4 replicates × 2 P application-rates) for the observed values. Mean of observed value (Mean Obs), mean of predicted value (Mean Pred), number of predicted and observed data pairs (n), normalized mean error (NME), normalized root mean square error (NRMSE), model efficiency (EF), coefficient of determination (R2), percentage lack of precision (PLP), and percentage lack of accuracy (PLA).

2.3.2.3 N amount exported in forage yield

Mean of observed values of N amount exported in forage yield was similar to the predicted ones (97 ±49 and 96 ±34 kg N ha^{-1}, respectively) for the first harvest. The model NRMSE was small (22%), with a low bias (NME= 2%), a substantial R^2 and high EF (0.84 and 0.8, respectively) (Figure 2.3). For the second harvest, the model underestimated the N amount exported in forage (mean of observed and predicted values of 20 ±16 and 12 ±17 kg N ha^{-1}, respectively, with NME of 39%). The NRMSE was very high (117%) with a very weak R^2 (0.03) and a negative EF (-1.1) (Figure 2.3). The model errors were mainly associated to dispersion error (PLP = 72%) for N exported.

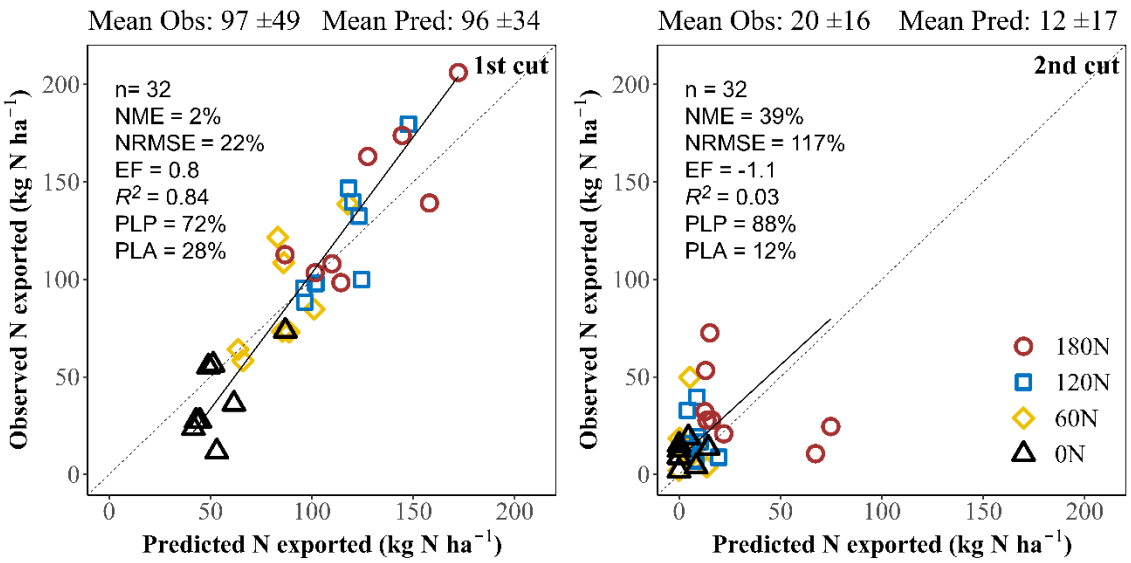

Figure 2.3 Observed versus predicted N exported in forage yield for the 1st and 2nd harvest as a function of N appl ication rates. Each point is an average of 8 measurements (=4 replicates × 2 P application-rates) for the observed values. Mean of observed value (Mean Obs), mean of predicted value (Mean Pred), number of predicted and observed data pairs (n), normalized mean error (NME), normalized root mean square error (NRMSE), model efficiency (EF), coefficient of determination (R2), percentage lack of precision (PLP), and percentage lack of accuracy (PLA).

2.3.3 STICS ability to reproduce the effect of agricultural practices and climatic variables

STICS was able to satisfactorily simulate the production attributes for the first harvest (Figures 2.1, 2.2, 2.3, 2.4; Table 2.6). STICS ability to reproduce the effect of N application rates on forage yield, N concentration and N amount exported in forage yield for the first harvest is presented in Figure 2.4 and Table 2.6. The model correctly simulated the positive effect of N application rates on harvested forage biomass, which was observed in the experiment. It reproduced with accuracy the forage yield for 60N, 120N and 180N treatments (with |NME| ranging from 0 to 3%, NRMSE < 17%, and high EF and R^2), but it overestimated forage yield without N fertilization (NME = -57%), especially in years when yields observed in the field were very low (Figure 2.4a). Furthermore, the model reproduced the significant decrease in forage yields observed in 2003, 2004, 2005 and 2006 (Figure 2.4a). STICS correctly simulated the positive effect of N application rates on N concentration in forage yield, with NME of 2, -4, -7 and 6%, respectively (Figure 2.4b, Table 2.6). In addition, the NRMSE were small (16, 15, 12, and 13%, respectively). Generally, STICS reproduced the positive effect of N application rates on N amount exported in forage yield (Figure 2.4c). However, the model tended to overestimate the N exported for 0N treatment. The model NRMSE was high (53%), with a large bias (NME= -38%), and a weak R^2 and EF = -0.1, for the N amount exported in forage yield without N fertilization. For the other N application rates treatments, the model NRMSE were small (ranging from 16 to 22%) with a low bias (|NME| < 9%), a moderate R^2, and a satisfactorily EF (Table 2.6).

Table 2.6 Performance evaluation of STICS for timothy forage yield (Mg DM ha^{-1}), N concentration in forage (NC forage) (g N kg^{-1} DM) and N amount exported in forage yield (N exported) [kg N ha^{-1}] for the 2 annual harvests for eight successive production years. Number of predicted and observed data pairs (n = 8), mean of observed value (Mean Obs), mean of predicted value (Mean Pred), normalized mean error (NME), normalized root mean square error (NRMSE), model efficiency (EF) and coefficient of determination (R^2).

N rate	Variables	Mean Obs	Mean Pred	NME (%)	NRMSE (%)	EF	R^2	Slope	Intercept
First harvest									
0N	Forage yield	2.4	4.1	-57	61	-1.0	0.72	1.1	-2.0
	NC forage	16.3	15.9	2	16	-0.3	0.19	0.9	1.9
	N exported	39	54	-38	53	-0.1	0.45	1.4	-36.6
60N	Forage yield	4.9	5.1	-3	14	0.78	0.79	1.1	-0.9
	NC forage	18.5	19.3	-4	15	-1.28	0.11	0.7	5.1
	N exported	90	87	4	22	0.48	0.51	1.7	-54.0
120N	Forage yield	5.7	5.7	0	13	0.79	0.76	1.2	-1.1
	NC forage	21.9	23.5	-7	12	-0.72	0.69	0.6	8.3
	N exported	123	116	5	16	0.59	0.73	1.9	-92.1
180N	Forage yield	5.8	6.0	-3	17	0.69	0.70	1.3	-2.2
	NC forage	24.4	23.0	6	13	-0.27	0.15	1.3	-5.1
	N exported	139	126	8	17	0.58	0.68	1.34	-32.1
Second harvest									
0N	Forage yield	0.5	0.4	19	62	-5.09	0.03	-0.4	0.7
	NC forage	20.9	10.2	51	54	-16.5	0.11	-1.5	36.5
	N exported	11	4	67	93	-2.44	0.02	1.1	6.9
60N	Forage yield	0.7	0.8	-2	99	-1.85	0.22	-1.1	1.5
	NCforage	21.1	11.8	44	47	-15.6	0.34	-1.7	40.7
	N exported	15	5	66	122	-0.59	0.01	-3.4	31.4
120N	Forage yield	0.9	1.2	-16	76	-2.85	0.21	-0.8	1.9
	NC forage	21.1	13.4	37	41	-18.8	0.07	-0.7	30.3
	N exported	19	9	52	86	-1.39	0.17	-2.4	41.3
180N	Forage yield	1.6	2.2	-31	109	-4.96	0.13	-0.6	2.9
	NC forage	22.5	16.9	25	31	-7.8	0.03	0.6	12.0
	N exported	34	29	13	112	-3.13	0.27	-0.8	56.2

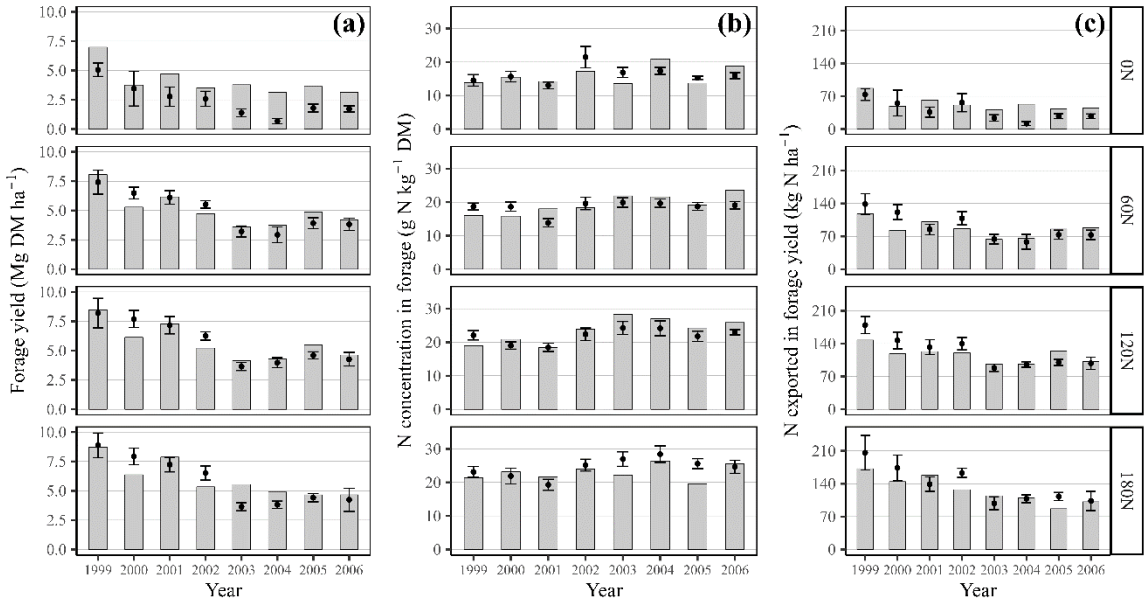

Figure 2.4 Annual mean of observed (dots) and predicted (grey bars) forage yield (a), N concentration in forage yield (b) and N exported in forage yield (c) from 1999 to 2006 at the first harvest as a function of N application rates. Bars on dots are standard deviation (n=8). 0N, 60N, 120N and 180N denoted application rates of 0, 60, 120 et 180 kg N ha^{-1} yr^{-1}, respectively.

STICS was not very good at simulating the production attributes for the 2nd harvest (Figures 2.1, 2.2, 2.3, 2.5; Table 2.6). The model underestimated forage yield and N exported for the first 2 years of production and overestimated them in 2004 and 2005. Very low aboveground biomass regrowth (leaves and stems) is simulated in 1999, 2000, 2001, 2003 and 2005 for the 0N treatment, and in 2000 and 2005 for the 60N treatment, so that forage harvests could not be carried out in the simulation (Figure 2.5a). The N concentrations were underestimated for all treatments (Figure 2.5b). For years without simulated harvests, the simulated N concentrations in the standing biomass were compared with the field-observed values.

Analysis of model residuals (observed value–predicted value) for the first harvest as a function of the cumulative rainfall, the mean temperature, and the sum GDD during the primary growth showed that model errors were not dependent on climatic variables (Figure 2.6). It seems that the N application rates explained most of the variability between observations and predictions. For the forage yield variable, predicted values were almost always higher than the observed values for the 0N treatment (Figure 2.6).

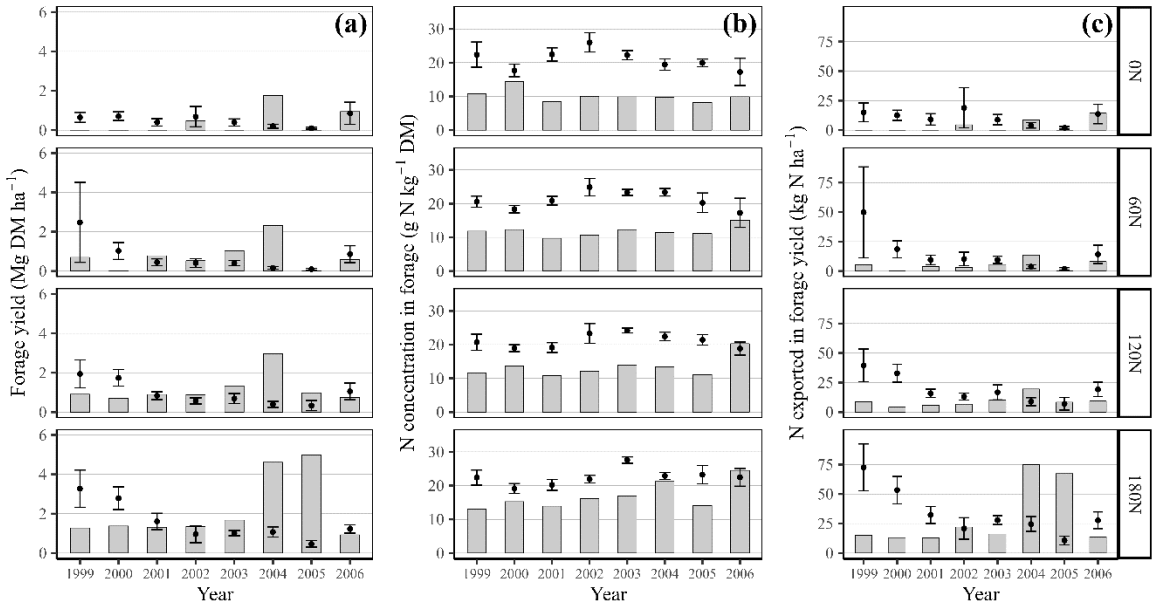

Figure 2.5 Annual mean of observed (dots) and predicted (grey bars) forage yield (a), N concentration in forage yield (b) and N exported in forage yield (c) from 1999 to 2006 at the second harvest as a function of N application rates. Bars on dots are standard deviation (n=8). 0N, 60N, 120N and 180N denoted application rates of 0, 60, 120 et 180 kg N ha^{-1} yr^{-1}, respectively.

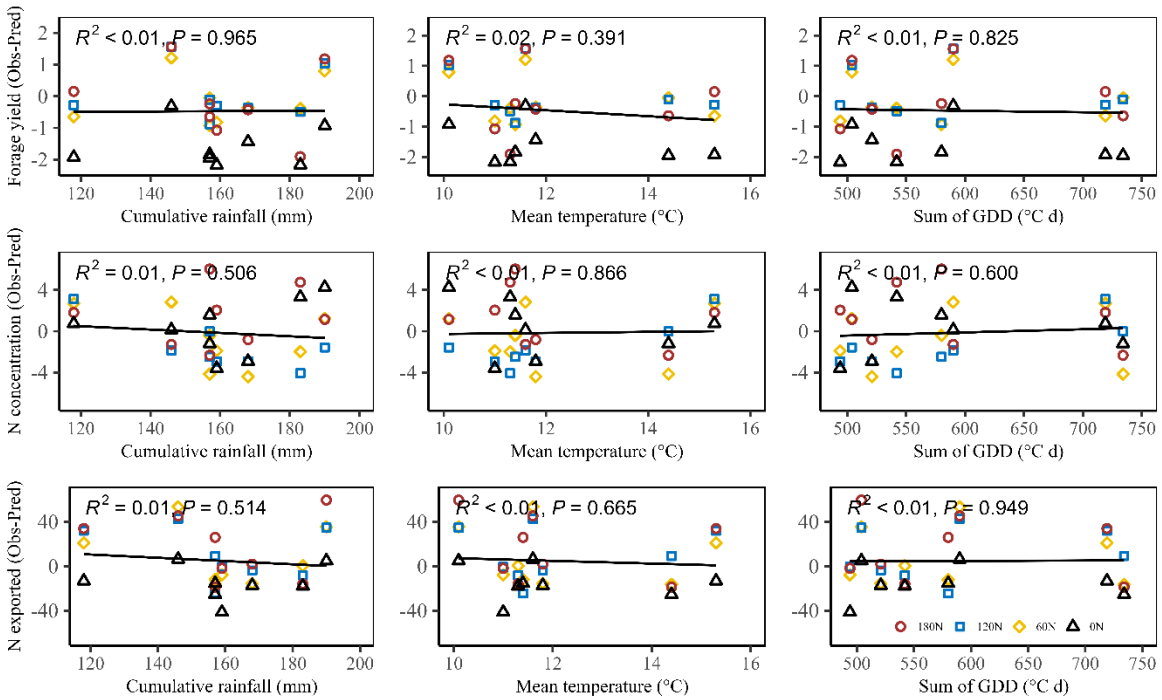

Figure 2.6 Difference between observed and predicted value of forage yield, N concentration in forage yield, and N amount exported in forage yield at the first harvest as a function of the cumulative rainfall, the mean temperature, and the sum of growing degree-days (GDD basis 0°C) during the primary growth (from 01 May to first harvest).

2.3.4 Variation of nitrogen nutrition index during growing cycle and level at harvest

The N nutrition index (NNI) value can fluctuate daily from 0.3 to N_{cmax}/N_c in STICS, with an NNI greater than or equal to 1.0 being the absence of stress. In general, the model outputs showed that the level of NNI variation during the growth cycle increased with N application rates (Figure 2.7). For the 0N treatment, the median of the variation of NNI exceeded 0.6 for only 2 years. The level of NNI at harvest increased also with the N fertilization application rates for all years, and it is in this aspect that stands out the difference between the 120N and 180N treatments (Figure 2.7). However, for the 180N treatment, the crop was always N-stressed during the primary growth cycle. Variations in crop NNI during the growth cycle (between May 1 and the date of the 1st harvest) did not reach the optimum value in all production years, despite the supply of 180 kg N ha^{-1} yr^{-1}.

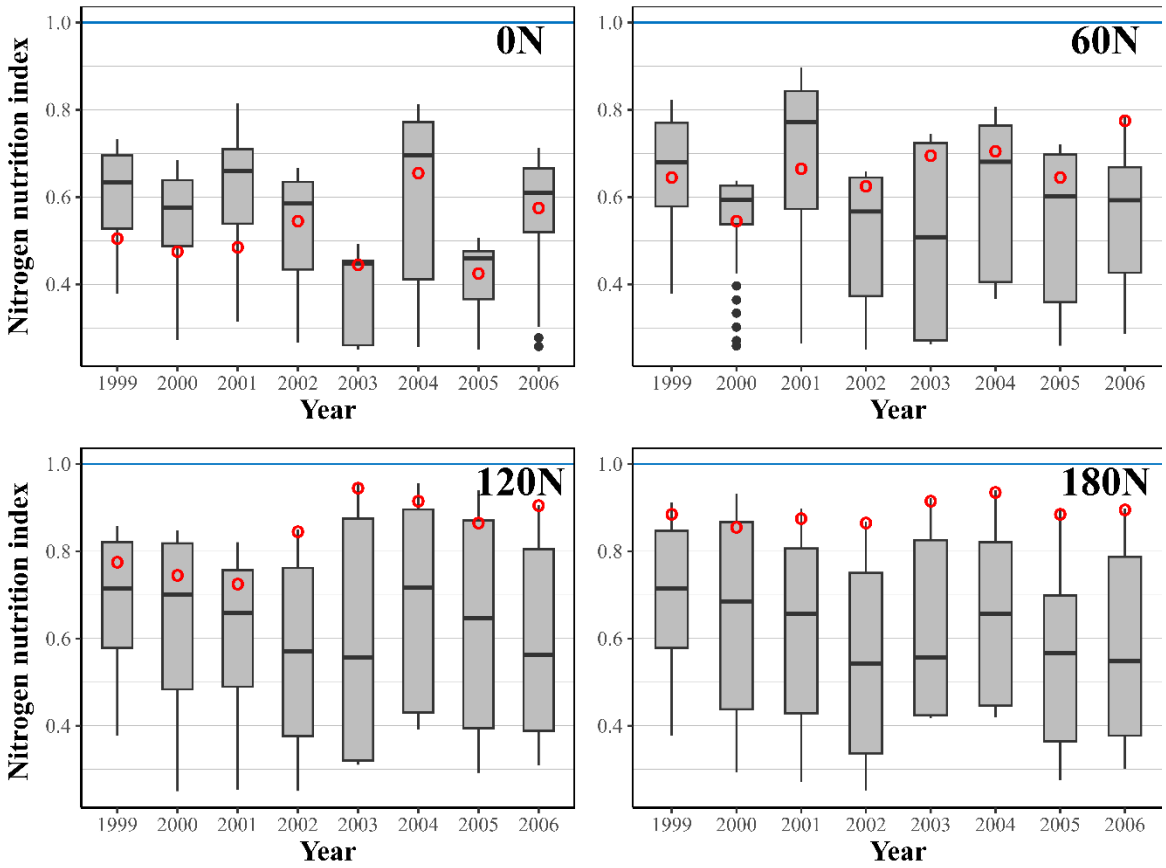

Figure 2.7 Level of simulated N nutrition index (NNI) at harvest (red symbol) and variation of simulated NNI (boxplot) during primary growth period (between 01 May and 1st harvest) according to N application rates. The blue horizontal line represents the optimal NNI threshold. The horizontal bold line represents the median. The bottom of the box is the first quartile and the top of the box the third quartile. Vertical bars represent the highest and lowest values occurring within the 1.5 interquartile range. Points represent outliers that are beyond this limit.

2.3.5 Relation between timothy forage yield and the metabolic reserve in the perennial organs before spring growth

Simulated values of restemp prior to spring growth activation were 3.3 Mg DM ha^{-1} for all treatments for the first year of production (Figure 2.8). Their values were generally above 2.2 Mg DM ha^{-1} for the first 4 years of production, except for the 0N, and 60N treatments in 2001. STICS simulated low metabolic reserve in the perennial organs for the last 4 years in which decline forage yields have been observed. Figure 2.8 showed that the simulated biomass of metabolic reserve in the perennial organs before the activation of growth has a relatively high explanatory power with regard to forage yield trends for the first harvest. The coefficient of determination of the linear regression of forage yields (1st harvest) as a function of the simulated biomass of the metabolic reserve in perennial organs was 71% (Figure 2.8).

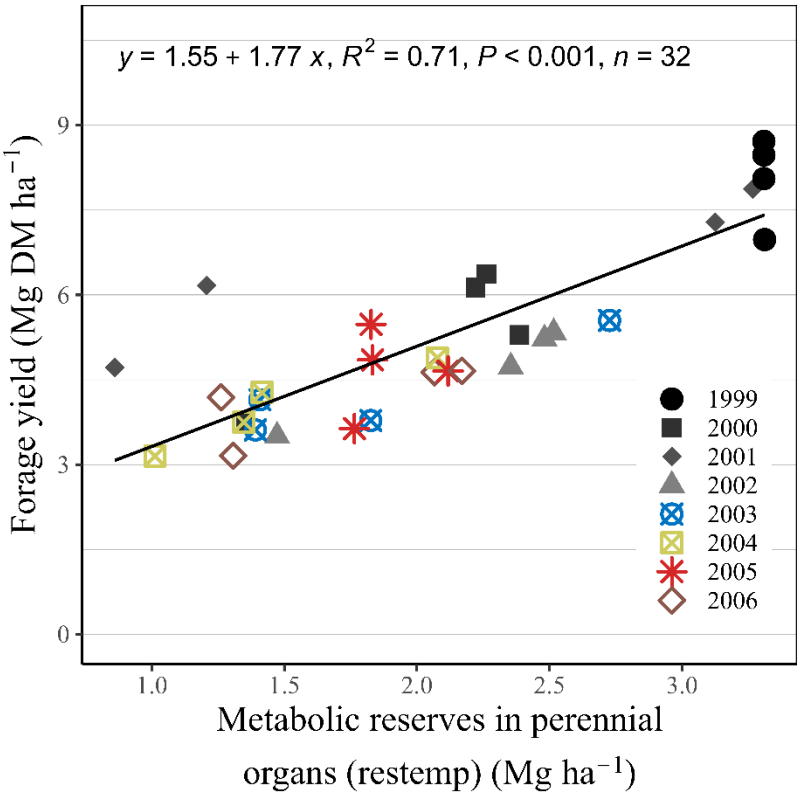

Figure 2.8 Relationship between timothy forage yield (1st harvest) and the metabolic reserves in the perennial organs prior to the primary growth cycle.

2.4 Discussion

2.4.1 General agronomic considerations

The average annual yield level obtained in this study (7.4 Mg DM ha^{-1} yr^{-1}) for the 8 production years with the 180N treatment is comparable to the yield level obtained in eastern Canada (7.8 Mg DM ha^{-1} yr^{-1}), but higher than that obtained in western regions where yields ranged between 5.0 and 6.0 Mg DM $ha^{-1}yr^{-1}$ (Jing et al., 2014). The results of the first harvest of this experiment have already been analysed and published (Bélanger et al., 2008). Using all the data from this same experiment, Bélanger et al. (2008) concluded that the maximum forage yield from the first harvest was reached at 120 kg N ha^{-1}. Analysis of the data from the first harvest in this chapter confirmed this result. According to the simulated NNI (Figure 2.7), the N nutrition was not at optimum levels, but it was nevertheless sufficient to obtain optimal yields since there was no significant difference between 120N and 180N treatments. Moreover, an additional N application rate would not be justified based on economic considerations: on strictly economic criteria, which consider the cost of fertilizer in relation to the yield gain, the 120N treatment may even be sufficient. For the second harvest, not

analysed by Bélanger et al. (2008), yields for some years were higher at 180 kg N ha^{-1} than at 120 kg N ha^{-1}.

From a nutritive point of view, the N concentration in the forage yield for some years for the first harvest was higher with 180 kg N ha^{-1} than with 120 kg N ha^{-1}. The N concentration for the 180N treatment for the first harvest varied between 19.3 and 28.4 g kg^{-1} DM depending on the year. The values of N concentration in timothy reported in the literature can vary widely (Kunelius et al., 2003; Michaud et al., 1998). Some studies reported that the N concentrations in timothy forage yield depend on cultivars (Kunelius et al., 2003). Other authors have also attributed variations in N concentration to dilution processes (Bélanger et al., 2001). Indeed, increasing N fertilization rates has a negative effect on DM digestibility by reducing the proportion of leaves in the forage (Deinum et al., 1968; Kunelius et al., 1976, Bélanger et al., 2001), yet timothy selected for high N concentration has a higher proportion of leaves (Brégard et al., 2000). According to Bélanger et al. (2001), the nutritive value of timothy is influenced indirectly by harvest dates, growing seasons, N fertilization, and cultivars, primarily through their impact on forage yield and the change in the ratio of its metabolic and structural components, with additionally a direct impact on each of these two components.

Given the negative relationship between yield and nutritive value for timothy (Bélanger et al., 2001), harvesting is ideally carried out at the development stage of heading to achieve a compromise between biomass yield gain and high-quality forage. This corresponds to a cumulative GDD of around 600-700°C d with a temperature basis of 0°C (Bélanger et al., 2008). Thus, the annual harvesting frequency is limited to two in the current climatic context of eastern Quebec and of Canada in general. In addition to not tolerating frequent defoliation (Kunelius et al., 2003), the two-harvest system also ensures that timothy regenerates the stand. However, a study conducted by Jing et al. (2014) has shown that with predicted climate change, an additional 3rd harvest per year could be possible, resulting in an increase in annual yield but a reduction in nutritive value. A timothy stand can last for many years, but certain measures must be taken to ensure solid stands, such as balanced fertilization (Bélanger et al., 1989). The 8 years of production in this study is already quite long because grasslands are often reseeded after 3-5 years of production. To avoid N deficiency during the first and especially during the second harvest, it is recommended to split the fertilizer application in two: one during the early growth period and the second just after the first harvest (Grant & Burgess, 1979). This study showed that the N amount exported annually by the forage yield was greater than the amount of N fertilizer applied, at least for the first 4 years for the 120N and 180N treatments. For example, for the 180N treatment, the N exported by summing the two harvests was 279 kg N ha^{-1} in 1999, 227 kg N ha^{-1} in 2000, 171 kg N ha^{-1} in 2001, and 184 kg N ha^{-1} in 2002 (Table 2.5). The N application rates therefore did not compensate for the N exported by the forage yields. This illustrates the importance of taking soil supply into account when calculating the N balance for managing N fertilization, with the aim of balancing N supply and crop needs.

2.4.3 Low performance of STICS for simulating the second harvest and the situations with a significant N deficiency in the first and second harvests without any N fertilization

The STICS predictions of forage yield for the second harvest, were poor with high bias (NME = -19%) but a large NRMSE (99%). This was to be expected, as previous studies of timothy simulation with STICS in eastern Canada have noted an overestimation of regrowth. Jégo et al. (2013) calculated NME from 13 to -111% and NRMSE from 63 to 121%, depending on the site location. Jing et al. (2017), who conducted a timothy simulation without annual reinitialization for 3 consecutive years, noted also a slight overestimation of the yield in the summer regrowth by STICS.

Running multi-year simulations without annual reinitialization did not improve the simulation of summer regrowth in this study, indicating that there was no significant advantage in improving the simulation of reserve dynamics with this simulation mode compared to the simulation with annual reinitialization (Jégo et al., 2013). The NRMSE value calculated for the second harvest was worse than those obtained by studies using the CATIMO model, with NRMSE < 30% (Jing et al., 2012, 2013). Improvements have been made to the simulation of crop reserves in the CATIMO model using the concept of reserve-dependent growth (Jing et al., 2012), whereas in the version of STICS used in this study, there is no compartmentation and simulation of reserve remobilization between non-perennial and perennial organs (Brisson et al., 2009). An improvement would be required on this aspect with STICS for timothy, by considering a distinction between the C and N content of non-perennial organs, perennial organs (rhizome and taproot) and roots, as well as the compartmentation of the C and N content of perennial and non-perennial organs into reserves remobilizable and structural parts. These modifications have already been calibrated for alfalfa and miscanthus and have enabled a more realistic simulation of regrowth by STICS (Strullu et al., 2014, 2020). The datasets used in this study did not allow the calibration of the new perennial crop formalism, recently available, for timothy. The next step in this research, to better simulate crop reserves, will be to mobilize timothy datasets including field measurements of the structural and metabolic C and N content of different plant parts (e.g. leaves, stem, perennial organ) during forage establishment and regrowth.

The performance evaluation showed that STICS poorly simulated the timothy forage yield and the N exported in forage yield for the 0N treatment (Figure 2.4, Table 2.6). The predicted values of forage yield (ranging from 3.2 to 7.0 Mg DM ha^{-1}) were higher than the observed values (ranging from 0.7 to 5.1 Mg DM ha^{-1}) for the 0N treatment. These differences may be due primarily to an overestimation of N mineralization in soil. In the absence of an actual measured value for the clay content of the soil, we have estimated at 180 g kg^{-1} by referring to the soil texture classification. Whereas in STICS, the clay content parameter has a significant influence on the potential decomposition rate of soil organic

matter (Beaudoin et al., 2022). Apart from measurement or modelling errors, they may also correspond to yield gaps not explained by STICS, due to pressure from bio-aggressors such as leaf diseases and weeds. It has been reported that crops grown under conditions of low N availability are susceptible to pathogenic diseases from facultative parasites (Dordas, 2008). Yet, in the case of timothy, few pathogens are known to cause significant yield losses and this crop is remarkably free of weeds, insects, diseases, and animal damage (Grant & Burgess, 1979). In addition, the overestimation of forage yield was particularly high over the last four years with the 0N treatment. However, it has been reported that N deficiency can also lead to a reduction in tillers density, and a too low tillers density could be the cause of lower yields, especially after several years (Lafarge & Loiseau, 2002). To date, STICS has not been able to take into account changes in the number of tillers over the years as a function of the level of N deficiency. The overestimation by STICS of biomass for the 0N treatment led to an overestimation of the N exported by the crop. In STICS, N uptake by the crop is closely linked to biomass simulation through the use of the dilution curve.

2.4.2 Good performance of STICS for simulating treatment with N fertilization and the first harvest

The performance evaluation showed that STICS was correctly able to simulate the timothy forage yield for the 60N, 120N and 180N for the primary growth without annual reinitialization with NRMSE ≤ 17%. However, the NRMSE calculated in our study, with the four treatments, for forage yield during primary growth remained undegraded with a value of 22%, comparable to that calculated for timothy simulated with the STICS crop-soil model in the study by Jégo et al. (2013) (NRMSE = 16% for all sites). We obtained further better NRMSE (15%) values if we only consider treatments with fertilization (Table 2.6). Our NRMSE values for the first harvest was slightly better than those reported in other studies using other crop model ranging between 21 and 31% (Bonesmo et al., 2005; Jing et al., 2012, 2013).

Concerning N in forage yield for the first harvest, STICS correctly reproduced the variability of the annual observed values. The NRMSE calculated in our study for the N concentration (14%) was in the same order of magnitude than that reported by the study of Jégo et al. (2013) (NRMSE from 10 to 30%), and in the same order or even better than values (16 to 54%) obtained with CATIMO model (Bonesmo et al., 2005; Jing et al., 2012, 2013). Meanwhile, predictions of N amount exported in forage yield were satisfactory and correctly reproduced the annual variability of observed data. However, it was observed that a slight overestimation of the N exported in forage yield can result in an overestimation of the N concentration in the forage (Figures 2.5b, 2.5c). The parameters of the critical N dilution curve proposed by Lemaire & Salette (1984), which were used in this simulation study, significantly improved the simulation results for N concentration in forage yield (Figure 2.2). With the default N dilution curve ($Nc= 5.7 \times (\text{Shoot Biomass})^{-0.33}$ proposed for timothy in STICS (Jégo

et al., 2013), the N concentration was overestimated by the model for the 60N, 120N and 180N treatments (data not shown). This study once again confirms the genericity of the model and the applicability of the N dilution curve from tall fescue to timothy (Lemaire & Salette, 1984), providing satisfactory results.

STICS also reproduced well the downward trend in timothy forage yield observed as a function of the age of the meadow for the first harvest. The results showed that this drop in yield over time was strongly correlated with the reduction in the metabolic reserve in the storage organs before the start of regrowth in the spring (Figure 2.8). Jing et al (2012) had demonstrated with the CATIMO model that this yield reduction was not due to variations in climatic conditions (temperature, radiation, precipitation). They mentioned the possibility of the accumulation of C and N reserves to explain this reduction in yield. Many authors have already stated that the accumulation of storage reserves in storage organs is crucial for winter maintenance and spring regrowth of perennial grasses (Teixeira et al., 2007; Sarath et al., 2014). For example, for Alfalfa, the forage production is mainly affected by the initial taproot C / N reserve levels (Meuriot et al., 2005). Nevertheless, some perennial plants, such as switchgrass, seem to readjust their source-sink strategy after reserve depletion to assimilate enough CO_2 to complete growth (Tejera-Nieves & Walker, 2023). As a result, a 30% reduction in switchgrass rhizome reserves did not reduce biomass yield (Tejera-Nieves & Walker, 2023). Despite this interesting insight, the cause of this decline in perennial reserve accumulation over time remains to be explored.

This work therefore constituted a validation of STICS for timothy under the pedoclimatic conditions of the eastern region of Canada for common agronomic situations. However, the results in this study suggested that the model does not work well in situations where N deficiency is particularly pronounced (with 0N treatment), implying a low level of N nutrition. It is important to mention that the absence of N fertilizer application (organic and/or inorganic) is not a standard practice in conventional farming. The 0N treatment was designed solely as a baseline for experimentation, enabling to see whether the different treatments had an effect or not.

With this study, STICS has already been evaluated with timothy cultivar Champ on 3 different soil textures: gravely sandy-loam, sandy loam and loam (Jégo et al., 2013; Jing et al., 2017). In addition, the STICS model has been evaluated mainly for timothy crop with annual reinitialization but has not been extensively tested for a continuous and long-term simulation. The present study represents an important advance in validating the applicability of the STICS model for long-term simulation of perennial forage systems in cold regions, especially in Quebec's agricultural regions. It also paves the way for future research aimed at using this model to improve the management of forage systems, particularly with regard to the winter survival of perennial crops in the context of global change.

2.5 Conclusion

The present study showed that the STICS model is validated for simulating timothy growth and N nutrition especially for the primary growth period in cold, humid continental climate. STICS is reliable for long-term simulation, without annual reinitialization, of forage yield, N concentration and N amount exported in crops in situations where N fertilizer is applied. The simulation of summer regrowth should be further improved, despite the better performance of the simulation with the activation of a formalism option to simulate root length expansion. With regard to yield decline in ageing timothy swards, this study confirmed the hypothesis that yield decline could be due to reduced accumulation of C reserves in the roots during the previous autumn. However, other factors should be explored to explain the cause of the decrease in C reserve in the perennial organs of perennial plants over time.

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GENERAL DISCUSSION AND CONCLUSION

F. General discussion

Spring barley (*Hordeum vulgare* L.) and timothy (*Phleum pratense* L.) are very important crops for the province of Quebec (Canada). Spring barley is used for livestock feed and malting. Its annual productivity averages 2-3 Mg DM ha^{-1}, which is not enough to meet local demand (Ministère de l'Agriculture, des Pêcheries et de l'Alimentation, 2020). Timothy grasslands are very prevalent in eastern Canada, as they provide high-quality forage for livestock. Timothy is by far the most important cultivated grass species in the province of Quebec. It occupies a significant proportion of the forage area and provides a high level of biomass production, around 9 t ha^{-1} $year^{-1}$ under the most favourable growing conditions.

The cold and humid continental climate of the province of Quebec, and more broadly of eastern Canada and other regions with similar conditions, induces specific growing conditions (e.g. short growing season from May to September/October, relatively low degree-day sums and radiation; poorly drained and acidic soils) that are very different from those encountered in temperate or tropical climate regions. These growing conditions are major constraints that significantly affect crop and soil functioning, and biomass production in agrosystems.

Modelling the functioning of agrosystems with soil-crop models, such as STICS and many others (Table A.1), allows us to understand how crops, soil and agronomic management interact in space and time. Models are useful and powerful tools that help agronomists, farmers, policymakers, and researchers to make decisions and recommendations on agronomic (e.g. fertilization, tillage, crop rotation) and the environmental (e.g. N leaching, greenhouse gas emissions) issues. Building of this type of soil-crop model often requires the simplification of agronomic reality in the field, to balance theory and practice, the complexity of the system studied, and the processes involved. Models generally integrate crop growth and development mechanisms in interaction with soil processes (e.g. water cycle, N transformations) and crop management practices.

Several models for simulating biomass production and crop N nutrition have been developed over the last few decades, but most of them are specific to temperate climatic conditions, the species grown in these regions and the associated agronomic practices. Generally, they are widely used to simulate these variables of interest only over a short period (one year or a few successive years, often with annual reinitialization) associated with a crop species.

The cumulative effects of different agronomic practices (e.g. fertilization, tillage, crop succession), observed under field conditions, confirm the need for long-term studies to analyze the performance of soil-crop models as a function of these practices.

The literature review revealed a lack of knowledge about the ability of these models to continuously simulate the behavior of soil-crop systems over long periods of time in the context of agricultural regions with a cold, humid continental climate, such as that found in the province of Quebec.

In this study, we calibrated and evaluated the performance of the STICS model for the long-term simulation of biomass production and associated N uptake under the growing conditions of Quebec's agricultural regions.

The general objective of this thesis was to study the genericity and the ability of the STICS soil-crop model to simulate over the long term annual and perennial crop systems with various N fertilization rates under the pedoclimatic conditions of Quebec's agricultural regions. The detailed objectives were as follows:

i) For the spring barley monoculture with cultivars selected for their adaptation to the pedoclimatic conditions of the Saguenay-Lac-Saint-Jean region, the aim was to carry out the statistical analysis of a set of annual data, collected over 31 years, on aboveground biomass, grain yield, N concentration and associated N uptake. Then, the second objective was to calibrate and evaluate the ability of STICS to predict the previous variables of interest over several decades without annual reinitialization, before comparing the two approaches. The underlying research question is therefore: are STICS long-term simulations better than simple statistical models?
ii) For timothy grassland cultivated for 8 consecutive years, the aim was first to assess the ability of STICS (without annual initialization) to predict biomass production and N uptake over this 8-year period when increasing N application rates were applied. Secondly, the aim was to explore with STICS the possible causes of the decreasing yield trend with years of cultivation of timothy.

The approach adopted in this thesis consisted of combining the results of field experiments with simulations produced by a model describing the functioning of agrosystems, i.e. STICS. Two experimental sites located in the province of Quebec, monitored, and managed by Agriculture and Agri-Food Canada, were selected for this thesis. We chose to work on species of economic importance to the region and for which multi-year data sets were available:

- the crop studied: spring barley or timothy;

- the duration of the experiment, over three decades for spring barley and 8 years for timothy, which represents a long cultivation period given that timothy grasslands are often reseeded after 3 or 4 years of production;
- the use of different treatments for N fertilization. Two types of N fertilization (mineral fertilizer applied at a rate of 70 kg N ha^{-1} yr^{-1} and liquid dairy manure applied at a rate of around 50 m^3 ha^{-1} yr^{-1} (corresponding to an average application of 107 kg N ha^{-1} yr^{-1}) for spring barley. Four levels of ammonium nitrate application rates (0, 60, 120, 180 kg N ha^{-1} yr^{-1}) for timothy;
- comprehensive databases of annual biomass production, plant N concentration and annual N uptake, which are the main variables of interest in this research.

For spring barley monoculture grown continuously over the period 1990 to 2020 (31 years), the STICS model was parameterized, calibrated, and evaluated by comparing the simulated values produced by STICS with the values observed under field conditions for two sources of N. The STICS validation with independent data could not be carried out in Chapter 1 of this thesis due to the lack of available data from other experimental sites, especially from Quebec's agricultural regions. However, in this general discussion section, the recent acquisition of a dataset from a site in the province of Alberta (Canada) has enabled an initial evaluation of STICS, adapted to Canadian growing conditions, outside the conditions of its calibration.

For timothy grasslands, the STICS evaluation steps for cultivars adapted to the climatic growing conditions of the province of Quebec have already been carried out by Jégo et al. (2013). This thesis aimed to complete and extend the study of the genericity of STICS by using a database with other cropping years from the same experimental site, where timothy biomass production and N nutrition were measured for four levels of N fertilization.

In this "general discussion" section, the main and new results of the two results chapters (chapter 1 on spring barley monoculture; chapter 2 on timothy grassland) are briefly recalled and discussed.

Two other results/discussion points also appear in this "general discussion" section. They correspond to work initiated within the framework of this thesis, but which could not be completed within the allocated timeframe. The first point concerns the first step in the long-term validation of STICS for spring barley grown under Canadian conditions, with independent dataset. The second point concerns the simulation of C and N stock in the tilled soil layer under 31 years of spring barley monoculture in the Normandin experiment setup.

F.1 Calibration and multi-year evaluation of STICS over long cropping periods

For the Normandin experimental site, the calibration of spring barley resulted in good agreement between simulated and observed values for biomass production and N nutrition variables. Good agreement was obtained between observed and predicted values of AGB, GY, NCAGB, NCG, NU and NAG for all dataset during 31 years of spring barley monoculture, with a small NME and an NRMSE value classified as good to fair (Table F.1). However, there was a greater dispersion for the plant N attributes (EF negative or close to 0). The annual variability of biomass and N accumulation in plant was generally well captured by STICS.

For the Harlaka experimental site, STICS performed well over 8 years for simulating the timothy forage yield for the first harvest, but it was not very good for the second harvest at summer regrowth (Table F.1). The overall correspondence between observed and predicted values was also satisfactory with regard to N concentration and the N amount in the biomass harvested for the first growth. STICS satisfactorily simulated the positive effect of N fertilization rate on harvested forage biomass, N concentration and on amount of exported N, except for the unfertilized treatment (Table F.1). Forage yield and N nutrition were overestimated by STICS with the 0N treatment. STICS reproduced well the decrease of the annual yield of timothy sward with years of cropping.

The calibration results in this study confirm the genericity of the STICS model and the relevance of the calibration procedure proposed for STICS and reported in previous studies (Guillaume et al., 2011; Jégo et al., 2010). The number of optimized STICS-parameters was low and concerned in particular parameters representing cultivar traits.

The availability of experimental data needed to calibrate cultivars across multiple sites is often limited. Data may be insufficient in terms of quality or quantity, so modelers often extrapolate site-specific calibration to a wider region (Fleisher et al., 2020). For example, Jégo et al. (2011) calibrated the maize cultivars adapted to a short growing season for the Mixedwood Plains ecozone in eastern Canada using a dataset from one site location that is representative of the study area. However, their evaluation results of the model with independent datasets showed that the definition of two cultivars is sufficient to achieve good predictions of yield, LAI, and biomass over a large geographical area (covering three degrees of latitude and 10 degrees of longitude).

The evaluation results obtained in this study are satisfactory, or even more than satisfactory. Especially since the simulations carried out in this study were performed over a long cropping period without annual reinitialization of the model. As an illustration, the results of our study are comparable to those of Yin et al. (2020) conducted in the northern region of France for long-term continuous simulations (a 34-year crop rotation experiment) of aboveground biomass, yield, N uptake and grain N of various crops (with |NME| = 2–10% and NRMSE = 19–25%). Compared to previous calibration

and performance evaluation studies with new crops or cultivars in the STICS or other models, our results provided a good to acceptable range of NME and NRMSE values. The satisfactory results obtained in this calibration and evaluation work under specific conditions and varied N fertilization management, confirm the STICS robustness (Coucheney et al., 2015).

In general, N export and uptake are more difficult to simulate accurately than aboveground biomass and yield and (Coucheney et al., 2015), which is in line with our results. This is mainly due to the complexity of the processes involved in the simulation of these variables. N export and uptake are not only linked to crop growth processes, but also to N transformations in the soil-plant system.

Although the results of this study are already satisfactory, there is still considerable scope for further improvement of the model to obtain more accurate results.

Table F.1 Overview of STICS performance criteria for the different variables of interest for spring barley and timothy. Number of predicted/observed data pairs (n), normalized mean error (NME), normalized root mean square error (NRMSE), model efficiency (EF).

Variables	n	NME	NRMSE	EF
Spring barley (31 years)				
AGB (Mg DM ha^{-1})	124	0	19	0.5
GY (Mg DM ha^{-1})	124	-2	22	0.5
NCAGB (g kg^{-1} DM)	96	-1	14	-0.4
NCG (g kg^{-1} DM)	96	-2	12	-0.4
NU (kg N ha^{-1})	96	-5	17	0.0
NAG (kg N ha^{-1})	96	-10	23	-0.2
Timothy (8 years)				
1st harvest				
Forage yield (Mg DM ha^{-1})	32	-9	22	0.7
NC forage (g kg^{-1} DM)	32	-1	14	0.5
N exported (kg N ha^{-1})	32	2	22	0.8
2nd harvest				
Forage yield (Mg DM ha^{-1})	32	-19	99	-2.4
NC forage (g kg^{-1} DM)	32	38	43	-13.5
N exported (kg N ha^{-1})	32	39	117	-1.1
0N treatment (1st harvest)				
Forage yield (Mg DM ha^{-1})	8	-57	61	-1.0
NC forage (g kg^{-1} DM)	8	2	16	-0.3
N exported (kg N ha^{-1})	8	-38	53	-0.1
60, 120 and 180N treatments (1st harvest)				
Forage yield (g kg^{-1} DM)	24	-2	15	0.8
NC forage (g kg^{-1} DM)	24	-1	13	0.3
N exported (kg N ha^{-1})	24	6	18	0.7

F.2 Validation of STICS for biomass production for spring barley

Chapter 1 presented the parameterization, calibration, and predictive performance of STICS to continuously simulate (without annual reinitialization) biomass production and N uptake for a spring barley monoculture grown at the Normandin experimental farm site over a 31-year period. To complete the study of the genericity of STICS for spring barley grown under cold and humid continental climate conditions, it was necessary to carry out the validation step using independent

data from other sites. The aim is to find out whether STICS is still relevant when the datasets used are obtained outside the conditions used for calibration.

F.2.1 Experimental site and new data

For this purpose, a database provided by Professor Miles Dyck, (Faculty of Agricultural, Life and Environmental Sciences - Renewable Resources Deptment, University of Alberta, Edmonton, AB, Canada) containing biomass production measurements from the “Breton Plots research” site, owned and operated by the University of Alberta, was used. This site is located near the town of Breton (lat. 53° 6′ 18″ N, long. 114° 28′ 25″ W) in central Alberta, roughly at 95 kilometres southwest of Edmonton. Within the Breton Plots research site, numerous long-term plot experiments have been conducted over the years (Dyck et al., 2012). At this site, the mean annual average temperature and precipitation, between 1981 and 2010, were of 3.4 °C and 602 mm, respectively.

The dataset included aboveground biomass and grain yield measurements for the spring barley cultivar "AC Lacombe" grown continuously from 2001 to 2019. The "AC Lacombe" cultivar is a six-row barley well adapted to the black and grey wooded soils of Western Canada. Seeding dates ranged from May 11 to June 9 in Breton, and the average annual fertilization rates at seeding were 90 kg N ha^{-1} yr^{-1}. Extreme climatic events (flooding or drought) prevented harvesting in 2011, 2013 and 2014. Because these extremes climatic events cannot be simulated by STICS, the continuous evaluation (without annual reinitialization) of the model performance with the newly calibrated parameters was therefore carried out considering the succession of 10 years of barley monoculture carried out from 2001 to 2010.

F.2.2 Agreement between observed and predicted values of aboveground biomass and grain yield

The statistical criterion for the observed vs. predicted comparison of spring barley AGB and GY production at the “Breton Plots research” site are presented in Figure F.1. The observed AGB values over 10 years of successive cropping ranged between 4.6 and 9.5 Mg DM ha^{-1} yr^{-1} with a mean of 7.2 ±1.7 Mg DM ha^{-1} yr^{-1} whereas the predicted AGB values ranged between 4.9 and 8.6 Mg DM ha^{-1} yr^{-1} with a mean of 6.5 ±1.1 Mg DM ha^{-1} yr^{-1}. The mean observed GY value for the 10 years of cropping was 3.8 ±0.7 Mg DM $ha^{-1}yr^{-1}$ with values ranging from 2.8 to 5.1 Mg DM ha^{-1} yr^{-1}. Meanwhile, the predicted GY ranged between 3.2 and 5.5 Mg DM ha^{-1} yr^{-1} with a mean of 4.1 ±0.7 Mg DM ha^{-1} yr^{-1}.

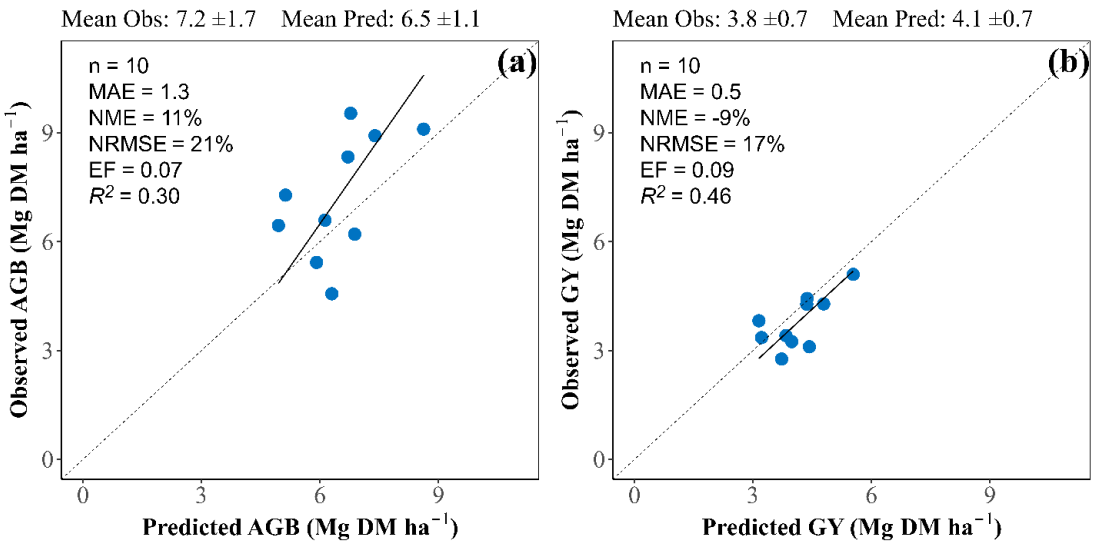

Figure F.1 Observed versus predicted (a) aboveground biomass (AGB) and (b) grain yield (GY) of spring barley cultivar « CV Lacombe » at the Breton Plots research site for the 2001-2010 period. Mean Obs: mean of observed values; Mean Pred: mean of predicted values; n: number of predicted/observed data pairs; MAE: mean absolute error; NME: normalized mean error; NRMSE: normalized root mean square error; EF: model efficiency; R^2: coefficient of determination (SMA).

The AGB and GY simulations based on data obtained at the “Breton plot research” were found to be satisfactory, as indicated by the low relative mean error (|NME| = 11% and 9%, respectively) and low normalized root mean square error (NRMSE = 21% and 17%, respectively). However, the EF was low but remained positive: 0.07 and 0.09 for AGB and GY, respectively. The calibration procedure carried out at the Normandin site produced validation results at “Breton Plots research” site that were acceptable in terms of NRMSE, but less so when the EF criteria was considered, indicating a higher dispersion.

Although both locations have a humid continental climate, the climates of Normandin and Breton are not quite the same. The average annual precipitation is 602 mm in Breton versus 850 mm in Normandin. The average annual temperature (over 30 years) is higher in Breton, with an annual average of 3.4 °C, compared to 2.0 °C in Normandin. These results confirm the observations of Kong et al. (1994) who found that the Chapais cultivar, originally from eastern Canada, can give excellent results across Canada, and even outperforms in the west. They also observed that eastern and western cultivars gave overall the same responses in terms of kernel weight, height, and maturity.

According to Affholder et al. (2012) and Fleisher et al. (2020), the calibration procedure against a local dataset can lead to confusion between phenotypic characteristics and production environment, and can result in crop parameter values that are location dependent. In this study, despite the use of

a single site to calibrate spring barley cultivars adapted to cold and humid continental regions, our calibration results were relevant and not impacted by this issue.

In conclusion, this first step of STICS validation for spring barley grown under Canadian climatic conditions, which has proved satisfactory, is already a good step forward. Further validation should be carried out with data from other sites for use in the agricultural regions of Quebec and more generally in eastern Canada., in particular to validate the simulation of spring barley N nutrition.

F.3 Evolution over 31 years of soil organic carbon and total nitrogen content under spring barley monoculture

STICS was tested for the simulation of soil organic C (SOC) and soil total N (STN) stock at 0-20 cm depth under 31 years of spring barley monoculture, including 2 types of tillage and 2 sources of N fertilizer.

F.3.1 Experimental site

The same long-term experimental setup initiated in 1989 at Agriculture and Agri-Food Canada's Normandin experimental farm is used in this study. The site is located in the Saguenay-Lac-Saint-Jean region of eastern Quebec, Canada (lat. 48° 50' N; long. 72° 33' W; alt. 137 m). The Labarre clay-loam soil in Normandin is classified as a humic gleysol (Humic Cryaquept). At the initiation of the experiment, in the first 15 cm, the soil contained 490 g kg^{-1} of clay and 430 g kg^{-1} of silt, with a pH_{water} of 5.6, and a bulk density of 1.36 g cm^{-3}. The initial soil organic C content is 26.1 g C kg^{-1}, while the initial soil organic N content is 1.7 g N kg^{-1}.

The experimental design was a factorial split-split-plot replicated four times with two types of crop rotation randomized into main plots (a continuous barley in monoculture and a 3-year cereal-perennial forage rotation), two tillage systems randomly assigned to subplots and two N sources randomly assigned to sub-subplots. Only the plots cropped with continuous barley in monoculture (16 plot units 10 m × 5 m in size) were considered in this study. Details of N application along with dates of seeding, harvest and tillage for each year are provided in Table 1.S2. The two tillage systems consisted of a moldboard plow operated to a 20-cm depth (MP) and a chisel plow to a 15-cm depth (CP), with tillage performed yearly in the fall after harvest. The two N sources were ammonium nitrate (MIN) and N-based liquid dairy manure (LDM), applied according to local recommendations. Before seeding, plots under the MIN treatment received 70 kg N ha^{-1} yr^{-1} as ammonium nitrate, 17.5 kg P ha^{-1} yr^{-1} as triple superphosphate, and 58 kg K ha^{-1} yr^{-1} as potassium chloride. For the LDM plots, about 50 m^3 ha^{-1} yr^{-1} of liquid dairy manure obtained from a local farm was applied in early spring, providing an average of 107 ±24 kg total N ha^{-1} yr^{-1}, 17 ±4 kg total P ha^{-1} yr^{-1}, and 119 ±29 kg total K ha^{-1} yr^{-1}. Annual

amounts of N applied as LDM from 1990 to 2020 are reported in Table 1.S2. Straw residues were returned to the soil after harvest.

F.3.2 Soil sampling and analysis

Soil samples were collected once per year after primary tillage in the fall, in 1993, then from 2001 to 2017. Soil samples (0–15 cm and 15–30 cm) were collected at three random locations in each plot, combined and sieved through a 6-mm sieve in the field and stored field moist at 4°C in plastic containers until analysis. Total soil C and N concentration (g kg^{-1}) was measured by dry combustion with a CNS analyzer (LECO, TRUSPEC, Leco Corp., St-Joseph, MI, USA) on air-dried soil, ground to pass a 0.5 mm sieve. In order to limit the bias that could be introduced in C and N gain or loss by soil compaction or fragmentation, total C and N concentration results were adjusted for soil bulk density using the equivalent soil mass approach (Ellert & Bettany, 1995). Carbonates in the soil samples were negligible, so total C was equal to organic C. Bulk density measurements were carried out only in 1989, 1993, 2002, 2010. Stainless steel cylinders were used to determine the bulk density of each layer: 5.5 cm in diameter and 3 cm in height for the top layer (0-15 cm), and 5 cm in diameter and 5 cm high for the deeper layers. The bulk density for the years for which we have no measured data was calculated as an average of the measured bulk density of two years, preceding and following, for which we have measurements. Soil organic C and total N were then calculated at a depth of 0-20 cm.

F.3.3 Observed versus predicted soil organic C and total N

STICS overestimated the evolution of SOC and STN stocks for LDM-CP and LDM-MP (Figure D.2). This could be due to an overestimation of the humified C from liquid dairy manure inputs, and to underestimation of the proportion of mineral N and the rate of organic N mineralization in LDM. The proportion of mineral N contained in the LDM was estimated at around 40%, as it was not measured. STICS predictions of SOC for MIN-CP and MIN-MP treatments were acceptable. However, it slightly overestimated final SOC for MIN-CP, and STN stocks for MIN-CP and MIN-CP. These overestimations could be explained partly by the fact that STICS underestimated the mineralization of organic matter for this study site, which had a very high soil clay content (490 g kg^{-1}). Apart from soil organic N content, temperature, and soil water content, the simulation of N mineralization in STICS is sensitive to soil characteristics, in particular clay and $CaCO_3$ content (Beaudoin et al., 2022). The accuracy of the simulation of the C/N ratio of residues returned to the soil is also very important for simulating the mineralization of organic residues and the subsequent release of N into the soil during the following crop growth cycles (Beaudoin et al., 2008; Yin et al., 2020). In this study, biomass growth and N nutrition were satisfactorily predicted by STICS, which indirectly indicated a correct simulation of the C/N ratio of the residues.

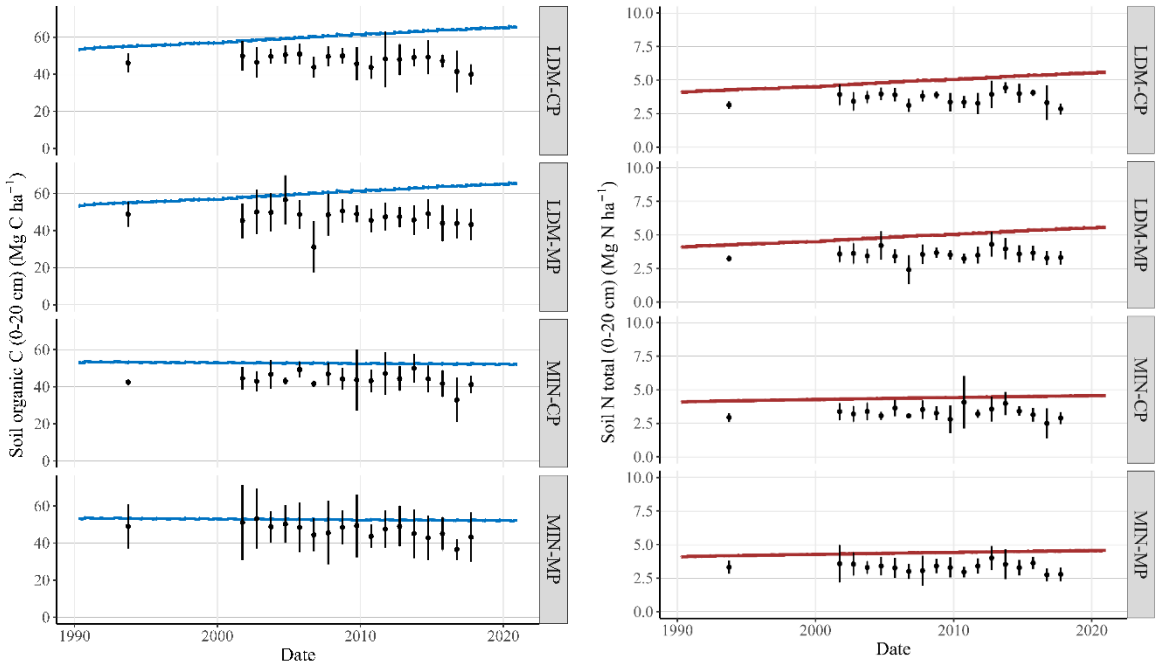

Figure F.2 Comparison of observed (dots) and predicted (blue line) (a) soil organic C and (b) soil total N from 1990 to 2020 for soil tillage and N fertilization source treatments. Dots are means. Bars on dots are standard deviation (n=4). LDM: liquid dairy manure; MIN: ammonium nitrate; MP: moldboard plow; CP: chisel plow.

On the other hand, Maillard et al. (2016) reported that in the long-term (21 years), yearly application of LDM resulted in an increase in SOC stocks in the upper soil layer. Thus, these deviations between observed and predicted values may also be attributable to the model structure (e.g., bulk density constant over time), model inputs (e.g., initialization), and the observed data uncertainty, as measurements and calculation of SOC and STN stocks can contain a lot of sources of uncertainties and bias (e.g. soil sampling equipment, depth of a respective soil layer, values conversion) (Poeplau et al., 2017; Sharma et al., 2020). As in our case in this study, soil sampling and analysis were carried out at 0-15 cm and 15-30 cm, but stocks were calculated and converted for a 0-20 cm depth (due to a constraint linked to model outputs). In addition, the bulk density was not systematically measured. In addition, we did not have The COS and STN stock values at the scale of the experimental units to initialize the simulation more accurately. This may have led to overestimation of the simulations from the outset.

We often tend to generalize that the biological activities of soil microorganisms are at their slowest when climatic conditions are most restrictive. However, in the context of Quebec, where the climate

is characterized by cold winters and long periods of frozen soil with permanent snow cover, the transformations of nitrogenous elements resulting from soil microbial activities appear to be considerable. Indeed, some authors have found that mineralization and nitrification processes can be observed in soils at near-zero or even negative temperatures (Clark et al., 2009). This situation can subsequently be favour to the release and loss of N, during the winter period. It is therefore essential to consider winter soil functioning in soil-crop models, to simulate the long-term dynamics of C and N stocks under humid continental climatic conditions.

Further investigations are required to refine these first results. The ability of STICS to simulate SOC dynamics under a cold and humid continental climate should be assessed against data from long-term experimental sites with complete soil datasets. Under temperate European conditions, studies have already demonstrated that STICS can effectively predict long-term SOC stocks in bare fallow and cropping systems (Clivot et al., 2020; Autret et al., 2020).

G. Conclusion and perspectives

STICS is a soil-crop model designed to simulate agro-environmental variables in agrosystems, mainly for temperate agropedoclimatic conditions. The aim of this thesis was to adapt STICS to agrosystems in cold and humid continental climates, and to analyze its genericity. In addition to the climatic context and the crops studied, the originality of this work also involved analyzing the performance of the model in simulating aboveground biomass production and N nutrition as a function of different N fertilization treatments over long periods continuously without annual reinitialization. Databases from two long-term field experiments were used, one from a 31-year spring barley monocrop, and the other from an 8-year timothy grassland.

For spring barley monoculture, after calibration of STICS with the Chapais cultivar, the values simulated each year for 31 years were close to the observed values of the variables of interest for both N treatments, but with greater dispersion for N uptake. STICS reproduced well the greater biomass production of the 70 kg N ha^{-1} yr^{-1} of mineral fertilizer treatment than the 107 kg N ha^{-1} yr^{-1} of liquid dairy manure treatment. However, STICS underestimated the simulation of biomass for the application of 70 kg N ha^{-1} yr^{-1}, whereas it overestimated them for the application of 107 kg N ha^{-1} yr^{-1} of LDM. These limitations of STICS are probably explained by weaknesses in considering the various terms of the N input/output balance (e.g. soil mineral N dynamics, leaching, emissions to the atmosphere) in the root zone, since the default parameters of STICS were used in the absence of local measurements.

For the 8 years of timothy, STICS performance was also good for plots fertilized with 60, 120 and 180 kg N ha^{-1} yr^{-1}. Annual forage production over 8 years was well simulated, although the model's performance was better for the simulation of the first harvest than for the second harvest, for which

biomass production was generally underestimated. On the other hand, in the absence of any N fertilization, the values predicted with STICS are much higher than those observed in the experimental setup.

These results confirm the overall good adaptability of STICS to a wide range of crops and cultivars, and to a variety of soil and climate conditions, and may explain the overall good performance of the STICS model in the current study. Apart from the very specific situation of not applying N fertilizer, a practice which is not representative of agricultural practices, STICS performance is therefore satisfactory for the two experimental sites studied.

However, the performance of the model could easily be improved by parameterizing the modules describing soil C and N transformations with local measurements (and not with default values established in temperate regions) representative of growing conditions in the province of Quebec. Indeed, many soil processes (e.g. mineralization of soil organic N and organic residues; nitrification; denitrification) are temperature-dependent, which will affect the supply of mineral N by the soil. Although STICS can run simulations in northern climates by adjusting the parameters of some of these processes, it is important to verify with field measurements that these adjustments are correct for growing conditions in the province of Quebec. Moreover, N uptake by a crop is the result of a compromise between soil N availability and crop N demand, which is estimated by a N dilution curve based on the aboveground biomass and dependent on the species. It would therefore be important to ensure that the N dilution curve is valid especially for the spring barley cultivars grown in these regions, to improve the model accuracy.

At the beginning of the thesis, other topics were also planned. For example, we intended to use the STICS model to simulate, over several decades, the effects of various climate change scenarios (increase in temperature, temperature sum and solar radiation) on yield and N nutrition. But here again, despite the interest of the matter, there was not enough time to explore such situations with STICS.

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Titre : Évaluation de la simulation à long terme sur STICS de la production de biomasse et de la nutrition azotée d'orge de printemps et de fléole des prés cultivés dans deux zones de production agricole du Québec (Canada)

Résumé : STICS est un modèle sol–culture basé sur les processus, initialement développé pour des conditions agropédoclimatiques des régions tempérées. Cette thèse vise à analyser et étendre l'application de STICS à deux cultures d'importance économique, l'orge de printemps et la fléole des prés, cultivées dans des conditions agropédoclimatiques de la province de Québec (climat continental froid et humide). L'objectif est également d'évaluer les performances prédictives du modèle sur des simulations à long terme. Outre le contexte climatique et les cultures étudiées, l'originalité de ce travail réside dans les simulations réalisées en continu, sans réinitialisation du modèle, sur de longues périodes. L'analyse des performances de STICS a porté sur la production de biomasse aérienne et l'absorption d'azote en fonction de différents traitements de fertilisation azotée. Deux essais agronomiques de longue durée ont été utilisés : (i) une monoculture d'orge de printemps (31 ans) et (ii) une prairie de fléole des prés (8 ans). Après la calibration de STICS pour l'orge de printemps, une concordance correcte entre les valeurs annuelles observées et simulées de toutes les variables d'intérêt a été obtenue sur une période de 31 ans, malgré une plus grande dispersion pour la nutrition azotée. Pendant les 8 années de culture de fléole, les performances de STICS sont satisfaisantes pour la simulation en continu du rendement et de la nutrition azotée à la croissance printanière, dans les situations où le niveau de stress azoté n'est pas très prononcé (60, 120 et 180 kg N ha^{-1} an^{-1}). Cette étude confirme la généricité du modèle STICS.

Mots clés : Modèle sol-culture STICS, expérimentations de longue durée, climat continental froid et humide, production de biomasse, nutrition azotée.

Title: Evaluation of STICS model performance for long-term simulation of biomass production and nitrogen nutrition of spring barley and timothy cultivated in two important agricultural regions in Québec (Canada)

Abstract: STICS is a process-based soil-crop model developed initially for temperate agropedoclimatic conditions. The objectives of this thesis were to analyze and extend the scope of application of STICS for two economically important crops, i.e. spring barley and timothy, grown under agropedoclimatic conditions in the province of Quebec (cold and humid continental climate), and to evaluate the predictive performance of the model on long-term simulations. In addition to the climatic context and the crops studied, the originality of this work also involved annual simulations, carried out continuously (without annual reinitialization) over long periods. Analysis of the long-term performance of STICS was carried out on aboveground biomass production and nitrogen (N) uptake as a function of different N fertilization treatments. We used databases from two field experiments: i) a 31-year spring barley monoculture; ii) an 8-year-old timothy prairie. For the 31 years of barley monoculture, after calibration of STICS, the simulated values correctly predict the observed values of the variables of interest for the different treatments, but with greater dispersion for N uptake. For the 8-year timothy grassland, the performance of STICS is satisfactory for continuous simulation of yield and N nutrition during spring growth, in situations where the level of N stress is not very pronounced (60, 120, and 180 kg N ha^{-1} per year). This study confirms the genericity of the STICS model.

Keywords: STICS soil-crop model, long-term field experiments, cold and humid continental climate, biomass production, nitrogen nutrition

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